Essays in Predictive and Causal Machine Learning

D I S S E R T A T I O N

of the University of St.Gallen, School of Management, Economics, Law, Social Sciences, International Afairs and Computer Science, to obtain the title of Doctor of Philosophy in Economics and Finance

submitted by

Gabriel Okasa

from

Slovakia

Approved on the application of

Prof. Dr. Michael Lechner

and

Prof. Dr. Martin Biewen

Dissertation no. 5206

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The University of St.Gallen, School of Management, Economics, Law, Social Sciences, International Afairs and Computer Science, hereby consents to the printing of the present dissertation, without hereby expressing any opinion on the views herein expressed.

St.Gallen, November 8, 2021

The President:

Prof. Dr. Bernhard Ehrenzeller

Dedicated To My Parents.

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St.Gallen, November 9, 2021 Gabriel Okasa

Contents

Summary

This dissertation consists of three chapters devoted to topics in predictive and causal machine learning. Common to all chapters is the synthesis of classical econometric methods and novel machine learning algorithms. Hence this doctoral thesis provides new insights into applications of machine learning for predictive tasks and for causal inference.

The frst chapter investigates the estimation of heterogeneous causal efects using machine learning. We focus on the meta-learning framework where the estimation of the causal parameter is decomposed into separate prediction tasks. Using synthetic and empirical simulations we study the fnite sample performance of meta-learners based on the Random Forest algorithm under diferent implementations using sample-splitting and cross-ftting procedures. The results imply that sample-splitting is benefcial in large samples for bias reduction but leads to an increase in variance, whereas cross-ftting keeps the bias low and successfully restores the full sample size efficiency. In contrast, the full-sample estimation is preferable in small samples when using machine learning. Additionally, we provide guidelines for applications of meta-learners in empirical studies depending on particular data characteristics such as treatment shares and sample size.

The second chapter considers the estimation of ordered choice models using machine learning. Similarly, as in the frst chapter, we focus on the Random Forest algorithm and develop a new machine learning estimator for models with ordered categorical outcome variable. The proposed Ordered Forest fexibly estimates the conditional ordered choice probabilities while taking the ordering information explicitly into account. In contrast to common machine learning estimators, it is not only suited for prediction tasks, but it also enables the estimation of marginal effects and conducting statistical inference, which provides additional interpretability as in classical econometric estimators. We conduct an extensive simulation study and fnd a good predictive performance, particularly in settings with nonlinearities and multicollinearity. Furthermore, we demonstrate the estimation of marginal efects and their standard errors in an empirical application.

The third chapter presents an empirical application based on the estimation of causal efects using machine learning. As in the previous two chapters, we rely on the Random Forest method and consider its causal variant, the Modifed Causal Forest. Following the rise of online dating, we study the efect of sport activity on partner choice by exploiting a unique dataset from an online dating platform. In particular, we estimate the causal efect of sport frequency on the contact chances, controlling for a large set of observable user characteristics. We fnd that for male users, doing sport on a weekly basis increases the probability to receive a frst message by more than 50%, in comparison to no sport activity. In contrast, we do not fnd such an evidence for female users. Moreover, the results indicate heterogeneity as for male users the efect increases with higher income.

Zusammenfassung

Die vorliegende Dissertation besteht aus drei Kapitel, welche sich dem prädiktiven und kausalen maschinellen Lernen widmen. Die Synthese von klassischen Methoden der Okonometrie und neuartigen ¨ Algorithmen des maschinellen Lernens ist allen Kapiteln gemeinsam. Somit bietet diese Doktorarbeit neue Erkenntnisse für die Anwendung von maschinellem Lernen für die Prädiktion und kausale Inferenz.

Das erste Kapitel untersucht die Schätzung heterogener kausaler Effekte mittels maschinellen Lernens. Wir fokussieren uns auf das Konzept des Meta-Learning, wobei die Schätzung kausaler Parameter in einzelne Prädiktionsmodelle aufgeteilt wird. Anhand von synthetischen und empirischen Simulationen analysieren wir die Eigenschaften der Meta-Learner in Stichproben mit begrenzter Anzahl an Beobachtungen, basierend auf dem Random Forest Algorithmus. Den Schwerpunkt legen wir hierbei auf verschiedene Implementierungen anhand von Sample-Splitting und Cross-Fitting Prozeduren. Die Ergebnisse belegen, dass Sample-Splitting in grossen Stichproben für die Verzerrungsreduktion hilfreich ist, jedoch führt dies gleichzeitig zu einer Varianzerhöhung. Ebenso reduziert Cross-Fitting in grossen Stichproben die Verzerrung, währenddessen die Effizienz erfolgreich wiederhergestellt wird. Demgegenüber ist bei Anwendung des maschinellen Lernens in kleinen Stichproben die Schätzung basierend auf der ganzen Stichprobe zu bevorzugen. Des Weiteren leiten wir Anwendungsempfehlungen für die Meta-Learner in empirischen Studien ab, die auf bestimmten Datenmerkmalen, wie Treatmentanteile und Stichprobengrösse, beruhen.

Das zweite Kapitel befasst sich mit der Schätzung von Ordered Choice Modellen mittels maschinellen Lernens. Ahnlich wie im ersten Kapitel betrachten wir den Random Forest Algorithmus und entwickeln einen neuen Schätzer für Modelle mit einer geordneten kategorischen abhängigen Variable. Die vorgeschlagene Ordered Forest Methode schätzt flexibel die bedingten geordneten Wahlwahrscheinlichkeiten, worin die Ordnungsinformation ausdrücklich berücksichtigt wird. Im Vergleich mit den gängigen Methoden des maschinellen Lernens, ist die Methode nicht nur für die Prädiktion geeignet, sondern ermöglicht auch die Schätzung marginaler Effekte sowie eine statistische Inferenzanalyse. Somit bietet sie eine zusätzliche Interpretierbarkeit, die auf den klassischen ökonometrischen Methoden beruht. Wir führen eine umfangreiche Simulationsstudie durch und stellen eine gute Vorhersagekraft fest, insbesondere in Szenarien mit Nichtlinearitäten und Multikollinearität. Ferner demonstrieren wir die Schätzung von marginalen Efekten und deren Standardfehler in einer empirischen Anwendung.

Das dritte Kapitel präsentiert eine empirische Anwendung gestützt auf die Schätzung von kausalen Efekten mittels maschinellen Lernens. Sowie in den vorherigen beiden Kapiteln, beziehen wir uns auf die Random Forest Methode und betrachten ihre Kausalversion, den Modifed Causal Forest. Nach dem Aufkommen des Online-Datings analysieren wir den Effekt der Sportaktivität auf die Partnerwahl durch die Nutzung eines einzigartigen Datensatzes einer Online-Dating Plattform. Insbesondere schätzen wir den kausalen Effekt der Häufigkeit des Sporttreibens auf die Kontaktchancen, unter Berücksichtigung einer grossen Anzahl von beobachtbaren Benutzercharakteristiken. Wir stellen fest, dass für männliche Benutzer das w¨ochentliche Sporttreiben die Wahrscheinlichkeit eine erste Nachricht zu erhalten um mehr als 50% erhöht, verglichen zu keiner sportlichen Aktivität. Andererseits finden wir keine solche Evidenz für weibliche Benutzer. Zugleich weisen die Ergebnisse eine Heterogenität auf, indem der Effekt für Männer mit einem höheren Einkommen steigt.

Chapter 1

Meta-Learners for Estimation of Causal Efects: Finite Sample Cross-Fit Performance

Abstract

Estimation of causal effects using machine learning methods has become an active research feld in econometrics. In this respect the meta-learning algorithms have gained considerable attention for estimation of heterogeneous causal efects. We study the fnite sample performance of various meta-learners for estimation of heterogeneous treatment efects, while explicitly focusing on the usage of sample-splitting and cross-ftting to reduce the overftting bias. In both synthetic and empirical simulations we fnd that the performance of the meta-learners in fnite samples greatly depends on the estimation procedure. The results imply that sample-splitting and cross-ftting are benefcial in large samples for bias reduction and efficiency of the meta-learners, respectively, whereas full-sample estimation is preferable in small samples. Furthermore, we derive practical recommendations for usage of specifc meta-learners in empirical studies depending on particular data characteristics such as treatment shares and sample size.

Keywords: Meta-learners, causal machine learning, heterogeneous treatment efects, Monte Carlo simulation, sample-splitting, cross-ftting.

JEL classifcation: C15, C18, C31.

1.1 Introduction

In recent years there has been a growing interest in the estimation of causal efects using machine learning algorithms, particularly in the feld of economics (Athey, [2018\)](#page-50-0). The newly emerging synthesis of machine learning methods with causal inference has a large potential for a more comprehensive estimation of causal efects (Lechner, [2018\)](#page-53-0). On the one hand, it enables a more fexible estimation of average efects which are of main interest in microeconometrics (Imbens & Wooldridge, [2009\)](#page-52-0). On the other hand, it advances the estimation beyond the average efects and allows for a systematic analysis of efect heterogeneity (Athey & Imbens, [2017\)](#page-50-1). Both of these aspects contribute to a better description of the causal mechanisms and thus to a possibly more efficient treatment allocation (Zhao, Zeng, Rush, & Kosorok, [2012;](#page-55-0) Kitagawa & Tetenov, [2018;](#page-52-1) Athey & Wager, [2021;](#page-50-2) Nie, Brunskill, & Wager, [2021\)](#page-53-1). Hence, applied researchers can greatly beneft from the usage of machine learning methods ranging from evaluation of public policies and business decisions to designing personalized interventions (Andini, Ciani, de Blasio, D'Ignazio, & Salvestrini, [2018;](#page-50-3) Bansak et al., [2018\)](#page-50-4).

Machine learning estimators as such are, however, primarily designed to tackle prediction problems and thus cannot be used off-the-shelf for causal inference. Therefore, new approaches for the estimation of causal parameters using machine learning emerged. Within the fast developing causal machine learning literature, one strand focused on direct modifcations of the existing machine learning algorithms that adjust the objective function for the estimation of causal effects. Such approach has led for example to the developments of Causal Trees (Athey & Imbens, [2016\)](#page-50-5) and Causal Forests (Wager & Athey, [2018;](#page-54-0) Lechner, [2018;](#page-53-0) Athey, Tibshirani, & Wager, [2019\)](#page-50-6). While these methods have well-established theoretical properties, they restrict the researcher in the choice of the machine learning method. Another strand of the causal machine learning literature thus proposed general procedures to decompose the causal problem into separate prediction problems that can be solved by standard machine learning algorithms and subsequently combined to estimate the causal parameters of interest. This approach has led to the development of meta-learners for the estimation of causal effects (see e.g. K¨unzel, Sekhon, Bickel, & Yu, [2019;](#page-53-2) Kennedy, [2020;](#page-52-2) or Nie & Wager, [2021\)](#page-53-3).

The meta-learners have received considerable attention for several reasons. First, the meta-learners do not modify the objective function of the machine learning methods but rather combine their pre-dictions in order to estimate the causal effect (Künzel et al., [2019\)](#page-53-2). This enables to directly leverage the superior prediction power of machine learning estimators. Second, the meta-learners are generic algorithms refraining from a specifc usage of any particular machine learning method. This allows to apply any suitable supervised learning method for the particular prediction problem at hand. Third, the meta-learners are attractive due to the ease of implementation using standard statistical software. This permits researchers to apply the meta-learners without any potential restrictions due to limited availability in software packages and enables tailored implementation for particular types of data. Despite the attractive features of the meta-learners, there is little guidance for applied researchers on how to choose from a variety of the meta-learners proposed in the literature, with lack of unifying simulation evidence for an assessment of the performance of the meta-learners in applied settings.

The complexity of the meta-learners varies widely and often hinges on the estimation of the nuisance functions such as the conditional mean of the outcome and the treatment, respectively (Chernozhukov et al., [2018\)](#page-51-0). The basic meta-learning algorithms include the S-learner and T-learner which besides the treatment efect function do not require estimation of any additional nuisance functions. However, the most prominent and widely used meta-learners in the literature consist of the X-learner (Künzel et al., [2019\)](#page-53-2), the DR-learner (Kennedy, [2020\)](#page-52-2), and the R-learner (Nie & Wager, [2021\)](#page-53-3), which all require estimation and combination of several nuisance functions to estimate the causal effect.^{[1](#page-16-0)} Due to the machine learning estimation of such nuisance functions the meta-learners are prone to the overftting bias, i.e. own observation bias. Therefore, sample-splitting has been proposed in the literature to reduce the overftting bias by using one part of the sample for estimation of the nuisance functions and the other part of the sample for estimation of the causal effect. In order to regain the full sample size effciency of the estimator cross-ftting repeats the estimation by swapping the samples and averaging the estimated causal effects (Chernozhukov et al., [2018\)](#page-51-0). However, the usage of sample-splitting and cross-ftting is not well understood in practice and the specifc definitions of meta-learners differ substantially in their implementation of these procedures. Despite the ambiguous defnitions, there is a lack of simulation evidence concerned with the usage of sample-splitting and cross-ftting within the meta-learning framework and thus limited guidance for or against specifc implementations. Moreover, there appears to be limited knowledge about how the asymptotic arguments translate into fnite sample properties of the metalearners.

In this paper, we address both of the above issues and study the fnite sample properties of the machine learning based meta-learners for estimation of causal efects based on the specifc implementations using the full-sample, sample-splitting and cross-ftting procedures for varying sample sizes. We focus on evaluating the estimation of heterogeneous treatment efects as these provide the most detailed description of the underlying causal mechanisms and thus allow for a better assessment of the individualized impacts of an intervention. For this purpose, we review the most widely used meta-learning algorithms together with their theoretical estimation requirements with respect to sample-splitting and cross-fitting and identify their strengths and weaknesses. We conduct both synthetic and empirical simulations comparing the performance of the meta-learners in various settings featuring unequal treatment shares, non-linear functional forms and large-dimensional feature sets. Importantly, within the simulations we explicitly study the convergence performance of the meta-learners based on growing sample sizes up to 32′000 observations. Furthermore, we derive practical recommendations on the choice of specifc meta-learners and the respective estimation procedures for applied empirical work.

The results of our simulation experiments reveal that the choice of the estimation procedure has a large impact on the performance of the machine learning based meta-learners in fnite samples. For sufficiently large samples we provide evidence for the theoretical arguments of bias reduction via samplesplitting and cross-ftting, while for smaller samples we observe adverse efects of these procedures when using machine learning. The results show that, if computation time is not a constraint, cross-ftting is always preferable to sample-splitting as it keeps the bias low, while successfully reducing the variance of the estimators even in small samples. Additionally, the results imply heterogeneous impacts of the estimation procedures on the performance of the meta-learners. The X-learner's performance is quite stable regardless of the estimation procedure, whereas the performance of the R-learner and DR-learner is more sensitive to the choice of the estimation procedure. Assessing the performance of the particular meta-learners reveals a clear pattern. In empirical settings with highly imbalanced treatment shares, the X-learner performs best, irrespective of the sample size, while the DR-learner becomes unstable due to extreme propensity scores. For less imbalanced settings the X-learner's performance is still superior in smaller samples, however, it gets outperformed by the DR-learner in larger samples which exhibits the fastest convergence rate in its sample-splitting and cross-ftting version. In empirical settings with balanced treatment shares, the performance of the DR-learner or the R-learner is superior for any sample size considered. The results imply that the usage of less sophisticated S-learner for estimation of causal efects should be avoided, while the T-learner might be a reasonable choice in small samples.

¹Further examples of some meta-learners proposed in the literature consist of the U-learner and Y-learner (Stadie, Kunzel, Vemuri, & Sekhon, [2018\)](#page-54-1), or the IF-learner (Curth, Alaa, & van der Schaar, [2020\)](#page-51-1) and RA-learner (Curth & van der Schaar, [2021\)](#page-51-2).

This paper contributes to the causal machine learning literature in several ways. First, we provide a unifying simulation evidence of meta-learning algorithms for the estimation of heterogeneous causal efects in large-dimensional and highly non-linear settings based on synthetic and empirical simulations. Second, we explicitly study the meta-learners under the full-sample, sample-splitting and cross-ftting implementations, respectively and thereby provide evidence on the contrast between the asymptotic arguments and fnite sample properties. Third, we empirically investigate the convergence performance of the meta-learners by repeating the simulation experiments with growing sample sizes. Finally, we derive relevant practical recommendations for applied empirical work which are based on the particular observable data characteristics.

This paper is organized as follows. We briefy discuss the related literature in Section [1.1.1.](#page-17-0) Section [1.2](#page-18-0) introduces the notation, the parameters of interest and their identifcation. Section [1.3](#page-20-0) reviews the considered meta-learners and the estimation procedures. Section [1.4](#page-30-0) describes the synthetic as well as empirical simulations and presents the corresponding results. The main fndings of the study are discussed in Section [1.5.](#page-44-0) Section [1.6](#page-47-0) concludes. Further details including descriptive statistics, an exhaustive summary of the main and supplementary results as well as a computation time analysis are provided in Appendices [1.A,](#page-56-1) [1.B](#page-65-0) and [1.C,](#page-78-0) respectively.

1.1.1 Literature

In general the literature on the fnite sample properties of causal machine learning estimators under a unified framework seems to be rather scarce. An exception in the econometric literature^{[2](#page-17-1)} is Knaus, Lechner, and Strittmatter [\(2021\)](#page-53-4) who study a wide range of estimators for heterogeneous as well as (group) average treatment efects, including direct estimators as well as some meta-learners in an Empirical Monte Carlo Study as developed in Huber, Lechner, and Wunsch [\(2013\)](#page-52-3) and Lechner and Wunsch [\(2013\)](#page-53-5). Knaus et al. [\(2021\)](#page-53-4) fnd no estimator to perform uniformly best, but notice that estimators which model both the outcome as well as the treatment process are substantially more robust throughout all data generating processes considered, which can be observed in our simulations as well. Among the metalearners considered, the DR-learner and the R-learner perform especially well in terms of the root mean squared error. Moreover, using the Random Forest as a base learner turns out to be more stable with better statistical properties in contrast to using the Lasso, particularly in smaller samples, which also motivates the usage of the Random Forest in our simulations. However, although both meta-learners are implemented with cross-ftting, an explicit consideration of diferent sample-splitting or cross-ftting schemes is missing. Curth and van der Schaar [\(2021\)](#page-51-2) focus directly on meta-learning algorithms for estimation of heterogeneous treatment effects, but refrain from studying sample-splitting and cross-ftting procedures and rely fully on the full-sample estimation. In this regard, Zivich and Breskin [\(2021\)](#page-55-1) study the performance of treatment efect estimators based on cross-ftting, including some meta-learners as well. Similarly to Knaus et al. [\(2021\)](#page-53-4) they fnd the DR-learner with an ensemble machine learning base learners together with cross-ftting to perform the best among all considered estimators, both in comparison to cases without cross-ftting and to parametric base learners. However, Zivich and Breskin [\(2021\)](#page-55-1) study exclusively the estimation of average efects without examining convergence performance of the estimators, considering only a single sample size of 3 ′000 observations. Recently, Jacob [\(2020\)](#page-52-4) focuses on the estimation of heterogeneous treatment efects under various cross-ftting schemes for selected meta-learning algorithms. Also, in this simulation study the DR-learner together with the R-learner achieve consistently the best results. Nonetheless, Jacob [\(2020\)](#page-52-4) stresses the heterogeneous impacts of the particular sample-splitting and cross-ftting procedures on each meta-learner, which is documented in our

 $2\overline{\text{Wending et al. (2018) conduct similar empirical simulation study in medical context.}}$ $2\overline{\text{Wending et al. (2018) conduct similar empirical simulation study in medical context.}}$ $2\overline{\text{Wending et al. (2018) conduct similar empirical simulation study in medical context.}}$

simulations as well. Nevertheless, even though considering varying sample sizes within the simulation experiments, the considered sample sizes are limited to 2 ′000 observations. Overall, none of the above studies focuses directly on the convergence performance of the meta-learners under various estimation procedures which still remains an open question. To the best of our knowledge, this is the frst paper that empirically studies the convergence properties of the meta-learners under full-sample, sample-splitting and cross-ftting implementations with growing sample sizes up to several thousands of observations, reaching 32′000 in our simulations.

Besides the meta-learning framework, there has been also a substantial development of specifc causal estimators based on direct modifcations of particular machine learning algorithms. Especially, the treebased estimators have been studied extensively in this respect. These include the above-mentioned Causal Trees (Athey & Imbens, [2016\)](#page-50-5) as well as Causal Boosting (Powers et al., [2018\)](#page-53-6) and Causal Forests (Wager & Athey, [2018\)](#page-54-0) with the extensions of the Modifed Causal Forests (Lechner, [2018\)](#page-53-0) and the Generalized Random Forests (Athey et al., [2019\)](#page-50-6). These methods are based on the underlying predictive algorithms of Regression Trees (Breiman, Friedman, Olshen, & Stone, [1984\)](#page-50-7), Boosted Trees (Friedman, [2001\)](#page-51-3) and Random Forests (Breiman, [2001\)](#page-50-8), respectively. Furthemore, Bayesian versions of Regression Trees (Chipman, George, & McCulloch, [1998\)](#page-51-4) have been adapted for estimation of causal efects as well (Hill, [2011;](#page-52-5) Taddy, Gardner, Chen, & Draper, [2016;](#page-54-3) Hahn, Murray, & Carvalho, [2020\)](#page-51-5). Besides the estimators based on recursive partitioning, important causal adjustments have been applied in respect to regularization based estimators such as the Lasso (Qian & Murphy, [2011;](#page-53-7) Belloni, Chernozhukov, & Hansen, [2013;](#page-50-9) Tian, Alizadeh, Gentles, & Tibshirani, [2014\)](#page-54-4) or Lasso-augmented Support Vector Machines (Imai & Ratkovic, [2013\)](#page-52-6). Additionally, further machine learning algorithms such as the Nearest Neighbours (Fan, Lv, & Wang, [2018\)](#page-51-6) or Neural Networks (Johansson, Shalit, & Sontag, [2016;](#page-52-7) Shalit, Johansson, & Sontag, [2017;](#page-54-5) Schwab, Linhardt, & Karlen, [2018;](#page-54-6) Shi, Blei, & Veitch, [2019\)](#page-54-7) have been transformed towards causal inference as well. For a comprehensive overview of many of these estimators, we refer the interested reader to Athey and Imbens [\(2019\)](#page-50-10) or Jacob [\(2021\)](#page-52-8). In this paper, although we focus on the machine learning estimation of causal effects, we refrain from an analysis of these methods due to major conceptual diferences to the meta-learning framework and the lack of comparability in terms of the usage of sample-splitting and cross-ftting procedures.

1.2 Framework and Identifcation

In order to describe the efects of interest and their corresponding identifcation assumptions we rely on the potential outcome framework (Rubin, [1974\)](#page-53-8). We assume a population P from which a realization of N *i.i.d.* random variables is given consisting of a random sample $\{Y_i(1), Y_i(0), W_i, X_i\} \sim \mathcal{P}$. Here, we consider a binary treatment variable W_i that is equal to 1 for the treated group and equal to 0 for the control group, respectively. According to the treatment status we define the potential outcome $Y_i(1)$ under treatment for the case when $W_i = 1$ and correspondingly the potential outcome $Y_i(0)$ under control for $W_i = 0$. Additionally, we define a *p*-dimensional vector of exogenous pre-treatment covariates such that $X_i \in \mathbb{R}^p$. Given this definition we can characterize the *Individual Treatment Effect* (ITE) as follows:

$$
\xi_i = Y_i(1) - Y_i(0).
$$

However, the fundamental problem of causal inference is that we never observe both potential outcomes at the same time (Holland, [1986\)](#page-52-9). Hence, the observed outcomes are defned according to the observational rule as $Y_i = Y_i(W_i)$. The observed data then consists of the triple $\{Y_i, W_i, X_i\}_{1 \leq i \leq N}$. Nevertheless, it is still possible to identify the expectation of ξ_i under additional assumptions (compare Rubin, [1974;](#page-53-8) or Imbens & Rubin, [2015\)](#page-52-10). Thus, we shift the effect of interest towards the *Conditional Average Treatment* Effect (CATE) which takes the expectation of ξ_i , conditional on covariates X_i and is given as:

$$
\tau(x) = \mathbb{E}\big[\xi_i \mid X_i = x\big] = \mathbb{E}\big[Y_i(1) - Y_i(0) \mid X_i = x\big] = \mu_1(x) - \mu_0(x)
$$

where $\mu_1(x) = \mathbb{E}[Y_i(1) | X_i = x]$ and $\mu_0(x) = \mathbb{E}[Y_i(0) | X_i = x]$ are the response functions for potential outcomes under treatment and under control, respectively. In this paper we always refer to the CATE with conditioning on all observed exogeneous covariates and thus focusing on the fnest level of hetero-geneity (see e.g. Knaus et al., [2021\)](#page-53-4).^{[3](#page-19-0)} Künzel et al. [\(2019\)](#page-53-2) point out that the best estimator for $\tau(x)$ is also the best estimator for ξ_i in terms of the mean squared error (MSE).

In order to identify the efects of interest, we need a set of identifcation assumptions. We operate under the selection-on-observables strategy^{[4](#page-19-1)} (see e.g. Imbens & Rubin, [2015\)](#page-52-10) and assume that we observe all relevant confounders, i.e. all covariates X_i that jointly influence both the treatment W_i and the potential outcomes, $Y_i(0)$ and $Y_i(1)$. We state the following identification assumptions:

Assumption 1 (Conditional Independence) $(Y_i(0), Y_i(1)) \perp W_i | X_i = x, \forall x \in \text{supp}(X_i)$. Assumption 2 (Common Support) $0 < \mathbb{P}[W_i = 1 | X_i = x] < 1, \forall x \in \text{supp}(X_i)$. Assumption 3 (SUTVA) $Y_i = W_i \cdot Y_i(1) + (1 - W_i) \cdot Y_i(0)$.

Assumption 4 (Exogeneity) $X_i(0) = X_i(1)$.

According to Assumption [1,](#page-19-2) also referred to as the conditional ignorability or unconfoudedness assumption, we assume that the potential outcomes are independent of the treatment assignment once conditioned on the covariates, i.e. we assume that there are no hidden confounders. Assumption [2,](#page-19-3) also known as the overlap assumption, states that the conditional treatment probability is bounded away from 0 and 1 and thus it is possible to observe treated as well as control units for each realization of $X_i = x$. Assumption [3](#page-19-4) is known as the stable unit treatment value assumption and indicates that the observed treatment value for a unit is independent of the treatment exposure for other units, which rules out any general equilibrium or spillover efects between treated and controls. Lastly, Assumption [4](#page-19-5) specifes that the covariates are not infuenced by the treatment.[5](#page-19-6) Under these assumptions it follows that

$$
\tau(x) = \mathbb{E}[Y_i(1) - Y_i(0) | X_i = x]
$$
\n(1.2.1)

$$
= \mathbb{E}[Y_i(1) | X_i = x] - \mathbb{E}[Y_i(0) | X_i = x]
$$
\n(1.2.2)

$$
= \mathbb{E}[Y_i(1) | X_i = x, W_i = 1] - \mathbb{E}[Y_i(0) | X_i = x, W_i = 0]
$$
\n(1.2.3)

$$
= \mathbb{E}[Y_i \mid X_i = x, W_i = 1] - \mathbb{E}[Y_i \mid X_i = x, W_i = 0]
$$
\n(1.2.4)

and thus the CATE can be nonparametrically identifed from observable data (Hurwicz, [1950\)](#page-52-11).

³In general, the term CATE describes conditional average treatment effects on various aggregation levels. In our case, the CATE corresponds to the Individualized Average Treatment Effect (IATE). Additionally, researchers and especially policy makers might be interested in a low-dimensional heterogeneity level based on some pre-specifed heterogeneity covariates of interest, which are referred to as the Group Average Treatment Efects (GATEs). Such efects are, however, beyond the scope of our study and the interested reader is referred to Zimmert and Lechner [\(2019\)](#page-55-2), Jacob, Härdle, and Lessmann [\(2019\)](#page-52-12) and Semenova and Chernozhukov [\(2021\)](#page-54-8) for a theoretical analysis and to Knaus et al. [\(2021\)](#page-53-4) for simulation based results or to Cockx, Lechner, and Bollens [\(2019\)](#page-51-7), Knaus, Lechner, and Strittmatter [\(2020\)](#page-52-13), Hodler, Lechner, and Raschky [\(2020\)](#page-52-14) and Goller, Harrer, Lechner, and Wolf [\(2021\)](#page-51-8) for empirical applications estimating policy relevant GATEs.

⁴For estimation of heterogeneous effects under different identification strategies see e.g. Athey et al. [\(2019\)](#page-50-6), Bargagli Stoffi and Gnecco [\(2020\)](#page-50-11) and Biewen and Kugler [\(2021\)](#page-50-12) for the case of instrumental variables and Gulyas and Pytka [\(2020\)](#page-51-9) and Zimmert and Zimmert [\(2020\)](#page-55-3) for the case of diference-in-diferences.

⁵Analogously to the definition of potential outcomes, we denote potential covariates under control and under treatment as $X_i(0)$ and $X_i(1)$, respectively.

1.3 Meta-Learning Algorithms and Estimation Procedures

In the machine learning literature meta-learning represents algorithms that exploit knowledge about learning to improve the algorithm's performance, as generally defned by Vilalta and Drissi [\(2002\)](#page-54-9). These include various algorithms that learn to solve new task from prior learning experience, i.e. learning to learn (Schmidhuber, [1987;](#page-54-10) Thrun & Pratt, [1998\)](#page-54-11), algorithms that learn from multiple related tasks, i.e. multi-task learning (Caruana, [1997\)](#page-51-10), or algorithms that learn from multiple models solving identical task, i.e. ensemble learning (Dietterich, [2000\)](#page-51-11).^{[6](#page-20-1)} Recently, the meta-learning framework has been adopted within the causal machine learning literature for learning causal effects from multiple prediction models (see for example Künzel et al., [2019\)](#page-53-2), which could be termed accordingly as *causal learning*.

At a high level the meta-learners for estimation of heterogeneous causal efects are two-step algorithms. In the frst step they defne regression functions, in the causal machine learning literature often denoted as the nuisance functions (Chernozhukov et al., [2018;](#page-51-0) Kennedy, [2020\)](#page-52-2), which can be estimated by any suitable supervised learning method, i.e. the base learner. In the second step they use the estimated nuisance functions to construct an estimator for the causal efect, i.e. the meta-learner. Various metalearners then difer in the defnitions of the nuisance functions and their subsequent usage to obtain the fnal estimator for the causal efects. Depending on the algorithm complexity, some meta-learners require estimation of only one single model whereas other require estimation of multiple models. This raises the question of data usage within the estimation procedure and thus the possible need for sample-splitting and cross-ftting, respectively.[7](#page-20-2)

In general, the nuisance functions are defned as conditional expectations of various types. The most common types are the propensity score function and the response function. First, the propensity score is defined as the conditional probability of a binary treatment W_i given the covariates X_i as follows:

$$
e(x) = \mathbb{P}[W_i = 1 \mid X_i = x].
$$

In the causal inference literature the propensity score plays a central role (Rosenbaum & Rubin, [1983\)](#page-53-9) in many matching and reweighting methods to balance the distributions of treated and controls (see Hahn, [1998;](#page-51-12) and Huber et al., [2013,](#page-52-3) among others). Second, the response function is broadly defned as the conditional expectation of an outcome variable Y_i given a conditioning set of explanatory variables. The particular defnitions of the response function then difer in the specifcation of the conditioning set and the subset of the data used. For the meta-learners studied in this paper, the following defnitions of the response function are of interest:

$$
\mu(x, w) = \mathbb{E}[Y_i \mid X_i = x, W_i = w]
$$
\n(1.3.1)

$$
\mu(x) = \mathbb{E}[Y_i \mid X_i = x] \tag{1.3.2}
$$

where Equation [1.3.1](#page-20-3) defines the full response function with conditioning on both the covariates X_i as well as the treatment indicator W_i , while $\mu(x,1)$ and $\mu(x,0)$ describe the response functions with conditioning on the covariates X_i in the subpopulation under treatment $W_i = 1$ and under control $W_i = 0$, accordingly. Similarly, Equation [1.3.2](#page-20-4) defines the full response function with conditioning only on covariates. The meta-learners then use selected nuisance functions together with the available data as

 6 For a recent survey on meta-learning, see Vanschoren [\(2019\)](#page-54-12).

⁷Recently, related issue of data usage of the meta-learning algorithms with respect to splitting into training and validation set for the learning to learn domain has been discussed by Bai et al. [\(2020\)](#page-50-13) and Saunshi, Gupta, and Hu [\(2021\)](#page-53-10).

inputs for the estimation of the CATE function which can be generally denoted as follows:

$$
\tau(x) = \zeta(W_i, X_i, Y_i, e(x), \mu(x, w), \mu(x))
$$

where $\zeta(\cdot)$ is a function of the respective inputs, which is detailed for each particular meta-learning algorithm in Section [1.3.2.](#page-24-0) The problem arises when estimating the nuisance functions using fexible machine learning methods as these are prone to the overftting bias, i.e. the 'own observation bias'. The overftting bias emerges when the in-sample data is ftted too well such that the out-of-sample performance is compromised (see e.g. Hastie, Tibshirani, & Friedman, [2009,](#page-52-15) for a general discussion of the overfitting issue in machine learning). Hence, a single observation i can have a large influence on the predictions for covariates X_i as pointed out by Athey and Imbens [\(2019\)](#page-50-10). Chernozhukov et al. [\(2018\)](#page-51-0) and Newey and Robins [\(2018\)](#page-53-11) thus propose sample-splitting procedures that allow for elimination of such overftting biases.[8](#page-21-1)

1.3.1 Sample-Splitting and Cross-Fitting

Theoretical arguments express the need for sample-splitting when the causal estimator involves several estimation steps such as the estimation of nuisance functions. Within the meta-learning framework the nuisance functions are typically highly complex and potentially high-dimensional functions estimated by supervised machine learning methods such as penalized regression, tree-based methods, neural networks, etc. Using the same data sample for machine learning estimation of the nuisance function as well as for estimation of the causal efect leads to overftting which induces a bias in the CATE estimator. On a high level, the bias of the CATE estimator can generally be decomposed into an estimation error of learning the CATE function itself, and the estimation error in learning the nuisance functions, encompassing the overftting bias (see e.g. Kennedy, [2020\)](#page-52-2). Chernozhukov et al. [\(2018\)](#page-51-0) show that for the ATE estimation the overftting bias can be controlled by using sample-splitting, while Kennedy [\(2020\)](#page-52-2) and Nie and Wager [\(2021\)](#page-53-3) extend this concept for the CATE estimation. In that case one part of the sample is used to estimate the nuisance functions and the other part is used to estimate the causal effect.^{[9](#page-21-2)} As a result, the bias term stemming from overftting can be shown to be bounded and to converge to zero. Building upon this result, Newey and Robins [\(2018\)](#page-53-11) propose a diferent sample-splitting scheme called double sample-splitting. In this case, not only the nuisance functions are estimated together on a separate part of the sample but each single nuisance function is estimated on an own separate part of the sample. In practice, the training data is split into $M + 1$ equally sized parts, with M being the number of nuisance functions to estimate and the remaining part of the data serves for estimation of the causal efect. Newey and Robins [\(2018\)](#page-53-11) show that under the double sample-splitting the bias term converges to zero at a faster rate compared to standard sample-splitting where all nuisances are estimated on the same sample.^{[10](#page-21-3)} The double sample-splitting procedure has also been recently implemented by Kennedy [\(2020\)](#page-52-2) in the context of the DR-learner.

In general, the overftting bias could also be controlled for by restricting the complexity of the nuisance functions which would, however, prevent high-dimensional settings as well as usage of a variety

⁸Original ideas of using sample-splitting procedures to eliminate own observation bias stem from the literature on density estimation going back to Bickel [\(1982\)](#page-50-14), Bickel and Ritov [\(1988\)](#page-50-15) and Powell, Stock, and Stoker [\(1989\)](#page-53-12) among others.

⁹Sample-splitting procedures are frequently used in causal machine learning literature including Double Machine Learning (Chernozhukov et al., [2018\)](#page-51-0), Causal Forests (Wager & Athey, [2018;](#page-54-0) Lechner, [2018\)](#page-53-0) or the here-discussed meta-learners (Kennedy, [2020;](#page-52-2) Nie & Wager, [2021\)](#page-53-3).

 10 The intuition for this result comes from the observation that for estimators using multiple nuisance functions, such as the doubly robust estimators as e.g. the herein discussed DR-learner, the estimation error involves a product of the biases from the estimation of the M nuisance functions. This induces additional nonlinearity bias if all M nuisance functions are estimated using the same data, which gets effectively removed by using separate samples for estimation of each of the M functions. For more details see Newey and Robins [\(2018\)](#page-53-11) and Kennedy [\(2020\)](#page-52-2).

of machine learning estimators or ensembles of those.^{[11](#page-22-0)} Hence, the advantage of using sample-splitting is to allow for a high degree of complexity of the nuisance functions estimated by a wide class of machine learning estimators (Kennedy, [2020\)](#page-52-2).

It follows that, theoretically, sample-splitting prevents overftting and thus reduces the bias in the fnal causal estimator (Chernozhukov et al., [2018;](#page-51-0) Wager & Athey, [2018\)](#page-54-0). At the same time, however, the variance of the estimator increases as less data is efectively used for estimation. Cross-ftting (Chernozhukov et al., [2018\)](#page-51-0) and respectively double cross-ftting (Newey & Robins, [2018\)](#page-53-11) have been proposed in the literature in order to reduce the variance loss induced by sample-splitting. In this procedure, the roles of the data parts get switched such that each part has been used for both the estimation of nuisances as well as the causal efect estimation. The fnal CATE estimator is then an average of the separate efect estimators produced. This method can be further extended to use more than $M + 1$ splits denoted as K-fold cross-ftting (Chernozhukov et al., [2018\)](#page-51-0) with the fnal CATE estimator given as:

$$
\hat{\tau}(x) = \frac{1}{K} \sum_{k=1}^{K} \hat{\tau}_k(x)
$$

where $\hat{\tau}_k(x)$ is the CATE estimator based on the k-th fold.^{[12](#page-22-1)}

The above theoretical arguments have a direct impact on the implementation of various meta-learning algorithms. Under the double sample-splitting the more models have to be estimated within the metalearning algorithm, the more data splits are being implicitly induced, while the impact thereof in fnite samples is not clear *a priori* as pointed out by Newey and Robins [\(2018\)](#page-53-11). As such, the researcher faces a typical bias-variance trade-of with respect to sample-splitting. In order to illustrate the issue it is instructive to decompose the mean squared error (MSE) of a CATE estimator $\hat{\tau}(x)$:

$$
MSE\bigg(\hat{\tau}(x)\bigg) = Var\bigg(\hat{\tau}(x)\bigg) + \bigg(Bias\big(\hat{\tau}(x)\big)\bigg)^2.
$$

Naively using the full data sample for estimation of both the nuisance functions as well as the CATE function leads to a higher bias due to overftting but at the same time to lower variance as all available data is used for estimation. Using sample-splitting eliminates the overftting bias but results in higher variance due to less data being used for estimation. In contrast, cross-ftting both removes the overftting bias and reduces the variance by efectively using all the available information from the data for estimation. Figure [1.3.1](#page-23-0) illustrates this theoretical argument by contrasting the distributions of the CATE parameter under full-sample estimation, double sample-splitting and double cross-ftting, resulting from a Monte Carlo simulation based on a large training sample of 32′000 observations (further details on the metalearner and the simulation design are provided in Sections [1.3.2](#page-24-0) and [1.4,](#page-30-0) respectively). We observe that the theoretical arguments can be documented in fnite samples too. As such, the full sample version exhibits substantial bias due to overftting as its distribution is shifted away from the true value of the CATE parameter, but with a rather low variance. On the contrary, the double sample-splitting version successfully eliminates the overftting bias as the simulated distribution is centered around the true value of the CATE, however with much larger variance. Finally, the double cross-ftting version keeps the reduction in bias whilst having a much lower variance in comparison to the double sample-splitting version as the spread of the CATE distribution comes close to the full sample version, indicating the gain in efficiency of this procedure.

¹¹ For results in the context of the Lasso estimation under sparsity see Belloni, Chernozhukov, Fernandez-Val, and Hansen [\(2017\)](#page-50-16).

 12 Increasing the efficiency of a sample-splitting based estimator by swapping the roles of the data samples and averaging the resulting estimates goes back to Schick [\(1986\)](#page-54-13) in the context of estimation of semi-parametric models.

Figure 1.3.1: CATE distributions under full-sample, sample-splitting and cross-ftting estimation.

Note: Distributions of the CATE parameter under full-sample estimation (blue), double sample-splitting (red) and double cross-ftting (green) as a result of a Monte Carlo simulation. The CATE distributions are smoothed with the Gaussian kernel using the Silverman's bandwidth. The dashed black line defnes the true value of the CATE while the solid black line plots the normal distribution around the true parameter with variance of the estimated CATE distribution. The CATEs are estimated by the DR-learner based on a training sample of $N^T = 32'000$ observations with 250 simulation replications and predicted out-of-sample. Detailed description of the simulation design is given in Section [1.4,](#page-30-0) while a detailed description of the DR-learner is given in Section [1.3.2.](#page-24-0)

Apart from the illustrative example above, the empirical question remains the precise quantifcation of this bias-variance trade-of for various meta-learners and to what degree this might vary with diferent sample sizes. Diferent meta-learners use diferent nuisance functions in diferent ways which might have an infuence on the performance under the particular estimation procedures. Even though sample-splitting and cross-ftting help to eliminate the overftting bias, in fnite samples less data available for estimation might even lead to higher bias due to errors in learning the CATE function itself, especially for small sample sizes. In this paper we address this open question via Monte Carlo simulations and compare the performance of various meta-learners under full-sample, double sample-splitting and double cross-ftting procedure for several diferent sample sizes to shed more light onto the fnite sample properties. We follow Newey and Robins [\(2018\)](#page-53-11) and choose the double sample-splitting, respectively double cross-ftting procedure due to its theoretically faster convergence rates. Furthermore, we opt for the setting with equally sized $K = M + 1$ folds as suggested by Kennedy [\(2020\)](#page-52-2). Additionally, we always distinguish between the training and validation data. We use the training data for learning the nuisance function and the CATE function, including the double sample-splitting and double cross-ftting procedure, while we evaluate the CATEs on a set of new validation data. An illustration of the data usage under full-sample estimation, double sample-splitting and double cross-ftting procedure is provided in Figure [1.3.2.](#page-24-1)

Further motivation for the usage of sample-splitting and cross-ftting stems from the theoretical arguments for conducting statistical inference about the causal parameters of interest. As such, samplesplitting plays a crucial role in obtaining estimators that are not only approximately unbiased but also normally distributed which in turn allows for a valid construction of confdence intervals. In this vein, Chernozhukov et al. [\(2018\)](#page-51-0) provide results for the estimators of average treatment efect (ATE) that rely on sample-splitting and cross-ftting procedures. Semenova and Chernozhukov [\(2021\)](#page-54-8) and Zimmert and Lechner [\(2019\)](#page-55-2) extend this analysis for parametric and nonparametric estimators of group average treatment efects (GATEs), respectively. In the context of Causal Forests, Wager and Athey [\(2018\)](#page-54-0), Lechner [\(2018\)](#page-53-0), and Athey et al. [\(2019\)](#page-50-6) also rely on sample-splitting procedures termed 'honesty' to provide inference for causal efects on various levels of aggregation. Nonetheless, in the context of metalearning estimation of causal efects, there appears to be lack of unifying model-free theory for conducting statistical inference so far. One exception is the study by Künzel et al. [\(2019\)](#page-53-2) that analyses various

Figure 1.3.2: Illustration of the full-sample, sample-splitting and cross-ftting procedure.

Note: Illustration of the full-sample (left), double sample-splitting (middle) and double cross-ftting (right) procedures with $K = 3$ folds. The propensity score function is defined by $e(x)$, the response functions in general are denoted by $\mu(x)$ and the CATE function is characterized by $\tau(x)$. Subscripts for the nuisance functions and the CATE function correspond to the fold used for estimation, while the colors indicate the combination of the estimated functions across diferent folds.

versions of bootstrapping for estimation of standard errors for the CATEs. Recently, Jacob [\(2021\)](#page-52-8) makes use of such bootstrapping procedures to construct confdence intervals in an empirical application. Besides the computational burden, however, none of the bootstrapping procedures studied by Künzel et al. [\(2019\)](#page-53-2) seems to reliably provide accurate coverage rates. However, the meta-learners analyzed in Künzel et al. [\(2019\)](#page-53-2) do not make use of sample-splitting, which could potentially improve the performance of the bootstrapping for estimation of standard errors, given the insights from the related literature. While we do study the properties of the distribution of the CATEs within the simulation experiments in Section [1.4,](#page-30-0) we do not further analyse the estimation of standard errors mainly due to computational reasons and focus primarily on the point estimators. However, apart from the computational aspects, we note that combining sample-splitting and cross-ftting with bootstrapping for statistical inference about causal efects within the meta-learning framework might be a promising avenue for future research.

1.3.2 Meta-Learners

In the following, we review the meta-learning algorithms for estimation of heterogeneous treatment effects and discuss their advantages and disadvantages in particular empirical settings.

1.3.2.1 S-learner

The first meta-learning algorithm we investigate is the S-learner as denoted by Künzel et al. [\(2019\)](#page-53-2). According to their naming convention, S- stands for Single as this meta-learner involves only one single model, namely the full response function, $\mu(x, w)$, that needs to be estimated. In the epidemiology literature the S-learner is also sometimes referred to as g-computation (Robins, [1986;](#page-53-13) Snowden, Rose, & Mortimer, [2011\)](#page-54-14). The fnal causal efect is, in this case, obtained as a diference between predictions of the response function with setting the treatment indicator to, $W_i = 1$, and $W_i = 0$, respectively. The algorithm can be described as follows:[13](#page-25-0)

Input: Training Data: $\{(X_i, Y_i, W_i)\}^T$, Validation Data: $\{(X_i)\}^V$ Output: CATE: $\hat{\tau}_S(x) = \hat{E}[Y_i(1) - Y_i(0) | X_i = x]$ begin RESPONSE FUNCTION: estimate: $\mu(x, w) = E[Y_i \mid X_i = x, W_i = w]$ in $\{(X_i, Y_i, W_i)\}^T$; CATE FUNCTION; define: $\hat{\tau}_S(x) = \hat{\mu}(x, 1) - \hat{\mu}(x, 0);$ predict: $\hat{\tau}_S(X_i) = \hat{\mu}(X_i, 1) - \hat{\mu}(X_i, 0)$ in $\{(X_i)\}^V$ end

As can be seen from Algorithm [1,](#page-25-1) the S-learner does not assign any special role to the treatment indicator W_i within the estimation procedure and uses it only *post hoc* in the computation of the causal effect. Thus, if the treatment indicator is not strongly predictive for the outcome the S-learner will tend to estimate a zero treatment efect.[14](#page-25-2) Nevertheless, the S-learner will perform particularly well if the true CATE function is indeed zero, i.e. if $\tau(x) = 0$, which has also been documented in the simulation experiments of Künzel et al. [\(2019\)](#page-53-14). For the forest based S-learner, Künzel (2019) proposes a modification of the algorithm such that it shrinks towards the ATE instead of zero by performing a Ridge regression in the final leaves of the trees within the forest.^{[15](#page-25-3)} In our simulations, we study a simpler modification of the forest based S-learner by always including the treatment indicator in the random subset of covariates when determining the splits. By doing so, we always give the S-learner the chance to split on the treatment indicator which might potentially alleviate the zero-bias issue. We will henceforth denote such learner as the SW-learner, where the W refects the enforcement of the treatment indicator into the splitting set of covariates. We discuss the behaviour of the SW-learner more closely throughout the simulation results in Section [1.4.3.](#page-37-0) Furthermore, notice that the Algorithm [1](#page-25-1) consists of only one nuisance function that needs to be estimated and thus does not require any sample-splitting or cross-ftting within the training sample induced by multiple nuisance functions, hence it always has access to the full sample of the training data.[16](#page-25-4)

¹³As a matter of notation, we refer to the training data used for model estimation with superscript ^T as $\{(X_i, Y_i, W_i)\}^T$ and the validation data used for effect prediction with superscript ^V as $\{(X_i)\}^V$.

 14 Künzel et al. [\(2019\)](#page-53-2) argue that the S-learner is actually biased towards zero.

 15 For a detailed explanation of this procedure see Künzel [\(2019\)](#page-53-14).

 16 Nevertheless, an optional additional sample-splitting or cross-fitting could potentially improve the performance of the Slearner by reducing the possible overftting of the base learner as such. This is, however, beyond the scope of our analysis and is left for future research.

1.3.2.2 T-learner

The T-learner is another common and widely used meta-learner that we investigate in our study. In the literature it is sometimes also called as the *basic* (Lechner, [2018\)](#page-53-0), *plug-in* (Kennedy, [2020\)](#page-52-2) or naive (Nie & Wager, [2021\)](#page-53-3) CATE estimator. According to Künzel et al. [\(2019\)](#page-53-2), T- stands for Two as this meta-learner involves two models that need to be estimated, defined by the treatment indicator W_i . These are namely the response function in the treated sample, $\mu(x, 1)$, and the response function in the control sample, $\mu(x, 0)$. This is in contrast to the above S-learner which pools the two response functions into a single one. However, similarly to the S-learner the causal efect is computed as a diference in predictions of the two response functions, which is motivated by the identifcation result as in Equation $(1.2.4)$. The algorithm can be summarized as follows:^{[17](#page-26-0)}

Algorithm 2: T-learner

Input: Training Data: $\{(X_i, Y_i, W_i)\}^T$, Validation Data: $\{(X_i)\}^V$ **Output:** CATE: $\hat{\tau}_T(X_i) = \hat{E}[Y_i(1) - Y_i(0) | X_i = x]$ begin RESPONSE FUNCTIONS; estimate: $\mu(x, 1) = E[Y_i | X_i = x, W_i = 1]$ in $\{(X_i, Y_i)\}_{W_i=1}^T$; estimate: $\mu(x, 0) = E[Y_i \mid X_i = x, W_i = 0]$ in $\{(X_i, Y_i)\}_{W_i=0}^T$; CATE FUNCTION; define: $\hat{\tau}_T(x) = \hat{\mu}(x, 1) - \hat{\mu}(x, 0);$ predict: $\hat{\tau}_T(X_i) = \hat{\mu}(X_i, 1) - \hat{\mu}(X_i, 0)$ in $\{(X_i)\}^V$ end

Hence the T-learner uses the treatment indicator to split the estimation of the response function into two parts. This procedure is expected to work particularly well if the CATE function is complicated and there are no common trends in the response functions. This phenomenon fnds supportive evidence in several simulation studies (see for example Künzel et al., [2019;](#page-53-2) Jacob, [2020;](#page-52-4) Curth & van der Schaar, [2021;](#page-51-2) or Nie & Wager, [2021\)](#page-53-3). Nonetheless, it is expected to work rather poorly if the CATE function is simple, as the response functions are not trained jointly and thus their diference might be unstable (Lechner, [2018;](#page-53-0) Kennedy, [2020;](#page-52-2) Nie & Wager, [2021\)](#page-53-3). In terms of the estimation of the nuisance functions, the T-learner behaves similarly to the S-learner, as only the response functions need to be estimated to compute the CATE. As such no additional sample-splitting induced by multiple nuisance functions is required as the response functions are themselves estimated on separate samples defned by treated and control.[18](#page-26-1)

1.3.2.3 X-learner

The above mentioned problems of the T-learner are aggravated if the treatment assignment is highly unbalanced, meaning that the vast majority of observations in the sample belongs to only one treatment status. Künzel et al. [\(2019\)](#page-53-2) therefore propose the X-learner which addresses this issue. The X-learner builds on the T-learner and, as such, first estimates the two response functions $\mu(x, 1)$ and $\mu(x, 0)$. It then uses these estimates to impute the unobserved individual treatment effects for the treated, $\tilde{\xi}_i^1$, and the control, $\tilde{\xi}_i^0$. The imputed effects are in turn used as pseudo-outcomes to estimate the treatment effects in

¹⁷Notationwise, we refer to a subset of the data defined by a specific value of the variable as for example $W_i = 1$ by a subscript as $\{(X_i, Y_i)\}_{W_i=1}$.

¹⁸Again, this does not preclude that an optional sample-splitting or cross-fitting might be beneficial for the same reason as in the case of the S-learner (Jacob, [2020,](#page-52-4) provides some results on this issue for the T-learner). Using an honest forest as a base learner would also add an implicit sample-splitting procedure, however, this is not analysed herein.

the treated sample, $\tau(x, 1)$, and the control sample, $\tau(x, 0)$, respectively. The final CATE estimate $\tau(x)$ is then a weighted average of these treatment effect estimates weighted by the propensity score, $e(x)$.^{[19](#page-27-0)} Thus the X-learner additionally uses the information from the treated to learn about the controls and vice-versa in a Cross regression style, hence the X term in its naming label. The learning algorithm can be detailed as follows:

Algorithm 3: X-learner

Input: Training Data: $\{(X_i, Y_i, W_i)\}^T$, Validation Data: $\{(X_i)\}^V$ **Output:** CATE: $\hat{\tau}_X(X_i) = \hat{E}[Y_i(1) - Y_i(0) | X_i = x]$ begin RESPONSE FUNCTIONS; estimate: $\mu(x, 1) = E[Y_i | X_i = x, W_i = 1]$ in $\{(X_i, Y_i)\}_{W_i=1}^T$; estimate: $\mu(x, 0) = E[Y_i \mid X_i = x, W_i = 0]$ in $\{(X_i, Y_i)\}_{W_i=0}^T$; IMPUTED EFFECTS; predict: $\tilde{\xi}_i^1 = Y_i - \hat{\mu}(X_i, 0)$ in $\{(X_i, Y_i)\}_{W_i=1}^T$; predict: $\tilde{\xi}_i^0 = Y_i - \hat{\mu}(X_i, 1)$ in $\{(X_i, Y_i)\}_{W_i=0}^T$; TREATMENT EFFECTS: estimate: $\tau(x, 1) = E[\tilde{\xi}_i^1 | X_i = x, W_i = 1]$ in $\{(X_i, Y_i)\}_{W_i=1}^T$; estimate: $\tau(x, 0) = E[\tilde{\xi}_i^0 | X_i = x, W_i = 0]$ in $\{(X_i, Y_i)\}_{W_i=0}^T$; PROPENSITY SCORE; estimate: $e(x) = P[W_i = 1 | X_i = x]$ in $\{(X_i, W_i)\}^T$; CATE FUNCTION: define: $\hat{\tau}_X(x) = \hat{e}(x) \cdot \hat{\tau}(x,0) + (1 - \hat{e}(x)) \cdot \hat{\tau}(x,1);$ predict: $\hat{\tau}_X(X_i) = \hat{e}(X_i) \cdot \hat{\tau}(X_i, 0) + (1 - \hat{e}(X_i)) \cdot \hat{\tau}(X_i, 1)$ in $\{(X_i)\}^V$ end

According to Algorithm [3,](#page-27-1) the X-learner, in contrast to the T-learner, frstly uses the response functions for imputing the unobserved individual treatment efects instead of directly estimating the CATE. Secondly, these imputed individual treatment efects are used for estimating the CATE and reweighted by the propensity scores. The reweighting helps to put more weight on the treatment efects which have been estimated more precisely, i.e. the ones coming from the larger treated or control sample, respectively. For this reason, the X-learner is expected to work particularly well in unbalanced settings, which is often the case in practice as the share of treated might be restricted fnancially or otherwise (see Gerber, Green, & Larimer, [2008;](#page-51-13) Broockman & Kalla, [2016;](#page-51-14) or Goller, Lechner, Moczall, & Wolf, [2020,](#page-51-15) for such unbalanced empirical settings). Furthermore, by directly estimating the treatment efects in the second step it enables the estimator to learn structural properties of the CATE function from the data and is thus expected to work well if the CATE function is approximately linear or sparse (Künzel et al., 2019). In simulations of Künzel et al. (2019) (2019) the X-learner performs reasonably well even in other nonfavourable settings. Notice further that Algorithm [3](#page-27-1) requires more estimation steps than the previous two meta-learners. Additionally to the estimation of the response functions, the X-learner requires the estimation of the treatment efect functions as well as the propensity score function. This raises the question of possible overftting and hence the need for sample-splitting and cross-ftting, respectively. However, there is theoretically no explicit requirement for sample-splitting in the case of the X-learner

 19 In the original definition of the X-learner, the estimation of the propensity score is not exactly specified as it could be any weighting function in general. However, in practice the estimation of the propensity score is recommended (Künzel et al., [2019\)](#page-53-2).

when estimating the nuisance functions, apart from training and validation data split (Künzel et al., [2019\)](#page-53-2). Yet, it might well be that the sample-splitting and further cross-ftting have a non-negligible infuence on the performance of the learner in fnite samples. We address this issue by implementing the double sample-splitting and double cross-ftting version of the X-learner in the simulation study. For the case of the full-sample estimation we use the out-of-bag predictions of the underlying forest as estimates of the nuisance functions. The out-of-bag predictions are based on the observations that have been left 'out of the bag' when drawing bootstrap samples to estimate the trees of the forest (Hastie et al., [2009\)](#page-52-15). Such observations, however, randomly appear both as training as well as validation observations and thus such out-of-bag predictions are neither the classical in-sample ftted values nor proper out-of-sample predictions.[20](#page-28-0)

1.3.2.4 DR-learner

Although the X-learner makes use of the estimation of multiple nuisance functions, it does not provide the double robustness property which exploits the fact that the estimator remains consistent if either the response function or the propensity score function is misspecifed (Kennedy, Ma, McHugh, & Small, [2017;](#page-52-16) Lee, Okui, & Whang, [2017\)](#page-53-15). Recently, Kennedy [\(2020\)](#page-52-2) proposed the DR-learner where DR symbolizes the Double Robustness property of the learner. The DR-learner constructs a doubly robust score in the frst estimation stage and estimates the CATE in the second stage. There have been many other versions of the DR-learner proposed in the literature, but these were restricted to a particular estimator used in the second stage and are thus not part of the meta-learning framework. For example, Semenova and Chernozhukov [\(2021\)](#page-54-8) propose a linear estimation of the CATE function, whereas a local-constant estimation is proposed by Zimmert and Lechner [\(2019\)](#page-55-2) and Fan, Hsu, Lieli, and Zhang [\(2020\)](#page-51-16), which works well for the estimation of GATEs, i.e. for low-dimensional conditioning set. The main advantage of the DR-learner in comparison to the other versions lies in the general model-free second stage with sharper error bounds and weaker conditions for oracle efficiency (see Kennedy, [2020,](#page-52-2) for details). How-ever, common to all versions in the literature is the estimation of the doubly robust score^{[21](#page-28-1)} by machine learning methods in the frst stage also known as Double Machine Learning (Chernozhukov et al., [2018\)](#page-51-0). For a comprehensive overview of the CATE estimators building on the doubly robust score see Knaus [\(2020\)](#page-52-17). The specifc algorithm for the DR-learner is then defned as follows:

 $^{20}\rm{We}$ use the out-of-bag predictions for all meta-learners within our analysis.

²¹ Also called efficient score or efficient influence function in the literature (Robins & Rotnitzky, [1995;](#page-53-16) Hahn, [1998\)](#page-51-12).

Algorithm 4: DR-learner

Input: Training Data: $\{(X_i, Y_i, W_i)\}^T$, Validation Data: $\{(X_i)\}^V$ **Output:** CATE: $\hat{\tau}_{DR}(x) = \hat{E}[Y_i(1) - Y_i(0) | X_i = x]$ begin RESPONSE FUNCTIONS: estimate: $\mu(x, 1) = E[Y_i \mid X_i = x, W_i = 1]$ in $\{(X_i, Y_i)\}_{W_i=1}^T$; estimate: $\mu(x, 0) = E[Y_i \mid X_i = x, W_i = 0]$ in $\{(X_i, Y_i)\}_{W_i=0}^T$; PROPENSITY SCORE; estimate: $e(x) = P[W_i = 1 | X_i = x]$ in $\{(X_i, W_i)\}^T$; PSEUDO OUTCOME; predict: $\hat{\psi}_i = \frac{W_i(X_i - \hat{\mu}(X_i, 1))}{\hat{e}(X_i)} - \frac{(1 - W_i)(Y_i - \hat{\mu}(X_i, 0))}{1 - \hat{e}(X_i)} + \hat{\mu}(X_i, 1) - \hat{\mu}(X_i, 0) \text{ in } \{(X_i, Y_i, W_i)\}^T;$ CATE FUNCTION: estimate: $\tau_{DR}(x) = E[\hat{\psi}_i | X_i = x]$ in $\{(X_i, Y_i, W_i)\}^T$; predict: $\hat{\tau}_{DR}(X_i) = \hat{E}[\hat{\psi}_i | X_i = x]$ in $\{(X_i)\}^V$ end

As can be seen in Algorithm [4](#page-29-0) above, the DR-learner estimates the very same nuisance functions, $\mu(x, 0), \mu(x, 1)$ and $e(x)$, as the X-learner but uses them in a completely different manner. It combines the nuisance functions as well as the outcome and treatment data in a doubly robust way to construct the pseudo-outcome ψ_i , i.e. the doubly robust score. The score is then regressed on the covariates to estimate the fnal CATE function. Therefore, the DR-learner can also adapt to structural properties of the CATE such as smoothness or sparsity. For this reason the DR-learner is expected to work well in similar situations as the X-learner with a more balanced treatment assignment, as too extreme propensity scores might possibly yield the estimator unstable (Huber et al., [2013;](#page-52-3) Powers et al., [2018\)](#page-53-6), especially in high dimensions (D'Amour, Ding, Feller, Lei, & Sekhon, [2021\)](#page-51-17). Moreover, it should have an additional advantage over the X-learner thanks to its double robustness property. The simulations of Kennedy [\(2020\)](#page-52-2) also suggest a faster convergence rate of the DR-learner in comparison to the X- and T-learner. In order to achieve the optimal rates the DR-learner explicitly requires the double sample-splitting as defned by Newey and Robins [\(2018\)](#page-53-11), while the double cross-ftting procedure remains optional. Theoretically it is not clear how important the role of the optional cross-ftting is for the DR-learner in fnite samples and how much of the efficiency loss due to sample-splitting can be thereby regained. In order to shed light on this issue we investigate the implementations of the DR-learner with double sample-splitting, double cross-ftting, as well as a version with full-sample estimation.

1.3.2.5 R-learner

Yet another approach of frst estimating nuisance functions and then using them to learn the treatment efects stems from the literature on partially linear model originally developed by Robinson [\(1988\)](#page-53-17). Nie and Wager [\(2021\)](#page-53-3) build on these ideas to fexibly estimate heterogeneous treatment efects and develop the R-learner, where the R stands for the recognition of the contribution of Robinson (1988) as well as for the Residualization approach. In the first step, the R-learner estimates the full response function, $u(x)$, similarly to the S-learner but without conditioning on the treatment indicator, as well as the propensity score function $e(x)$. It then residualizes the outcome and the treatment by the predictions of the response and the propensity score function, respectively, to construct a modifed outcome. In the second step, the R-learner regresses the modifed outcome on the covariates, weighted by the squared

residualized treatment^{[22](#page-30-1)}, i.e. $(W_i - \hat{e}(X_i))^2$, to estimate the CATE function (Schuler, Baiocchi, Tibshirani, & Shah, [2018\)](#page-54-15). Analogous transformation of the outcome is also used by the Causal Forest of Athey et al. [\(2019\)](#page-50-6) termed local centering, or in the G-estimation for sequential trials by Robins [\(2004\)](#page-53-18). The full estimation procedure of the R-learner can be summarized as follows:

Algorithm 5: R-learner

Input: Training Data: $\{(X_i, Y_i, W_i)\}^T$, Validation Data: $\{(X_i)\}^V$ **Output:** CATE: $\hat{\tau}_R(x) = \hat{E}[Y_i(1) - Y_i(0) | X_i = x]$ begin RESPONSE FUNCTION; estimate: $\mu(x) = E[Y_i \mid X_i = x]$ in $\{(X_i, Y_i)\}^T$; PROPENSITY SCORE; estimate: $e(x) = P[W_i = 1 | X_i = x]$ in $\{(X_i, W_i)\}^T$; MODIFIED OUTCOME: predict: $\hat{\phi}_i = \frac{\left(Y_i - \hat{\mu}(X_i)\right)}{\left(\frac{V_i - \hat{\mu}(X_i)}{\sigma}\right)}$ $\frac{(Y_i-\mu(X_i))}{(W_i-\hat{e}(X_i))}$ in $\{(X_i,Y_i,W_i)\}^T$; CATE FUNCTION; estimate: $\tau_R(x) = E[\hat{\phi}_i \mid X_i = x]$ weighted by $(W_i - \hat{e}(X_i))^2$ in $\{(X_i, Y_i, W_i)\}^T$; predict: $\hat{\tau}_R(X_i) = \hat{E}[\hat{\phi}_i \mid X_i = x]$ in $\{(X_i)\}^V$ end

As follows from Algorithm [5,](#page-30-2) the R-learner separates the estimation into two steps. First, it eliminates the spurious correlations between the response function $\mu(x)$ and the propensity score function $e(x)$ and second, it optimizes the CATE function $\tau_R(x)$. From this standpoint the R-learner follows a related estimation scheme as the DR-learner and is expected to work well in similar settings where the nuisance functions as well as the CATE function might have a high degree of complexity. A possible advantage of the R-learner over the DR-learner might stem from the additional weighting which reduces the impact of extreme propensity scores as pointed out by Jacob [\(2021\)](#page-52-8). In their simulation experiments, Nie and Wager [\(2021\)](#page-53-3) show good performance of the R-learner in settings with complicated nuisance functions and rather simple CATE function. Furthermore, for the theoretical results Nie and Wager [\(2021\)](#page-53-3) explicitly require sample-splitting and cross-ftting, respectively. In particular, they advocate for a 5- or 10-fold cross-ftting procedure as defned by Chernozhukov et al. [\(2018\)](#page-51-0). In order to examine the importance of the cross-ftting in fnite samples we compare the performance of the R-learner as in the above cases with full-sample estimation, double sample-splitting and double cross-ftting, respectively.

1.4 Simulation Study

We study the fnite sample performance of meta-learners for estimation of heterogeneous treatment efects based on Random Forests (Breiman, [2001;](#page-50-8) see also Biau & Scornet, [2016,](#page-50-17) for a comprehensive introduction). The focus of the Monte Carlo study lies in an assessment of the infuence of sample-splitting and cross-ftting in the causal efect estimation. For this purpose we compare the above discussed metalearners estimated with full-sample, double sample-splitting, and double cross-ftting. We rely on the Random Forest as the base learner for all meta-learners for several reasons. First, diferent meta-learners

 22 An estimation procedure without the weighting step is in literature referred to as the U-learner (Stadie et al., [2018;](#page-54-1) Künzel et al., [2019;](#page-53-2) Nie & Wager, [2021\)](#page-53-3). However, such estimator turned out to be quite unstable in the simulation experiments in Nie and Wager [\(2021\)](#page-53-3) as well as in those of Künzel et al. [\(2019\)](#page-53-2) and will thus not be considered further in our analysis.

require estimation of diferent nuisance functions which involve diferent types of outcome variables. As such, the response functions mostly involve a continuous outcome variable whereas the propensity score function includes a binary outcome. Hence, when using Random Forests no additional adjustments need to be done in terms of estimation as it automatically estimates probabilities in case of binary outcome and expected values in case of continuous outcomes, respectively. This is in contrast to linear learners such as the Lasso (Tibshirani, [1996\)](#page-54-16), Ridge (Hoerl & Kennard, [1970\)](#page-52-18) or Elastic Net (Zou & Hastie, [2005\)](#page-55-4) where the estimator needs to be modifed using appropriate link function for proper probability estimation (see for example Hastie et al., [2009,](#page-52-15) for the Logit-Lasso). Second, Random Forest is a local nonparametric method which does not need any data pre-processing to fexibly learn the underlying functional form from the data (Hastie et al., [2009\)](#page-52-15). Thus, Random Forest is able to approximate any function with diferent degrees of complexity which is often the case in treatment efect estimation where the nuisance functions tend to be rather difcult complex functions while the CATE function itself is often simple and sparse (Künzel et al., [2019;](#page-53-2) Kennedy, [2020\)](#page-52-2). This is again an advantage in comparison to the linear learners mentioned above which become more fexible once an augmented covariate set consisting of polynomials and interactions is created and thus can be regarded as global nonparametric methods (Hastie et al., [2009\)](#page-52-15). Third, in contrast to other fexible state-of-the-art machine learners such as Neural Networks the theoretical properties of Random Forest are better understood which makes it less of a black-box method and thus more amenable to conduct statistical inference (see Meinshausen, [2006;](#page-53-19) Biau, [2012;](#page-50-18) Wager, Hastie, & Efron, [2014;](#page-54-17) Wager, [2014;](#page-54-18) Scornet, Biau, & Vert, [2015;](#page-54-19) Mentch & Hooker, [2016;](#page-53-20) Wager & Athey, [2018;](#page-54-0) Athey et al., [2019,](#page-50-6) for a discussion of statistical properties of Random Forests). Additionally, another reason why we do not use the Lasso and the linear learners as such is due to a substantial increase in variance as they are prone to outliers as documented in the simulation studies of Jacob [\(2020\)](#page-52-4) as well as Knaus et al. [\(2021\)](#page-53-4). Lastly, from the practical standpoint there is a vast variety of fast and reliable software implementations of Random Forests which makes it easy to use for practitioners.[23](#page-31-0)

In order to objectively evaluate the performance and the robustness of diferent meta-learners in estimating heterogeneous treatment efects with regard to the double sample-splitting and double crossftting, we design several simulation scenarios. On the one hand, for each meta-learner we construct such a data generating process (DGP) that suits the particular advantages of the respective meta-learner, i.e. we design a simulation scenario where each meta-learner is expected to work best. Hence, we are able to check if the particular meta-learner outperforms the others and how big the performance discrepancies are for the other meta-learners in comparison to the expected best performing meta-learner. On the other hand, we design a challenging scenario where none of the meta-learners has a priori an explicit advantage, which serves as our main simulation design of interest. Thus we can compare the performance of the meta-learners in an objective manner and quantify the deviations to their respective best performance cases. Furthermore, common to all DGPs is the observational study design, i.e. there is always selection into treatment and thus all considered meta-learners have to deal with confounding and not only with modelling the treatment efect itself. Moreover, in contrast to many simulation studies where the nuisances are simple low-dimensional functions (Wager & Athey, [2018;](#page-54-0) Künzel et al., [2019;](#page-53-2) Kennedy, [2020\)](#page-52-2), we model all nuisance functions as highly non-linear but sparse functions with largedimensional covariate space to both challenge the potential of the machine learning methods, though still largely obeying the theory induced limitations. For other challenging simulation designs see also Jacob [\(2020\)](#page-52-4) or Zivich and Breskin [\(2021\)](#page-55-1) as well as Lechner [\(2018\)](#page-53-0) and Knaus et al. [\(2021\)](#page-53-4) for the Empiri-

 23 In our simulations we use the R-package ranger which provides a fast C++ implementation of Random Forests, particularly suited for high-dimensional data (Wright & Ziegler, [2017\)](#page-55-5). Further options include the grf package written by Tibshirani et al. [\(2018\)](#page-54-20), the forestry package by Künzel, Liu, Saarinen, Tang, and Sekhon [\(2020\)](#page-53-21) or the randomForest package by Liaw and Wiener [\(2002\)](#page-53-22).

cal Monte Carlo Simulations. Importantly, in order to study the approximate convergence rates of the meta-learners we repeat each simulation scenario several times with increasing training sample sizes using $N^T = \{500, 2'000, 8'000, 32'000\}$. We emphasize that the considered sample sizes substantially exceed the ones from previous simulation studies devoted to the analysis of sample-splitting methods, which were limited to 2'000 (Jacob, [2020\)](#page-52-4) and 3'000 (Zivich & Breskin, [2021\)](#page-55-1) observations, respectively. Furthermore, the large samples enable us to study the performance of the meta-learners in settings in which the application of machine learning methods is arguably more relevant. We choose to always quadruple the sample size, which allows us to easily benchmark the results with the parametric \sqrt{N} rate, in which case the estimation error is expected to halve with each increase of the sample size. We then evaluate the performance measures on a validation set with sample size of $N^V = 10'000$ to reduce the prediction noise as is usual in many Monte Carlo studies (Janitza, Tutz, & Boulesteix, [2016;](#page-52-19) Hornung, [2019;](#page-52-20) Lechner & Okasa, [2019;](#page-53-23) Jacob, [2020;](#page-52-4) Knaus et al., [2021\)](#page-53-4). Lastly, in terms of the tuning parameters for the Random Forest base-learner we stick to the default, in the literature commonly used settings, corresponding to 1'000 trees, the number of randomly chosen split variables set to the square root of number of features, and the minimum leaf size equal to $5.^{24}$ $5.^{24}$ $5.^{24}$ Finally, for each DGP we simulate the training data $R = \{2'000, 1'000, 500, 250\}$ times in total, where we use $2'000$ replications for the smallest sample size and decrease the number of replications down to 250 for the largest sample size, due to computational reasons.[25](#page-32-2)

1.4.1 Performance Measures

For the evaluation of the performance of the considered meta-learners with regard to the samplesplitting and cross-ftting in detail, we employ several evaluation measures. First, to assess the overall estimator performance we compute the root mean squared error for each observation i from the validation sample over the R simulation replications:^{[26](#page-32-3)}

$$
RMSE(\hat{\tau}(X_i)) = \sqrt{\frac{1}{R}\sum_{r=1}^{R} (\tau(X_i) - \hat{\tau}^r(X_i))^2}.
$$

Next, we decompose the root mean squared error and evaluate the bias and variance component separately to contrast the theoretically expected asymptotic behaviour of sample-splitting and cross-ftting with the fnite sample properties. Hence, we additionally compute the mean absolute bias:

$$
|BIAS(\hat{\tau}(X_i))| = \frac{1}{R} \sum_{r=1}^{R} |\tau(X_i) - \hat{\tau}^r(X_i)|
$$

as well as the standard deviation of the treatment efects:

$$
SD(\hat{\tau}(X_i)) = \sqrt{\frac{1}{R} \sum_{r=1}^{R} (\hat{\tau}^r(X_i) - \frac{1}{R} \sum_{r=1}^{R} \hat{\tau}^r(X_i))}
$$
.

 24 We refrain from cross-validation or other tuning parameter optimization procedures due to computational constraints. We recommend such optimization in the applied work as it might considerably improve the performance of the estimator (see Curth $\&$ van der Schaar, [2021,](#page-51-2) for an evidence based on Neural Networks), however, for the purposes of the simulation study it would not change the relative ranking of the meta-learners as each of them uses the very same base learner.

 25 Notice, however, that we only halve the number of replications while quadrupling the sample size and as such we may limit a possible deterioration of the performance in terms of the simulation error. A similar strategy for balancing the precision and the computational burden has been used in the simulations by Lechner [\(2018\)](#page-53-0) or Knaus et al. [\(2021\)](#page-53-4). Detailed results on the simulation error are provided in Appendix [1.B.2.](#page-70-0)

 26 We take the square root of the MSE to have the same scale as for the other performance measures, i.e. the absolute bias and the standard deviation.

Furthermore, inspired by the simulation study of Knaus et al. [\(2021\)](#page-53-4) we also compute the Jarque-Bera statistic (Jarque & Bera, [1980;](#page-52-21) Bera & Jarque, [1981\)](#page-50-19) to test for the normality of the treatment efect predictions:[27](#page-33-1)

$$
JB(\hat{\tau}(X_i)) = \frac{R}{6} \bigg(S(\hat{\tau}(X_i))^2 + \frac{1}{4} (K(\hat{\tau}(X_i)) - 3)^2 \bigg)
$$

where $S(\hat{\tau}(X_i))$ and $K(\hat{\tau}(X_i))$ is the skewness and the kurtosis of the R treatment effect predictions for observation i , respectively. As a matter of presentation for CATEs, we report the mean values of the RMSE, absolute bias, standard deviation and the Jarque-Bera statistic over N^V validation observations.^{[28](#page-33-2)} Additionally, we provide evaluation of further performance measures in Appendix [1.B.2.](#page-70-0)

1.4.2 Simulation Design

In the general simulation design we follow Künzel et al. (2019) and specify the response functions for potential outcomes under treatment, $\mu_1(x)$, and control, $\mu_0(x)$, the propensity score, $e(x)$, and the treatment effect function, $\tau(x)$, respectively. First, we simulate a p-dimensional matrix of covariates $X_i \in \mathbb{R}^p$ drawing from the uniform distribution, as previously used in simulations of Wager and Athey (2018) , Künzel et al. (2019) or Nie and Wager (2021) among others, such that:

$$
X_i \sim \mathcal{U}\big([0,1]^{n \times p}\big)
$$

and defining the correlation structure according to Falk [\(1999\)](#page-51-18) using a random correlation matrix Σ_n generated by the method of Joe (2006) .^{[29](#page-33-3)} Second, we specify the response functions and simulate the potential outcomes as:

$$
Y_i(0) = \mu_0(X_i) + \epsilon_i(0)
$$

$$
Y_i(1) = \mu_1(X_i) + \epsilon_i(1)
$$

with errors $\epsilon_i(0), \epsilon_i(1) \stackrel{iid}{\sim} \mathcal{N}(0, 1)$ that are independent of the covariates X_i . Third, we define the propensity score function and simulate the treatment assignment according to:

$$
W_i \sim Bern\big(e(X_i)\big)
$$

and use the observational rule to set the observed outcomes such that:

$$
Y_i = W_i \cdot Y_i(1) + (1 - W_i) \cdot Y_i(0)
$$

to complete the observable triple $\{(X_i, Y_i, W_i)\}$. The subsequent simulation designs then differ only with respect to how the corresponding functions, namely $\mu_0(x), \mu_1(x), e(x)$ and $\tau(x)$ are specified. For all of our simulations we defne the response function under non-treatment according to the well-known Friedman function [\(1991\)](#page-51-19) to create a difficult yet standardized setting, which has been used also in the simulations of Nie and Wager [\(2021\)](#page-53-3), as follows:

$$
\mu_0(x) = \sin(\pi \cdot x_1 \cdot x_2) + 2 \cdot (x_3 - \frac{1}{2})^2 + x_4 + \frac{1}{2} \cdot x_5 \tag{1.4.1}
$$

²⁷See Thadewald and Büning [\(2007\)](#page-54-21) for a discussion of the Jarque-Bera test and its comparison to other tests for normality. ²⁸As such, we define the average RMSE as $\overline{RMSE} = \frac{1}{N} \sum_{i=1}^{N} RMSE(\hat{\tau}(X_i))$ and analogously for the remaining performance measures. Additionally, for the Jarque-Bera statistic we report also the share of CATEs from the validation sample for which the normality gets rejected at the 5% confdence level. For details, see Appendix [1.B.2.](#page-70-0)

 29 For a detailed correlation heat map of the covariates and further descriptive statistics of the simulated datasets see Appendix [1.A.](#page-56-1)

hence efectively creating a highly non-linear but sparse response function which is challenging to estimate on its own.[30](#page-34-0) The response function under treatment is then defned simply as:

$$
\mu_1(x) = \mu_0(x) + \tau(x)
$$

while we vary the specification of the treatment effect function $\tau(x)$ throughout our simulation designs. Lastly, we model the propensity score function similarly to Wager and Athey [\(2018\)](#page-54-0) and Künzel et al. [\(2019\)](#page-53-2) using the β distribution with parameters 2 and 4 such that:

$$
e(x) = \alpha \bigg(1 + \beta_{2,4} (f(x)) \bigg) \tag{1.4.2}
$$

while the scale parameter α controls the share of treated in the sample and at the same time helps to bound the resulting probabilities away from 0 and 1 and thus to avoid extreme propensity scores which might yield some meta-learners using such propensities for reweighting unstable (Huber et al., [2013;](#page-52-3) Powers et al., [2018\)](#page-53-6). We additionally make the propensity score dependent on features X_i of dimension p^e in a non-linear fashion using the functional form specification of Nie and Wager [\(2021\)](#page-53-3) and set:

$$
f(x) = \sin(\pi \cdot x_1 \cdot x_2 \cdot x_3 \cdot x_4)
$$

which creates a non-linear setting that is challenging to model as opposed to, e.g. polynomial transformations alone. Similarly, such non-linear transformations for the propensity scores using the sine function have been used also in simulations by Lechner [\(2018\)](#page-53-0) and Knaus et al. [\(2021\)](#page-53-4).

General Settings	
Number of DGPs Number of Replications R	6 $\{2'000, 1'000, 500, 250\}$
Training Sample N^T Validation Sample N^V	$\{500, 2'000, 8'000, 32'000\}$ 10'000
DGP Settings	
Covariate Space Dimension p	100
Signal Covariates in Response Function p^{μ}	5
Signal Covariates in Propensity Score Function p^e	4
Signal Covariates in Treatment Function p^{τ}	$\{0, 1, 2, 3\}$
Forest Settings	
Number of Trees	1'000
Random Subset of Split Covariates	
Minimum Leaf Size	5

Table 1.4.1: Overview of the Simulation Study

As a matter of notation we refer to p as the dimension of the covariate space, p^{μ} , p^e and p^{τ} as the dimension of the signal covariates in the response function, the propensity score function, and the CATE function, respectively. We set the aforementioned dimensions as follows: $p = 100$, $p^{\mu} = 5$, $p^e = 4$ and p^{τ} varies with forthcoming simulation designs. We note that such large-dimensional covariate set is quite unique as the majority of simulation studies relies on low-dimensional covariate sets (see e.g. Künzel et al., [2019;](#page-53-2) Jacob, [2020;](#page-52-4) or Nie & Wager, [2021\)](#page-53-3).[31](#page-34-1) We further defne the sets of covariates such that $X^{p^{\tau}} \subset X^{p^e} \subset X^{p^u} \subset X^p$. By doing so we make it difficult for the meta-learners to accurately fit the

³⁰Note that π refers to the mathematical constant, i.e. $\pi \approx 3.14$.

 31 An exception is the simulation study of Powers et al. [\(2018\)](#page-53-6) who explicitly study the estimation of heterogeneous treatment effects in high-dimensions.

functions and eliminate the spurious correlations between the response and propensity score functions. Moreover, it also becomes challenging to disentangle the confounding efects from the actual treatment efect heterogeneity which the herein discussed meta-learners are specifcally designed for. Finally, a general overview of the simulation study is provided in Table [1.4.1.](#page-34-2)

1.4.2.1 Simulation 1: balanced treatment and constant zero CATE

The frst simulation design features our complicated sparse non-linear nuisance functions as defned above in Equations [\(1.4.1\)](#page-33-4) and [\(1.4.2\)](#page-34-3) in contrast to a very simple CATE function. In fact, the treatment efect here is defned as being constant and equal to zero:

$$
\tau(x) = 0
$$

with a balanced treatment assignment with the scaling factor $\alpha = \frac{1}{4}$ which results in approximately 50% treated and 50% of control units. Such DGP with zero CATE serves as a benchmark and should implicitly suit the S-learner as the treatment indicator is not predictive for the outcome. Nevertheless the other meta-learners with the exception of the T-learner should be also capable of capturing the true zero efect as this is often a showcase example when motivating the particular meta-learners as well as simulating their performance (see Künzel et al., [2019;](#page-53-2) Kennedy, [2020;](#page-52-2) and Nie & Wager, [2021,](#page-53-3) for details).

1.4.2.2 Simulation 2: balanced treatment and complex nonlinear CATE

In the second simulation design we keep the balanced treatment allocation but feature a highly complex and non-linear CATE function resulting from a completely disjoint DGPs for the response function under treatment and under control. As such the response function under control is defned according to Equation [\(1.4.1\)](#page-33-4), while the response function under treatment is defned as a non-zero constant, i.e. $\mu_1(x) = 1$. The CATE is then defined as:

$$
\tau(x) = \mu_1(x) - \mu_0(x).
$$

Such simulation setups have been previously used also in Künzel et al. [\(2019\)](#page-53-2) or in Nie and Wager [\(2021\)](#page-53-3). In this case the response functions, $\mu_0(x)$ and $\mu_1(x)$, are uncorrelated and thus there is no advantage in pooling those two together. Rather, estimating these two functions separately is the best strategy as there is nothing additional to learn from the other treatment group. For this reason, the T-learner should perform best here, however the meta-learners which also estimate the response functions separately such as the X- and DR-learner are expected to perform well too. Clearly, other meta-learners such as the Sand R-learner which estimate the pooled response function have a disadvantage as they frst need to learn the disjoint structure.

1.4.2.3 Simulation 3: highly unbalanced treatment and constant non-zero CATE

In our third simulation design we change the scaling factor in the propensity score function to $\alpha = \frac{1}{12}$ such that we generate approximately 15% treated units.^{[32](#page-35-0)} We then model the treatment effect

 32 In contrast to Künzel et al. [\(2019\)](#page-53-2) we do not specify the treatment imbalance as extreme as 1% treated mostly for computational reasons. Due to our smallest sample size of $N = 500$ used in the simulations and the double sample-splitting procedure, it might occasionally happen that the estimated propensity scores would be exactly zero which would prevent estimation of the DR-learner as well as the R-learner due to the division by zero when constructing the pseudo-outcomes. In our specifcation, even with the share of the treated being 16.77% in expectation, the aforementioned issue with zero propensity scores still might occur. In such cases, we redraw the sample to ensure at least 15% of treated. However, this
as a constant as for example in Kennedy [\(2020\)](#page-52-0) or Nie and Wager [\(2021\)](#page-53-0) and thus create a scenario with highly complicated nuisance functions and very simple CATE function given as:

$$
\tau(x) = 1.
$$

Accordingly, the X-learner should perform best in this scenario given the high imbalance in the treatment assignment and the sparse CATE function at the same time. In contrast, other meta-learners using the propensity score for reweighting such as the DR- and R-learner might perform worse due to potentially extreme propensity scores close to the $\{0,1\}$ bounds. Furthermore, the T-learner is clearly disadvantaged in this scenario due to the high treatment imbalance as well as due to the simple CATE function, whereas the S-learner is not expected to work particularly well either due to the relatively bigger efect size bounded away from zero.

1.4.2.4 Simulation 4: unbalanced treatment and simple CATE

In our fourth simulation design we model the CATE function similarly to the above design as a simple non-zero constant and combine it with an indicator function as also used by Künzel et al. [\(2019\)](#page-53-1) to add more structure to the CATE. As such we defne the treatment efect as:

$$
\tau(x) = 1 + 1 \cdot \mathbb{1}(x_1 > 0.5)
$$

and otherwise keep the DGP same as in the third design while only increasing the share of treated to roughly 25% as is the case in the simulations of Nie and Wager [\(2021\)](#page-53-0) by setting $\alpha = \frac{1}{8}$. By doing so we should theoretically shift the advantage from the X-learner more onto the DR-learner as both metalearners are motivated by complex nuisance functions and a simple CATE function with the diference of the X-learner being designed particularly for highly unbalanced treatment allocation. Also the R-learner is expected to perform relatively well in this scenario due to the less unbalanced treatment shares, whereas the S- and T-learner are not expected to perform well for the same reasons as in the above situations.

1.4.2.5 Simulation 5: unbalanced treatment and linear CATE

The ffth simulation design features the same nuisance functions and treatment share as the fourth design, however, here instead of the indicator function we model the treatment efect as a low-dimensional linear function as:

$$
\tau(x) = 1 + \frac{1}{2}x_1 + \frac{1}{2}x_2
$$

as used in one of the simulation designs of Nie and Wager [\(2021\)](#page-53-0) where the R-learner performed best and as such it is also expected to have an advantage here. Yet again the X- and DR-learner should perform comparatively well in this setting while the S- and T-learner not so much for the very same reasons as stated above.

1.4.2.6 Main Simulation: unbalanced treatment and nonlinear CATE

In the last simulation design we create arguably the most challenging scenario in which none of the meta-learners has an a priori advantage and thus presents our main simulation design of interest. In this case not only the nuisances but also the CATE itself is modelled as a smooth non-linear function of a

occurs only a handful of times out of 2000 draws in total and only for the smallest sample size considered. Nie and Wager [\(2021\)](#page-53-0) also use similar restrictions on the propensity scores in their simulations due to the very same issue.

slightly larger dimension than in the previous settings, i.e. $p^{\tau} = 3$. Following Wager and Athey [\(2018\)](#page-54-0) we specify the CATE function as follows:

$$
\tau(x) = 1 + \frac{4}{p^{\tau}} \sum_{j=1}^{p^{\tau}} \left(\frac{1}{1 + e^{-12(x_j - 0.5)}} - \frac{1}{2} \right).
$$

We further keep the treatment share equal to about 25% and the nuisance functions as previously specified as well. Hence, the meta-learners need to frst account for the moderately imbalanced treatment shares, second accurately estimate the complex nuisance functions and disentangle their correlation, and third separate the treatment efect heterogeneity from the selection efects by precisely estimating the non-linear CATE function.

1.4.3 Simulation Results

For the analysis of the simulation results we focus on the Main Simulation design with unbalanced treatment assignment and nonlinear CATE function as this is arguably the most challenging simulation design which does not a priori create conditions that would be advantageous for any of the considered meta-learners. We then summarize the results for the rest of the simulation designs for which we provide the detailed results in Appendix [1.B.1.](#page-65-0) Supplementary results providing additional measures, including the simulation error, bias, skewness, kurtosis, share of CATEs for which the normality has been rejected, as well as the correlation and variance ratio of the estimated and the true CATEs are presented in Appendix [1.B.2.](#page-70-0)

1.4.3.1 Results of Main Simulation: unbalanced treatment and nonlinear CATE

The performance of the meta-learners in the Main Simulation is depicted in Table [1.4.2.](#page-37-0) We report the results for the average values of the RMSE, absolute bias, standard deviation and the Jarque-Bera test statistic over the $N^V = 10'000$ predicted CATEs from the validation sample. Figure [1.4.1](#page-38-0) details the performance of the meta-learners implemented in the full-sample, double sample-splitting and double cross-ftting versions.

 $RMSE$ |BIAS| SD JB 500 2000 8000 32000 500 2000 8000 32000 500 2000 8000 32000 500 2000 8000 32000 S 0.878 0.749 0.651 0.570 0.867 0.739 0.641 0.560 **0.108 0.096 0.091 0.088** 7.140 2.888 2.173 1.936
S-W 0.765 0.634 0.533 0.462 0.717 0.602 0.508 0.443 0.261 0.190 0.149 0.125 **2.086** 2.106 2.019 1.931 S-W 0.765 0.634 0.533 0.462 0.717 0.602 0.508 0.443 0.261 0.190 0.149 0.125 2.086 2.106 2.019 1.931 T 0.766 0.634 0.533 0.462 0.719 0.602 0.509 0.442 0.260 0.190 0.149 0.125 2.603 2.085 2.016 1.924 X-F 0.743 0.618 0.517 0.442 0.711 0.597 0.500 0.427 0.200 0.141 0.117 0.103 3.490 2.230 2.034 1.857 X-S 0.820 0.707 0.591 0.499 0.779 0.684 0.574 0.484 0.244 0.164 0.125 0.107 5.146 2.680 2.157 1.929 X-C 0.794 0.693 0.582 0.494 0.770 0.680 0.571 0.482 0.171 0.114 0.097 0.092 3.984 2.322 1.964 1.827 DR-F 0.817 0.659 0.542 0.463 0.764 0.627 0.518 0.443 0.285 0.194 0.149 0.126 141.106 40.528 5.490 2.172 DR-S 1.053 0.825 0.579 0.445 0.906 0.731 0.521 0.403 0.640 0.433 0.281 0.206 567.501 458.729 159.041 36.504 DR-C 0.880 0.727 0.523 0.409 0.809 0.680 0.490 0.383 0.359 0.255 0.179 0.143 52.224 38.216 12.644 3.162 R-F 0.815 0.679 0.590 0.529 0.746 0.632 0.554 0.499 0.346 0.251 0.201 0.172 4.583 3.499 2.225 1.983 R-S 0.932 0.788 0.659 0.580 0.833 0.721 0.613 0.546 0.468 0.333 0.243 0.195 3.959 3.365 2.666 2.028 R-C 0.825 0.725 0.621 0.554 0.779 0.694 0.597 0.533 0.261 0.196 0.155 0.136 2.416 2.184 2.036 1.959 Note: The results for the \overline{RMSE} , $\overline{|BIAS|}$, \overline{SD} and \overline{JB} show the mean values of the root mean squared error, absolute bias, standard deviation

Table 1.4.2: CATE Results for Main Simulation

and the Jarque-Bera test statistic of all 10′000 CATE estimates from the validation sample. The critical values for the JB test statistic are 5.991 and 9.210 at the 5% and 1% level, respectively. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively. Bold numbers indicate the best performing meta-learner for given measure and sample size.

Starting with the most simple S-learner, we observe a competitive performance in terms of the average RMSE for the smaller sample sizes which, however, disappears for larger sample sizes. Taking

Figure 1.4.1: CATE Results for Main Simulation

Note: The results for \overline{RMSE} , \overline{BIAS} , and \overline{SD} show the mean values of the root mean squared error, absolute bias, and standard deviation of all 10′000 CATE estimates from the validation sample. The fgure shows the results based on the increasing training samples of {500, 2 ′000, 8 ′000, 32′000} observations displayed on the log scale. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

a closer look at the results reveals that the competitive performance of the S-learner stems mainly from the very low standard deviation while being substantially biased. Indeed, the variance of the S-learner is the smallest among all meta-learners for all sample sizes. This is mainly due to its tendency to predict efects close to zero if the treatment indicator is not strongly predictive for the outcome as pointed out by Künzel et al. [\(2019\)](#page-53-1). This explains also the high bias of this estimator as the CATEs vary between −1 and 3 with only a small proportions of the CATEs being equal to zero (see Figure [1.A.6](#page-62-0) in Appendix [1.A](#page-56-0) for details). Nevertheless, the Jarque-Bera test does not indicate evidence against the normality of the predicted CATE distribution, on average.

Considering the modifed version of the S-learner with enforcement of the treatment indicator into the forest splitting set, i.e. the SW-learner, we notice almost identical performance to the one of the T-learner. This result can be explained by an observation that once the SW-learner fnds the split based on the treatment indicator early within the trees it mimics the disjoint structure of the T-learner. The rest of the recursive partitioning is then very similar to the one of the T-learner which has been also documented for the case of the S-learner in the simulation experiments conducted by Künzel et al. [\(2019\)](#page-53-1). As a result, it seems that enforcing the treatment indicator into the splitting set helps to alleviate the high bias of the S-learner to some degree, however, it increases the variance of the estimator at the same time. Nevertheless, the bias-variance trade-of in this case results in lower average RMSE in comparison to the S-learner and the SW-learner might thus be preferred over the simple S-learner, when using Random Forest as a base learner. Overall, the SW- and T-learner are very competitive in the smaller sample sizes both in terms of the average RMSE as well as the average absolute bias. However, with access to more training data these two learners do not improve fast enough and are outperformed by the more sophisticated learners in the largest sample size consisting of 32′000 observations. Concerning the distribution of the predicted CATEs there seems to be on average no statistical evidence against the normality, neither for the SW-learner nor for the T-learner.

In contrast to the above mentioned meta-learners the X-learner makes use of the additional estimation of nuisance functions. In its full-sample version the X-learner performs best in terms of the average RMSE for all sample sizes, except the largest one. The good RMSE performance stems partly from the relatively low bias and partly from the relatively low variance of the estimator as the X-learner exhibits the smallest average absolute bias for the smaller sample sizes (500 and 2′000), while having one of the lowest average standard deviations throughout all sample sizes. Interestingly, we only partly document the theoretical properties regarding the sample-splitting and cross-ftting procedures. As such, the full-sample version is the best performing one in terms of the average RMSE as well as in terms of the average absolute bias across all sample sizes, which is a pattern observed in the simulation experiments of Jacob [\(2020\)](#page-52-1) as well. Accordingly, the sample-splitting version exhibits not only higher values of the average standard deviation but also higher values of the average absolute bias. Nevertheless, we observe that the crossfitting version successfully regains the efficiency lost due to sample-splitting as it exhibits steadily lower variance than the sample-splitting version and even lower variance than the full-sample version, while having a bias of roughly the same magnitude as the sample-splitting version. As for the distribution of the predicted CATEs, on average, we do not observe evidence for deviations from normality for any of the versions of the X-learner. Additionally, we do not observe any major diferences in the speed of convergence between the diferent versions as can be seen in Figure [1.4.1.](#page-38-0) Moreover, the absolute diferences in the performance measures among the diferent versions are small in comparison to other meta-learners using nuisance functions. Albeit rather surprising at the frst sight, the explanation for this phenomenon comes presumably from the diferent usage of the propensity score by the X-learner in comparison to the R- and DR-learner. As such, the R- and DR-learner use the propensity score together with the response functions to construct a new pseudo-outcome which is subsequently used to estimate the CATEs. In contrast, the X-learner uses merely the response functions to create the pseudo-outcome, while the propensity score is used only to reweight the final CATE estimates and thus it does not enter into any additional estimation step. Therefore, the X-learner might be less prone to overftting bias which would partly justify the full-sample estimation as described in Künzel et al. $(2019)^{33}$ $(2019)^{33}$ $(2019)^{33}$ $(2019)^{33}$

Assessing the performance of the DR-learner reveals some interesting insights. The frst observation is that the cross-ftting version performs best of all meta-learners in terms of the average RMSE for the largest sample size of 32′000 observations. This comes mainly from the low bias of this estimator as the average absolute bias is the lowest among all learners for the two largest sample sizes, while the average standard deviation is relatively high. However, looking at the average value of the Jarque-Bera statistic suggests evidence against the normality of the predicted CATEs for all but the largest sample size. Inspecting the results more closely reveals that the issue stems from heavy tails of the CATE distributions. The extreme values of the predicted CATEs are mainly caused by the propensity scores which are close to the $\{0,1\}$ bounds. Similar issues of the DR-learner due to extreme propensity scores have also been documented in the simulation experiments of Knaus et al. [\(2021\)](#page-53-2) as well as in the empirical application of Knaus [\(2020\)](#page-52-2). The second observation is that for the DR-learner we clearly see how the theoretical arguments of sample-splitting and cross-ftting translate into the fnite sample properties of the estimator. However, these can be documented only for large sample sizes. As such, the bias of the sample-splitting version is smaller than the one of the full-sample version in the largest sample size, while the bias of the cross-ftted version is even slightly lower than the sample-splitting version and is lower than the bias in the full-sample version for both the largest (32′000) and the second largest (8′000) sample considered. For the smaller sample sizes (500 and 2 ′000) we see that the reduction in the overftting bias is not large enough in comparison to the bias stemming from the estimation of the CATE function. As such, for small sample sizes the additional splitting of the sample does not leave enough

³³ Nonetheless, this insight might still substantiate the need for sample-splitting, although only with two folds instead of three as used here.

observations to learn the non-linear structure of the CATE. Considering the variance of the estimator, we also observe the theoretically expected pattern. The full-sample version of the DR-learner exhibits the smallest average standard deviation throughout all sample sizes, while the standard deviation for the sample-splitting version is roughly twice as high. Nevertheless, the cross-ftting version successfully reduces the standard deviation for all sample sizes and comes close to the full-sample version, efectively regaining the lost efciency of the estimator due to sample-splitting. Overall, in terms of the average RMSE this bias-variance trade-off results in favourable performance of the sample-splitting version in the largest and of the cross-ftting version in the two largest samples in comparison to the full-sample version. Considering the distribution of the predicted CATEs we see that the heavy tails problem due to extreme propensity scores is the worst for the sample-splitting version, where even in the second largest sample size of 8'000 observations, the normality is rejected for more than 50% of the predicted CATEs from the validation sample (compare the supplementary results in Appendix [1.B.2\)](#page-70-0). This stems from the smaller samples used for estimation of the propensity scores which are more likely to yield extreme values under imbalanced treatment assignment. We also observe that this issue is less pronounced for the full-sample version. The third and the last observation is yet the probably most noticeable pattern across all performance measures, namely the fast convergence of the sample-splitting and cross-ftting version of the DR-learner which is substantially faster in comparison to all other meta-learners as can be seen in Figure [1.4.1.](#page-38-0) As such the DR-learner performs almost worst of all, both in terms of the average RMSE and average absolute bias for the smallest sample size of 500 observations, but almost best of all for the largest sample size of 32′000 observations. This provides evidence that the DR-learner is able to learn a highly complex CATE function once enough data becomes available and additionally highlights the need for sample-splitting and cross-ftting in order to achieve the theoretically described optimal performance (Kennedy, [2020\)](#page-52-0).

The performance of the R-learner is competitive with the other meta-learners especially in smaller samples, particularly for the full-sample version. In the smallest sample size of 500 observations the R-learner outperforms the DR-learner in terms of the average RMSE, irrespective of the estimation procedure. However, with growing sample sizes the performance evens out and eventually for the largest sample size of $32'000$ observations the R-learner lags behind the majority of the estimators. This is in contrast to previous results from simulations of Jacob [\(2020\)](#page-52-1) and Knaus et al. [\(2021\)](#page-53-2) where the Rlearner exhibits rather good performance, albeit studied only in smaller samples. The decomposition of the RMSE shows that while the full-sample version of the R-learner exhibits rather low bias, it sufers from a higher variance as can be seen in Figure [1.4.1.](#page-38-0) Nonetheless, the distributions of the predicted CATEs do not show on average deviations from the normal distribution. This is contrary to the DRlearner and illustrates the advantage of the additional weighting step. As such, even though the R-learner uses the propensity scores for reweighting to construct the modifed outcome, it successfully manages to downweight the modifed outcomes based on extreme propensity scores to alleviate the heavy tails issues observed in the case of the DR-learner. In particular, even for the sample-splitting version of the Rlearner the share of predicted CATEs for which the normality is rejected is an order of magnitude lower in comparison to the DR-learner (see Appendix [1.B.2](#page-70-0) for details). In terms of the estimation procedure, we observe a similar pattern as for the X-learner in a sense that the full-sample version performs better with respect to the average RMSE and absolute bias, while the cross-ftting version helps to reduce the variance of the estimator not only in comparison to the sample-splitting version but even in comparison to the full-sample version. The sample-splitting version exhibits higher values of the average absolute bias and standard deviation for all sample sizes considered, while the convergence rates are approximately same as for the full-sample and the cross-ftting version. Hence, there is a lack of indication that the overftting type of bias reduction could become relevant in bigger samples. Similarly to the DR-learner,

also for the R-learner the diferences between the diferent estimation procedures seem to be higher than those for the X-learner which is again presumably due to the diferent usage of the propensity scores.

Inspecting the results for the rest of the simulation designs reveals further insights and helps to generalize the fndings from the main and most challenging simulation design discussed above.

1.4.3.2 Results of Simulation 1: balanced treatment and constant zero CATE

Within the benchmark Simulation 1 with zero constant CATE the S-learner, as expected, performs best with respect to all performance measures across all sample sizes (see Table [1.B.1](#page-65-1) in Appendix [1.B.1\)](#page-65-0). However, the results reveal poor statistical properties of the S-learner as it appears to be substantially biased and inconsistent as the absolute bias as well as standard deviation increase with growing sample size.^{[34](#page-41-0)} In general, the performance of the S-learner is, in all simulation designs, plagued by the substantially higher bias than all the other meta-learners, partially accompanied by the consistency issues. The SW-learner is afected by the same issues as the S-learner in Simulation 1 but manages to substantially reduce the bias for the rest of the simulation designs and is generally close to the performance of the T-learner as seen in the Main Simulation.

1.4.3.3 Results of Simulation 2: balanced treatment and complex nonlinear CATE

In Simulation 2 with balanced treatment and complex nonlinear CATE we also observe, as expected, a very good RMSE performance of the T-learner throughout all sample sizes (see Table [1.B.2](#page-66-0) in Appendix [1.B.1\)](#page-65-0). However, it exhibits quite high variance which is mostly due to the fact that it estimates two completely disjoint response functions for estimating the CATE. Furthermore, in this design the R-learner in its full-sample version performs particularly well, which comes rather as a surprise as it pools the two disjoint response functions within the estimation procedure. Nevertheless, the R-learner achieves even lower bias than the T-learner for large samples, but with rather high variance which is a pattern observed across all simulation designs.

1.4.3.4 Results of Simulation 3: highly unbalanced treatment and constant non-zero CATE

Simulation 3 features a highly unbalanced treatment assignment and a constant CATE for which the X-learner performs best as expected, throughout all sample sizes and irrespective of the estimation procedure (see Table [1.B.3](#page-67-0) in Appendix [1.B.1\)](#page-65-0). Indeed, the diferences between the particular versions, i.e. full-sample, sample-splitting and cross-ftting, are quite small which is in contrast to the R- and DR-learner confrming the insights from the Main Simulation. Within this highly unbalanced design the estimation of the propensity score function plays a key role as in this case the estimated propensity scores can get quite often very close to zero. This, however, does not afect the performance of the X-learner as it uses the propensity scores in a fundamentally different way and even the most extreme $\{0, 1\}$ scores would be indeed admissible as pointed out by Künzel et al. [\(2019\)](#page-53-1). On the contrary, the results show that such extreme propensity scores make now both the R-learner and the DR-learner unstable, with the instability being particularly pronounced in the latter meta-learner. In the case of the DR-learner the

 $34A$ closer look on the estimation results reveals the reason for this phenomenon. With small sample sizes, the underlying trees of the S-learner's forest are quite shallow and barely split on the treatment indicator resulting in quite homogeneous CATE predictions which are very close to the actual zero efect. However, as the sample size increases, the chance of splits based on the treatment indicator increases which results in more heterogeneous efect predictions spread around zero. Accordingly, the bias as well as the standard deviation increase. Similar consistency issues of the forest-based S-learner seem to appear also in the simulations of Künzel et al. [\(2019\)](#page-53-1) where the MSE rises with growing sample size for some designs and only stabilizes with very big sample sizes.

heavy tail problem of the CATE distribution is aggravated by more unbalanced treatment assignment as can be seen based on the Jarque-Bera statistic and also on the higher variance of the estimator. While the R-learner manages to avoid this issue by downweighting the observations with extreme propensity scores in less unbalanced settings, it is not fully able to do so when the imbalance is very high and there is potentially a large proportion of propensity scores close to 1. This translates into the higher values of the Jarque-Bera statistic as well as to higher variance and higher bias, too. These issues lead ultimately to bad performance in terms of the average RMSE for both the R- and DR-learner.

1.4.3.5 Results of Simulation 4: unbalanced treatment and simple CATE

In Simulation 4 the imbalance in the treatment assignment is less pronounced which should partly reduce the propensity score issues for the R- and DR-learner. Within this simulation design we observe similar patterns as for the Main Simulation. For the small and medium sized samples the X-learner in the full-sample version performs best in terms of the average RMSE, while it gets outperformed by the DRlearner in its cross-ftting version in the largest sample-size. While the R-learner's performance is quite competitive in smaller samples, it lags behind in larger samples as observed in other simulation designs. As a general pattern, the X-learner remains quite stable with respect to the estimation procedure whereas the DR-learner in its sample-splitting and cross-ftting version exhibits substantially faster convergence than the competing estimators. Nonetheless, based on the Jarque-Bera statistic, the heavy tail issue is less pronounced but still present as can be seen in Table [1.B.4](#page-68-0) in Appendix [1.B.1.](#page-65-0)

1.4.3.6 Results of Simulation 5: unbalanced treatment and linear CATE

Lastly, in Simulation 5 the CATE function gets more involved, while the treatment assignment remains unchanged. The results once again resemble the general pattern (for details see Table [1.B.5](#page-69-0) in Appendix [1.B.1\)](#page-65-0). As such the R-learner is competitive mainly in the smaller sample sizes, in this case best performing in the cross-ftting version. The DR-learner in the sample-splitting and cross-ftting version exhibits faster convergence rates, however, in this case the considered sample sizes are not large enough to outperform the X-learner. The X-learner exhibits again little diferences regarding the estimation procedure and outperforms the other meta-learners in all performance measures across all sample-sizes.

1.4.4 Empirical Simulation

In order to compare the performance of the meta-learners outside a completely synthetic design of the above simulations we apply the estimators in an arguably more realistic setting using an augmented real dataset. For this purpose we use the data from the data challenge of the 2018 Atlantic Causal Inference Conference (2018 ACIC henceforth). This data is particularly suitable for a comparison of the meta-learners for two reasons. First, the data is based on a randomized control trial in education, namely the National Study of Learning Mindsets (NSLM) by Yeager et al. [\(2019\)](#page-55-0), and thus provides us with a real data example. Second, the dataset has been augmented to an observational setting with measured confounding and known treatment efects (Carvalho, Feller, Murray, Woody, & Yeager, [2019\)](#page-51-0) which enables us to evaluate the performance of the meta-learners for the estimation of CATEs.

The dataset includes a total of 10′391 observations with 10 covariates, a simulated continuous outcome and a binary treatment, while the share of treated is approximately 25% .^{[35](#page-42-0)} The variables are

 35 The dataset can be retrieved online from [GitHub.](https://github.com/grf-labs/grf/blob/master/experiments/acic18/synthetic_data.csv) We neglect here the information about the additional school ID for simplicity and comparability reasons.

described in Table [1.A.1](#page-63-0) in Appendix [1.A.2.](#page-63-1) Additionally, to create a more challenging large-dimensional setting, similar to the synthetic simulations, we augment the dataset further with $p = 90$ uniformly distributed covariates, i.e. $X_{11,...,100} \sim \mathcal{U}([0,1]^{n \times p})$ with the same correlation structure as used within the synthetic simulations.^{[36](#page-43-0)} At a high level, we are interested in estimating the treatment effects of an intervention to foster a belief to develop intelligence in students on a measure of student achievement, conditional on observed covariates. The CATEs were generated according to the following specifcation:

$$
\tau(x) = 0.228 + 0.05 \cdot \mathbb{1}(x_1 < 0.07) - 0.05 \cdot \mathbb{1}(x_2 < -0.69) - 0.08 \cdot \mathbb{1}(c_1 \in 1, 13, 14)
$$

while the conditional independence assumption holds by construction, the confounding has a complicated functional form. For a detailed description of the data generating process used for the augmentation see Carvalho et al. [\(2019\)](#page-51-0).

Similarly as in the synthetic simulations we estimate the heterogeneous treatment efects with all meta-learners and evaluate their performance with regard to the point estimates. For this purpose we perform an empirical simulation study inspired, among others, by Lechner [\(2018\)](#page-53-3) and Künzel et al. [\(2019\)](#page-53-1) where we first, set apart a validation set of size $N = 1'000$ observations, and second, sample $R = \{2'000, 1'000, 500\}$ training sets each of sizes $N = \{500, 2'000, 8'000\}$ observations from the remaining data. We omit the biggest sample of $N = 32'000$ observations due to the size restrictions of the dataset. We report mean performance measures in a similar fashion as in the previous simulation experiments.

1.4.4.1 Results of Empirical Simulation

The CATE results of the Empirical Simulation for all meta-learners are summarized in Table [1.4.3,](#page-44-0) while Figure [1.4.2](#page-44-1) provides details on the meta-learners in the full-sample, double sample-splitting and double cross-ftting versions.

The results reveal a similar picture to the synthetic simulations in general, with the largest similarities to Simulation 3 and 5 in particular. Accordingly, the X-learner achieves the best performance in terms of the average RMSE as well as average absolute bias in all considered sample-sizes, regardless of the estimation procedure. This emphasizes the good performance of the X-learner in settings with unbalanced treatment assignment and sparse CATE function with structural properties. In the largest sample size of 8′000 observations, also the DR- and R-learner come close to the performance of the X-learner in terms of the average RMSE, while the simpler SW- and T-learner are competitive mainly in the smaller sample sizes. We also observe a slightly faster convergence of the sample-splitting and cross-ftting version of the DR-learner as in the synthetic simulations, however, the limited sample size in this case does not allow for a sufficiently large improvement to outperform the X-learner. Given the smaller sample sizes in the empirical simulation, we are not able to detect the bias-variance trade-of and the sample-splitting versions always exhibit higher values of the average RMSE, average absolute bias and average standard deviation. This is particularly noticeable for the smallest sample size of 500 observations as there is essentially not enough data left after splitting to learn the correct CATE function. For all meta-learners the cross-ftting versions then always perform better in terms of the variance reduction and even lead to a lower bias in comparison to the sample-splitting versions. These results accentuate the fact that the benefts of sample-splitting in removing the overftting bias become apparent only for sufficiently large samples. Additionally, we see larger discrepancies between the estimation versions of the DR- and R-learner in comparison to very stable performance of the X-learner, similarly as in the synthetic simulations. Lastly, the results on the distribution of the predicted CATEs resemble those of

 36 For more detailed descriptive statistics of the augmented empirical dataset including correlation heat map of the covariates see Appendix [1.A.2.](#page-63-1)

the synthetic simulations with the heavy tail problem of the DR-learner in its sample-splitting version as well as deviations from normality of the S- and SW-learner.

Table 1.4.3: CATE Results for Empirical Simulation

		RMSE			BIAS			\overline{SD}			\overline{JB}				
	500	2000	8000	500	2000	8000	500	2000	8000	500	2000	8000			
S	0.175	0.127	0.093	0.171	0.121	0.090		0.035 0.035	0.023	165.803	7.372	2.054			
S-W	0.131	0.109	0.078	0.106	0.090	0.070	0.121	0.084	0.037	57.438	2.065	1.903			
т	0.150	0.111	0.079	0.122	0.092	0.071	0.127	0.084	0.037	2.050	2.047	2.082			
$X-F$	0.112	0.082	0.056	0.092		0.069 0.052	0.089	0.056	0.021	2.043	1.941	2.078			
$X-S$	0.129	0.093	0.069	0.105	0.078	- 0.060	0.104	0.067	0.040	2.129	2.594	2.004			
$X-C$		0.103 0.077 0.055				0.087 0.067 0.052	0.072		0.044 0.017		1.652 1.794	1.935			
$DR-F$	0.147	0.105	0.070	0.119	0.087	0.063	0.125	0.078	0.033	7.134	3.377	2.001			
$DR-S$	0.256	0.180	0.123	0.201	0.143	0.101	0.242	0.162	0.097	68.837	46.173	6.196			
$DR-C$	0.159	0.116	0.078	0.128	0.096	0.071	0.135	0.088	0.037	6.334	5.329	2.969			
$R-F$	0.183	0.131	0.089	0.146	0.107	0.078	0.167	0.109	0.051	3.819	3.862	2.027			
$R-S$	0.237	0.174	0.123	0.189	0.140	0.100	0.224	0.158	0.099	3.490	3.494	3.117			
$R-C$	0.144	0.109	0.076	0.117	0.091	0.068	0.123	0.084	0.037	2.060	2.222	2.225			

Note: The results for the \overline{RMSE} , \overline{BIAS} , \overline{SD} and \overline{JB} show the mean values of the root mean squared error, absolute bias, standard deviation and the Jarque-Bera test statistic of all 1'000 CATE estimates validation sample. The critical values for the JB test statistic are 5.991 and 9.210 at the 5% and 1% level, respectively. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively. Bold numbers indicate the best performing meta-learner for given measure and sample size.

Figure 1.4.2: CATE Results for Empirical Simulation

Note: The results for \overline{RMSE} , \overline{BIAS} , and \overline{SD} show the mean values of the root mean squared error, absolute bias, and standard deviation of all 1′000 CATE estimates from the validation sample. The fgure shows the results based on the increasing training samples of {500, 2 ′000, 8 ′000} observations displayed on the log scale. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.5 Discussion

Given the results of our synthetic and empirical simulations there are several important fndings for the estimation of heterogeneous causal efects by the meta-learners and the associated usage of samplesplitting and cross-ftting which are relevant for applied empirical work.

1.5.1 Meta-Learners

In general, the results suggest that meta-learners that directly model both the outcome equations and the selection process perform better, especially in larger samples, which is in line with the insights from the previous literature (see e.g. Knaus et al., [2021\)](#page-53-2). Meta-learners modelling only the outcome equations are competitive only in smaller samples and tend to perform poorly in larger samples as they fail to properly account for the selection into treatment.

In particular, we do not recommend the usage of the S-learner for estimation of heterogeneous causal efects due to empirically documented undesirable statistical properties such as high bias and consistency issues. The herein studied modifcation of the S-learner, the SW-learner, alleviates the high bias of the S-learner, however, it does not solve the consistency issues. Hence, enforcing the treatment variable into the splitting set of the forest does not constitute an attractive option for estimation of causal efects. In contrast, the T-learner does not sufer from high bias or any consistency issues and has a stable performance as it uses the full data sample without the need of sample-splitting due to potential overftting. Hence, the T-learner might be an interesting option, if a large sample is not available for the empirical analysis. Related simulation studies (Jacob, [2020;](#page-52-1) Knaus et al., [2021\)](#page-53-2) fnd also relatively competitive performance of the T-learner, especially with the Random Forest as a base learner.

Among the meta-learners based on the estimation of nuisance functions, the X-learner performs very well not only in settings with highly unbalanced but also in less unbalanced treatment shares with simple CATEs and demonstrates the theoretically argued capability to learn such CATE structures (Künzel et al., [2019\)](#page-53-1). Moreover, the X-learner exhibits a quite stable performance across all simulation designs with low bias and very low variance, even in small samples. Additionally, due to its particular usage of the propensity scores, the X-learner is not too sensitive to the choice of the estimation procedure. As such, both the full-sample version and the cross-ftting version of the X-learner are viable options, regardless of the sample size. For these reasons, we recommend to use the X-learner for CATE estimation if the researcher is facing a situation with very low number of treated units as well as in less unbalanced settings with potentially limited sample size. In contrast to the X-learner, the DR-learner performs particularly well in settings with nonlinear and complex CATEs if large enough samples are available. However, it tends to be unstable in small samples with unbalanced treatment assignment due to extreme propensity scores, which relates to the results of Jacob [\(2020\)](#page-52-1) and Knaus et al. [\(2021\)](#page-53-2). Additionally, for the DRlearner the choice of the estimation procedure is crucial as its sample-splitting and cross-ftting version exhibits the fastest convergence rates of all meta-learners which highlights the theoretical arguments provided in Kennedy [\(2020\)](#page-52-0). According to the simulation evidence, we advice to employ the cross-ftting version of the DR-learner for the CATE estimation in settings with rather balanced treatment assignment and when large sample is available. Recently, Knaus [\(2020\)](#page-52-2) proposed the normalized DR-learner, that addresses the problem of unstable CATE predictions due to extreme propensity scores which might be a viable option for smaller sample sizes and settings with unbalanced treatment shares. Lastly, the simulation evidence suggests that the R-learner is in comparison to the DR-learner less prone to unstable performance due to extreme propensity scores. However, its performance is competitive only in smaller samples, while the empirically approximated speed of convergence is slower than the one of the DR-learner and seems to depend on the CATE complexity as theoretically argued by Nie and Wager [\(2021\)](#page-53-0). With respect to the estimation procedure we do not fnd a clear-cut evidence in favour of a particular version as both the full-sample as well as the cross-ftting version exhibit comparably good performance. Based on this evidence, the R-learner might be an attractive option for estimation of CATEs if the treatment is not too imbalanced and if only a small sample is available. For comparable sample sizes, Knaus et al. [\(2021\)](#page-53-2) also fnd the R-learner to have good performance in a variety of settings.

Overall, we point out that based on the simulation evidence, for all meta-learners the approximate convergence rates appear to be substantially slower than the parametric rate of \sqrt{N} . This is expected given the insights from previous literature that the estimation of more granular heterogeneous efects is a more difcult task in comparison to the estimation of average efects (compare e.g. Lechner, [2018;](#page-53-3) or Knaus et al., [2021\)](#page-53-2). However, we note that the approximate convergence rates difer considerably among the meta-learners and their specifc implementations as documented in our simulation experiments.

1.5.2 Estimation Procedures

Our simulation evidence suggests that using the full sample for estimation of both the nuisance functions as well as the CATE function leads to a remarkably good performance in terms of both bias and variance in fnite samples. Recently, Curth and van der Schaar [\(2021\)](#page-51-1) also point out that the fullsample estimation seems to work better in practice, especially for small samples. In theory, we would expect lower variance yet higher bias due to overftting (Chernozhukov et al., [2018\)](#page-51-2). The possible reason for this phenomenon might in our case be due to the out-of-bag predictions of the forest that we use throughout the simulation experiments. Even though these predictions are not out-of-sample per se they are not directly based on the observations used for estimation and as such might help to alleviate the overftting problem when using full sample (compare Athey & Imbens, [2019,](#page-50-0) for a discussion of out-of-bag predictions in Random Forests). In the causal machine learning literature, such out-of-bag predictions are for example also used in the case of the Generalized Random Forest for the residualization (Athey et al., [2019\)](#page-50-1), similar to the one used in the R-learner. In contrast to the full-sample estimation, using the double sample-splitting for the estimation of the nuisance functions, we efectively use only one third of the available data. Theoretically, we should observe a smaller bias but higher variance of the estimators. However, in almost all cases we observe both higher bias as well as higher variance, particularly for the small sample sizes. Nonetheless, we document the expected bias-variance trade-of for the largest sample sizes. This stems mainly from the fact that using only a third of the smaller samples does not allow a sensible machine learning estimation of the highly non-linear nuisance functions featured in our simulations. However, especially for the DR-learner we do observe faster convergence rates for the samplesplitting version which is compatible with the theoretical convergence arguments (Newey & Robins, [2018;](#page-53-4) Kennedy, [2020\)](#page-52-0). Hence, it seems to be the case that in order to beneft from the double sample-splitting the training sample must be of sufficient size, otherwise the full sample estimation achieves a better performance. Lastly, the double cross-ftting for estimation of the nuisance components efectively uses all the available information from the data and substantially reduces the variance of the estimators, while keeping the bias low at the same time. This comes at the price of longer computation time in comparison to the sample-splitting procedure as the estimation is repeated several times. Nevertheless, the computation time of the cross-ftting procedure is on average comparable with the full-sample estimation (see Appendix [1.C](#page-78-0) for details).

Based on the above simulation evidence, it seems reasonable to always use the full-sample estimation together with out-of-bag predictions (if available) when a relatively small sample is available to the applied researcher, whereas to use the double cross-ftting procedure when a relatively large data is accessible, regardless of the choice of a meta-learner. On the contrary, the simulations do not provide any evidence for an advantageous usage of the double sample-splitting over the double cross-ftting, apart from the computational aspects.

1.6 Conclusion

We investigate the fnite sample performance of the meta-learners for the estimation of heterogeneous causal efects with focus on the specifc estimation implementations related to data usage. In particular, we examine the properties of double sample-splitting and double cross-ftting as defned by Newey and Robins [\(2018\)](#page-53-4) in contrast to using full sample for estimation. For this purpose, we review several metalearning algorithms for estimation of causal efects and discuss their advantages and disadvantages in particular empirical settings. We conduct an extensive simulation study with data generating processes involving highly non-linear functional forms and large-dimensional feature space to challenge the machine learning algorithms, while keeping the treatment efect specifcations well-structured. Furthermore, we perform an empirical simulation based on an augmented real dataset to refect an actual empirical setting. Moreover, we repeat the simulation experiments for increasing sample sizes to empirically study the convergence properties of the meta-learners. Based on our simulation evidence, we provide a guideline for empirical researchers and practitioners to better inform the decisions of applying certain method and estimation procedure for their particular research objectives.

The results of our simulation study show that the choice of the estimation procedure can indeed largely impact the performance of the meta-learners in fnite samples. On the one hand, we provide an empirical evidence for the theoretical arguments of the bias-variance trade-of related to sample-splitting and cross-fitting which, however, become apparent only if sufficiently large samples are used. On the other hand, we document the adverse efects of these procedures in small samples, when using machine learning. Therefore, we argue that in empirical studies based on small samples, applied researchers should use the full sample for machine learning estimation of both the nuisance functions as well as the treatment efect function as the overftting bias is in such cases of secondary importance. However, for empirical analyses with access to large data samples, we advocate for the usage of the double cross-ftting for the estimation of treatment efects as the overftting bias here becomes of primary importance. The double cross-ftting procedure then efectively reduces this overftting bias and successfully preserves the full sample size effciency of the estimator. Moreover, if computation time is not a constraint, we discourage applied researchers to use the double sample-splitting procedure due to substantial increase in variance, while having no benefit over the double cross-fitting in terms of bias reduction.

In contrast to the typical drawbacks of simulation studies, the particular design of our simulation experiments with varying sample size and varying treatment shares allows us to draw relevant conclusions that are not solely dependent on the particular specifcation of the data generating processes, but rely on the data characteristics that an applied researcher can observe without imposing arbitrary assumptions. In particular, the simulation evidence implies a clear advantage for the X-learner, when a researcher is confronted with highly unbalanced treatment shares. This fnding holds irrespective of the sample size at hand and as such we recommend the usage of X-learner for estimation of heterogeneous treatment efects whenever the share of treated or controls is around 15% or less. With less unbalanced treatment shares at around 25% of treated or controls, the size of the available sample becomes decisive. For smaller samples with only few hundred observations (500 and 2'000), the simulation evidence again favours the usage of the X-learner. However, for bigger samples with several thousand observations (8′000 and 32′000), our fndings favour the DR-learner as it can successfully learn highly complex treatment efect function if enough data is available. Finally, with perfectly balanced treatment shares, the sample size matters less. In such cases, the DR-learner as well as the R-learner are both the preferred estimators. However, we advise against the usage of these two methods in highly imbalanced settings as their performance becomes unstable due to extreme propensity scores. Finally, concerning the simpler meta-learners, we explicitly argue against the usage of the S-learner by applied researchers for estimation of heterogeneous

treatment efects due to the herein empirically documented undesirable statistical properties, while the T-learner might be a reasonable choice in small samples with balanced treatment shares.

Even though we shed light on certain fnite sample issues of applying diferent estimation procedures when using meta-learners for estimation of heterogeneous causal efects, our fndings raise new relevant questions. Most importantly, the question of conducting statistical inference about the estimated heterogeneous treatment efects is worth further investigations. Based on the insights in this paper it would be of interest to investigate the performance of the bootstrapping for estimation of standard errors as studied by Künzel et al. [\(2019\)](#page-53-1) for meta-learners based on the double sample-splitting and double cross-fitting procedures. Moreover, a comparison of such bootstrapping inference procedure for meta-learners and the approaches used in the Causal Forest literature such as the bootstrap of little bags in the Generalized Random Forest (Athey et al., [2019\)](#page-50-1) or the weight-based inference as in the Modifed Causal Forest (Lechner, [2018\)](#page-53-3) would be desirable. Furthermore, the performance diference in the point estimation using the out-of-bag vs. in-sample predictions could provide additional insights on the benefts of samplesplitting and cross-ftting procedures and hence to assess the robustness of our results to diferent types of base learners. Finally, a further simulation comparison between the X-learner, the DR-learner and its normalized version as proposed by Knaus [\(2020\)](#page-52-2) for highly imbalanced settings would be of interest.

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Appendix

1.A Descriptive Statistics

1.A.1 Synthetic Simulations

This appendix provides the descriptive statistics for the data generated in the six main simulation designs discussed in the main text. For each simulation design we plot the distribution of the observed realized outcomes, Y_i , as well as the potential outcomes, $Y_i(0)$ and $Y_i(1)$. Furthermore, we provide the distribution of the treatment indicator, W_i , together with the propensity score distribution under treatment and under control to visualize the overlap condition. Lastly, we plot the distribution of the true treatment effects, $\tau(X_i)$. Moreover, the plots include a correlation heat map for the covariates X_i . The respective fgures for each simulation design are listed below.

1.A.1.1 Simulation 1: balanced treatment and constant zero CATE

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1.A.1.2 Simulation 2: balanced treatment and complex nonlinear CATE

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1.A.1.3 Simulation 3: highly unbalanced treatment and constant non-zero CATE

1.A.1.4 Simulation 4: unbalanced treatment and simple CATE

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Figure 1.A.5: Descriptive Statistics for the Validation Data in Simulation 5

Figure 1.A.6: Descriptive Statistics for the Validation Data in Main Simulation

1.A.2 Empirical Simulation

This appendix provides a comprehensive overview of the variables in the augmented real dataset as well as descriptive statistics thereof. Similarly to the results from the main simulation, we plot the distribution of the observed realized outcomes, Y_i , as well as the distribution of the treatment indicator, W_i . Analogously, we plot the distribution of the true treatment effects, $\tau(X_i)$ together with the correlation heat map for the covariates X_i . The respective figures for the distributions of the potential outcomes and the propensity scores under treatment and under control are omitted due to missing data availability for these quantities. The corresponding fgures and tables are listed below.

Table 1.A.1: Variable description of the 2018 ACIC dataset. Source: Carvalho, Feller, Murray, Woody, and Yeager [\(2019\)](#page-51-0).

Variable	Description
Υ	outcome measure of achievement recorded post-treatment (continuous variable)
W	treatment indicating receipt of the intervention (binary variable)
S ₃	student's self-reported expectations for success in the future, a proxy for prior achievement, measured prior to random assignment (ordered categorical variable)
C1	student's race/ethnicity (unordered categorical variable)
C ₂	student's identified gender (binary variable)
C ₃	student's first generation status, i.e. first in family to go to college (binary variable)
XC	urbanicity of the school, i.e. rural, suburban, etc. (unordered categorical variable)
X1	school-level mean of students' fixed mindsets, reported prior to random assignment (contin- uous variable)
X2	school achievement level, measured by test scores and college preparation for the previous 4 cohorts of students (continuous variable)
X3	school racial/ethnic minority composition, i.e. percentage of student body that is Black,
	Latino, or Native American (continuous variable)
X4	school poverty concentration, i.e. percentage of students who are from families whose in- comes fall below the federal poverty line (continuous variable)
X5	School size, i.e. total number of students in all four grade levels in the school (continuous variable)

Figure 1.A.7: Descriptive Statistics for the Validation Data in Empirical Simulation

1.B Simulation Results

1.B.1 Main Results

1.B.1.1 Simulation 1: balanced treatment and constant zero CATE

RMSE |BIAS| SD JB 500 2000 8000 32000 500 2000 8000 32000 500 2000 8000 32000 500 2000 8000 32000 S 0.008 0.009 0.013 0.018 0.005 0.006 0.010 0.014 0.007 0.008 0.012 0.016 21102.232 3656.421 285.128 12.451 S-W 0.037 0.038 0.049 0.059 0.023 0.025 0.036 0.047 0.033 0.040 0.047 20410.604 4973.704 364.501 12.494 S-W 0.037 0.038 0.049 0.059 0.023 0.025 0.036 0.047 0.033 0.032 0.040 0.047 20410.604 4973.704 364.501 12.494 T 0.225 0.168 0.128 0.101 0.180 0.135 0.103 0.082 0.206 0.149 0.109 0.083 2.071 2.280 2.000 1.912 X-F 0.160 0.111 0.080 0.059 0.128 0.089 0.065 0.048 0.142 0.095 0.067 0.048 1.689 2.442 2.068 2.002 X-S 0.186 0.127 0.091 0.067 0.149 0.103 0.074 0.055 0.162 0.106 0.073 0.053 1.916 2.152 2.180 2.125 X-C 0.152 0.106 0.075 0.054 0.123 0.087 0.062 0.045 0.120 0.075 0.052 0.036 1.293 2.393 2.023 1.982 DR-F 0.209 0.146 0.105 0.079 0.167 0.117 0.084 0.064 0.196 0.135 0.095 0.070 4.677 18.496 17.015 7.978 DR-S 0.343 0.241 0.170 0.122 0.272 0.191 0.135 0.097 0.335 0.235 0.166 0.119 5.548 15.737 30.661 41.289 DR-C 0.207 0.147 0.103 0.074 0.166 0.118 0.082 0.059 0.194 0.137 0.097 0.070 2.606 3.632 9.329 13.029 R-F 0.261 0.192 0.145 0.114 0.208 0.153 0.116 0.092 0.249 0.180 0.132 0.102 5.911 23.800 26.134 14.008 R-S 0.334 0.243 0.181 0.137 0.265 0.193 0.144 0.109 0.321 0.232 0.168 0.124 3.192 5.140 15.179 15.980 R-C 0.208 0.156 0.118 0.092 0.166 0.125 0.096 0.075 0.186 0.135 0.098 0.072 2.117 2.586 3.209 3.779

Table 1.B.1: CATE Results for Simulation 1

Note: The results for the \overline{RMSE} , \overline{BIAS} , \overline{SD} and \overline{JB} show the mean values of the root mean squared error, absolute bias, standard deviation and the Jarque-Bera test statistic of all 10'000 CATE estimate 9.210 at the 5% and 1% level, respectively. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-fitting versions, for given measure and sample size.

Note: The results for \overline{RMSE} , \overline{BIAS} , and \overline{SD} show the mean values of the root mean squared error, absolute bias, and standard deviation of all 10′000 CATE estimates from the validation sample. The fgure shows the results based on the increasing training samples of {500, 2 ′000, 8 ′000, 32′000} observations displayed on the log scale. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.B.1.2 Simulation 2: balanced treatment and complex nonlinear CATE

			\overline{RMSE}				BIAS				\overline{SD}			\overline{JB}				
	500	2000	8000	32000	<i>500</i>	2000	8000	<i>32000</i>	500	2000		8000 32000	<i>500</i>	2000		8000 32000		
^S			0.527 0.442 0.374	0.326	0.522	0.434	0.366	0.317			0.055 0.068 0.066	0.064	711.571 17.960		4.186	2.537		
S-W			0.463 0.357 0.303 0.265			0.431 0.328	0.280	0.246	0.177	0.151	0.120	0.099	268.394	2.900	2.520	2.207		
				0.434 0.358 0.303 0.265		0.392 0.328	0.280	0.246	0.204		0.154 0.120	0.099	2.206		2.464 2.466 2.250			
$X-F$	0.432	0.377	0.331	0.296	0.407	0.361	0.318	0.285	0.143	0.103	0.083	0.072	1.915		2.167 1.936	- 1.906		
$X-S$			0.460 0.411 0.362	0.321	0.432	0.393	0.349	0.310	0.160	0.110	0.085	0.073		2.048 2.046 2.156 1.957				
$X-C$	0.443		0.400 0.356	0.317	0.424	0.389	0.347	0.309	0.119	0.082		0.068 0.062	1.417	2.139		1.955 1.900		
DR-F	0.439		0.366 0.312	0.276	0.399	0.338	0.291	0.259	0.197	0.144	0.113	0.095	3.392	2.919	2.104	- 1.936		
DR-S			0.534 0.439 0.355	0.297	0.461	0.388	0.318	0.270	0.328	0.236	0.173	0.136	5.134	8.959	4.011	2.371		
DR-C	0.451		0.388 0.322	0.276	0.413	0.361	0.302	0.259	0.193	0.146	0.114	0.095	2.498	2.525	2.158	1.980		
$R-F$	0.458	0.373	0.307	0.266	0.404		0.333 0.277 0.241		0.251	0.188	0.146	0.122	4.201	4.206	2.437	2.021		
$R-S$	0.529		0.439 0.356	0.298	0.458	0.389	0.319	0.269	0.318	0.236		0.178 0.140	2.989	3.550	4.630	-3.400		
$R-C$	0.449	0.388	0.322	0.274	0.413	0.361	0.301	0.256	0.187	0.145	0.116	0.097	2.195	2.280	2.107	1.940		

Table 1.B.2: CATE Results for Simulation 2

Note: The results for the \overline{RMSE} , \overline{BIAS} , \overline{SD} and \overline{JB} show the mean values of the root mean squared error, absolute bias, standard deviation and the Jarque-Bera test statistic of all 10'000 CATE estimates from the validation sample. The critical values for the JB test
statistic are 5.991 and 9.210 at the 5% and 1% level, respectively. Additionally, Xindicate the best performing meta-learner for given measure and sample size.

Figure 1.B.2: CATE Results for Simulation 2

Note: The results for \overline{RMSE} , $\overline{|BIAS|}$, and \overline{SD} show the mean values of the root mean squared error, absolute bias, and standard deviation of all 10′000 CATE estimates from the validation sample. The fgure shows the results based on the increasing training samples of {500, 2 ′000, 8 ′000, 32′000} observations displayed on the log scale. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.B.1.3 Simulation 3: highly unbalanced treatment and constant non-zero CATE

			RMSE				BIAS				\overline{SD}			\overline{JB}						
	500	2000		8000 32000	500	2000	8000	<i>32000</i>	<i>500</i>	2000	8000	<i>32000</i>	500	2000	8000	32000				
S	0.645	0.475	0.359	0.279	0.638	0.468	0.352	0.272		0.099 0.084	0.072	0.062	2.888	2.667	2.111	1.981				
S-W	0.246	0.191	0.146	0.111	0.197	0.154	0.119	0.091	0.233	0.163	0.121	0.090	4.611	2.281	2.385	1.993				
	0.244	0.191	0.146	0.111	0.195	0.154	0.119	0.091	0.227	0.164	0.121	0.090	2.806	2.271	2.243	1.964				
$X-F$	0.180	0.123	0.090	0.068	0.144	0.098	0.072	0.054	0.175	0.118	0.085	0.061	3.663	2.552	4.441	2.820				
$X-S$	0.226	0.149	0.110	0.078	0.180	0.119	0.087	0.062	0.219	0.143	0.104	0.072	2.367	2.678	3.058	3.192				
$X-C$				0.159 0.102 0.073 0.054				0.127 0.081 0.059 0.043	0.150		0.092 0.064 0.046		6.541	1.969	2.263	1.994				
$DR-F$	0.287	0.202	0.146	0.110	0.222	0.158	0.116	0.089	0.279	0.188	0.129	0.093	3060.536		812.294 244.016	38.545				
DR-S	0.649	0.502	0.334	0.218	0.475	0.365	0.250	0.168	0.645	0.498	0.329	0.213	1276.433	1496.545 795.711		258.858				
$DR-C$	0.364	0.290	0.197	0.131	0.282	0.223	0.153	0.104	0.359	0.283	0.189	0.124	112.249		149.500 126.268	43.274				
$R-F$	0.441	0.366	0.293	0.243	0.348	0.287	0.232	0.195	0.435	0.354	0.273	0.215	14.590	27.616	19.045	8.171				
$R-S$	0.573	0.461	0.366	0.285	0.453	0.363	0.288	0.227	0.570	0.454	0.353	0.264	7.887	12.474	18.638	11.149				
$R-C$	0.295	0.262	0.220	0.184	0.235	0.208	0.176	0.150	0.289	0.249	0.199	0.152	2.822	3.570	4.324	3.162				

Table 1.B.3: CATE Results for Simulation 3

Note: The results for the \overline{RMSE} , \overline{BIAS} , \overline{SD} and \overline{JB} show the mean values of the root mean squared error, absolute bias, standard deviation and the Jarque-Bera test statistic of all 10′000 CATE estimates from the validation sample. The critical values for the JB test statistic are 5.991 and 9.210 at the 5% and 1% level, respectively. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-fitting versions, for given measure and sample size.

Figure 1.B.3: CATE Results for Simulation 3

Note: The results for \overline{RMSE} , $\overline{|BIAS|}$, and \overline{SD} show the mean values of the root mean squared error, absolute bias, and standard deviation of all 10′000 CATE estimates from the validation sample. The fgure shows the results based on the increasing training samples of {500, 2 ′000, 8 ′000, 32′000} observations displayed on the log scale. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.B.1.4 Simulation 4: unbalanced treatment and simple CATE

			\overline{RMSE}				BIAS				\overline{SD}			\overline{JB}		
	500	2000	8000	<i>32000</i>	<i>500</i>	2000	8000	<i>32000</i>	<i>500</i>	2000		8000 32000	500	2000	8000	<i>32000</i>
^S	0.834	0.616	0.472	0.370	0.825		0.606 0.462	0.361		0.105 0.090	0.078	0.069	1.935	2.120	2.075	1.951
S-W	0.443	0.336	0.258	0.206			0.390 0.300 0.233	0.187	0.229	0.162	0.120	0.093	2.575	2.330	2.124	1.957
T.	0.443	0.335	0.258	0.206			0.390 0.300 0.233	0.187	0.229	0.163	0.120	0.093	2.552	2.278	2.130	1.938
$X-F$	0.428 0.329 0.247			0.191	0.394		0.308 0.233	0.180	0.171			0.114 0.083 0.064	3.731	2.312	2.210	1.978
$X-S$	0.501	0.399	0.307	0.232	0.456	0.375	0.291	0.220	0.213		0.136 0.097	0.073	6.602	2.762	2.298	2.113
$X-C$	0.477	0.385	0.300	0.227	0.453	0.374	0.292	0.220	0.148			0.091 0.068 0.055	5.617	2.026		2.023 1.898
DR-F	0.510	0.369	0.275	0.214	0.454	0.334	0.251	0.196	0.249		0.165 0.117	0.088		116.949 156.252		41.933 5.158
DR-S	0.728	0.537	0.339	0.230	0.591	0.445	0.279	0.190	0.549		0.377 0.247	0.171			497.136 530.045 407.510 97.233	
DR-C	0.565	0.435		0.269 0.182	0.493	0.388		0.236 0.159	0.308	0.215		0.145 0.104	51.595	50.726		42.424 15.770
$R-F$	0.537	0.426	0.349	0.293		0.454 0.364	0.303	0.258	0.337		0.250 0.192	0.151	8.764	13.754	7.349	2.839
$R-S$	0.653	0.521	0.412	0.338	0.539	0.438	0.352	0.294	0.460		$0.332 \quad 0.245$	0.184	7.025	6.592	7.512	5.029
$R-C$	0.524	0.440	0.361	0.303	0.469	0.402	0.333	0.282	0.246		0.185 0.142	0.113	2.700	2.900		2.732 2.318

Table 1.B.4: CATE Results for Simulation 4

Note: The results for the \overline{RMSE} , $\overline{[BIAS]}$, \overline{SD} and \overline{JB} show the mean values of the root mean squared error, absolute bias, standard deviation and the Jarque-Bera test statistic of all 10⁷000 CATE estimates from the validation sample. The critical values for the JB test statistic are 5.991
and 9.210 at the 5% and 1% level, respectively. Additionally, X-F, DR-F, meta-learner for given measure and sample size.

Figure 1.B.4: CATE Results for Simulation 4

Note: The results for \overline{RMSE} , $\overline{|BIAS|}$, and \overline{SD} show the mean values of the root mean squared error, absolute bias, and standard deviation of all 10′000 CATE estimates from the validation sample. The fgure shows the results based on the increasing training samples of {500, 2 ′000, 8 ′000, 32′000} observations displayed on the log scale. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.B.1.5 Simulation 5: unbalanced treatment and linear CATE

			\overline{RMSE}				BIAS				\overline{SD}			\overline{JB}				
	<i>500</i>	2000	8000	<i>32000</i>	<i>500</i>	2000	8000	32000	<i>500</i>	2000	8000	32000	<i>500</i>	2000	8000	32000		
S	0.823	0.606	0.461	0.358	0.817	0.599	0.454	0.351	0.101	0.087	0.075	0.066	1.796	2.150	2.057	1.986		
S-W	0.305	0.244	0.196	0.164	0.255	0.209	0.170	0.145	0.222	0.159	0.117	0.089	2.457	2.189	2.054	1.957		
T	0.305	0.244	0.196	0.164	0.255	0.209	0.171	0.145	0.222	0.159	0.117	0.089	2.497	2.173	2.026	1.936		
$X-F$			0.237 0.178 0.137 0.109				0.200 0.154 0.120 0.097		0.164	0.110	0.078	0.058	3.329	2.228	2.102	2.022		
$X-S$	0.276	0.210	0.163	0.126	0.230	0.181	0.143	0.112	0.202		0.130 0.092	-0.067	6.639	2.811	2.296	2.421		
$X-C$	0.231	0.182	0.144	0.114	0.200	0.165	0.132	0.105				0.139 0.086 0.061 0.046	4.474	2.014	2.004	2.037		
$DR-F$		0.314 0.248	0.203	0.166	0.258	0.212	0.179	0.148	0.237	0.159	0.112	0.084		123.780 364.063 249.515		26.116		
DR-S	0.556	0.413	0.298	0.215	0.428	0.322	0.239	0.176	0.515	0.362	0.242	0.167		453.484 685.910 651.725 174.087				
$DR-C$	0.354	0.280	0.217	0.162	0.287	0.232	0.185	0.140	0.289	0.205	0.140	0.099	50.509	61.849	72.770	22.771		
$R-F$	0.392	0.312	0.254	0.223	0.314	0.253	0.211	0.190	0.339	0.253	0.187	0.146	12.888	28.931	17.700	4.568		
$R-S$	0.500	0.388	0.305	0.248	0.398	0.311	0.248	0.206	0.457	0.336	0.246	0.179	9.107	10.173	16.684	12.581		
$R-C$	0.311	0.262	0.222	0.194	0.256	0.219	0.191	0.172	0.241	0.185	0.139	0.104	2.925	3.617	3.874	3.072		

Table 1.B.5: CATE Results for Simulation 5

Note: The results for the \overline{RMSE} , $\overline{[BIAS]}$, \overline{SD} and \overline{JB} show the mean values of the root mean squared error, absolute bias, standard deviation and the Jarque-Bera test statistic of all 10⁷000 CATE estimates from the validation sample. The critical values for the JB test statistic are 5.991
and 9.210 at the 5% and 1% level, respectively. Additionally, X-F, DR-F, meta-learner for given measure and sample size.

Figure 1.B.5: CATE Results for Simulation 5

Note: The results for \overline{RMSE} , $\overline{|BIAS|}$, and \overline{SD} show the mean values of the root mean squared error, absolute bias, and standard deviation of all 10′000 CATE estimates from the validation sample. The fgure shows the results based on the increasing training samples of {500, 2 ′000, 8 ′000, 32′000} observations displayed on the log scale. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.B.2 Supplementary Results

This appendix provides supplementary results based on additional performance measures, complementing those from Section [1.4.1.](#page-32-0) To understand the simulation noise and thus the precision the average RMSE is measured with, we compute the standard error of the average RMSE following Knaus et al. [\(2021\)](#page-53-5) as:

$$
SE(\overline{RMSE}) = \sqrt{\frac{1}{R} \sum_{r=1}^{R} \left(\frac{1}{N^V} \sum_{i=1}^{N^V} \left(\tau(X_i) - \hat{\tau}^r(X_i) \right)^2 - \overline{RMSE} \right)^2}.
$$

Additionally, besides the absolute bias, we evaluate also the bias without the absolute value given by:

$$
BIAS(\hat{\tau}(X_i)) = \frac{1}{R} \sum_{r=1}^{R} \left(\tau(X_i) - \hat{\tau}^r(X_i) \right)
$$

We further evaluate also the components of the Jarque-Bera statistic separately, namely the skewness, i.e. $S(\hat{\tau}(X_i))$ and the kurtosis, i.e. $K(\hat{\tau}(X_i))$ defined by:

$$
S(\hat{\tau}(X_i)) = \frac{\frac{1}{R} \sum_{r=1}^{R} (\hat{\tau}^r(X_i) - \frac{1}{R} \sum_{r=1}^{R} \hat{\tau}^r(X_i))^3}{\left(\frac{1}{R} \sum_{r=1}^{R} (\hat{\tau}^r(X_i) - \frac{1}{R} \sum_{r=1}^{R} \hat{\tau}^r(X_i))^2\right)^{3/2}} \quad \text{and} \quad K(\hat{\tau}(X_i)) = \frac{\frac{1}{R} \sum_{r=1}^{R} (\hat{\tau}^r(X_i) - \frac{1}{R} \sum_{r=1}^{R} \hat{\tau}^r(X_i))^4}{\left(\frac{1}{R} \sum_{r=1}^{R} (\hat{\tau}^r(X_i) - \frac{1}{R} \sum_{r=1}^{R} \hat{\tau}^r(X_i))^2\right)^2}.
$$

As in the main simulation results, we report the averages of the above measures over the validation sample N^V . Complementary to the average values of the Jarque-Bera statistic presented in the main text, herein we report the share of CATEs for which the normality gets rejected at the 5% level. In order to further evaluate the performance on the replication level we compute the correlation between the true and the estimated treatment efects given by:

$$
CORR = \frac{1}{R} \sum_{r=1}^{R} \left(\rho(\tau, \hat{\tau}^r) \right)
$$

where τ is a vector of size N^V containing the true treatment effects from the validation sample and $\hat{\tau}^r$ is a vector of size N^V containing the estimated treatment effects for the validation sample at the replication r, while $\rho(\cdot)$ denotes the correlation function. Similarly, we compute also the variance ratio of the true and the estimated treatment efects as follows:

$$
VAR = \frac{1}{R} \sum_{r=1}^{R} \left(\frac{Var(\hat{\tau}^r)}{Var(\tau)} \right)
$$

where $Var(\cdot)$ denotes the variance. The full results including the main and the supplementary performance measures are listed in Tables [1.B.6](#page-71-0) - [1.B.12](#page-77-0) below.

1.B.2.1 Simulation 1: balanced treatment and constant zero CATE

		\overline{RMSE}				$SE(\overline{RMSE})$					BIAS				\overline{BIAS}		\overline{SD}				
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	
S	0.008	0.009	0.013	0.018	0.005	0.005	0.006	0.004	0.005	0.006	0.010	0.014	-0.003	-0.004	-0.006	-0.008	0.007	0.008	0.012	0.016	
S-W	0.037	0.038	0.049	0.059	0.028	0.024	0.024	0.015	0.023	0.025	0.036	0.047	-0.017	-0.020	-0.028	-0.033	0.033	0.032	0.040	0.047	
T.	0.225	0.168	0.128	0.101	0.046	0.024	0.013	0.007	0.180	0.135	0.103	0.082	-0.087	-0.072	-0.060	-0.048	0.206	0.149	0.109	0.083	
$X-F$	0.160	0.111	0.080	0.059	0.054	0.026	0.014	0.006	0.128	0.089	0.065	0.048	-0.074	-0.055	-0.041	-0.029	0.142	0.095	0.067	0.048	
$X-S$	0.186	0.127	0.091	0.067	0.071	0.034	0.018	0.008	0.149	0.103	0.074	0.055	-0.090	-0.071	-0.053	-0.037	0.162	0.106	0.073	0.053	
X-C	0.152	0.106	0.075	0.054	0.068	0.034	0.018	0.008	0.123	0.087	0.062	0.045	-0.092	-0.074	-0.052	-0.036	0.120	0.075	0.052	0.036	
$DR-F$	0.209	0.146	0.105	0.079	0.044	0.021	0.011	0.006	0.167	0.117	0.084	0.064	-0.072	-0.055	-0.043	-0.032	0.196	0.135	0.095	0.070	
$DR-S$	0.343	0.241	0.170	0.122	0.071	0.029	0.013	0.006	0.272	0.191	0.135	0.097	-0.069	-0.045	-0.030	-0.017	0.335	0.235	0.166	0.119	
$DR-C$	0.207	0.147	0.103	0.074	0.046	0.020	0.009	0.004	0.166	0.118	0.082	0.059	-0.072	-0.050	-0.029	-0.015	0.194	0.137	0.097	0.070	
$R-F$	0.261	0.192	0.145	0.114	0.039	0.020	0.012	0.006	0.208	0.153	0.116	0.092	-0.077	-0.066	-0.058	-0.048	0.249	0.180	0.132	0.102	
$R-S$	0.334	0.243	0.181	0.137	0.073	0.032	0.018	0.010	0.265	0.193	0.144	0.109	-0.089	-0.072	-0.064	-0.055	0.321	0.232	0.168	0.124	
$R-C$	0.208	0.156	0.118	0.092	0.050	0.026	0.015	0.008	0.166	0.125	0.096	0.075	-0.092	-0.077	-0.065	-0.054	0.186	0.135	0.098	0.072	
		\overline{SKEW}			\overline{KURT}						$JB\%$				CORR				VARR		
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	<i>2000</i>	8000	<i>32000</i>	500	2000	8000	32000	
S	2.638	1.809	0.929	0.307	17.334	10.674	5.654	3.539	1.000	1.000	1.000	0.539									
$S-W$	2.744	2.171	1.150	0.339	17.212	12.179	6.003	3.493	1.000	1.000	1.000	0.586									
T	0.005	-0.009	-0.004	-0.008	3.016	3.038	3.006	2.983	0.058	0.075	0.052	0.044									
$X-F$	0.010	-0.030	-0.001	-0.022	2.990	3.058	3.002	2.985	0.028	0.091	0.055	0.051									
$X-S$	0.017	-0.023	0.003	-0.008	2.951	3.023	3.029	3.003	0.036	0.066	0.063	0.060									
X-C	0.002	-0.040	0.003	-0.018	2.985	3.061	3.006	2.986	0.010	0.086	0.052	0.049									
$DR-F$	-0.008	-0.031	-0.020	-0.010	3.112	3.235	3.196	3.100	0.211	0.253	0.154	0.086									
$DR-S$	-0.009	-0.040	-0.060	-0.040	3.150	3.308	3.410	3.359	0.271	0.359	0.274	0.164									
$DR-C$	-0.013	-0.031	-0.039	-0.019	3.054	3.099	3.158	3.128	0.102	0.158	0.152	0.099									
$R-F$	0.017	0.015	0.013	0.007	3.145	3.296	3.256	3.147	0.275	0.296	0.181	0.104									
$R-S$	0.027	0.009	0.014	0.012	3.077	3.161	3.251	3.222	0.150	0.216	0.211	0.132									
$R-C$	0.003	0.003	0.001	0.008	3.024	3.065	3.081	3.067	0.065	0.092	0.104	0.083									

Table 1.B.6: CATE Results for Simulation 1

Note: The results for the \overline{RMSE} , $\overline{[BIAS]}$, \overline{BIAS} , $\overline{S}\overline{D}$, \overline{SKEW} , and \overline{KURT} show the mean values of the root mean squared error, absolute bias, bias, standard deviation, skewness and kurtosis of al estimates from the validation sample. $SE(\overline{RMSE})$ depicts the standard error of the average RMSE and JB% presents the share of CATEs for which the Jarque-Bera test has been rejected at the 5% level. The results for CORR and V ARR show the values of the correlation and variance ratio between the true and the estimated CATEs over all replications. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-fitting versions, respectively.
1.B.2.2 Simulation 2: balanced treatment and complex nonlinear CATE

			RMSE				$SE(\overline{RMSE})$				$ \overline{BIAS }$				\overline{BIAS}			\overline{SD}		
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S	0.527	0.442	0.374	0.326	0.114	0.092	0.075	0.064	0.522	0.434	0.366	0.317	-0.369	-0.258	-0.190	-0.143	0.055	0.068	0.066	0.064
$S-W$	0.463	0.357	0.303	0.265	0.084	0.050	0.045	0.041	0.431	0.328	0.280	0.246	-0.159	-0.036	-0.029	-0.023	0.177	0.151	0.120	0.099
	0.434	0.358	0.303	0.265	0.056	0.049	0.045	0.041	0.392	0.328	0.280	0.246	-0.040	-0.034	-0.029	-0.023	0.204	0.154	0.120	0.099
$X-F$	0.432	0.377	0.331	0.296	0.069	0.066	0.061	0.056	0.407	0.361	0.318	0.285	-0.031	-0.022	-0.017	-0.012	0.143	0.103	0.083	0.072
$X-S$	0.460	0.411	0.362	0.321	0.071	0.071	0.067	0.061	0.432	0.393	0.349	0.310	-0.041	-0.029	-0.021	-0.015	0.160	0.110	0.085	0.073
$X-C$	0.443	0.400	0.356	0.317	0.076	0.075	0.070	0.063	0.424	0.389	0.347	0.309	-0.042	-0.032	-0.022	-0.014	0.119	0.082	0.068	0.062
$DR-F$	0.439	0.366	0.312	0.276	0.058	0.053	0.048	0.044	0.399	0.338	0.291	0.259	-0.032	-0.026	-0.021	-0.016	0.197	0.144	0.113	0.095
$DR-S$	0.534	0.439	0.355	0.297	0.059	0.050	0.044	0.038	0.461	0.388	0.318	0.270	-0.027	-0.017	-0.013	-0.008	0.328	0.236	0.173	0.136
$DR-C$	0.451	0.388	0.322	0.276	0.060	0.057	0.050	0.044	0.413	0.361	0.302	0.259	-0.030	-0.021	-0.013	-0.006	0.193	0.146	0.114	0.095
$R-F$	0.458	0.373	0.307	0.266	0.052	0.045	0.039	0.034	0.404	0.333	0.277	0.241	-0.039	-0.034	-0.030	-0.027	0.251	0.188	0.146	0.122
$R-S$	0.529	0.439	0.356	0.298	0.060	0.050	0.043	0.038	0.458	0.389	0.319	0.269	-0.042	-0.036	-0.033	-0.030	0.318	0.236	0.178	0.140
$R-C$	0.449	0.388	0.322	0.274	0.061	0.058	0.050	0.044	0.413	0.361	0.301	0.256	-0.045	-0.040	-0.034	-0.028	0.187	0.145	0.116	0.097
			SKEW				KURT				$JB\%$				$CORR$			VARR		
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S	-1.172	-0.282	-0.138	-0.087	4.608	3.106	3.021	3.003	1.000	0.832	0.206	0.087	0.430	0.737	0.850	0.890	772.103	31.143	11.674	6.871
S-W	-0.820	-0.054	-0.003	0.003	3.494	3.015	3.027	2.999	1.000	0.116	0.075	0.058	0.490	0.728	0.846	0.896	51.036	5.794	4.379	3.494
T	0.000	-0.007	0.002	0.004	3.030	3.043	3.025	3.002	0.070	0.085	0.072	0.057	0.465	0.722	0.846	0.896	6.865	5.692	4.382	3.492
$X-F$	0.001	-0.012	0.007	0.001	3.010	3.026	2.984	2.971	0.045	0.067	0.045	0.043	0.458	0.723	0.847	0.891	20.826	14.657	8.854	5.962
$X-S$	0.008	-0.014	0.011	-0.007	2.931	3.022	3.006	2.981	0.043	0.058	0.062	0.050	0.266	0.553	0.785	0.868	25.303	22.204	13.868	8.249
$X-C$	0.000		0.007	-0.006						0.065	0.045	0.045	0.391	0.677	0.835	0.886	55.123	33.303	15.678	8.554
		-0.022			2.993	3.029	2.983	2.975	0.015											
$DR-F$	-0.003	-0.013	-0.000	0.000	3.082	3.054	3.002	2.976	0.151	0.100	0.052	0.046	0.429	0.707	0.842	0.891	7.946	6.991	5.202	4.024
$DR-S$	-0.002	-0.021	-0.009	-0.010	3.135	3.199	3.090	3.016	0.247	0.249	0.113	0.063	0.224	0.455	0.718	0.841	3.595	4.565	4.468	3.649
$DR-C$	-0.006	-0.017	-0.005	0.001	3.057	3.047	3.005	2.978	0.099	0.087	0.056	0.051	0.359	0.628	0.828	0.895	9.232	8.713	5.869	4.112
$R-F$	0.012	0.006	0.015	0.010	3.107	3.086	3.018	2.986	0.200	0.132	0.064	0.050	0.398	0.668	0.824	0.884	4.473	4.449	3.642	3.005
$R-S$ $R-C$	0.014 0.001	0.003 0.002	0.017 0.013	0.011 0.017	3.072 3.033	3.108 3.033	3.073 3.000	3.008 2.983	0.130 0.069	0.151 0.074	0.097 0.053	0.059 0.048	0.227 0.363	0.456 0.630	0.716 0.828	0.840 0.897	3.805 9.803	4.558 8.713	4.304 5.702	3.512 3.970

Table 1.B.7: CATE Results for Simulation 2

Note: The results for the \overline{RMSE} , \overline{BIAS} , \overline{BIS} , $\overline{S}\overline{D}$, \overline{SKEW} , and \overline{KURT} show the mean values of the root mean squared error, absolute bias, bias, standard deviation, skewness and kurtosis of al from the validation sample. $SE(\overline{RMSE})$ depicts the standard error of the average RMSE and JB% presents the share of CATEs for which the Jarque-Bera test has been rejected at the 5% level. The results for CORR and V ARR show the values of the correlation and variance ratio between the true and the estimated CATEs over all replications. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.B.2.3 Simulation 3: highly unbalanced treatment and constant non-zero CATE

		RMSE					$SE(\overline{RMSE})$				BIAS				\overline{BIAS}				\overline{SD}	
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S	0.645	0.475	0.359	0.279	0.077	0.043	0.025	0.014	0.638	0.468	0.352	0.272	0.638	0.468	0.352	0.272	0.099	0.084	0.072	0.062
$S-W$	0.246	0.191	0.146	0.111	0.059	0.025	0.015	0.009	0.197	0.154	0.119	0.091	-0.045	-0.050	-0.042	-0.032	0.233	0.163	0.121	0.090
T	0.244	0.191	0.146	0.111	0.053	0.025	0.015	0.008	0.195	0.154	0.119	0.091	-0.057	-0.050	-0.041	-0.032	0.227	0.164	0.121	0.090
$X-F$	0.180	0.123	0.090	0.068	0.060	0.024	0.012	0.006	0.144	0.098	0.072	0.054	-0.041	-0.033	-0.025	-0.016	0.175	0.118	0.085	0.061
$X-S$	0.226	0.149	0.110	0.078	0.095	0.040	0.019	0.007	0.180	0.119	0.087	0.062	-0.058	-0.042	-0.034	-0.021	0.219	0.143	0.104	0.072
$X-C$	0.159	0.102	0.073	0.054	0.074	0.031	0.015	0.007	0.127	0.081	0.059	0.043	-0.053	-0.043	-0.033	-0.021	0.150	0.092	0.064	0.046
$DR-F$	0.287	0.202	0.146	0.110	0.058	0.022	0.012	0.007	0.222	0.158	0.116	0.089	-0.049	-0.040	-0.029	-0.017	0.279	0.188	0.129	0.093
$DR-S$	0.649	0.502	0.334	0.218	0.204	0.093	0.039	0.018	0.475	0.365	0.250	0.168	-0.052	-0.038	-0.025	-0.007	0.645	0.498	0.329	0.213
$DR-C$	0.364	0.290	0.197	0.131	0.075	0.032	0.016	0.008	0.282	0.223	0.153	0.104	-0.048	-0.036	-0.026	-0.005	0.359	0.283	0.189	0.124
$R-F$	0.441	0.366	0.293	0.243	0.048	0.028	0.022	0.020	0.348	0.287	0.232	0.195	0.032	0.040	0.043	0.048	0.435	0.354	0.273	0.215
$R-S$	0.573	0.461	0.366	0.285	0.141	0.057	0.034	0.025	0.453	0.363	0.288	0.227	0.032	0.038	0.042	0.044	0.570	0.454	0.353	0.264
$R-C$	0.295	0.262	0.220	0.184	0.044	0.022	0.017	0.019	0.235	0.208	0.176	0.150	0.030	0.041	0.043	0.046	0.289	0.249	0.199	0.152
		SKEW					\overline{KURT}				$JB\%$				CORR				<i>VARR</i>	
	500	2000	8000	32000	<i>500</i>	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S.	0.060	0.062	0.037	0.027	2.991	3.007	2.999	2.983	0.113	0.101	0.059	0.052								
$S-W$	-0.070	-0.005	-0.011	-0.003	3.102	3.039	3.028	2.988	0.277	0.075	0.067	0.049								
T	-0.024	-0.007	-0.009	-0.003	3.062	3.042	3.024	2.987	0.121	0.076	0.067	0.046								
$X-F$	-0.055	-0.015	-0.023	-0.004	3.080	3.069	3.111	3.035	0.186	0.095	0.123	0.068								
$X-S$	-0.017	0.030	-0.012	-0.010	3.085	3.074	3.095	3.083	0.084	0.107	0.110	0.091								
X-C	-0.101	-0.014	-0.025	-0.001	3.127	3.020	3.021	2.998	0.430	0.053	0.067	0.049								
$DR-F$	-0.006	-0.035	-0.041	-0.020	5.349	4.944	3.984	3.340	0.949	0.674	0.337	0.147								
$DR-S$	-0.011	-0.070	-0.096	-0.095	6.502	7.416	6.268	4.523	1.000	0.995	0.817	0.397								
$DR-C$	-0.033	-0.047	-0.056	-0.055	4.033	4.468	4.258	3.538	0.996	0.928	0.557	0.229								
$R-F$	-0.026	-0.025	-0.012	0.006	3.325	3.511	3.375	3.159	0.658	0.542	0.282	0.121								
$R-S$	0.035	-0.003	-0.018	-0.005	3.222	3.382	3.464	3.292	0.468	0.520	0.378	0.183								
$R-C$	-0.015	-0.011	-0.006	0.009	3.067	3.129	3.159	3.086	0.117	0.173	0.178	0.105								

Table 1.B.8: CATE Results for Simulation 3

Note: The results for the \overline{RMSE} , $\overline{[BIAS]}$, \overline{BIAS} , $\overline{S}\overline{D}$, \overline{SKEW} , and \overline{KURT} show the mean values of the root mean squared error, absolute bias, bias, standard deviation, skewness and kurtosis of al estimates from the validation sample. $SE(\overline{RMSE})$ depicts the standard error of the average RMSE and $JB\%$ presents the share of CATEs for which the Jarque-Bera test has been rejected at the 5% level. The results for CORR and V ARR show the values of the correlation and variance ratio between the true and the estimated CATEs over all replications. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-fitting versions, respectively.

1.B.2.4 Simulation 4: unbalanced treatment and simple CATE

		RMSE					$SE(\overline{RMSE})$				BIAS				\overline{BIAS}			\overline{SD}		
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S	0.834	0.616	0.472	0.370	0.121	0.106	0.091	0.076	0.825	0.606	0.462	0.361	0.825	0.605	0.458	0.354	0.105	0.090	0.078	0.069
$S-W$	0.443	0.336	0.258	0.206	0.049	0.032	0.024	0.020	0.390	0.300	0.233	0.187	-0.077	-0.071	-0.059	-0.048	0.229	0.162	0.120	0.093
Т	0.443	0.335	0.258	0.206	0.049	0.033	0.024	0.020	0.390	0.300	0.233	0.187	-0.076	-0.071	-0.059	-0.048	0.229	0.163	0.120	0.093
$X-F$	0.428	0.329	0.247	0.191	0.040	0.026	0.017	0.011	0.394	0.308	0.233	0.180	-0.061	-0.052	-0.038	-0.027	0.171	0.114	0.083	0.064
$X-S$	0.501	0.399	0.307	0.232	0.052	0.031	0.020	0.014	0.456	0.375	0.291	0.220	-0.077	-0.064	-0.050	-0.034	0.213	0.136	0.097	0.073
$X-C$	0.477	0.385	0.300	0.227	0.033	0.021	0.015	0.010	0.453	0.374	0.292	0.220	-0.079	-0.067	-0.048	-0.034	0.148	0.091	0.068	0.055
$DR-F$	0.510	0.369	0.275	0.214	0.046	0.033	0.020	0.013	0.454	0.334	0.251	0.196	-0.064	-0.055	-0.038	-0.027	0.249	0.165	0.117	0.088
DR-S	0.728	0.537	0.339	0.230	0.122	0.059	0.030	0.016	0.591	0.445	0.279	0.190	-0.055	-0.050	-0.034	-0.014	0.549	0.377	0.247	0.171
$DR-C$	0.565	0.435	0.269	0.182	0.043	0.035	0.021	0.012	0.493	0.388	0.236	0.159	-0.069	-0.054	-0.030	-0.010	0.308	0.215	0.145	0.104
$R-F$	0.537	0.426	0.349	0.293	0.046	0.030	0.021	0.015	0.454	0.364	0.303	0.258	-0.029	-0.022	-0.012	-0.005	0.337	0.250	0.192	0.151
$R-S$	0.653	0.521	0.412	0.338	0.092	0.049	0.032	0.023	0.539	0.438	0.352	0.294	-0.035	-0.032	-0.019	-0.014	0.460	0.332	0.245	0.184
$R-C$	0.524	0.440	0.361	0.303	0.032	0.026	0.018	0.015	0.469	0.402	0.333	0.282	-0.039	-0.030	-0.018	-0.011	0.246	0.185	0.142	0.113
		\overline{SKEW}					\overline{KURT}				$JB\%$				CORR			VARR		
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S	0.015	0.028	0.030	0.019	3.010	3.000	2.993	2.976	0.050	0.056	0.056	0.047	0.598	0.816	0.904	0.942	24.819	10.142	5.669	3.726
S-W	-0.027	-0.003	-0.001	-0.005	3.047	3.026	3.002	2.982	0.101	0.076	0.058	0.044	0.507	0.763	0.878	0.926	4.538	3.298	2.466	2.002
T	-0.027	-0.005	-0.002	-0.006	3.044	3.025	3.003	2.977	0.094	0.076	0.060	0.044	0.509	0.764	0.878	0.927	4.528	3.295	2.467	1.994
$X-F$	-0.064	-0.017	-0.010	-0.013	3.065	3.020	3.006	2.966	0.192	0.076	0.068	0.048	0.644	0.877	0.952	0.977	9.886	5.412	3.200	2.330
$X-S$	-0.071	-0.027	-0.009	-0.014	3.185	3.066	3.038	2.992	0.426	0.112	0.073	0.057	0.337	0.734	0.909	0.963	14.543	9.199	4.845	2.973
$X-C$	-0.103	-0.029	-0.017	-0.010	3.089	2.962	2.996	2.959	0.374	0.049	0.052	0.042	0.496	0.850	0.945	0.975	31.636	11.894	5.217	3.047
$DR-F$	-0.058	-0.059	-0.034	-0.011	3.848	3.745	3.319	3.054	0.798	0.443	0.200	0.073	0.242	0.717	0.894	0.949	4.993	4.567	3.159	2.400
$DR-S$	-0.067	-0.115	-0.101	-0.076	5.197	5.478	4.775	3.768	0.999	0.933	0.587	0.267	0.061	0.324	0.742	0.892	1.351	1.832	1.821	1.578
$DR-C$	-0.026	-0.054	-0.059	-0.047	3.683	3.762	3.578	3.234	0.958	0.710	0.371	0.146	0.107	0.498	0.870	0.948	3.482	4.144	2.451	1.768
$R-F$	-0.018	-0.007	-0.002	0.001	3.215	3.280	3.152	3.031	0.443	0.342	0.165	0.067	0.251	0.524	0.712	0.825	2.355	2.844	2.901	2.686
$R-S$	0.049	0.024	0.010	0.003	3.182	3.217	3.212	3.106	0.412	0.314	0.211	0.110	0.105	0.308	0.564	0.739	1.873	2.403	2.835	2.879
$R-C$	-0.028	0.000	0.002	-0.004	3.053	3.076	3.060	3.016	0.110	0.118	0.098	0.066	0.174	0.476	0.731	0.846	5.354	5.714	4.761	3.722

Table 1.B.9: CATE Results for Simulation 4

Note: The results for the \overline{RMSE} , $\overline{[BIAS]}$, \overline{BIAS} , $\overline{S}\overline{D}$, \overline{SKEW} , and \overline{KURT} show the mean values of the root mean squared error, absolute bias, bias, standard deviation, skewness and kurtosis of al estimates from the validation sample. $SE(\overline{RMSE})$ depicts the standard error of the average RMSE and JB% presents the share of CATEs for which the Jarque-Bera test has been rejected at the 5% level. The results for CORR and V ARR show the values of the correlation and variance ratio between the true and the estimated CATEs over all replications. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-fitting versions, respectively.

1.B.2.5 Simulation 5: unbalanced treatment and linear CATE

		RMSE					$SE(\overline{RMSE})$				$\overline{BIAS }$				\overline{BIAS}				\overline{SD}	
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S	0.823	0.606	0.461	0.358	0.069	0.043	0.031	0.028	0.817	0.599	0.454	0.351	0.817	0.599	0.454	0.351	0.101	0.087	0.075	0.066
$S-W$	0.305	0.244	0.196	0.164	0.046	0.029	0.021	0.017	0.255	0.209	0.170	0.145	-0.076	-0.067	-0.054	-0.044	0.222	0.159	0.117	0.089
Т	0.305	0.244	0.196	0.164	0.046	0.029	0.021	0.017	0.255	0.209	0.171	0.145	-0.076	-0.068	-0.055	-0.044	0.222	0.159	0.117	0.089
$X-F$	0.237	0.178	0.137	0.109	0.044	0.026	0.017	0.014	0.200	0.154	0.120	0.097	-0.062	-0.052	-0.038	-0.028	0.164	0.110	0.078	0.058
$X-S$	0.276	0.210	0.163	0.126	0.068	0.032	0.021	0.015	0.230	0.181	0.143	0.112	-0.074	-0.065	-0.050	-0.034	0.202	0.130	0.092	0.067
$X-C$	0.231	0.182	0.144	0.114	0.049	0.030	0.022	0.017	0.200	0.165	0.132	0.105	-0.078	-0.067	-0.048	-0.034	0.139	0.086	0.061	0.046
$DR-F$	0.314	0.248	0.203	0.166	0.041	0.025	0.023	0.020	0.258	0.212	0.179	0.148	-0.064	-0.054	-0.038	-0.027	0.237	0.159	0.112	0.084
$DR-S$	0.556	0.413	0.298	0.215	0.136	0.053	0.024	0.016	0.428	0.322	0.239	0.176	-0.053	-0.051	-0.034	-0.014	0.515	0.362	0.242	0.167
$DR-C$	0.354	0.280	0.217	0.162	0.054	0.024	0.019	0.016	0.287	0.232	0.185	0.140	-0.068	-0.053	-0.030	-0.010	0.289	0.205	0.140	0.099
$R-F$	0.392	0.312	0.254	0.223	0.038	0.023	0.020	0.019	0.314	0.253	0.211	0.190	-0.021	-0.016	-0.009	-0.003	0.339	0.253	0.187	0.146
$R-S$	0.500	0.388	0.305	0.248	0.105	0.042	0.024	0.020	0.398	0.311	0.248	0.206	-0.023	-0.024	-0.014	-0.010	0.457	0.336	0.246	0.179
$R-C$	0.311	0.262	0.222	0.194	0.037	0.022	0.021	0.023	0.256	0.219	0.191	0.172	-0.028	-0.021	-0.013	-0.007	0.241	0.185	0.139	0.104
		SKEW					\overline{KURT}				$JB\%$				CORR				VARR	
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S.	0.004	0.030	0.027	0.026	2.981	2.998	2.991	2.984	0.034	0.062	0.054	0.050	0.211	0.415	0.561	0.672	6.435	4.582	4.002	3.502
$S-W$	-0.024	-0.005	-0.007	-0.012	3.045	3.023	3.000	2.988	0.087	0.067	0.054	0.048	-0.035	0.115	0.332	0.524	1.094	1.571	2.232	2.654
T.	-0.024	-0.005	-0.006	-0.008	3.045	3.025	2.996	2.981	0.091	0.065	0.053	0.047	-0.034	0.115	0.331	0.524	1.093	1.573	2.230	2.652
$X-F$	-0.056	-0.015	-0.008	-0.012	3.061	3.020	3.015	2.987	0.163	0.067	0.059	0.051	0.202	0.481	0.728	0.849	2.966	3.413	3.225	2.767
$X-S$	-0.063	-0.025	-0.013	-0.016	3.202	3.087	3.032	3.009	0.442	0.120	0.075	0.063	0.093	0.270	0.563	0.780	3.071	3.496	3.862	3.255
$X-C$	-0.081	-0.026	-0.011	-0.021	3.101	2.960	2.999	2.983	0.260	0.047	0.051	0.054	0.154	0.400	0.713	0.861	7.940	7.788	6.045	3.922
$DR-F$	-0.064	-0.072	-0.047	-0.026	3.874	4.167	3.685	3.167	0.803	0.500	0.250	0.101	-0.038	0.013	0.159	0.442	0.965	1.702	2.879	3.695
$DR-S$	-0.073	-0.121	-0.132	-0.113	5.095	5.798	5.324	4.050	0.998	0.933	0.601	0.285	-0.012	0.016	0.101	0.345	0.251	0.361	0.691	1.205
$DR-C$	-0.029	-0.062	-0.077	-0.061	3.678	3.871	3.805	3.335	0.957	0.750	0.407	0.167	-0.012	0.030	0.167	0.515	0.664	1.013	1.885	2.627
$R-F$	-0.028	-0.017	-0.002	-0.007	3.282	3.454	3.273	3.069	0.563	0.445	0.203	0.082	0.004	0.055	0.114	0.150	0.400	0.631	1.037	1.510
$R-S$	0.043	0.020	0.004	-0.010	3.234	3.309	3.373	3.229	0.525	0.438	0.302	0.154	-0.014	0.016	0.063	0.124	0.310	0.419	0.680	1.134
$R-C$	-0.029	-0.002	-0.002	-0.001	3.064	3.117	3.124	3.055	0.129	0.165	0.146	0.081	-0.027	0.024	0.102	0.193	0.923	1.223	1.840	2.659

Table 1.B.10: CATE Results for Simulation 5

Note: The results for the \overline{RMSE} , \overline{BIAS} , \overline{BIAS} , \overline{SDS} , \overline{SKEW} , and \overline{KUR} show the mean values of the root mean squared error, absolute bias, bias, standard deviation, skewness and kurtosis of all 10' estimates from the validation sample. $SE(\overline{RMSE})$ depicts the standard error of the average RMSE and JB% presents the share of CATEs for which the Jarque-Bera test has been rejected at the 5% level. The results for CORR and VARR show the values of the correlation and variance ratio between the true and the estimated CATEs over all replications. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.B.2.6 Main Simulation: unbalanced treatment and nonlinear CATE

		RMSE					$SE(\overline{RMSE})$				BIAS				\overline{BIAS}				\overline{SD}	
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S	0.878	0.749	0.651	0.570	0.203	0.169	0.142	0.121	0.867	0.739	0.641	0.560	0.578	0.413	0.305	0.229	0.108	0.096	0.091	0.088
$S-W$	0.765	0.634	0.533	0.462	0.123	0.107	0.093	0.082	0.717	0.602	0.508	0.443	-0.135	-0.121	-0.099	-0.081	0.261	0.190	0.149	0.125
T.	0.766	0.634	0.533	0.462	0.123	0.107	0.093	0.081	0.719	0.602	0.509	0.442	-0.139	-0.121	-0.099	-0.081	0.260	0.190	0.149	0.125
$X-F$	0.743	0.618	0.517	0.442	0.128	0.111	0.095	0.082	0.711	0.597	0.500	0.427	-0.124	-0.102	-0.077	-0.060	0.200	0.141	0.117	0.103
$X-S$	0.820	0.707	0.591	0.499	0.137	0.127	0.109	0.093	0.779	0.684	0.574	0.484	-0.147	-0.123	-0.096	-0.073	0.244	0.164	0.125	0.107
$X-C$	0.794	0.693	0.582	0.494	0.144	0.132	0.112	0.095	0.770	0.680	0.571	0.482	-0.151	-0.126	-0.095	-0.072	0.171	0.114	0.097	0.092
$DR-F$	0.817	0.659	0.542	0.463	0.126	0.112	0.097	0.085	0.764	0.627	0.518	0.443	-0.116	-0.095	-0.067	-0.049	0.285	0.194	0.149	0.126
$DR-S$	1.053	0.825	0.579	0.445	0.133	0.097	0.076	0.064	0.906	0.731	0.521	0.403	-0.102	-0.085	-0.053	-0.021	0.640	0.433	0.281	0.206
$DR-C$	0.880	0.727	0.523	0.409	0.118	0.112	0.088	0.072	0.809	0.680	0.490	0.383	-0.118	-0.088	-0.049	-0.017	0.359	0.255	0.179	0.143
$R-F$	0.815	0.679	0.590	0.529	0.112	0.101	0.095	0.090	0.746	0.632	0.554	0.499	-0.115	-0.100	-0.081	-0.066	0.346	0.251	0.201	0.172
$R-S$	0.932	0.788	0.659	0.580	0.120	0.110	0.100	0.095	0.833	0.721	0.613	0.546	-0.126	-0.117	-0.095	-0.081	0.468	0.333	0.243	0.195
$R-C$	0.825	0.725	0.621	0.554	0.130	0.123	0.110	0.102	0.779	0.694	0.597	0.533	-0.131	-0.115	-0.094	-0.077	0.261	0.196	0.155	0.136
		SKEW					\overline{KURT}				$JB\%$				CORR				VARR	
	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000	500	2000	8000	32000
S	0.115	0.071	0.047	0.024	3.006	2.966	2.990	2.968	0.466	0.115	0.062	0.045	0.624	0.831	0.904	0.934	92.890	27.182	12.760	7.598
S-W	-0.024	-0.016	-0.011	-0.026	3.004	2.999	2.988	2.967	0.055	0.056	0.054	0.044	0.524	0.798	0.891	0.922	13.575	8.180	5.033	3.633
T	-0.035	-0.017	-0.014	-0.027	3.035	2.996	2.986	2.967	0.097	0.055	0.051	0.044	0.514	0.798	0.891	0.922	13.471	8.176	5.034	3.626
$X-F$	-0.060	-0.030	-0.017	-0.023	3.054	2.984	2.985	2.950	0.171	0.064	0.049	0.040	0.664	0.894	0.950	0.967	24.558	11.070	6.021	4.070
$X-S$	-0.067	-0.030	-0.028	-0.019	3.143	3.047	3.002	2.964	0.323	0.106	0.060	0.045	0.367	0.754	0.919	0.957	38.577	21.499	9.669	5.561
$X-C$	-0.079	-0.042	-0.021	-0.021	3.064	2.953	2.987	2.944	0.209	0.066	0.049	0.037	0.530	0.852	0.946	0.966	79.900	27.087	10.181	5.644
$DR-F$	-0.106	-0.073	-0.034	-0.022	3.915	3.381	3.081	2.982	0.827	0.366	0.119	0.052	0.317	0.770	0.912	0.948	13.371	10.505	6.196	4.273
$DR-S$	-0.143	-0.216	-0.148	-0.084	5.350	5.320	4.033	3.317	1.000	0.947	0.526	0.189	0.095	0.406	0.812	0.918	3.696	4.807	3.992	2.940
$DR-C$	-0.080	-0.111	-0.075	-0.044	3.678	3.629	3.243	3.034	0.960	0.668	0.243	0.085	0.162	0.580	0.899	0.950	9.167	9.660	4.855	3.102
$R-F$	-0.009	-0.006	-0.013	-0.018	3.126	3.077	3.012	2.982	0.233	0.128	0.063	0.049	0.368	0.692	0.832	0.890	7.963	7.751	6.147	4.980
$R-S$	0.031	0.018	0.002	-0.009	3.107	3.097	3.048	2.992	0.207	0.151	0.082	0.054	0.166	0.449	0.732	0.846	6.605	7.982	7.305	6.036
$R-C$	-0.021	-0.006	-0.014	-0.020	3.043	3.018	3.003	2.966	0.088	0.063	0.052	0.042	0.271	0.624	0.843	0.902	17.941	15.725	9.647	6.705

Table 1.B.11: CATE Results for Main Simulation

Note: The results for the \overline{RMSE} , \overline{BIAS} , \overline{BIS} , $\overline{S}\overline{D}$, \overline{SKEW} , and \overline{KURT} show the mean values of the root mean squared error, absolute bias, bias, standard deviation, skewness and kurtosis of al from the validation sample. $SE(\overline{RMSE})$ depicts the standard error of the average RMSE and JB% presents the share of CATEs for which the Jarque-Bera test has been rejected at the 5% level. The results for CORR and V ARR show the values of the correlation and variance ratio between the true and the estimated CATEs over all replications. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

1.B.2.7 Empirical Simulation

		\overline{RMSE}			$SE(\overline{RMSE})$			BIAS			\overline{BIAS}			\overline{SD}	
	500	2000	8000	500	2000	8000	500	2000	8000	500	2000	8000	500	2000	8000
S	0.175	0.127	0.093	0.025	0.015	0.009	0.171	0.121	0.090	0.171	0.119	0.085	0.035	0.035	0.023
$S-W$	0.131	0.109	0.078	0.031	0.014	0.011	0.106	0.090	0.070	-0.011	-0.050	-0.043	0.121	0.084	0.037
T	0.150	0.111	0.079	0.027	0.014	0.011	0.122	0.092	0.071	-0.063	-0.053	-0.044	0.127	0.084	0.037
$X-F$	0.112	0.082	0.056	0.029	0.014	0.011	0.092	0.069	0.052	-0.056	-0.045	-0.036	0.089	0.056	0.021
$X-S$	0.129	0.093	0.069	0.041	0.019	0.011	0.105	0.078	0.060	-0.065	-0.054	-0.043	0.104	0.067	0.040
$X-C$	0.103	0.077	0.055	0.035	0.018	0.013	0.087	0.067	0.052	-0.065	-0.054	-0.043	0.072	0.044	0.017
$DR-F$	0.147	0.105	0.070	0.026	0.014	0.010	0.119	0.087	0.063	-0.061	-0.051	-0.042	0.125	0.078	0.033
$DR-S$	0.256	0.180	0.123	0.055	0.023	0.011	0.201	0.143	0.101	-0.066	-0.056	-0.047	0.242	0.162	0.097
$DR-C$	0.159	0.116	0.078	0.031	0.015	0.011	0.128	0.096	0.071	-0.068	-0.057	-0.046	0.135	0.088	0.037
$R-F$	0.183	0.131	0.089	0.022	0.011	0.009	0.146	0.107	0.078	-0.051	-0.043	-0.034	0.167	0.109	0.051
$R-S$	0.237	0.174	0.123	0.046	0.021	0.011	0.189	0.140	0.100	-0.058	-0.049	-0.042	0.224	0.158	0.099
$R-C$	0.144	0.109	0.076	0.026	0.013	0.010	0.117	0.091	0.068	-0.058	-0.050	-0.040	0.123	0.084	0.037
		\overline{SKEW}			\overline{KURT}			$JB\%$			CORR			VARR	
	500	2000	8000	500	2000	8000	500	2000	8000	500	2000	8000	500	2000	8000
S	0.671	0.178	0.031	3.310	2.998	2.988	1.000	0.511	0.051	0.050	0.135	0.328	10.481	2.315	1.666
S-W	0.394	0.014	0.007	2.838	2.979	2.984	1.000	0.049	0.040	0.061	0.162	0.359	0.562	0.331	0.448
T	0.002	0.007	0.001	3.001	2.986	2.995	0.055	0.056	0.058	0.058	0.158	0.357	0.200	0.323	0.447
$X-F$	0.007	0.013	0.007	3.006	2.981	2.999	0.053	0.049	0.055	0.103	0.223	0.458	0.542	0.748	0.912
$X-S$	0.020	0.022	0.007	3.024	3.045	2.993	0.063	0.100	0.045	0.058	0.134	0.297	0.544	0.716	0.981
$X-C$	0.009	0.011	0.007	2.987	2.964	2.982	0.028	0.027	0.049	0.094	0.197	0.393	1.327	1.527	1.665
$DR-F$	0.012	0.008	0.001	3.100	3.025	2.986	0.209	0.105	0.054	0.059	0.139	0.372	0.209	0.388	0.645
$DR-S$	0.013	0.016	0.006	3.678	3.476	3.130	0.906	0.472	0.161	0.031	0.066	0.161	0.065	0.110	0.220
$DR-C$	0.018	0.014	-0.009	3.158	3.095	3.055	0.318	0.190	0.098	0.053	0.113	0.251	0.185	0.309	0.564
$R-F$	-0.012	-0.009	-0.006	3.068	3.042	2.990	0.179	0.125	0.047	0.072	0.145	0.306	0.105	0.188	0.320
$R-S$	-0.002	-0.015	-0.006	3.090	3.083	3.052	0.166	0.154	0.109	0.040	0.080	0.174	0.074	0.116	0.212
$R-C$	0.002	-0.006	-0.007	3.004	2.987	3.023	0.053	0.060	0.062	0.068	0.139	0.275	0.219	0.333	0.545

Table 1.B.12: CATE Results for Empirical Simulation

Note: The results for the \overline{RMSE} , $\overline{[BIAS]}$, \overline{BIAS} , \overline{SD} , \overline{SKEW} , and \overline{KURT} show the mean values of the root mean squared error, absolute bias, bias, standard deviation, skewness and kurtosis of all 1'000 CATE estimates from the validation sample. $SE(\overline{RMSE})$ depicts the standard error of the average RMSE and JB% presents the share of CATEs for which the Jarque-Bera test has been rejected at the 5% level. The results for CORR and V ARR show the values of the correlation and variance ratio between the true and the estimated CATEs over all replications. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-fitting versions, respectively.

1.C Computation Time

In order to assess the computational trade-ofs among diferent estimation schemes as well as diferent meta-learners we evaluate the computational time for each meta-learner and each estimation scheme for each sample size over 10 replications of the Main Simulation to illustrate the performance. The results are summarized in Table [1.C.1](#page-78-0) and Figure [1.C.1](#page-78-1) below.

1.C.1 Main Simulation: unbalanced treatment and nonlinear CATE

			MEAN				SD.				MIN				MAX	
	<i>500</i>	2000	8000	32000	500	2000	<i>8000</i>	32000	<i>500</i>	2000	<i>8000</i>	<i>32000</i>	<i>500</i>	2000	8000	32000
S.	1.492	8.786		53.385 252.165		0.039 0.991	9.777	0.551	1.440			7.110 43.000 251.050	1.560	9.860		67.790 252.810
S-W	1.416	6.730		39.117 263.195		0.051 1.015	5.804	4.636	1.330			4.890 31.920 250.630	1.500	8.050		49.950 267.140
T.	1.203	6.168		38.933 238.932		0.043 0.880	5.982	26.988	1.110			4.460 29.530 162.260	1.260	7.540		47.340 249.560
X-F		2.894 16.512		92.803 658.892			0.081 1.303 10.148	49.316				2.770 14.070 80.950 531.960			2.980 17.590 106.570 687.320	
X-S	0.915	4.233		28.863 185.232		0.074 0.380	3.061	21.873	0.760			3.500 25.830 145.250	1.000	4.640		35.250 215.630
X-C		3.027 14.353		89.644 627.236		0.265 0.657	9.687	91.057				2.790 13.300 79.280 405.540			3.470 15.720 103.810 721.920	
		DR-F 2.262 15.998		94.615 576.230				0.129 0.696 16.618 120.102				2.080 14.920 57.130 323.300			2.490 17.040 113.820 676.650	
		DR-S 0.836 4.292		30.218 214.072			0.189 0.345 5.321	36.595	0.580			3.780 26.640 160.380	1.200	4.940		42.280 277.320
				DR-C 2.684 17.272 105.261 664.728			0.596 3.941 14.058	60.375				2.150 12.770 88.690 572.030			4.300 22.850 128.400 744.670	
$R-F$		2.058 10.588		78.830 530.529			0.594 1.430 18.923	78.864	0.840			8.750 28.900 354.890		2.450 13.020		91.270 603.520
$R-S$	0.919	6.514		31.234 208.910			0.429 2.084 7.845	49.782	0.530			4.420 21.340 154.770		2.100 10.440		43.750 308.480
$R-C$		2.177 11.934		72.912 435.450				0.080 1.230 23.239 140.374	2.020			9.240 53.290 312.420			2.250 12.970 134.670 780.560	
												<i>Note:</i> The results for the MEAN, SD, MIN, and MAX show the values of the mean, standard deviation, minimum and maximum for the				
												computation time in seconds based on 10 simulation replications. The computation time includes both the estimation as well as the prediction				
												task. No multithreading used within the estimation of meta-learners. Additionally, X-F, DR-F, R-F denote the full-sample versions of the				
												meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-fitting versions, respectively.				

Table 1.C.1: Computation Time Results for Main Simulation

Note: The results for the MEAN, SD, MIN, and MAX show the values of the mean, standard deviation, minimum and maximum for the computation time in seconds based on 10 simulation replications. The fgure shows the results based on the increasing training samples of {500, 2 ′000, 8 ′000, 32′000} observations displayed on the log scale. Additionally, X-F, DR-F, R-F denote the full-sample versions of the meta-learners, while X-S, DR-S, R-S and X-C, DR-C, R-C denote the sample-splitting and cross-ftting versions, respectively.

Chapter 2

Random Forest Estimation of the Ordered Choice Model

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Abstract

In this paper we develop a new machine learning estimator for ordered choice models based on the random forest. The proposed *Ordered Forest* flexibly estimates the conditional choice probabilities while taking the ordering information explicitly into account. In addition to common machine learning estimators, it enables the estimation of marginal efects as well as conducting inference and thus provides the same output as classical econometric estimators. An extensive simulation study reveals a good predictive performance, particularly in settings with non-linearities and near-multicollinearity. An empirical application contrasts the estimation of marginal efects and their standard errors with an ordered logit model.

Keywords: Ordered choice models, random forests, probabilities, marginal efects, machine learning.

JEL classifcation: C14, C25, C40.

2.1 Introduction

Many empirical models deal with categorical dependent variables which have an inherent ordering. In such cases the outcome variable is measured on an ordered scale such as level of education defned by primary, secondary and tertiary education or income coded into low, middle and high income level. Further examples include survey outcomes on self-assessed health status (bad, good, very good, see e.g. Case, Lubotsky, & Paxson, [2002;](#page-107-0) or Murasko, [2008\)](#page-109-0), level of life satisfaction and happiness (Boes, Staub, & Winkelmann, [2010;](#page-107-1) and Boes & Winkelmann, [2010\)](#page-107-2) or political opinions (do not agree, agree, strongly agree, see e.g. Jackson & Darrow, [2005;](#page-108-0) or Jackman, [2009\)](#page-108-1) as well as grades, scores and various ratings and valuations (see Butler, Finegan, & Siegfried, [1998;](#page-107-3) Hamermesh & Parker, [2005;](#page-108-2) Afonso, Gomes, & Rother, [2009;](#page-107-4) or Gogas, Papadimitriou, & Agrapetidou, [2014,](#page-108-3) for some further examples). Moreover, even sports outcomes resulting in loss, draw and win are part of such modelling framework (e.g. Goller, Knaus, Lechner, & Okasa, [2018\)](#page-108-4). So far, the ordered probit or ordered logit model represent workhorse models in such cases. The main advantage of these models is the ease of estimation, usually done by maximum likelihood. However, the major disadvantage are the strong parametric assumptions which are imposed for convenience rather than derived from any substantive knowledge about the application. Unfortunately, the desired marginal efects are sensitive to these assumptions. Although there is a large literature on how to generalize these assumptions in case of binary choice models (Matzkin, [1992;](#page-109-1) Ichimura, [1993;](#page-108-5) Klein & Spady, [1993\)](#page-108-6), or multinomial (unordered) choice models (Lee, [1995;](#page-109-2) Fox, [2007\)](#page-108-7), limited work has been done for ordered choice models (Lewbel, [2000;](#page-109-3) Klein & Sherman, [2002;](#page-108-8) also see Stewart, [2005,](#page-109-4) for an overview).

In this paper, we exploit recent advances in the machine learning literature to develop an estimator for conditional choice probabilities as well as marginal efects together with inference procedures when the outcome variable has an ordered categorical nature. The proposed Ordered Forest estimator is based on the regression random forest algorithm as introduced by Breiman [\(2001\)](#page-107-5) and makes use of cumulative probability predictions based on binary indicators of respective ordered categories to fexibly estimate the single choice probabilities of the particular ordered category, conditional on covariates. Furthermore, to analyze the relationship of the ordered choice probabilities with the covariates, the Ordered Forest exploits numerical derivative approximations for estimation of the mean marginal efects and marginal efects at mean as the typical quantities of interest in the feld of discrete choice models (see e.g. Greene & Hensher, [2010\)](#page-108-9). Finally, in order to quantify the estimation uncertainty of the above parameters, the Ordered Forest adapts the weight-based inference proposed by Lechner [\(2018\)](#page-109-5) using the asymptotic results of Wager and Athey [\(2018\)](#page-110-0) for the consistency and normality of random forest predictions for the case of ordered categorical outcomes. Thus Ordered Forest estimator provides not only the point estimate for the conditional choice probabilities and the corresponding marginal effects, but also an estimate for the respective standard errors.

We investigate the predictive performance of the estimator by comparing it to classical and other competing methods via a large-scale Monte Carlo simulation study as well as using real datasets. The results from the synthetic simulation reveal good performance of the Ordered Forest in fnite samples throughout all simulation designs, including high-dimensional settings. In particular, the superior performance of the estimator over the parametric ordered logit becomes apparent when dealing with nonlinear functional forms and near-multicollinearity among covariates. Furthermore, the Ordered Forest outperforms the competing forest-based estimators in the most complex simulation designs. Additionally, the results from the empirical evaluation further confrm the good predictive performance of the estimator in real datasets. Lastly, an empirical application demonstrates the estimation of the marginal efects and the associated inference procedure. The empirical results highlight the value of the additional fexibility in the efect estimation of relevant economic parameters. Moreover, to enable the usage of the method by applied researchers a free software implementation of the Ordered Forest estimator has been developed in R (R Core Team, [2018\)](#page-109-6) and is provided in an R-package orf (Lechner & Okasa, [2019\)](#page-109-7) available at the official [CRAN](https://CRAN.R-project.org/package=orf) repository.^{[1](#page-82-0)}

This paper contributes to the econometric as well as machine learning literature in several ways. In terms of econometrics, this paper develops a new estimator of the ordered choice models based on a machine learning algorithm. The proposed Ordered Forest estimator improves on the classical parametric models such as ordered logit and ordered probit models by allowing ex-ante flexible functional forms as well as allowing for a larger covariate space. The latter is a feature of many machine learning methods, but is typically absent from standard econometrics. In terms of machine learning, this paper develops a new type of random forest estimator adapted to ordered categorical outcomes. As such, the proposed Or-dered Forest extends the classical regression forests as developed by Breiman [\(2001\)](#page-107-5) and Wager and Athey [\(2018\)](#page-110-0) specifically for estimation of ordered choice models and thus expands the forest-based estimators for particular econometric models such as for example the survival forest (Hothorn, Lausen, Benner, $\&$ Radespiel-Tröger, [2004\)](#page-108-10) designed for estimation of survival models or the quantile regression forest (Meinshausen, [2006\)](#page-109-8) for estimation of conditional quantiles. Additionally to the above forest-based estimators, the Ordered Forest further advances machine learning methods with the estimation of marginal efects and the inference thereof, a feature of many parametric models, but generally missing in the machine learning literature. Hence, our contribution is twofold. First, with respect to the literature on parametric estimation of the ordered choice models, the Ordered Forest represents a fexible estimator without any parametric assumptions, while providing essentially the same information as an ordered parametric model. Second, with respect to the machine learning literature, the Ordered Forest achieves more precise estimation of ordered choice probabilities, while adding estimation of marginal efects as well as statistical inference thereof.

This paper is organized as follows. Section [2.2](#page-82-1) discusses the related literature concerning parametric and machine learning methods for the estimation of ordered choice models. Section [2.3](#page-85-0) reviews the random forest algorithm and its theoretical properties. In Section [2.4](#page-87-0) the Ordered Forest estimator is introduced including the estimation of the conditional choice probabilities, marginal efects and the inference procedure. The Monte Carlo simulation is presented in Section [2.5.](#page-92-0) Section [2.6](#page-101-0) shows an empirical application. Section [2.7](#page-105-0) concludes. Further details regarding estimation methods, the simulation study and the empirical application are provided in Appendices [2.A,](#page-111-0) [2.B](#page-114-0) and [2.C,](#page-143-0) respectively.

2.2 Literature

In econometrics, the ordered probit and ordered logit models are widely used when there are ordered response variables (McCullagh, [1980\)](#page-109-9). These models build on the latent regression model assuming an underlying continuous outcome Y_i^* as a linear function of regressors X_i with unknown coefficients β , while assuming that the latent error term u_i follows the standard normal or the logistic distribution. Furthermore, the ordered discrete outcome Y_i represents categories that cover a certain range of the latent continuous Y_i^* and is determined by unknown threshold parameters α_m . Formally, in the case of the ordered logit the latent model is defned as:

$$
Y_i^* = X_i'\beta + u_i, \qquad (u_i \mid X_i) \sim Logistic(0, \pi^2/3)
$$
\n(2.2.1)

¹Additionally, an implementation of the estimator in GAUSS is available [online](https://www.michael-lechner.eu/statistical-software/) and on ResearchGate. A Python version of the estimator focused on prediction exercise is available on [GitHub](https://github.com/okasag/OrderedForest).

with unknown threshold parameters $\alpha_0 < \alpha_1 < ... < \alpha_M$ such that:

$$
Y_i = m \quad \text{if} \quad \alpha_{m-1} < Y_i^* \le \alpha_m \quad \text{for} \quad m = 1, \dots, M,\tag{2.2.2}
$$

where the coefficients and the thresholds are commonly estimated via maximum likelihood with the delta method or bootstrapping used for inference. Notice, that the outer thresholds are $\alpha_0 = -\infty$ and $\alpha_M = \infty$. The above latent model is also often motivated by the quantity of interest, i.e. the conditional choice probabilities which are given by:

$$
P[Y_i = m \mid X_i = x] = \Lambda \left(\alpha_m - X_i' \beta \right) - \Lambda \left(\alpha_{m-1} - X_i' \beta \right),\tag{2.2.3}
$$

where the link function $\Lambda(\cdot)$ is the logistic cdf mapping the real line onto the unit interval. Thus, the estimated probabilities are bounded between 0 and 1. The marginal efects are further given as partial derivative of the probabilities in $(2.2.3)$ as:

$$
\frac{\partial P[Y_i = m \mid X_i = x]}{\partial x^k} = \left[\lambda (\alpha_{m-1} - X_i' \beta) - \lambda (\alpha_m - X_i' \beta) \right] \beta_k,
$$
\n(2.2.4)

where x^k is the k-th element of X_i and β_k is the corresponding coefficient, while $\lambda(\cdot)$ being the logistic pdf.

Although such models are relatively easy to estimate, they impose strong parametric assumptions which hinder the fexibility of these models. Apart from the assumptions about the distribution of the error term, further functional form assumptions are being imposed. As is clear from [\(2.2.1\)](#page-82-2), the coefficients β are constant across the outcome classes which is often labelled as the parallel regression assumption (Williams, [2016\)](#page-110-1). This infexibility afects both the estimation of the choice probabilities as well as the estimation of marginal effects. For these reasons, generalizations of these models have been proposed in the literature in order to relax some of the assumptions. An example of such models is the generalized ordered logit model (McCullagh & Nelder, [1989\)](#page-109-10), where the parallel regression assumption is abandoned. Boes and Winkelmann [\(2006\)](#page-107-6) provide an excellent overview of several other generalized parametric models. However, all of these models retain some of the distributional assumptions which limit their modelling fexibility.

Besides the standard econometric literature on parametric specifcations of ordered choice models (for an overview see Agresti, [2002;](#page-107-7) or Boes & Winkelmann, [2006\)](#page-107-6), a new strand of literature devoted to relaxing the parametric assumptions by using novel machine learning methods is emerging. Particularly, the tree-based methods have gained considerable attention. Although the classical CART algorithms introduced by Breiman, Friedman, Olshen, and Stone [\(1984\)](#page-107-8) are very powerful in both regression as well as in classifcation (see Loh, [2011,](#page-109-11) for a review), there is a need for adjustment when predicting ordered response. In the case of regression, the discrete nature of the outcome is not being taken into account and in the case of classifcation, the ordered nature of the outcome is not being taken into account. For these reasons, a strand of the literature focused particularly on adjustments towards ordered classifcation rather than regression which excludes the estimation of the conditional probabilities as is the case in the parametric ordered choice models. For example, Kramer, Widmer, Pfahringer, and De Groeve [\(2001\)](#page-109-12) propose a simple procedure for constructing a distance-sensitive classifcation learner using post-processing classifcation rules. Another approach suggested in the literature is to modify the splitting criterion directly. In particular, the usage of alternative impurity measures as opposed to the Gini coefficient in case of classifcation trees have been suggested, namely the generalized Gini criterion (Breiman et al., [1984\)](#page-107-8) or the ordinal impurity function (Piccarreta, [2008\)](#page-109-13). Both of these measures put higher penalty on misclassifcation the more distant the predicted category is from the true one. It follows that the above methods focus on estimating ordered classes rather than estimating ordered class probabilities, as is the focus of this paper.

The above ideas, however, have not been much used in practice. The reason might be the well-known drawbacks of single trees which sufer from unstable splits and a lack of smoothness (Hastie, Tibshirani, & Friedman, [2009\)](#page-108-11). A natural extension of the CART algorithms is the random forest frst introduced by Breiman [\(2001\)](#page-107-5). However, the random forest algorithm as well as CART is primarily suitable for either regression or classifcation exercises. As such, appropriate modifcations of the standard random forest algorithm are desired in order to predict conditional probabilities of discrete outcomes while taking the ordering nature into account. Hothorn, Hornik, and Zeileis [\(2006b\)](#page-108-12) propose a random forest algorithm building on their conditional inference framework for recursive partitioning which can also deal with ordered outcomes. The diference to standard regression forests lies in a diferent splitting criterion using a test statistic where the conditional distribution at each split is based on permutation tests (for details see Strasser & Weber, [1999;](#page-110-2) and Hothorn et al., [2006b\)](#page-108-12). Their proposed ordinal forest regression assumes an underlying latent continuous response Y_i^* as is the case in standard ordered choice models. Hothorn et al. [\(2006b\)](#page-108-12) define a score vector $s(m) \in \mathbb{R}^M$, with $m = 1, ..., M$ observed ordered classes. This scores refect the distances between the classes. The authors suggest to set the scores as midpoints of the intervals of Y_i^* which define the classes. As the underlying Y_i^* is unobserved, such a suggestion results in $s(m) = m$ and ordinal forest regression collapses to a standard forest regression as pointed out by Janitza, Tutz, and Boulesteix [\(2016\)](#page-108-13).[2](#page-84-0) However, although the tree building step coincides, the prediction step difers as the estimates are the choice probabilities calculated as the proportions of the respective outcome classes falling into the same leaf instead of averages of the outcomes. As such, for each leaf within a tree, the prediction is computed for each value of the ordered categorical outcome as its share within the leaf, resulting in a probability predictions between 0 and 1. This is in contrast to standard prediction procedures, which would compute an average of all values of the ordered categorical outcome. Nevertheless, after computing the single-tree predictions as the relative frequencies of the ordered outcomes, the forest estimates of the conditional choice probabilities $\hat{P}[Y_i = m \mid X_i = x]$ are computed by taking the averages of the choice probabilities produced by each tree, i.e. the same aggregation scheme as in a regression forest. Hornung [\(2019a\)](#page-108-14) points out that setting $s(m) = m$ implies inherently assuming that the class widths, i.e. the adjacent intervals of the continuous outcome variable Y_i^* determining the descrete outcome Y_i are of the same length. This, however, does not have to hold in general and these intervals might not follow any particular pattern.^{[3](#page-84-1)} In order to address this issue, Hornung [\(2019a\)](#page-108-14) proposes an ordinal forest method, which optimizes these interval widths by maximizing the out-of-bag (OOB) prediction performance of the forests.[4](#page-84-2) However, on the contrary to the approach of Hothorn et al. [\(2006b\)](#page-108-12), the forest algorithm used is based on the forest as developed by Breiman [\(2001\)](#page-107-5), while the primary target is to predict the ordinal class and the choice probabilities are obtained as relative frequencies of trees predicting the particular class. As such, each tree predicts the most probable value of the ordered categorical outcome. Thereupon, the forest prediction for the conditional choice probability is computed as the share of trees predicting the particular categorical value of the ordered outcome. This is in contrast to the estimation scheme by Hothorn et al. [\(2006b\)](#page-108-12), where the probability prediction step occurs at the level of trees, instead of at the level of forest as is the case here. Hornung [\(2019a\)](#page-108-14) shows better prediction performance of such ordinal forests which optimize the class widths of Y_i^* in comparison to the conditional forests. Without the optimization step, the author denotes such forest as the naive

²Janitza et al. [\(2016\)](#page-108-13) perform also a simulation study to test the robustness of the suggested score values by setting $s(m) = m^2$, but do not find any significant differences to simple $s(m) = m$.

³Recently, Buri and Hothorn [\(2020\)](#page-107-9) and Tutz [\(2021\)](#page-110-3) proposed score-free methods based on random forests that do not rely on the underlying continuous intervals of the observed ordered classes.

⁴This approach could be regarded as semiparametric as it uses the nonparametric structure of the trees and assumes a particular parametric distribution (standard normal) within its optimization procedure.

ordinal forest.[5](#page-85-1)

While both of the discussed approaches take the ordering information of the outcomes into account, they focus mainly on prediction and variable importance without considering estimation of the marginal efects or the associated inference for the efects which are a fundamental part of the classical econometric ordered choice models. In addition, although both of these methods demonstrate good predictive performance, none of them provides theoretical guarantees with regards to the distribution of these predictions. Further, it is worth to mention that in practice both methods sufer from considerable computational costs. In case of the conditional forest, the additional permutation tests that need to be performed to evaluate the test statistic at each split result in a considerably longer computation time. For the ordinal forest, the additional optimization step for the class widths requires a prior estimation of a large number of forests (1000 by default) which also leads to a substantially longer computation time (see Tables [2.B.26](#page-141-0) and [2.B.27](#page-142-0) in Appendix [2.B.4](#page-140-0) for further details).

There is also a strand of literature which is concerned with the estimation of ordered outcome models in high-dimensional settings based on regularization methods. Examples of this approach include penalized ordered outcome models by Wurm, Rathouz, and Hanlon [\(2017\)](#page-110-4) who make use of a standard ordered logit/probit regression while introducing an elastic net penalization term. Harrell [\(2015\)](#page-108-15) describes a cumulative logit model with a ridge type of penalty. Archer et al. [\(2014\)](#page-107-10) implement the GMIFS (generalized monotone incremental forward stagewise) algorithm for penalized ordered outcome models which is similar to the Lasso type penalty. However, although the penalized models can deal with high dimensions, when the true model is relatively "sparse", they nevertheless belong to a specifc parametric class such as the ordered logit/probit (see Hastie et al., [2009\)](#page-108-11). Such models can only become more fexible, and thus partially relax the parametric assumptions when generating a large number of polynomials and interactions of available covariates prior to estimation. It follows that these models use a global approximation of the functional form and cannot learn it adaptively as tree-based approaches do. In contrast, random forests do not impose parametric assumptions and can learn any arbitrary relationship in a nonparametric way by locally adaptive estimation in small neighbourhoods of the data. It follows that random forests use a local approximation of the functional form, without any need for prior pre-processing of the data. As such, random forests are nonlinear in covariates and although there are no specifc statistical tests to fnd such a random forest structure, essentially random forests can approximate any structure, including a global linear structure, if a sufficient amount of data is provided. For these reasons, the remainder of this paper focuses on the forest-based methods.

2.3 Random Forests

Random forests as introduced by Breiman [\(2001\)](#page-107-5) became quickly a very popular prediction method thanks to its good prediction accuracy, while being relatively simple to tune. Further advantages of random forests as a nonparametric technique are the high degree of fexibility and ability to deal with large number of predictors, while coping better with the curse of dimensionality problem in comparison to classical nonparametric methods such as kernel or local linear regression (see for example Racine, [2008\)](#page-109-14). Random forests are based on bootstrap aggregation, i.e. the so-called bagging of single regression (or classifcation) trees where the covariates considered for each next split within a tree are selected at random. More precisely, the random forest algorithm draws a bootstrap sample $Z_i^*(X_i, Y_i)$ of size N from the available training data for $b = 1, ..., B$ bootstrap replications. For each bootstrapped sample, a random-forest tree \hat{T}_b is grown by recursive partitioning until the minimum leaf size is reached. At each

 $5A$ more detailed description of the conditional as well as the ordinal forest is provided in Appendix [2.A.2](#page-112-0) and [2.A.3,](#page-113-0) respectively.

of the splits, m out of p covariates chosen at random are considered. After all B trees are grown in this fashion, the regression random forest estimate of the conditional mean $E[Y_i | X_i = x]$ is the ensemble of the trees:

$$
\hat{RF}^{B}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{T}_{b}(x) \quad \text{with} \quad \hat{T}_{b}(x) = \frac{1}{|\{i : X_{i} \in L_{b}(x)\}|} \sum_{\{i : X_{i} \in L_{b}(x)\}} Y_{i}, \quad (2.3.1)
$$

where $L_b(x)$ denotes a leaf containing x. Single trees, if grown sufficiently deep, have a low bias, but fairly high variance. By averaging over many single trees with randomly choosing the set of observations and split covariates, the variance of the estimator is being reduced substantially. First, the variance reduction is achieved through bagging. The higher the number of bootstrap replications, the lower the variance. Second, the variance is further reduced through the random selection of covariates. The lower is the number of considered covariates for a split, the more is the correlation between the trees reduced and consequently, the bigger is the variance reduction of the average (Hastie et al., [2009\)](#page-108-11).

Another attractive feature of random forests is the weighted average representation of the fnal estimate of the conditional mean $E[Y_i \mid X_i = x]$. As such we can rewrite the random forest prediction as follows:

$$
\hat{RF}^{B}(x) = \sum_{i=1}^{N} \hat{w}_{i}(x)Y_{i},
$$
\n(2.3.2)

where the weights are defned as:

$$
\hat{w}_{b,i}(x) = \frac{\mathbf{1}(\{X_i \in L_b(x)\})}{|\{i : X_i \in L_b(x)\}|} \quad \text{with} \quad \hat{w}_i(x) = \frac{1}{B} \sum_{b=1}^B \hat{w}_{b,i}(x). \tag{2.3.3}
$$

As such the forest weights $\hat{w}_i(x)$ are again an average over all single tree weights. These tree weights capture if the training example X_i falls into the leaf $L_b(x)$ scaled by the size of that leaf. Notice, that the weights are locally adaptive. Intuitively, random forests resemble the classical nonparametric kernel regression with an adaptive, data-driven bandwidth and with limited curse of dimensionality. One can show that in the regression case, the random forest estimate as defined in $(2.3.1)$ is equivalent to the weighting estimate defned in [\(2.3.2\)](#page-86-1). This weighting perspective of random forests has been frstly suggested by Hothorn et al. [\(2004\)](#page-108-10) and Meinshausen [\(2006\)](#page-109-8) in the scope of survival and quantile regression, respectively. Recently, Athey, Tibshirani, and Wager [\(2019\)](#page-107-11) point out the usefulness of the random forest weights in various estimation tasks. In this spirit, we will later on in Section [2.4.3](#page-90-0) use the forest induced weights explicitly for inference as has been recently suggested by Lechner [\(2018\)](#page-109-5).

Besides the huge popularity of random forests for prediction, the statistical literature focused on establishing asymptotic properties of random forests as well (Meinshausen, [2006;](#page-109-8) Biau, [2012;](#page-107-12) Scornet, Biau, & Vert, [2015;](#page-109-15) Mentch & Hooker, [2016\)](#page-109-16). A major step towards formally valid inference has been done in a recent work by Wager [\(2014\)](#page-110-5) and Wager and Athey [\(2018\)](#page-110-0) who prove consistency and asymptotic normality of random forest predictions, under some modifcations of the standard random forest algorithm. These modifcations concern both the tree-building procedure as well as the tree-aggregation scheme. First, the tree aggregation is now done using subsampling without replacement instead of bootstrapping. Second, the tree building procedure introduces the major and crucial condition of so-called honesty as first suggested by Athey and Imbens [\(2016\)](#page-107-13). A tree is honest, if it does not use the same responses for both, placing splits and estimating the within-leaf predictions. This can be achieved by the so-called double-sample trees, which split the random subsample of training data $Z_i^*(X_i, Y_i)$ into two disjoint sets of the same size, while the one is used for placing splits and the other one for estimating

the predictions. Furthermore, for the consistency it is essential that the size of the leaves L of the trees becomes small relative to the sample size as N gets large.^{[6](#page-87-1)} This is achieved by introducing some randomness in choosing the splitting variables. Particularly, each covariate receives a minimum amount of positive chance of a split. Such constructed tree is then said to be a random-split tree. Additionally, the trees are required to be α -regular, meaning that after each split, both of the child nodes contain at least a fraction α of the training data (specifically, $\alpha \leq 0.2$ is required). Lastly, trees have to be symmetric in a sense that the order of the training data is independent of the predictor output. Overall, apart from subsampling and honesty the above conditions are not particularly binding and do not fundamentally deviate from the standard regression random forest. Lastly, some additional regularity conditions need to be satisfied for the asymptotic arguments to hold. In particular, the data $Z_i(X_i, Y_i) \in [0,1]^p \times \mathbb{R}$ comes from *i.i.d.* sampling, the p-dimensional covariates $X_i \sim \mathcal{U}([0,1]^p)$ are independently and uniformly distributed, the conditional means $E[Y_i \mid X_i = x]$ and $E[Y_i^2 \mid X_i = x]$ are Lipschitz-continuous, the variance is bounded away from zero, $Var[Y_i | X_i = x] > 0$, and the number of subsampling replications is large enough to eliminate the Monte Carlo effects, while an appropriate scaling of the subsample size s_N is ensured.[7](#page-87-2) Then, under the above assumptions, the random forest predictions can be shown to be (pointwise) asymptotically Gaussian and unbiased. We use this result to provide an inference procedure for the marginal effects of the Ordered Forest discussed in Section [2.4.3.](#page-90-0)

2.4 Ordered Forest Estimator

The general idea of the *Ordered Forest* estimator is to provide a flexible alternative for estimation of ordered choice models that can deal with a large-dimensional covariate space. As such, the main goal is the estimation of conditional ordered choice probabilities, i.e. $P[Y_i = m \mid X_i = x]$ as well as marginal efects, i.e. the changes in the estimated probabilities in association with changes in covariates. Correspondingly, the variability of the estimated efects is of interest and therefore a method for conducting statistical inference is provided as well. The latter two features go beyond the traditional machine learning estimators which focus solely on the prediction exercise, and complement the prediction with the same econometric output as the traditional parametric estimators.

2.4.1 Conditional Choice Probabilities

The main idea of the estimation of the ordered choice probabilities by a random forest algorithm lies in the estimation of cumulative, i.e. nested probabilities based on binary indicators. As such, for an i.i.d random sample of size $N(i = 1, ..., N)$, consider an ordered outcome variable $Y_i \in \{1, ..., M\}$ with ordered classes m. Then the binary indicators are given as $Y_{m,i} = \mathbf{1}(Y_i \leq m)$ for outcome classes $m = 1, ..., M-1$. First, the ordered model is transformed into multiple overlapping binary models which are estimated by random forests yielding the predictions for the cumulative probabilities, i.e $\hat{Y}_{m,i} = \hat{P}[Y_{m,i} = 1 | X_i = x].$ Second, the estimated cumulative probabilities are diferenced to isolate the respective class probabilities $P_{m,i} = P[Y_i = m \mid X_i = x]$. Hence the estimate for the conditional probability of the m-th ordered class

 $6Wager$ and Athey [\(2018\)](#page-110-0) point out that the leaves need to be relatively small in all dimensions of the covariate space. This implies that the high-dimensional settings are not considered and hence the theoretical asymptotic results might not hold in such settings.

 7 The condition of uniformity of covariates is due to simplicity and is not particularly binding as the result holds also with a density bounded away from zero and infnity as argued by Wager and Athey [\(2018\)](#page-110-0). Furthermore, the Lipschitz-continuity of the conditional mean appears not too restrictive as the random forest estimates have in general smooth response surfaces when $B \to \infty$, i.e. the number of bootstrap or subsampling iterations goes to infinity (Bühlmann & Yu, [2002\)](#page-107-14). Lastly, the appropriate scaling of the subsample size s_N does not affect the asymptotic normality, but violations might lead to asymptotic bias as pointed out by Wager and Athey [\(2018\)](#page-110-0). For a detailed description of the conditions as well as of the proof, see Wager and Athey [\(2018\)](#page-110-0).

is given by subtracting two adjacent cumulative probabilities as $\hat{P}_{m,i} = \hat{Y}_{m,i} - \hat{Y}_{m-1,i}$. Formally, the proposed estimation procedure can be described as follows:

1. Create $M-1$ binary indicator variables such as

$$
Y_{m,i} = \mathbf{1}(Y_i \le m) \quad \text{for} \quad m = 1, ..., M - 1,\tag{2.4.1}
$$

where m is known and given by the definition of the dependent variable.

2. Estimate regression random forest for each of the $M-1$ indicators as

$$
P[Y_{m,i} = 1 \mid X_i = x] = \sum_{i=1}^{N} w_{m,i}(x) Y_{m,i} \quad \text{for} \quad m = 1, ..., M - 1,
$$
 (2.4.2)

where the forest weights are defined as $w_{m,i}(x) = \frac{1}{B} \sum_{b=1}^{B} w_{m,b,i}(x)$ with trees weights given by $w_{m,b,i}(x) = \frac{\mathbf{1}\left(\left\{X_i \in L_{b,m}(x)\right\}\right)}{\left\{\left\{i:X_i \in L_{b,m}(x)\right\}\right\}}$ with leaves $L_{b,m}(x)$ for a total of B trees.

3. Obtain forest predictions for each of the $M-1$ indicators as

$$
\hat{Y}_{m,i} = \hat{P}[Y_{m,i} = 1 \mid X_i = x] = \sum_{i=1}^{N} \hat{w}_{m,i}(x) Y_{m,i} \quad \text{for} \quad m = 1, ..., M - 1,
$$
\n(2.4.3)

where $\hat{Y}_{m,i}$ are estimated cumulative probabilities.

4. Compute ordered probabilities for each distinct class as

$$
\hat{P}_{m,i} = \hat{Y}_{m,i} - \hat{Y}_{m-1,i} \qquad \text{for} \qquad m = 2, ..., M \qquad (2.4.4)
$$

with

$$
\hat{Y}_{M,i} = 1
$$
 and $\hat{P}_{1,i} = \hat{Y}_{1,i}$ (2.4.5)

and

$$
\hat{P}_{m,i} = 0 \t\t \text{if} \t\t \hat{P}_{m,i} < 0 \t\t (2.4.6)
$$

$$
\hat{P}_{m,i} = \frac{\hat{P}_{m,i}}{\sum_{m=1}^{M} \hat{P}_{m,i}} \quad \text{for} \quad m = 1, ..., M,
$$
\n(2.4.7)

where equation [\(2.4.4\)](#page-88-0) makes use of the cumulative (nested) probability feature. As such, the predicted values of two subsequent binary indicator variables $Y_{m,i}$ are subtracted from each other to isolate the probability of the higher order class.^{[8](#page-88-1)} In equation $(2.4.5)$ the first part is given by construction as follows from the indicator function [\(2.4.1\)](#page-88-3) that all values of Y_i fullfil the condition for $m = M$ and from the fact that cumulative probabilities must add up to 1. The second part defnes the probability of the lowest value of the ordered outcome variable. This follows directly from the random forest estimation as the created indicator variable $Y_{1,i}$ describes the very lowest value of the ordered outcome classes and as such, no modifcation of its predicted value is necessary to obtain a valid probability prediction. Line [\(2.4.6\)](#page-88-4) ensures that the computed probabilities from [\(2.4.4\)](#page-88-0) do not become negative. This might occasionally happen especially if the respective outcome classes comprise of very few observations. This issue is wellknown also from the generalized ordered logit model where the parallel regression assumption is relaxed (see McCullagh & Nelder, [1989,](#page-109-10) p. 155). However, even though it is possible in theory, growing honest

⁸Similar transformations of an ordered model into multiple binary models have been proposed in the classifcation literature. Kwon, Han, and Lee [\(1997\)](#page-109-17) introduce the so-called ordinal pairwise partitioning method in the context of neural networks. Yet the closest to our work is the approach by Frank and Hall [\(2001\)](#page-108-16) who make use of the cumulative model explicitly.

trees seems to largely prevent this from happening in practice. Lastly, in case if negative predictions should occur and thus being set to zero, [\(2.4.7\)](#page-88-5) defnes a normalization step to ensure that all class probabilities sum up to 1. Notice, that such an approach requires estimation of $M-1$ forests in the training data, which might appear to be computationally expensive. However, given that most empirical problems involve a rather limited number of outcome classes (usually not exceeding 10 distinct classes) and the relatively fast estimation of standard regression forest^{[9](#page-89-0)} without any additional permutation test nor optimization steps needed as is the case for the conditional or the ordinal forests, respectively, the here proposed procedure shall be computationally advantageous (see Tables [2.B.26](#page-141-0) and [2.B.27](#page-142-0) in Appendix [2.B.4\)](#page-140-0).

2.4.2 Marginal Efects

After estimating the conditional ordered choice probabilities, it is of interest to investigate how the estimated probabilities are associated with covariates, i.e. how the changes in the covariates translate into changes in the probabilities. Typical measures for such relationships in standard nonlinear econometrics are the marginal, or, partial efects. Thus, for nonlinear models, including ordered choice models, two fundamental measures are of common interest, mean marginal effects and marginal effects at the mean of the covariates.^{[10](#page-89-1)} These quantities are feasible also in the case of the *Ordered Forest* estimator. Due to the character of the ordered choice model, the marginal efects on all probabilities of diferent values of the ordered outcome classes are estimated, i.e. $P[Y_i = m | X_i = x]$. In the following, let us define the marginal effect for an element x^k of X_i as follows:

$$
ME_i^{k,m}(x) = \frac{\partial P[Y_i = m \mid X_i^k = x^k, X_i^{-k} = x^{-k}]}{\partial x^k},\tag{2.4.8}
$$

with X_i^k and X_i^{-k} denoting the elements of X_i with and without the k-th element, respectively.^{[11](#page-89-2)} Next, let us defne the marginal efect for categorical variables as a discrete change in the following way:

$$
ME_i^{k,m}(x) = P[Y_i = m \mid X_i^k = \lceil x^k \rceil, X_i^{-k} = x^{-k} \rceil - P[Y_i = m \mid X_i^k = \lfloor x^k \rfloor, X_i^{-k} = x^{-k}], \tag{2.4.9}
$$

where $\lceil \cdot \rceil$ and $\lceil \cdot \rceil$ denote upper and lower integer values, respectively, such that a difference of one unit is respected. Notice, that in the case of a binary variable this leads to the respective probabilities being evaluated at $\lceil x^k \rceil = 1$ and $\lceil x^k \rceil = 0$ as is usual for ordered choice models. From the above definitions of marginal efects, we obtain the desired quantity of interest, i.e. the marginal efect at mean by evaluating $ME_i^{k,m}(x)$ at the population mean of X_i , for which the sample mean is a natural proxy. The mean marginal effect is obtained by taking sample averages of $ME_i^{k,m}(x)$, i.e. $\frac{1}{N} \sum_{i=1}^{N} ME_i^{k,m}(x)$.

Having formally defned the desired marginal efects, the next issue is the estimation of these efects. For the case of binary and categorical covariates X^k , this appears straightforward as the estimated Ordered Forest model provides predicted values for all probabilities at all values x^k . As such, the estimate $\hat{ME}_i^{k,m}$ $\binom{n}{i}$ of marginal effects defined in equation [\(2.4.9\)](#page-89-3) remains as a difference of the two conditional probabilities estimated by the Ordered Forest. However, it is less obvious for continuous variables, where derivatives are needed. As the estimates of the choice probabilities are averaged leaf means, the marginal efect is not explicit and not diferentiable. In the nonparametric literature Stoker [\(1996\)](#page-110-6) and Powell and Stoker [\(1996\)](#page-109-18), among others, are directly concerned with estimating average derivatives. However, these

 $\overline{^{9}}$ The computational speed of the regression forests depends on many tuning parameters, of which the number of bootstrap replications, i.e. grown trees is the most decisive one.

¹⁰One can evaluate the marginal effect at any arbitrarily chosen value. The default option is usually the mean or the median. ¹¹As a matter of notation, capitals denote random variables, whereas small letters refer to the particular realizations of the random variable.

methods lack convenience of estimation and have thus not been widely adopted by empirical researchers.^{[12](#page-90-1)} Therefore, we approximate the derivative by a discrete analogue based on the defnition of a derivative as follows:

$$
\hat{ME}_i^{k,m}(x) = \frac{\hat{P}[Y_i = m \mid X_i^k = x^{kU}, X_i^{-k} = x^{-k}] - \hat{P}[Y_i = m \mid X_i^k = x^{kL}, X_i^{-k} = x^{-k}]}{x^{kU} - x^{kL}}
$$
(2.4.10)

$$
=\frac{\hat{P}_{m,i}(x^{kU})-\hat{P}_{m,i}(x^{kL})}{x^{kU}-x^{kL}},
$$
\n(2.4.11)

with x^{kU}, x^{kL} defined as $x^{kU} = x^k + h \cdot \sigma(x^k)$ and $x^{kL} = x^k - h \cdot \sigma(x^k)$, while ensuring that the support of x^k is respected, and where $\sigma(\cdot)$ denotes standard deviation and h controls the window size for evaluating the marginal effect. We recommend to set $h = 0.1$ to achieve accurate evaluation at the margin.^{[13](#page-90-2)} Hence, the approximation targets the marginal change in the value of the covariate X_i^k . Notice, that such an estimation of marginal efects is much more demanding exercise than solely predicting the choice probabilities. Therefore, it is expected that considerably more subsampling iterations are needed for a good performance.

2.4.3 Inference

The building block of the *Ordered Forest* are the estimates of conditional probabilities such as $P[Y_{m,i} = 1 | X_i = x]$. Particularly, the *Ordered Forest* makes use of linear combinations of such probability estimates made by the random forest for both the conditional ordered choice probabilities as well as for the corresponding marginal effects. Therefore, for conducting inference on these quantities, it is sufficient to ensure that the underlying estimates of conditional probabilities are asymptotically normally distributed. Here, we combine the results of Wager and Athey [\(2018\)](#page-110-0) and Lechner [\(2018\)](#page-109-5). First, we use the asymptotic results of Wager and Athey [\(2018\)](#page-110-0) who show that the consistency and normality of random forest predictions hold also when dealing with binary outcomes, and thus also hold for probability predictions of type $P[Y_{m,i} = 1 | X_i = x]$. Hence, the final *Ordered Forest* estimates for the conditional ordered choice probabilities and the marginal effects, based on a forest algorithm respecting the conditions discussed in Section [2.3,](#page-85-0) inherit the consistency and normality properties. Second, we adapt the inference procedure for random forests as developed by Lechner [\(2018\)](#page-109-5) to estimate the variance of the conditional ordered choice probabilities and the corresponding marginal effects.

The here proposed method for conducting approximate inference of the estimated marginal efects utilizes the weight-based representation of random forest predictions and adapts the weight-based infer-ence proposed by Lechner [\(2018\)](#page-109-5) for the case of the *Ordered Forest* estimator.^{[14](#page-90-3)} The main condition for conducting weight-based inference is to ensure that the weights and the outcomes are independent. In general, the weights are functions of the covariates for the observation i and the training data. In order to estimate the variance of the marginal efects successfully, the conditioning set of the weights must be reduced. Therefore, if the observation i is not part of the training data and there is i.i.d. sampling, then the weights depend only on the observation i and are furthermore independent of the outcomes (for a formal analysis, see Lechner, [2018\)](#page-109-5). This is achieved through sample splitting where one half of the sample is used to build the forest, and thus to determine the weights, and the other half to estimate

 12 The issues range from estimation difficulty, possibly non-standard distribution of the estimator, to ambiguous choices of nuisance parameters.

¹³We have additionally experimented with $h = 0.5$ and $h = 1$ which resulted in incrementally larger effect sizes. Generally, the lower the window size h , the more local the effect and the higher the window size h , the more global the effect becomes. As Burden and Faires [\(2011\)](#page-107-15) point out, the window size h should not be chosen too small due to the instability of the numerical derivative approximations. In the software implementation in the R package orf, users can control this parameter by changing the argument window. See Lechner and Okasa [\(2019\)](#page-109-7) for more details.

¹⁴See also Lechner [\(2002\)](#page-109-19) and Imbens and Abadie [\(2006\)](#page-108-17) for related approaches

the efects using the respective outcomes. Notice that this condition goes beyond honesty as defned in Wager and Athey [\(2018\)](#page-110-0) as this requires not only estimating honest trees but estimating honest forest as a whole. The reason for this is the fact that the weights are not based on the estimated trees, but on the estimated forest. Therefore, to ensure independence between the weights and outcomes, the honesty condition must be w.r.t. to the forest and it is not sufficient to build honest trees only. This comes, however, at the expense of the efficiency of the estimator as less data are effectively used. Nevertheless, the simulation evidence in Lechner [\(2018\)](#page-109-5) suggests that this efficiency loss is small, if present at all.^{[15](#page-91-0)}

Since the *Ordered Forest* estimator is based on differences of random forest predictions for adjacent outcome categories, also the covariance term enters the variance formula of the final estimator^{[16](#page-91-1)} as opposed to the Modifed Causal Forests developed in Lechner [\(2018\)](#page-109-5). Further, the estimation of marginal effects is based on differences of single *Ordered Forest* predictions which also needs to be taken into account.^{[17](#page-91-2)} Let us first rewrite the marginal effects in terms of weighted means of the outcomes as follows:

$$
\hat{M}E_{i}^{k,m}(x) = \frac{\hat{P}_{m,i}(x^{kU}) - \hat{P}_{m,i}(x^{kL})}{x^{kU} - x^{kL}}
$$
\n
$$
= \frac{1}{x^{kU} - x^{kL}} \cdot \left(\left[\sum_{i=1}^{N} \hat{w}_{i,m}(x^{kU}) Y_{i,m} - \sum_{i=1}^{N} \hat{w}_{i,m-1}(x^{kU}) Y_{i,m-1} \right] - \left[\sum_{i=1}^{N} \hat{w}_{i,m}(x^{kL}) Y_{i,m} - \sum_{i=1}^{N} \hat{w}_{i,m-1}(x^{kL}) Y_{i,m-1} \right] \right)
$$
\n
$$
= \frac{1}{x^{kU} - x^{kL}} \cdot \left(\left[\sum_{i=1}^{N} \hat{w}_{i,m}(x^{kU}) Y_{i,m} - \sum_{i=1}^{N} \hat{w}_{i,m}(x^{kL}) Y_{i,m} \right] - \left[\sum_{i=1}^{N} \hat{w}_{i,m-1}(x^{kU}) Y_{i,m-1} - \sum_{i=1}^{N} \hat{w}_{i,m-1}(x^{kL}) Y_{i,m-1} \right] \right)
$$
\n
$$
= \frac{1}{x^{kU} - x^{kL}} \cdot \left(\sum_{i=1}^{N} \tilde{w}_{i,m}(x^{kU}x^{kL}) Y_{i,m} - \sum_{i=1}^{N} \tilde{w}_{i,m-1}(x^{kU}x^{kL}) Y_{i,m-1} \right),
$$

where $\tilde{w}_{i,m}(x^{kU}x^{kL}) = \hat{w}_{i,m}(x^{kU}) - \hat{w}_{i,m}(x^{kL})$, and $\tilde{w}_{i,m-1}(x^{kU}x^{kL}) = \hat{w}_{i,m-1}(x^{kU}) - \hat{w}_{i,m-1}(x^{kL})$ are the new weights defning the marginal efect. As such the quantity of interest for inference becomes the variance of the above expression given as:

$$
Var\left(\hat{ME}_{i}^{k,m}(x)\right) = Var\left(\frac{1}{x^{kU} - x^{kL}} \cdot \left(\sum_{i=1}^{N} \tilde{w}_{i,m}(x^{kU}x^{kL})Y_{i,m} - \sum_{i=1}^{N} \tilde{w}_{i,m-1}(x^{kU}x^{kL})Y_{i,m-1}\right)\right)
$$

$$
= Var\left(\frac{\sum_{i=1}^{N} \tilde{w}_{i,m}(x^{kU}x^{kL})Y_{i,m}}{x^{kU} - x^{kL}}\right) + Var\left(\frac{\sum_{i=1}^{N} \tilde{w}_{i,m-1}(x^{kU}x^{kL})Y_{i,m-1}}{x^{kU} - x^{kL}}\right)
$$

$$
- 2 \cdot Cov\left(\frac{\sum_{i=1}^{N} \tilde{w}_{i,m}(x^{kU}x^{kL})Y_{i,m}}{x^{kU} - x^{kL}}; \frac{\sum_{i=1}^{N} \tilde{w}_{i,m-1}(x^{kU}x^{kL})Y_{i,m-1}}{x^{kU} - x^{kL}}\right),
$$

which suggests the following estimator for the variance:^{[18](#page-91-3)}

$$
\begin{split} &\hat{Var}\bigg(\hat{ME}_{i}^{k,m}(x)\bigg) = \frac{N}{N-1} \cdot \frac{1}{(x^{kU} - x^{kL})^2}.\\ &\cdot \bigg(\sum_{i=1}^{N}\bigg(\tilde{w}_{i,m}(x^{kU}x^{kL})Y_{i,m} - \frac{1}{N}\sum_{i=1}^{N}\tilde{w}_{i,m}(x^{kU}x^{kL})Y_{i,m}\bigg)^2 + \sum_{i=1}^{N}\bigg(\tilde{w}_{i,m-1}(x^{kU}x^{kL})Y_{i,m-1} - \frac{1}{N}\sum_{i=1}^{N}\tilde{w}_{i,m-1}(x^{kU}x^{kL})Y_{i,m-1}\bigg)^2\\ &- 2\cdot \sum_{i=1}^{N}\bigg(\tilde{w}_{i,m}(x^{kU}x^{kL})Y_{i,m} - \frac{1}{N}\sum_{i=1}^{N}\tilde{w}_{i,m}(x^{kU}x^{kL})Y_{i,m}\bigg) \cdot \bigg(\tilde{w}_{i,m-1}(x^{kU}x^{kL})Y_{i,m-1} - \frac{1}{N}\sum_{i=1}^{N}\tilde{w}_{i,m-1}(x^{kU}x^{kL})Y_{i,m-1}\bigg)\bigg), \end{split}
$$

 15 The so-called cross-fitting to avoid the efficiency loss as suggested by Chernozhukov et al. [\(2018\)](#page-107-16) does not appear to be applicable here as the independence of the weights and the outcomes would not be ensured.

¹⁶One could avoid the covariance term with an additional sample split, which might, however, further lead to a decreased efficiency of the estimator.

¹⁷Notice, that for outcome classes $m = 1$ and $m = M$, the variance formula simplifies substantially.

 18 Here, we estimate the variance with sample counterparts. An alternative approach, as in Lechner [\(2018\)](#page-109-5), would be to first apply the law of total variance and, second, estimate the conditional moments by nonparametric methods. However, due to the presence of the covariance term the conditioning set contains 2 variables which causes the convergence rate to decrease and hence such variance estimation might even result in less precise estimates, depending on the sample size.

where for the marginal effects at the mean of the covariates the weights $\tilde{w}_{i,m}(x^{kU}x^{kL})$ and the scaling factor $1/(x^{kU}-x^{kL})^2$ are evaluated at the respective sample means, whereas for the mean marginal effects the average of the weights $\frac{1}{N} \sum_{i=1}^{N} \tilde{w}_{i,m}(x^{kU} x^{kL})$ and of the scaling factor $1/(\frac{1}{N} \sum_{i=1}^{N} (x^{kU} - x^{kL}))^2$ is used. Notice also the fact that the scaling factor drops out in the case of categorical covariates. According to the simulation study in Lechner [\(2018\)](#page-109-5) the weight-based inference in case of the Modifed Causal Forests tends to be rather conservative for the individual efects and rather accurate for aggregate efects. The results from the here conducted empirical application resemble this pattern where inference for the marginal efects at the mean of the covariates is more conservative in comparison to inference for the mean marginal efects (see also Appendix [2.C.2](#page-144-0) for a comparison).

2.5 Monte Carlo Simulation

In order to investigate the finite sample performance of the proposed *Ordered Forest* estimator, we perform a Monte Carlo simulation study comparing competing estimators for ordered choice models based on the random forest algorithm. As a parametric benchmark, we take the ordered logistic regression. The considered models are specifcally the following: (i) ordered logit (McCullagh, [1980\)](#page-109-9), (ii) naive ordinal forest (Hornung, [2019a\)](#page-108-14), (iii) ordinal forest (Hornung, [2019a\)](#page-108-14), (iv) conditional forest (Hothorn et al., [2006b\)](#page-108-12), and (v) Ordered Forest as developed in Section [2.4.](#page-87-0) Within the simulation study the Ordered Forest estimator is analyzed more closely to study the fnite sample performance of the estimator depending on the particular forest building schemes and the way the ordering information is being taken into account. Regarding the former we study the Ordered Forest based on the standard random forest as in Breiman [\(2001\)](#page-107-5), i.e. with boostrapping and without honesty as well as based on the adjusted random forest as in Wager and Athey [\(2018\)](#page-110-0), i.e. with subsampling and with honesty. Regarding the latter we study an alternative approach for estimating the conditional choice probabilities which could be labelled as a 'multinomial' forest. In that case, the ordering information is not being taken into account and the probabilities of each category are estimated directly. The details of this approach are provided in Appendix [2.A.1.](#page-111-1) Given this, the *Ordered Forest* estimator should perform better than the multinomial forest in terms of the prediction accuracy thanks to the incorporation of additional information from the ordering of the outcome classes.

Monte Carlo	
observations in training set	200 (800)
observations in testing set	10000
replications	100
covariates with effect	15
trees in a forest	1000
randomly chosen covariates	
minimum leaf size 19	

Table 2.5.1: General Settings of the Simulation

General settings regarding the sample size, the number of replications, as well as forest-specifc tuning parameters for the Monte Carlo simulation are depicted in Table [2.5.1.](#page-92-2) Furthermore, a detailed description of the software implementation of the respective estimators as well as the software specifc tuning parameters are discussed in Appendix [2.B.4.](#page-140-0)

 19 Due to the conceptual differences of the conditional forests, an alternative stopping rule ensuring growing deep trees is chosen. See details in Appendix [2.B.4.](#page-140-0)

2.5.1 Data Generating Process

In terms of the data generating process, we built upon an ordered logit model as defned in [\(2.2.1\)](#page-82-2) and [\(2.2.2\)](#page-83-1). As such we simulate the underlying continuous latent variable Y_i^* as a linear function of regressors X_i , while drawing the error term u_i from the logistic distribution. Then, the continuous outcome Y_i^* is discretized into an ordered categorical outcome Y_i based on the threshold parameters α_m ^{[20](#page-93-0)} Furthermore, the intercept term is fixed to zero, i.e. $\beta_0 = 0$ and thus the thresholds are relative to this value of the intercept. As a result, such DGP captures the probability of the latent variable Y_i^* falling into a particular class given the location defned by the deterministic component of the model together with its stochastic component (Carsey & Harden, [2013\)](#page-107-17).

In simulations of the data generating process, diferent numbers of possible discrete ordered classes are considered, particularly $M = \{3, 6, 9\}$ which corresponds to the simulation set-up used in Janitza et al. [\(2016\)](#page-108-13) and Hornung [\(2019a\)](#page-108-14). Further, both equal class widths, i.e. equally spaced threshold parameters α_m , as well as randomly spaced thresholds, while still preserving the monotonicity of the discrete outcome Y_i , are considered. For the latter, the threshold quantiles are drawn from the uniform distribution, i.e. $\alpha_m^q \sim U(0, 1)$ and ordered afterwards. For the former, the threshold quantiles are equally spaced between 0 and 1 depending on the number of classes. The β coefficients are specified as having fixed coefficient size, namely $\beta_1, ..., \beta_5 = 1, \beta_6, ..., \beta_{10} = 0.75$ and $\beta_{11}, ..., \beta_{15} = 0.5$ as is also the case in Janitza et al. [\(2016\)](#page-108-13) and Hornung [\(2019a\)](#page-108-14). Moreover, an option for nonlinear efects is introduced, too. As such, the covariates do not enter the functional form linearly, but are given by a sine function $sin(2X_i)$ as for example in Lin, Li, and Sun [\(2014\)](#page-109-20), which is hard to model as opposed to other nonlinearities such as polynomials or interactions. The set of covariates X_i is drawn from the multivariate normal distribution with zero mean and a pre-specified variance-covariance matrix Σ , i.e. $X_i \sim \mathcal{N}(0, \Sigma)$, where Σ is specified either as an identity matrix and as such implying zero correlation between regressors, or it is specifed to have a specific correlation structure between regressors 21 as follows:

$$
\rho_{i,j} = \begin{cases}\n1 & \text{for } i = j \\
0.8 & \text{for } i \neq j; i, j \in \{1, 3, 5, 7, 9, 11, 13, 15\} \\
0 & \text{otherwise}\n\end{cases}
$$

which is inspired by the correlation structure from the simulations in Janitza et al. [\(2016\)](#page-108-13) and Hornung [\(2019a\)](#page-108-14). Further, an option to include additional variables with zero efect is implemented as well. As such, another 15 covariates are added to the covariate space with $\beta_{16} = ... = \beta_{30} = 0$ from which 10 are again drawn from the normal distribution with zero mean and unit variance, i.e. $X_{i,0}^c \sim \mathcal{N}(0,1)$ and 5 are dummies drawn from the binomial distribution, i.e. $X_{i,0}^d \sim \mathcal{B}(0.5)$. As the performance of the *Ordered* Forest estimator in high-dimensional settings is of particular interest, due to yet not fully understood theoretical properties in such settings, we include an option for additionally enlarging the covariate space with 1000 zero effect covariates $X_{i,0} \sim \mathcal{N}(0,1)$, effectively creating a setting with $p >> N$. In the high-dimensional case the ordered logit is excluded from the simulations for obvious reasons. Overall, considering all the possible combinations for specifying the DGP, we end up with 72 different DGPs.^{[22](#page-93-2)}

²⁰The thresholds are determined beforehand according to fixed threshold quantiles α_m^q of a large sample of $N = 1'000'000$ observations of the latent Y_i^* from the very same DGP to reflect the realized outcome distribution and then used afterwards in the simulations as a part of the deterministic component.

 21 Note that with a too high multicollinearity, the ordered logit model breaks down. With restricting the level of multicollinearity, the logit model can be still reasonably compared to the other competing methods.

²²For the low-dimensional setting we have $n = 4$ options for the DGP settings, out of which we can choose from none to all of them, whereby the ordering does not matter, we end up with 16 possible combinations as given by the formula $\sum_{r=0}^{n} {n \choose r}$, each for 3 possible numbers of outcome classes resulting in 48 different DGPs. For the high-dimensional setting we have $n = 3$ options as the additional noise variables are always considered. This for all 3 distinct numbers of outcome classes yields 24 diferent DGPs.

For all of them we simulate a training dataset of size $N = 200$ and a testing dataset of size $N = 10'000$ for evaluating the prediction performance of the considered methods. We simulate the large testing set for three main reasons. First, the large testing set enables us to reduce the prediction noise and thus provides a more reliable measure for average out-of-sample performance of the estimators. Second, the large testing set also helps to reduce the simulation noise and thus to obtain more precise estimates for the performance measures. Third, we choose the large testing set to ensure further comparability with the simulation studies performed by Janitza et al. [\(2016\)](#page-108-13) and Hornung [\(2019a\)](#page-108-14). Note that such a large testing set is also common choice in many other simulation studies (see e.g. Jacob, [2020;](#page-108-18) or Knaus, Lechner, & Strittmatter, [2021\)](#page-109-21). Further, we focus more closely on the simulation designs corresponding to the least and the most complex DGPs for which we simulate also a training set of size $N = 800$. The former DGP (labelled as simple DGP henceforth) corresponds exactly to an ordered logit model as in [\(2.2.1\)](#page-82-2) with equal class widths, uncorrelated covariates with linear efects and without any additional zero efect variables. The latter DGP (labelled as complex DGP henceforth) features random class widths, correlated covariates with nonlinear efects and additional zero efect variables. For each replication, we estimate the model on the training set and evaluate the predictions on the testing set, for all tested methods.

2.5.2 Evaluation Measures

In order to properly evaluate the prediction performance we use two measures of accuracy, namely the mean squared error (MSE) and the ranked probability score (RPS). The former evaluates the error of the estimated conditional choice probabilities as a squared diference from the true values of the conditional choice probabilities. Given our simulation design, we know these true values, which are given as in equation [\(2.2.3\)](#page-83-0). Hence, we can defne the Monte Carlo average MSE as:

$$
AMSE = \frac{1}{R} \sum_{j=1}^{R} \frac{1}{N} \sum_{i=1}^{N} \frac{1}{M} \sum_{m=1}^{M} \left(P[Y_{i,j} = m \mid X_{i,j} = x] - \hat{P}[Y_{i,j} = m \mid X_{i,j} = x] \right)^2,
$$

where j refers to the j-th simulation replication, while R being the total number of replications. The second measure, the RPS as developed by Epstein [\(1969\)](#page-108-19) is arguably the prefered measure for the evaluation of probability forecasts for ordered outcomes as it takes the ordering information into account (see Gneiting & Raftery, [2007;](#page-108-20) and Constantinou & Fenton, [2012\)](#page-107-18). The Monte Carlo average RPS can be defned as follows:

$$
ARPS = \frac{1}{R} \sum_{j=1}^{R} \frac{1}{N} \sum_{i=1}^{N} \frac{1}{M-1} \sum_{m=1}^{M} \left(P[Y_{i,j} \leq m \mid X_{i,j} = x] - \hat{P}[Y_{i,j} \leq m \mid X_{i,j} = x] \right)^2,
$$

where on the contrary to the MSE, the difference between the cumulative choice probabilities is measured. The RPS can be seen as a generalization of the Brier Score (Brier, [1950\)](#page-107-19) for multiple, ordered outcomes. As such, it measures the discrepancy between the predicted cumulative distribution function and the true one. Nevertheless, although the ordering information is taken into account, the relative distance between the classes is not refected as pointed out by Janitza et al. [\(2016\)](#page-108-13).

2.5.3 Simulation Results

For the sake of brevity, here we focus mainly on the simulation results obtained for the simple and for the complex DGP, while the results for all 72 DGPs are provided in Appendix [2.B.2.](#page-124-0) Figures [2.5.1](#page-95-0) and [2.5.2](#page-96-0) summarize the results for the low-dimensional setting for the simple and the complex DGP, respectively. Similarly, Figures [2.5.3](#page-97-0) and [2.5.4](#page-98-0) present the results for the simple and the complex DGP for the high-dimensional setting. The upper panels of the fgures show the ARPS, the preferred accuracy measure, whereas the lower panels show the AMSE as a complementary measure. Within the fgures the transparent boxplots in the background show the results for the smaller sample size along with the bold boxplots in the foreground showing the results for the bigger sample size. From left to right the fgures present the results for 3, 6 and 9 outcome classes, respectively. The fgures compare the prediction accuracy of the ordered logit, naive ordinal forest, ordinal forest, conditional forest, Ordered Forest and the multinomial forest, where the asterisk ([∗]) denotes the honest version of the last two forests considered. Further tables with more detailed results and statistical tests for mean diferences in the prediction errors are listed in Appendix [2.B.1.](#page-114-1)

Figure 2.5.1: Simulation Results: Simple DGP & Low Dimension

Note: Figure summarizes the prediction accuracy results based on 100 simulation replications. The upper panel contains the ARPS and the lower panel contains the AMSE. The boxplots show the median and the interquartile range of the respective measure. The transparent boxplots denote the results for the small sample size, while the bold boxplots denote the results for the big sample size. From left to right the results for 3, 6, and 9 outcome classes are displayed.

In the low-dimensional setting with the simple DGP it is expected that the ordered logistic regression should perform best in terms of both the AMSE as well as the ARPS. Indeed, we do observe this results in Figure [2.5.1](#page-95-0) as the ordered logit model performs unanimously best out of the considered models, reaching almost zero prediction error. Among the fexible forest-based estimators, the proposed Ordered Forest belongs to those better performing methods in terms of both accuracy measures. The honest versions of the forests lag behind what points at the efficiency loss due to the additional sample splitting. Overall, the ranking of the estimators stays stable with regards to the number of outcome categories. Additional pattern common to all estimators is the lower prediction error and increased precision with growing sample size.

Figure 2.5.2: Simulation Results: Complex DGP & Low Dimension

Note: Figure summarizes the prediction accuracy results based on 100 simulation replications. The upper panel contains the ARPS and the lower panel contains the AMSE. The boxplots show the median and the interquartile range of the respective measure. The transparent boxplots denote the results for the small sample size, while the bold boxplots denote the results for the big sample size. From left to right the results for 3, 6, and 9 outcome classes are displayed.

In the case of the complex DGP, the performance of the fexible forest-based estimators is expected to be better in comparison to the parametric ordered logit. This can be seen in Figure [2.5.2](#page-96-0) as the ordered logit lags behind the majority of the fexible methods in both accuracy measures. The somewhat higher prediction errors of the naive and the ordinal forest compared to the other forest-based methods might be due to their diferent primary target which are the ordered classes instead of the ordered probabilities as is the case for the other methods. In this respect the conditional forest exhibits considerably good prediction performance. The Ordered Forest outperforms the competing forest-based estimators in terms of the ARPS throughout all outcome class scenarios and also in terms of the AMSE in two scenarios, being outperformed only by the conditional forest in case of 9 outcome classes. Interestingly, the multinomial forest performs very well across all scenarios. However, it is consistently worse than the Ordered Forest with bigger discrepancy between the two the more outcome classes are considered. This points to the value of the ordering information and the ability of the Ordered Forest to utilize it in the estimation. With regards to the sample size, we observe the same pattern as in Figure [2.5.1.](#page-95-0)

Figure 2.5.3: Simulation Results: Simple DGP & High Dimension

Note: Figure summarizes the prediction accuracy results based on 100 simulation replications. The upper panel contains the ARPS and the lower panel contains the AMSE. The boxplots show the median and the interquartile range of the respective measure. The transparent boxplots denote the results for the small sample size, while the bold boxplots denote the results for the big sample size. From left to right the results for 3, 6, and 9 outcome classes are displayed.

Considering the high-dimensional setting for the case of the simple DGP, we see in Figure [2.5.3](#page-97-0) that the Ordered Forest slightly lags behind the other methods, except the scenarios with 3 outcome classes. In comparison, the conditional forest performs best in terms of the ARPS as well as in terms of the AMSE. Also the naive and the ordinal forest exhibit better performance compared to the previous simulation designs. However, it should be noted that the overall diferences in the magnitude of the prediction errors are much lower within this simulation design as compared to the previous designs. Further, taking a closer look at the ARPS results of the multinomial forest we clearly see that in the simple ordered design the ignorance of the ordering information really harms the predictive performance of the estimator the more outcome classes are considered. Additionally, it is interesting to see that the performance gain due to a bigger sample size seems to be much less for the honest version of the forests in the high-dimensional setting as opposed to the low-dimensional setting.

Figure 2.5.4: Simulation Results: Complex DGP & High Dimension

Note: Figure summarizes the prediction accuracy results based on 100 simulation replications. The upper panel contains the ARPS and the lower panel contains the AMSE. The boxplots show the median and the interquartile range of the respective measure. The transparent boxplots denote the results for the small sample size, while the bold boxplots denote the results for the big sample size. From left to right the results for 3, 6, and 9 outcome classes are displayed.

Lastly, the case of the complex DGP in the high-dimensional setting as in Figure [2.5.4](#page-98-0) shows some interesting patterns. In general, all of the methods exhibit good predictive performance as the loss in the prediction accuracy due to the high-dimensional covariate space is small. Additionally, although dealing with the most complex design, no substantial loss in the prediction accuracy can be observed in comparison to the less complex designs. This fact demonstrates the ability of the random forest algorithm as such to efectively cope with highly nonlinear functional forms even in high dimensions. Further, it seems that the role of the sample size is of particular importance in this complex design. On the contrary to the previous designs, where the prediction accuracy increases almost by a constant amount for all estimators and thus does not change their relative ranking, here it does not hold anymore. First, some estimators seem to learn faster than others, i.e. to have a faster rate of convergence. As such in the small sample size the Ordered Forest has in some settings higher values of the ARPS as well as the AMSE than the conditional forest, however manages to outperform the conditional forest in the bigger training sample. This becomes most apparent in the case of 9 outcome classes. Here, the median of the ARPS is almost the same for the two methods based on the small training sample, but signifcantly lower for the Ordered Forest based on the larger training sample.[23](#page-98-1) Second, for the ordinal forest the prediction accuracy even worsens with the bigger training sample, which might hint on possible convergence issues. This might possibly come from the fact that the estimator comprises multiple distinct optimization and partly nonlinear transformation steps that are tied together, but lack formal asymptotic arguments to analyse the impacts and propagation of the estimation errors into the fnal point estimator. Overall, the Ordered Forest achieves the lowest ARPS as well as AMSE within this design, closely followed by the

 23 See Appendix [2.B.1](#page-114-1) for the detailed results of the statistical tests conducted.

conditional and the multinomial forest. However, the generally good performance of the conditional forest might be due to a different type of the stopping criterion, which enables growing very deep trees that are possibly deeper than the classical Breiman [\(2001\)](#page-107-5) trees with pre-specifed minimum leaf size and as such might achieve lower bias which is then refected in the lower values of ARPS as well as of AMSE.

In addition to the four main simulation designs discussed above, we also inspect all 72 diferent DGPs to analyze the performance and the sensitivity of the *Ordered Forest* to the particular features of the simulated DGPs (for details see Appendix [2.B.2\)](#page-124-0). In case of both the low-dimensional setting, as well as the high-dimensional setting, the *Ordered Forest* performs particularly well if there are nonlinear efects accompanied by near-multicollinearity of regressors as such as well as together with additional noise variables or randomly spaced thresholds. Furthermore, the honest version of the Ordered Forest achieves consistently lower prediction accuracy in both settings. It seems that in small samples the increase in variance due to honesty dominates the reduction in the bias of the estimator. In order to further investigate the impact of the honesty feature in bigger samples as well as the convergence of the Ordered Forest, we quadruple the size of the training set once again and repeat the main simulation for the Ordered Forest and its honest version with $N = 3'200$ observations (see Appendix [2.B.1](#page-114-1) for the full results). Firstly, for both versions we observe that with growing sample size the prediction errors get lower and the precision increases. However, the rate of convergence seems to be slower than the parametric rate of \sqrt{N} . Secondly, we observe the same pattern as in the smaller sample sizes, namely slightly lower prediction accuracy for the honest version of the Ordered Forest which stays roughly constant across all simulation designs. Hence, even in the biggest sample the additional variance dominates the bias reduction. However, it should be noted that for a prediction exercise honesty is an optional choice, while if inference is of interest, honesty becomes binding.

2.5.4 Empirical Results

Additionally to the above synthetic simulations, we explore the performance of the Ordered Forest estimator based on real datasets^{[24](#page-99-0)} previously used in Janitza et al. (2016) and Hornung $(2019a)$. Table [2.5.2](#page-99-1) summarizes the features of the datasets and the descriptive statistics are provided in Appendix [2.B.3.1.](#page-137-0) We compare our estimator in terms of the prediction accuracy to all the estimators used in the above Monte Carlo simulation.

		Datasets Summary				
Dataset	Sample Size	Outcome	Class Range			Covariates
Wine Quality	4893	Quality Score	1 (moderate)		6 (high)	
Mammography	412	Visits History	1 (never)	\sim	3 (over year)	b.
Nhanes	1914	Health Status	1 (excellent)		5 (poor)	26
Vlbw	218	Physical Condition	(threatening)	-	9 (optimal)	10
Support Study	798	Disability Degree	(none)		5 (fatal)	15

Table 2.5.2: Description of the Datasets

Similarly to Hornung [\(2019a\)](#page-108-14) we evaluate the prediction accuracy based on a repeated cross-validation in order to reduce the dependency of the results on the particular training and test sample splits. As such we perform a 10-fold cross-validation on each dataset, i.e. we randomly split the dataset in 10 equally sized folds and use 9 folds for training the model and 1 fold for validation. This process is repeated such that each fold serves as a validation set exactly once. Lastly, we repeat this whole procedure 10 times

 24 The here proposed algorithm has been already applied and is in use for predicting match outcomes in football, see Goller et al. [\(2018\)](#page-108-4) and [SEW Soccer Analytics](https://sew.unisg.ch/de/empirische-wirtschaftsforschung/sports-economics-research-group/soccer-analytics) for details.

and report average accuracy measures. The results of the cross-validation exercise for the ARPS as well as the AMSE are summarized in Figures [2.5.5](#page-100-0) and [2.5.6,](#page-101-1) respectively. Similarly as for the simulation results Appendix [2.B.3](#page-137-1) contains more detailed statistics.

Figure 2.5.5: Cross-Validation: ARPS

Note: Figure summarizes the prediction accuracy results in terms of the ARPS based on 10 repetitions of 10-fold crossvalidation for respective datasets. The boxplots show the median and the interquartile range of the respective measure.

The main diference in evaluating the prediction accuracy in comparison to the simulation study is the fact that we do not observe the underlying ordered class probabilities, but only the realized ordered classes. This afects the computation of the accuracy measures and it can be expected that the prediction errors are somewhat higher in comparison to the simulation data, which is also the case here. Overall, the results imply a substantial heterogeneity in the prediction accuracy across the considered datasets. On the one hand, the parametric ordered logit does well in small samples $(vlbw)$ whereas the forest-based methods are somewhat lagging behind. This is not surprising as a lower precision in small samples is the price to pay for the additional fexibility. On the other hand, in the largest sample (winequality) the ordered logit is clearly the worst performing method and all forest-based methods perform substantially better. With respect to the *Ordered Forest* estimator we observe relatively high prediction accuracy for three datasets (mammography, supportstudy, winequality) and relatively low prediction accuracy for two datasets (nhanes, vlbw) in comparison to the competing methods. The good performance in the winequality and the *supportstudy* dataset is expected due to the large samples available. In case of the mammography dataset, even when smaller in sample size, the Ordered Forest maintains the good prediction performance, with its honest version doing even better. The worse performance for the vlbw dataset might be due to the small sample size. However, the honest version of the Ordered Forest performs rather well. The relatively poor performance in the case of the *nhanes* dataset comes rather at surprise as the sample size is rather large. Nevertheless, here the diferences among all estimators are very small in magnitude, in fact the smallest among the considered datasets. Overall, the empirical results provide

an evidence for a good predictive performance of the new Ordered Forest estimator based on various real datasets.

Figure 2.5.6: Cross-Validation: AMSE

Note: Figure summarizes the prediction accuracy results in terms of the AMSE based on 10 repetitions of 10-fold crossvalidation for respective datasets. The boxplots show the median and the interquartile range of the respective measure.

2.6 Empirical Application

For an analysis of the relationship between the covariates and the predicted ordered choice probabilities we estimate the marginal effects for the *Ordered Forest* and compare these to the marginal effects estimated by the ordered logit. We estimate both common measures for marginal efects, i.e. the mean marginal efects as well as the marginal efects at covariate means. The main diference between the ordered logit and the *Ordered Forest* is the fact that the *Ordered Forest* does not use any parametric link function in the estimation of the marginal efects and as such does not impose any functional form on these estimates. As a result, the *Ordered Forest* does neither fix the sign of the marginal effects estimates nor revert it exactly once within the class range as is the case for the ordered logit (the so-called 'single crossing' feature, see i.e. Boes & Winkelmann, [2006;](#page-107-6) or Greene & Hensher, [2010\)](#page-108-9) but rather estimates these in a data-driven manner. Nevertheless, the Ordered Forest, same as the ordered logit, still ensures that the marginal efects across the class range sum up to zero (being more likely to be in some particular classes must imply being less likely to be in some other classes). As such the Ordered Forest not only enables a more fexible estimation of the ordered choice probabilities but also of the marginal efects.

In order to showcase the *Ordered Forest* estimation of marginal effects, we revisit the question of self-assessed health status and its relationship with socio-economic characteristics as for example analyzed previously by Case et al. [\(2002\)](#page-107-0) and Murasko [\(2008\)](#page-109-0). In our empirical application we analyze the dataset from the 2009 National Health Interview Survey (NHIS) used in Angrist and Pischke [\(2014\)](#page-107-20) which includes an ordered categorical outcome indicating a self-assessed health status. The specifc survey

question of interest reads as: 'Would you say your health in general is excellent, very good, good, fair, or poor?' and is coded on an ordered scale ranging from 1 (poor) to 5 (excellent). We examine how the ordered choice probabilities of the self-assessed health status difer for individuals with and without a coverage by private health insurance (see Levy & Meltzer, [2008,](#page-109-22) for a review of insurance efects on health) as well as how these probabilities vary with further socio-demographic characteristics, namely age, race and family size as well as economic characteristics, namely education, employment status and family income. The considered dataset is well-suited for demonstrating the evaluation of marginal efects for several reasons. First, the dataset features an ordered categorical outcome with 5 distinct ordered categories, which are unevenly distributed and thus challenging for estimating the associated marginal efects. Second, the dataset includes both continuous as well as categorical covariates which enables an exhaustive demonstration of the evaluation of marginal efects for various variable types. Third, the dataset contains more than 18′000 observations which allows for a precise estimation of the marginal effects. The descriptive statistics for the considered dataset are presented in Appendix $2.C.1.^{25}$ $2.C.1.^{25}$ $2.C.1.^{25}$ $2.C.1.^{25}$ We follow the data preparation of Angrist and Pischke [\(2014\)](#page-107-20) and discard all observations with missing values and retain only individuals from single family households and those of age between 26 and 59 years as those do not yet qualify for the public health insurance program Medicare.

First of all, in order to describe the diferences in the health status based on the health insurance we inspect the ordered class probabilities for the self-reported health status for individuals with and without a private health insurance contract. The descriptive results are reported in Table [2.6.1](#page-102-1) below, including statistical evidence for the diferences between the two groups. The descriptive evidence suggests that individuals with health insurance have a higher probability to be in excellent or very good health condition and at the same time have a lower probability to be in good or fair health condition. This evidence is both statistically precise and economically relevant. Furthermore, individuals with health insurance seem to have also a lower probability to be in poor health condition. However the evidence for that is less pronounced, both in statistical as well as in economic terms.

		NHIS Dataset			
			Health Insurance		
Health Status	Yes	No	Diff	tValue	pValue
Poor	1.07	1.51	-0.44	-1.84	6.61
Fair	4.81	10.19	-5.38	-9.28	0.00
Good	23.26	35.14	-11.88	-12.66	0.00
Very good	36.31	27.54	8.77	9.70	0.00
Excellent	34.55	25.62	8.93	10.08	0.00
N	15816	2974			

Table 2.6.1: Diferences in Health Status based on Health Insurance: NHIS Dataset

Next, in order to investigate the diferences in the health status based on the health insurance we estimate the ordered choice probabilities for the self-reported health status conditional on having a private health insurance contract and further socio-economic characteristics using the Ordered Forest and the ordered logit and evaluate the corresponding marginal efects. Table [2.6.2](#page-103-0) contains the estimated mean marginal efects for each outcome class for all covariates together with the associated standard errors, t-values, p-values as well as conventional signifcance levels for both the Ordered Forest as well as the ordered logit.[26](#page-102-2)

 25 The dataset is freely accessible from the R-package stevedata (Miller, [2021\)](#page-109-23) or in the data appendix of Angrist and Pischke [\(2014\)](#page-107-20) available [online](http://masteringmetrics.com/wp-content/uploads/2015/01/Data.zip).

 26 The results for the marginal effects at mean are available in Appendix [2.C.2.](#page-144-0)

In general, we see similar patterns in terms of the effect sizes and effect direction for both the Ordered Forest and the ordered logit. However, we do observe more variability in terms of the efect direction in case of the Ordered Forest as we would also expect given the fexibility arguments discussed above. In terms of uncertainty of the efects the weight-based inference seems to be slightly more conservative than the delta method used in the ordered logit. Nevertheless, the Ordered Forest also detects very precise efects which are not discovered by the ordered logit.

Dataset				Ordered Forest					Ordered Logit		
Variable	Class		Effect Std.Error t-Value p-Value					Effect Std.Error t-Value p-Value			
Health Insurance	1	0.23	0.08	2.89	0.38	$***$	-0.11	0.05	-2.19	2.85	$**$
	$\overline{2}$	-0.95	0.49	-1.93	$5.35\,$	\ast	-0.49	$0.22\,$	-2.22	2.68	$***$
	3	-4.51	1.99	-2.27	$2.33\,$	$***$	-1.32	0.59	-2.25	2.44	$\ast\ast$
	4	4.44	$1.80\,$	2.47	$1.35\,$	$***$	$0.02\,$	0.03	$\,0.65\,$	51.88	
	5	0.78	2.47	0.32	75.21		1.90	0.83	2.29	2.22	$***$
Female	$\overline{1}$	-0.19	0.12	-1.59	11.16		$0.02\,$	0.03	0.68	49.85	
	$\overline{2}$	$0.05\,$	$0.31\,$	0.17	86.56		$0.10\,$	0.14	0.68	49.81	
	3	$0.52\,$	0.70	0.74	45.99		$0.26\,$	0.39	0.68	49.80	
	$\overline{4}$	0.44	$0.86\,$	0.52	$60.63\,$		$0.00\,$	$0.01\,$	$0.59\,$	55.20	
	$\bf 5$	-0.82	1.16	-0.70	48.08		-0.39	0.57	-0.68	49.80	
Non White	$\overline{1}$	0.38	0.15	2.57	1.02	$**$	0.36	$0.05\,$	7.02	0.00	$***$
	$\overline{2}$	$0.57\,$	0.42	1.36	17.53		$1.60\,$	0.20	7.89	0.00	$***$
	3	$5.97\,$	1.12	5.32	0.00	$***$	$4.10\,$	0.48	$8.57\,$	$0.00\,$	$***$
	$\overline{4}$	-4.23	1.09	-3.87	0.01	$***$	-0.26	0.08	-3.12	0.18	***
	$\bf 5$	-2.69	$1.57\,$	-1.72	8.57	\ast	-5.81	0.65	-8.87	0.00	***
Age	$\overline{1}$	0.04	0.01	4.22	0.00	$***$	$0.04\,$	0.00	12.60	0.00	$***$
	$\,2$	$0.15\,$	$0.03\,$	5.09	0.00	$***$	$0.20\,$	$0.01\,$	19.77	0.00	$***$
	$\boldsymbol{3}$	$0.45\,$	0.07	6.07	$0.00\,$	$***$	$0.54\,$	0.02	23.87	$0.00\,$	$***$
	4	-0.01	0.09	-0.13	89.49		$0.01\,$	0.01	1.24	21.54	
	$\bf 5$	-0.62	0.12	-5.10	$0.00\,$	$***$	-0.78	0.03	-24.15	$0.00\,$	$***$
Education	$\overline{1}$	0.00	0.00	0.41	68.03		-0.11	$0.01\,$	-11.61	0.00	$***$
	$\sqrt{2}$	-0.01	0.00	-1.73	8.42	\ast	-0.51	0.03	-16.80	0.00	$***$
	3	-0.02	$\rm 0.01$	-2.80	$0.52\,$	***	-1.39	$0.07\,$	-18.94	$0.00\,$	***
	$\overline{4}$	$0.00\,$	$0.01\,$	0.71	48.08		-0.02	$\rm 0.02$	-1.23	21.83	
	$\bf 5$	0.02	0.01	2.57	1.03	$***$	$2.04\,$	0.11	18.85	$0.00\,$	$***$
Family Size	$\overline{1}$	0.00	0.00	0.32	74.77		-0.01	$\overline{0.01}$	-0.81	42.01	
	$\overline{2}$	-0.00	$0.01\,$	-0.21	83.33		-0.04	0.05	-0.81	41.95	
	3	-0.06	$0.02\,$	-3.49	$0.05\,$	$***$	-0.12	0.14	-0.81	41.93	
	$\overline{4}$	-0.03	$\rm 0.02$	-1.78	$7.51\,$	\ast	-0.00	$0.00\,$	-0.67	50.41	
	5	0.10	0.02	4.97	0.00	$***$	0.17	0.21	0.81	41.94	
Employed	$\overline{1}$	-3.99	0.50	-7.94	0.00	$***$	-0.42	0.06	-7.30	0.00	$***$
	$\overline{2}$	-3.81	0.73	-5.19	$0.00\,$	$***$	-1.86	$0.23\,$	-8.21	0.00	$***$
	3	2.58	$1.15\,$	2.25	2.44	$***$	-4.77	0.53	-8.98	0.00	$***$
	$\overline{4}$	4.37	$1.24\,$	3.51	$0.04\,$	***	0.39	0.11	3.55	0.04	***
	$\bf 5$	$0.84\,$	1.82	0.46	$64.34\,$		$6.66\,$	$0.71\,$	$\ \, 9.42$	0.00	$***$
Income	$\overline{1}$	-0.11	0.04	-3.00	0.27	$***$	-0.00	0.00	-12.07	0.00	$***$
	$\overline{2}$	-0.46	0.14	-3.27	$0.11\,$	$***$	-0.00	$0.00\,$	-17.73	0.00	$***$
	3	-0.06	$0.51\,$	-0.12	$90.68\,$		-0.00	0.00	-20.61	$0.00\,$	$***$
	$\overline{4}$	0.36	0.37	0.97	33.42		-0.00	0.00	-1.24	21.41	
	5	$0.27\,$	0.45	0.61	$54.03\,$		0.00	0.00	20.96	$0.00\,$	$***$

Table 2.6.2: Mean Marginal Efects: NHIS Dataset

Significance levels correspond to: $***$, $< 0.01,***$, $< 0.05, *$, < 0.1 .

Notes: Table shows the comparison of the mean marginal effects in % points between the Ordered Forest and the ordered logit. The efects are estimated for all classes, together with the corresponding standard errors, t-values and p-values. The standard errors for the Ordered Forest are estimated using the weight-based inference and for the ordered logit are obtained via the delta method.

In particular, inspecting the variable of interest, namely the indicator for private health insurance, we immediately see the additional flexibility of the *Ordered Forest*. While both methods estimate positive marginal efects of having a private health insurance on the probability of being in very good or excellent health condition and negative marginal effects for being in good or fair health condition, the Ordered Forest estimates also a positive efect for being in poor health condition, whereas the ordered logit is

forced to estimate a negative efect due to its above-mentioned single-crossing property. As such, the Ordered Forest estimates a non-monotonic efect of having a private health insurance across the class probabilities. The results suggest that on one hand individuals with health insurance are less likely to be in good or fair health condition by 4.51 or 0.95 % points, respectively. On the other hand, individuals with health insurance are more likely to be in very good or excellent health condition by 4.44 or 0.78 % points, respectively, but they are also more likely to be in poor health condition by 0.23 % points. As the decision to sign up for a private health insurance is not random, i.e. the data comes from a non-experimental setting, it is not possible to uncover the causal efect without strong assumptions. One might, however, argue that based on the partial correlation evidence, due to the regular medical care and prevention the health insurance increases the likelihood of being in rather good health condition, but also that individuals with rather poor health condition are more likely to sign up for a private health insurance to cover up for the expected medical care costs. As can be seen, the Ordered Forest enables for such a non-monotonic efects analysis, while the ordered logit does not permit such mechanism to take place at all. Overall, in terms of efect sizes, for both estimators we observe smaller magnitudes in comparison to the unconditional diferences presented in Table [2.6.1.](#page-102-1) However, the efect sizes estimated by the Ordered Forest are slightly bigger than those of the ordered logit. With regards to the statistical uncertainty around the estimated marginal efects, both methods exhibit similar level of precision.

Inspecting the efects of the additional conditioning variables, we see that neither the Ordered Forest nor the ordered logit fnd evidence for gender infuencing the health class probabilities as the estimated efects are of small magnitude and lack statistical precision. In contrast, both methods estimate a higher probability of being in poor, fair or good health condition and conversely a lower probability of being in very good or excellent health condition for people of color, an efect that is sizeable and statistically precise. In this case, we note the slightly more conservative standard errors of the Ordered Forest. Furthermore, both methods estimate a higher likelihood of being in rather bad health condition and a lower likelihood of being in rather good health condition for increasing age with similar efect sizes as well as with similar statistical precision. In terms of education, there seem to be a positive relationship with regard to the probability of being in an excellent health condition. However, this efect is less pronounced for the Ordered Forest considering both the efect size and the precision in comparison to the ordered logit. The same positive relationship can be observed also for the family size and although the economic relevance of this efect is rather small, the Ordered Forest estimates this efect with high statistical precision, whereas the ordered logit does not fnd statistical evidence in this respect. Considering the employment status, both methods estimate lower likelihood of being in rather bad health condition and a higher likelihood of being in good health condition with comparable efect sizes as well as statistical precision. Lastly, the Ordered Forest and the ordered logit both estimate a positive relationship with regards to the income level. As such, individuals with higher income are less likely to be in rather bad health condition and more likely to be in rather good health condition. In case of the *Ordered Forest*, the efect sizes are slightly larger, but with lower statistical precision, fnding relevant evidence only for the negative efects on the fair and poor health status, whereas in case of the ordered logit the statistical precision is higher, however with efectively estimating a zero efect. This might be due to the somewhat higher collinearity between the education and income level (0.45) , which suggests a better handling of near-multicollinearity among covariates of the *Ordered Forest* as has been documented in the simulation study. Overall, however, the main advantage of the estimation of the marginal efects by the Ordered Forest stems from a more fexible, data-driven approximation of possible nonlinearities in the functional form.

2.7 Conclusion

In this paper, we develop and apply a new machine learning estimator of the econometric ordered choice models based on the random forest algorithm. The Ordered Forest estimator is a fexible alternative to parametric ordered choice models such as the ordered logit or ordered probit which does not rely on any distributional assumptions and provides essentially the same output as the parametric models, including the estimation of the marginal efects as well as the associated inference. The proposed estimator utilizes the fexibility of random forests and can thus naturally deal with nonlinearities in the data and with a large-dimensional covariate space, while taking the ordering information of the categorical outcome variable into account. Hence, the estimator fexibly estimates the conditional ordered choice probabilities without restrictive assumptions about the distribution of the error term, or other assumptions such as the single index and constant threshold assumptions as is the case for the parametric ordered choice models (see Boes & Winkelmann, [2006,](#page-107-6) for a discussion of these assumptions). Further, the estimator allows also the estimation of the marginal efects, i.e. how the estimated conditional ordered choice probabilities vary with changes in covariates. The weighted representation of these efects enables the weight-based inference as suggested by Lechner [\(2018\)](#page-109-5). The fact that the estimator comprises of linear combinations of random forest predictions ensures that the theoretical guarantees of Wager and Athey [\(2018\)](#page-110-0) are satisfed. Additionally, a free software implementation of the Ordered Forest estimator is available in the R-package orf on the official [CRAN](https://CRAN.R-project.org/package=orf) repository to enable the usage of the method by applied researchers.

The performance of the *Ordered Forest* estimator is studied and compared to other competing estimators in an extensive Monte Carlo simulation as well as using real datasets. The simulation results suggest good performance of the estimator in fnite samples, including also high-dimensional settings. The advantages of the machine learning estimation compared to a parametric method become apparent when dealing with near-multicollinearity and highly nonlinear functional forms. In such cases all of the considered forest-based estimators perform better than the ordered logit in terms of the prediction accuracy. Among the forest-based estimators the *Ordered Forest* proposed in this paper performs well throughout all simulated DGPs and outperforms the competing methods in the most complex simulation designs. The empirical evidence using real datasets supports the fndings from the Monte Carlo simulation. Additionally, the estimation of the marginal efects as well as the inference procedure seems to work well in the presented empirical example.

Despite the attractive properties of the Ordered Forest estimator, many interesting questions are left open. Particularly, a further extension of the Monte Carlo simulation to study the sensitivity of the Ordered Forest in respect to tuning parameters of the underlying random forest as well as in respect to diferent simulation designs would be of interest. Similarly, the performance of the estimator with and without honesty for larger sample sizes should be further investigated. Also, the optimal choice of the size of the window for evaluating the marginal efects would be worth to explore. Additionally, besides the theoretical guarantees for the point estimator, a rigorous asymptotic analysis of the weight-based inference procedure for the estimation of standard errors would be benefcial to describe the exact theoretical properties. Lastly, it would be of great interest to see more real data applications of the Ordered Forest estimator such as for example in Kim, Lym, and Kim [\(2021\)](#page-108-21), especially for large samples.

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Appendix

2.A Other Machine Learning Estimators

2.A.1 Multinomial Forest

Considering the Ordered Forest estimator a possible modifcation for models with categorical outcome variable without an inherent ordering appears to be straightforward. Instead of estimating cumulative probabilities and afterwards isolating the respective class probabilities, we can estimate the class probabilities $P_{m,i} = P[Y_i = m \mid X_i = x]$ directly. As such the binary outcomes are now constructed to indicate the particular outcome classes separately. Then the random forest predictions for each class yield the conditional choice probabilities which need to be afterwards normalized to sum up to 1. Formally, consider (un)ordered categorical outcome variable $Y_i \in \{1, ..., M\}$ with classes m and sample size $N(i = 1, ..., N)$. Then, the estimation procedure can be described as follows:

1. Create M binary indicator variables such as

$$
Y_{m,i} = \mathbf{1}(Y_i = m) \quad \text{for} \quad m = 1, ..., M. \tag{2.A.1}
$$

where m is known and given by the definition of the dependent variable.

2. Estimate regression random forest for each of the M indicators as

$$
P[Y_{m,i} = 1 \mid X_i = x] = \sum_{i=1}^{N} w_{m,i}(x) Y_{m,i} \quad \text{for} \quad m = 1, ..., M,
$$
 (2.A.2)

where the forest weights are defined as $w_{m,i}(x) = \frac{1}{B} \sum_{b=1}^{B} w_{m,b,i}(x)$ with trees weights given by $w_{m,b,i}(x) = \frac{\mathbf{1}\left(\left\{X_i \in L_{b,m}(x)\right\}\right)}{\left|\left\{i: X_i \in L_{b,m}(x)\right\}\right|}$ with leaves $L_{b,m}(x)$ for a total of B trees.

3. Obtain forest predictions for each of the M indicators as

$$
\hat{Y}_{m,i} = \hat{P}[Y_{m,i} = 1 \mid X_i = x] = \sum_{i=1}^{N} \hat{w}_{m,i}(x) Y_{m,i} \quad \text{for} \quad m = 1, ..., M,
$$
\n(2.A.3)

where $\hat{Y}_{m,i}$ are estimated probabilities. 4. Compute probabilities for each class as

$$
\hat{P}_{m,i} = \hat{Y}_{m,i} \qquad \text{for} \qquad m = 1, ..., M \qquad (2.A.4)
$$

$$
\hat{P}_{m,i} = \frac{\hat{P}_{m,i}}{\sum_{m=1}^{M} \hat{P}_{m,i}} \quad \text{for} \quad m = 1, ..., M,
$$
\n(2.A.5)

where the equation $(2.A.4)$ defines the probabilities of all M classes and subsequent equation $(2.A.5)$ ensures that the probabilities sum up to 1 as this might not be the case otherwise. Similarly to the

Ordered Forest estimator, also the multinomial forest is a linear combination of the respective forest predictions and as such also inherits the theoretical properties stemming from random forest estimation as described in Section [2.3](#page-85-0) of the main text.

2.A.2 Conditional Forest

The conditional forest as discussed in Section [2.2](#page-82-0) of the main text is grown with the so-called conditional inference trees. The main idea is to provide an unbiased way of recursive splitting of the trees using a test statistic based on permutation tests (Strasser & Weber, [1999\)](#page-110-0). To describe the estimation procedure, consider an ordered categorical outcome $Y_i \in (1, ..., M)$ with ordered classes m and sample size $N(i = 1, ..., N)$. Further, define binary case weights $w_i \in \{0, 1\}$ which determine if the observation is part of the current leaf. Then, the algorithm developed by Hothorn et al. [\(2006b\)](#page-108-0) can be described as follows:

1. Test the global null hypothesis of independence between any of the P covariates and the outcome, for the particular case weights, given a bootstrap sample Z_b . Afterwards, select the p-th covariate $X_{i,p}$ with the strongest association with the outcome Y_i , or stop if the null hypothesis cannot be rejected. The association is measured by a linear statistic T given as:

$$
T_p(Z_b, w) = \sum_{i=1}^{N} w_i g_p(X_{i,p}) h(Y_i),
$$
\n(2.A.6)

where $g_p(\cdot)$ and $h(\cdot)$ are specific transformation functions.

2. Split the covariate sample space \mathcal{X}_p into two disjoint sets $\mathcal I$ and $\mathcal J$ with adapted case weights $w_i\mathbf{1}(X_{i,p}\in\mathcal{I})$ and $w_i\mathbf{1}(X_{i,p}\in\mathcal{J})$ determining the observations falling into the subset \mathcal{I} and $\mathcal{J},$ respectively. Then, the split is chosen by evaluating a two-sample statistic as a special case of [2.A.6:](#page-112-0)

$$
T_p^{\mathcal{I}}(Z_b, w) = \sum_{i=1}^{N} w_i \mathbf{1}(X_{i,p} \in \mathcal{I}) h(Y_i)
$$
 (2.A.7)

for all possible subsets $\mathcal I$ of the covariate sample space $\mathcal X_p$.

3. Repeat steps [1](#page-112-0) and [2](#page-112-1) recursively with modifed case weights.

Hence, the above algorithm distinguishes between variable selection (step [1\)](#page-112-0) and splitting rule (step [2\)](#page-112-1), while both relying on the variations of the test statistic $T_p(Z_b, w)$. In practice, however, the distribution of this statistic under the null hypothesis is unknown and depends on the joint distribution of Y_i and $X_{i,p}$. For this reason, the permutation tests are applied to abstract from the dependency by fixing the covariates and conditioning on all possible permutations of the outcomes. Then, the conditional mean and covariance of the test statistic can be derived and the asymptotic distribution can be approximated by Monte Carlo procedures, while Strasser and Weber [\(1999\)](#page-110-0) proved its normality. Finally, variables and splits are chosen according to the lowest p-value of the test statistic $T_p(Z_b, w)$ and $T_p^{\mathcal{I}}(Z_b, w)$, respectively.

Besides the permutation tests, the choice of the tranformation functions $g_p(\cdot)$ and $h(\cdot)$ is important and depends on the type of the variables. For continuous outcome and covariates, identity transformation is suggested. For the case of an ordinal regression which is of interest here, the transformation function is given through the score function $s(m)$. If the underlying latent Y_i^* is unobserved, it is suggested that $s(m) = m$ and thus $h(Y_i) = Y_i$. Hence, in the tree building the ordered outcome is treated as a continuous one (Janitza et al., [2016\)](#page-108-1). Then, however, the leaf predictions are the choice probabilities computed as proportions of the outcome classes falling within the leaf, instead of ftting a within leaf constant. The fnal conditional forest predictions for the choice probabilities are the averaged conditional tree probability predictions. Such obtained choice probabilities are analyzed in the Monte Carlo study in Section [2.5](#page-92-0) of the main text.

2.A.3 Ordinal Forest

In the following, the algorithm for the ordinal forest as developed by Hornung [\(2019a\)](#page-108-2) is described. To begin with, consider an ordered categorical outcome $Y_i \in (1, ..., M)$ with ordered classes m and sample size $N(i = 1, ..., N)$. Then, for a set of optimization forests $b = 1, ..., B_{sets}$:

- 1. Draw M − 1 uniformly distributed variables $D_{b,m} \sim U(0, 1)$ and sort them according to their values. Further, set $D_{b,1} = 0$ and $D_{b,M+1} = 1$.
- 2. Define a score set $S_{b,m} = \{S_{b,1},...,S_{b,M}\}\$ with scores constructed as $S_{b,m} = \Phi^{-1}\left(\frac{D_{b,m}+D_{b,m+1}}{2}\right)$ for $m = 1, ..., M$, where $\Phi(\cdot)$ is the cdf of the standard normal.
- 3. Create a new continuous outcome $Z_{b,i} = (Z_{b,1},..., Z_{b,N})$ by replacing each class value m of the original ordered categorical Y_i by the m-th value of the score set $S_{b,m}$ for all $m = 1, ..., M$.
- 4. Use $Z_{b,i}$ as dependent variable and estimate a regression forest $RF_{S_{b,m}}$ with B_{prior} trees.
- 5. Obtain the out-of-bag (OOB) predictions for the continuous $Z_{b,i}$ and transform them into predictions for Y_i as follows: $\hat{Y}_{b,i} = m$ if $\hat{Z}_{b,i} \in [\Phi^{-1}(D_{b,m}, \Phi^{-1}(D_{b,m+1})]$ for all $i = 1, ..., N$.
- 6. Compute a performance measure for the given forest $\hat{RF}_{S_{b,m}}$ based on some performance function of type $f(Y_i, \hat{Y}_{b,i}).$

After estimating B_{sets} of optimization forests, take S_{best} of these which achieved the best performance according to the performance function. Then, construct the fnal set of uniformly distributed variables $D_1, ..., D_{M+1}$ as an average of those from S_{best} for $m = 1, ..., M+1$. Finally, form the optimized score set $S_m = \{S_1, ..., S_M\}$ with scores constructed as $S_m = \Phi^{-1}\left(\frac{D_m + D_{m+1}}{2}\right)$ for $m = 1, ..., M$. The continuous outcome $Z_i = (Z_1, ..., Z_N)$ is then similarly as in the optimization procedure constructed by replacing each m value of the original outcome Y_i by the m-th value of the optimized score set S_m for all $m = 1, ..., M$. Finally, estimate the regression forest RF_{final} using Z_i as the dependent variable. On one hand, the class prediction of such an ordinal forest is one of the M ordered classes which has been predicted the most by the respective trees of the forest. On the other hand, the probability prediction is obtained as a relative frequency of trees predicting the particular class. Such predicted choice probabilities are analyzed in the conducted Monte Carlo study in Section [2.5](#page-92-0) of the main text. Further, the so-called naive forest corresponds to the ordinal forest with omitting the above described optimization procedure.

2.B Simulation Study

2.B.1 Main Simulation Results

In the following Tables [2.B.1,](#page-115-0) [2.B.2,](#page-116-0) [2.B.3,](#page-117-0) [2.B.4](#page-118-0) and [2.B.5](#page-119-0) are summarized the simulation results presented in Section [2.5.3](#page-94-0) of the main text. Each table specifes the particular simulation design as follows: the column *Class* indicates the number of outcome classes, $Dim.$ specifies the dimension, DGP characterizes the data generating process as defned in the main text and Statistic contains summary statistics of the simulation results. In particular, the mean of the respective accuracy measure and its standard deviation. Furthermore, rows t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods. The alternative hypothesis is that the mean of the Ordered Forest is less than the mean of the other method to test if the Ordered Forest achieves signifcantly lower prediction error than the other considered methods. Furthermore, Figures [2.B.1,](#page-120-0) [2.B.2,](#page-121-0) [2.B.3](#page-122-0) and [2.B.4](#page-123-0) complement the results presented in Section [2.5.3](#page-94-0) of the main text for the simulations with the increased sample size.

2.B.1.1 ARPS: Sample Size $= 200$

Table 2.B.1: Simulation results: Accuracy Measure = ARPS $\&$ Sample Size = 200

Notes: Table reports the average measures of the RPS based on 100 simulation replications for the sample size of 200 observations. The frst column denotes the number of outcome classes. Columns 2 and 3 specify the dimension and the DGP, respectively. The fourth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods.

2.B.1.2 AMSE: Sample Size = 200

Table 2.B.2: Simulation results: Accuracy Measure = AMSE & Sample Size = 200

Notes: Table reports the average measures of the MSE based on 100 simulation replications for the sample size of 200 observations. The frst column denotes the number of outcome classes. Columns 2 and 3 specify the dimension and the DGP, respectively. The fourth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods.

2.B.1.3 ARPS: Sample Size $= 800$

Table 2.B.3: Simulation results: Accuracy Measure = ARPS $\&$ Sample Size = 800

Notes: Table reports the average measures of the RPS based on 100 simulation replications for the sample size of 800 observations. The frst column denotes the number of outcome classes. Columns 2 and 3 specify the dimension and the DGP, respectively. The fourth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods.

2.B.1.4 AMSE: Sample Size $= 800$

Table 2.B.4: Simulation results: Accuracy Measure = AMSE & Sample Size = 800

Notes: Table reports the average measures of the MSE based on 100 simulation replications for the sample size of 800 observations. The frst column denotes the number of outcome classes. Columns 2 and 3 specify the dimension and the DGP, respectively. The fourth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods.

2.B.1.5 ARPS & AMSE: Sample Size = 3200

		Simulation Design			ARPS		AMSE
Class	Dim.	DGP	Statistic	Ordered	Ordered*	Ordered	Ordered*
3	Low	Simple	mean st.dev. t-test wilcox-test	0.0373 0.0004	0.0670 0.0005 0.0000 0.0000	0.0376 0.0005	0.0591 0.0004 0.0000 0.0000
3	Low	Complex	mean st.dev. t-test wilcox-test	0.0285 0.0004	0.0415 0.0005 0.0000 0.0000	0.0243 0.0003	$_{0.0336}$ 0.0004 0.0000 0.0000
$\sqrt{3}$	High	Simple	mean st.dev. t-test wilcox-test	0.0956 0.0003	0.1069 0.0002 0.0000 0.0000	0.0798 0.0002	0.0872 0.0002 0.0000 0.0000
3	High	Complex	mean st.dev. t-test wilcox-test	0.0498 0.0004	0.0620 0.0005 0.0000 0.0000	0.0557 0.0005	$_{0.0653}$ 0.0005 0.0000 0.0000
6	Low	Simple	mean st.dev. t-test wilcox-test	0.0335 0.0004	0.0593 0.0004 0.0000 0.0000	0.0188 0.0002	0.0253 0.0001 0.0000 0.0000
6	Low	Complex	mean st.dev. t-test wilcox-test	0.0255 0.0003	0.0367 0.0004 0.0000 0.0000	0.0162 0.0002	0.0197 0.0002 0.0000 0.0000
$\,6$	High	Simple	mean st.dev. t-test wilcox-test	0.0825 0.0002	0.0923 0.0002 0.0000 0.0000	0.0314 0.0001	0.0335 0.0000 0.0000 0.0000
6	High	Complex	mean st.dev. t-test wilcox-test	0.0526 0.0004	0.0656 0.0004 0.0000 0.0000	0.0264 0.0002	0.0292 0.0001 0.0000 0.0000
$\boldsymbol{9}$	Low	Simple	mean st.dev. t-test wilcox-test	0.0321 0.0003	0.0565 0.0003 0.0000 0.0000	0.0110 0.0001	0.0136 0.0001 0.0000 0.0000
9	Low	Complex	mean st.dev. t-test wilcox-test	0.0244 0.0002	0.0350 0.0003 0.0000 0.0000	0.0098 0.0001	0.0110 0.0001 0.0000 0.0000
$\boldsymbol{9}$	High	Simple	mean st.dev. t -test wilcox-test	0.0783 0.0002	0.0875 0.0002 0.0000 0.0000	0.0165 0.0000	0.0172 0.0000 0.0000 0.0000
9	High	Complex	mean st.dev. t-test wilcox-test	0.0559 0.0004	0.0697 0.0004 0.0000 0.0000	0.0145 0.0001	0.0160 0.0001 0.0000 0.0000

Table 2.B.5: Simulation results: Accuracy Measure = $ARPS/AMSE \&$ Sample Size = 3200

Notes: Table reports the average measures of the RPS and MSE based on 100 simulation replications for the sample size of 3200 observations. The frst column denotes the number of outcome classes. Columns 2 and 3 specify the dimension and the DGP, respectively. The fourth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and the honest version of the Ordered Forest.

Figure 2.B.1: Ordered Forest Simulation Results: Simple DGP & Low Dimension

Note: Figure summarizes the prediction accuracy results based on 100 simulation replications. The upper panel contains the ARPS and the lower panel contains the AMSE. The boxplots show the median and the interquartile range of the respective measure. The transparent boxplots denote the results for the small sample size, the semi-transparent ones denote the medium sample size, while the bold boxplots denote the results for the big sample size. From left to right the results for 3, 6, and 9 outcome classes are displayed.

Figure 2.B.2: Ordered Forest Simulation Results: Complex DGP & Low Dimension

Note: Figure summarizes the prediction accuracy results based on 100 simulation replications. The upper panel contains the ARPS and the lower panel contains the AMSE. The boxplots show the median and the interquartile range of the respective measure. The transparent boxplots denote the results for the small sample size, the semi-transparent ones denote the medium sample size, while the bold boxplots denote the results for the big sample size. From left to right the results for 3, 6, and 9 outcome classes are displayed.

Figure 2.B.3: Ordered Forest Simulation Results: Simple DGP & High Dimension

Note: Figure summarizes the prediction accuracy results based on 100 simulation replications. The upper panel contains the ARPS and the lower panel contains the AMSE. The boxplots show the median and the interquartile range of the respective measure. The transparent boxplots denote the results for the small sample size, the semi-transparent ones denote the medium sample size, while the bold boxplots denote the results for the big sample size. From left to right the results for 3, 6, and 9 outcome classes are displayed.

Figure 2.B.4: Ordered Forest Simulation Results: Complex DGP & High Dimension

Note: Figure summarizes the prediction accuracy results based on 100 simulation replications. The upper panel contains the ARPS and the lower panel contains the AMSE. The boxplots show the median and the interquartile range of the respective measure. The transparent boxplots denote the results for the small sample size, the semi-transparent ones denote the medium sample size, while the bold boxplots denote the results for the big sample size. From left to right the results for 3, 6, and 9 outcome classes are displayed.

2.B.2 Complete Simulation Results

Tables [2.B.6](#page-125-0) to [2.B.17](#page-136-0) below summarize the simulation results for all 72 diferent DGPs, complementing the main results presented in Section [2.5.3](#page-94-0) of the main text. Each table specifes the particular simulation design as follows: the first column DGP provides the identifier for the data generating process. Columns 2 to 5 specify the particular characteristics of the respective DGP, namely if the DGP features additional noise variables $(noise)$, 15 in the low-dimensional case and 1000 in the high-dimensional case, nonlinear effects (nonlin), multicollinearity among covariates (multi), and randomly spaced thresholds (random). The sixth column Statistic contains summary statistics of the simulation results. In particular, the mean of the respective accuracy measure (mean) and its standard deviation (st.dev.). Furthermore, rows *t-test* and *wilcox-test* contain the *p*-values of the parametric *t*-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the *Ordered Forest* and all the other methods. The alternative hypothesis is that the mean of the Ordered Forest is less than the mean of the other method to test if the Ordered Forest achieves signifcantly lower prediction error than the other considered methods.

2.B.2.1 ARPS: Low Dimension with 3 Classes

Table 2.B.6: Simulation Results: Accuracy Measure $=$ ARPS & Low Dimension with 3 Classes

Notes: Table reports the average measures of the RPS based on 100 simulation replications for the sample size of 200 observations with 3 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namel t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods.

2.B.2.2 ARPS: Low Dimension with 6 Classes

Table 2.B.7: Simulation Results: Accuracy Measure $=$ ARPS & Low Dimension with 6 Classes

Notes: Table reports the average measures of the RPS based on 100 simulation replications for the sample size of 200 observations with 6 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namel

2.B.2.3 ARPS: Low Dimension with 9 Classes

Table 2.B.8: Simulation Results: Accuracy Measure $=$ ARPS & Low Dimension with 9 Classes

Notes: Table reports the average measures of the RPS based on 100 simulation replications for the sample size of 200 observations with 9 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namel t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods.

2.B.2.4 ARPS: High Dimension with 3 Classes

Table 2.B.9: Simulation Results: Accuracy Measure = ARPS & High Dimension with 3 Classes

Notes: Table reports the average measures of the RPS based on 100 simulation replications for the sample size of 200 observations with 3 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namely 1000 additional noise variables (noise), nonlinear effects (nonlin), multicollinearity among covariates (multi), and randomly spaced thresholds (random). The sixth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the $Ordered$ *Forest* and all the other methods.

2.B.2.5 ARPS: High Dimension with 6 Classes

Table 2.B.10: Simulation Results: Accuracy Measure = ARPS & High Dimension with 6 Classes

Notes: Table reports the average measures of the RPS based on 100 simulation replications for the sample size of 200 observations with 6 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namely 1000 additional noise variables (noise), nonlinear effects (nonlin), multicollinearity among covariates (multi), and randomly spaced thresholds (random). The sixth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the $Ordered$ *Forest* and all the other methods.

2.B.2.6 ARPS: High Dimension with 9 Classes

Table 2.B.11: Simulation Results: Accuracy Measure = ARPS & High Dimension with 9 Classes

Notes: Table reports the average measures of the RPS based on 100 simulation replications for the sample size of 200 observations with 9 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namely 1000 additional noise variables (noise), nonlinear effects (nonlin), multicollinearity among covariates (multi), and randomly spaced thresholds (random). The sixth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the $Ordered$ *Forest* and all the other methods.

2.B.2.7 AMSE: Low Dimension with 3 Classes

Table 2.B.12: Simulation Results: Accuracy Measure $=$ AMSE & Low Dimension with 3 Classes

Notes: Table reports the average measures of the MSE based on 100 simulation replications for the sample size of 200 observations with 3 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namel

2.B.2.8 AMSE: Low Dimension with 6 Classes

Table 2.B.13: Simulation Results: Accuracy Measure $=$ AMSE & Low Dimension with 6 Classes

Notes: Table reports the average measures of the MSE based on 100 simulation replications for the sample size of 200 observations with 6 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namel

2.B.2.9 AMSE: Low Dimension with 9 Classes

Table 2.B.14: Simulation Results: Accuracy Measure $=$ AMSE & Low Dimension with 9 Classes

Notes: Table reports the average measures of the MSE based on 100 simulation replications for the sample size of 200 observations with 9 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namel

2.B.2.10 AMSE: High Dimension with 3 Classes

Table 2.B.15: Simulation Results: Accuracy Measure = AMSE & High Dimension with 3 Classes

Notes: Table reports the average measures of the MSE based on 100 simulation replications for the sample size of 200 observations with 3 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namely 1000 additional noise variables (noise), nonlinear effects (nonlin), multicollinearity among covariates (multi), and randomly spaced thresholds (random). The sixth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the $Ordered$ *Forest* and all the other methods.

2.B.2.11 AMSE: High Dimension with 6 Classes

Table 2.B.16: Simulation Results: Accuracy Measure = AMSE & High Dimension with 6 Classes

Notes: Table reports the average measures of the MSE based on 100 simulation replications for the sample size of 200 observations with 6 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namely 1000 additional noise variables (noise), nonlinear effects (nonlin), multicollinearity among covariates (multi), and randomly spaced thresholds (random). The sixth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the $Ordered$ *Forest* and all the other methods.

2.B.2.12 AMSE: High Dimension with 9 Classes

Table 2.B.17: Simulation Results: Accuracy Measure = AMSE & High Dimension with 9 Classes

Notes: Table reports the average measures of the MSE based on 100 simulation replications for the sample size of 200 observations with 9 outcome classes. Columns 1 to 5 specify the DGP identifier and its features, namely 1000 additional noise variables (noise), nonlinear effects (nonlin), multicollinearity among covariates (multi), and randomly spaced thresholds (random). The sixth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the $Ordered$ *Forest* and all the other methods.

2.B.3 Empirical Results

In this section we present more detailed and supplementary results regarding the empirical results (Section [2.5.4\)](#page-99-0) discussed in the main text. In the following the descriptive statistics for the considered datasets and the results for the prediction accuracy are summarized.

2.B.3.1 Descriptive Statistics

Mammography Dataset										
variable	type	mean	sd	median	min	max				
$SYMPT*$	Categorical	2.97	0.95	3.00	1.00	4.00				
РB	Numeric	7.56	2.10	7.00	5.00	17.00				
$HIST*$	Categorical	1.11	0.31	1.00	1.00	2.00				
BSE^*	Categorical	1.87	0.34	2.00	1.00	2.00				
$DECT^*$	Categorical	2.66	0.56	3.00	1.00	3.00				
v^*	Categorical	1.61	0.77	$1.00\,$	1.00	3.00				

Table 2.B.18: Descriptive Statistics: mammography dataset

Table 2.B.19: Descriptive Statistics: nhanes dataset

		Nhanes Dataset				
variable	type	mean	sd	median	min	max
sex^*	Categorical	1.51	0.50	2.00	1.00	2.00
race^*	Categorical	2.87	1.00	3.00	1.00	5.00
country_of_birth*	Categorical	1.34	0.79	1.00	1.00	4.00
education*	Categorical	3.37	1.24	3.00	1.00	5.00
$martial_status^*$	Categorical	2.31	1.74	1.00	1.00	6.00
waistcircum	Numeric	100.37	16.37	99.40	61.60	176.70
Cholesterol	Numeric	196.89	41.59	193.00	97.00	432.00
WBCcount	Numeric	7.30	2.88	6.90	1.60	83.20
$AcuteIllness*$	Categorical	1.25	0.43	1.00	1.00	2.00
$depression^*$	Categorical	1.39	0.76	1.00	1.00	4.00
ToothCond*	Categorical	3.05	1.24	3.00	1.00	5.00
sleepTrouble*	Categorical	2.28	1.28	2.00	1.00	5.00
$wakeUp^*$	Categorical	2.41	1.30	2.00	1.00	5.00
cig^*	Categorical	1.51	0.50	2.00	1.00	2.00
diabetes*	Categorical	1.14	0.34	1.00	1.00	2.00
asthma [*]	Categorical	1.15	0.36	1.00	1.00	2.00
heartFailure*	Categorical	1.03	0.16	1.00	1.00	2.00
stroke*	Categorical	1.03	0.18	1.00	1.00	2.00
chronicBronchitis*	Categorical	1.07	0.26	1.00	1.00	2.00
alcohol	Numeric	3.93	20.18	2.00	0.00	365.00
heavyDrinker*	Categorical	1.17	0.37	1.00	1.00	2.00
$medicalPlaceToGo*$	Categorical	1.92	0.67	2.00	1.00	5.00
BPsys	Numeric	124.44	18.62	122.00	78.00	230.00
BP dias	Numeric	71.18	11.84	72.00	10.00	114.00
age	Numeric	49.96	16.68	50.00	20.00	80.00
BMI	Numeric	29.33	6.66	28.32	14.20	73.43
\mathbf{y}^*	Categorical	2.77	1.00	3.00	1.00	5.00

Supportstudy Dataset										
variable	type	mean	sd	median	min	max				
age	Numeric	62.80	16.27	65.29	20.30	100.13				
$sex*$	Categorical	1.54	0.50	2.00	1.00	2.00				
dzgroup^*	Categorical	3.23	2.48	2.00	1.00	8.00				
num.co	Numeric	1.90	1.34	2.00	0.00	7.00				
scoma	Numeric	12.45	25.29	0.00	0.00	100.00				
charges	Numeric	59307.91	86620.70	28416.50	1635.75	740010.00				
avtisst	Numeric	23.53	13.60	20.00	1.67	64.00				
$race*$	Categorical	1.36	0.88	1.00	1.00	5.00				
meanbp	Numeric	84.52	27.64	77.00	0.00	180.00				
wblc	Numeric	12.62	9.31	10.50	0.05	100.00				
hrt	Numeric	98.59	32.93	102.50	0.00	300.00				
resp	Numeric	23.60	9.54	24.00	0.00	64.00				
temp	Numeric	37.08	1.25	36.70	32.50	41.20				
crea	Numeric	1.80	1.74	1.20	0.30	11.80				
sod	Numeric	137.64	6.34	137.00	118.00	175.00				
v^*	Categorical	2.90	1.81	2.00	1.00	5.00				

Table 2.B.20: Descriptive Statistics: supportstudy dataset

Table 2.B.21: Descriptive Statistics: vlbw dataset

Vlbw Dataset										
variable	type	mean	sd	median	min	max				
$race*$	Categorical	1.57	0.50	2.00	1.00	2.00				
bwt	Numeric	1094.89	260.44	1140.00	430.00	1500.00				
inout*	Categorical	1.03	0.16	1.00	1.00	2.00				
$twn*$	Categorical	1.24	0.43	1.00	1.00	2.00				
lol	Numeric	7.73	19.47	3.00	0.00	192.00				
$mag\text{suffix}$	Categorical	1.18	0.39	1.00	1.00	2.00				
$meth^*$	Categorical	1.44	0.50	1.00	1.00	2.00				
toc^*	Categorical	1.24	0.43	1.00	1.00	2.00				
$delivery*$	Categorical	1.41	0.49	1.00	1.00	2.00				
$sex*$	Categorical	1.50	0.50	1.00	1.00	2.00				
y^*	Categorical	5.09	2.58	6.00	1.00	9.00				

Table 2.B.22: Descriptive Statistics: winequality dataset

2.B.3.2 Prediction Accuracy

Tables [2.B.23](#page-139-0) and [2.B.24](#page-139-1) summarize in detail the results of the prediction accuracy exercise using real datasets for the ARPS and the AMSE, respectively. The frst column Data specifes the dataset, the second column Class defnes the number of outcome classes of the dependent variable and the third column Size indicates the number of observations. Similarly to the simulation results, the column Statistic contains summary statistics and statistical tests results for the equality of means between the results of the Ordered Forest and all the other methods.

	Dataset Summary							Comparison of Methods			
Data	Class	Size	Statistic	Ologit	Naive	Ordinal	Cond.	Ordered	Ordered*	Multi	Multi*
mammography	3	412	mean st.dev. t-test wilcox-test	0.1776 0.0010 1.0000 1.0000	0.2251 0.0027 0.0000 0.0000	0.2089 0.0021 0.0000 0.0000	0.1767 0.0013 1.0000 1.0000	0.1823 0.0018	0.1766 0.0008 1.0000 1.0000	0.1826 0.0019 0.3999 0.3153	0.1767 0.0007 1.0000 1.0000
nhanes	5	1914	mean st.dev. t-test wilcox-test	0.1088 0.0004 1.0000 1.0000	0.1089 0.0003 1.0000 1.0000	0.1100 0.0004 0.9839 0.9738	0.1085 0.0001 1.0000 1.0000	0.1103 0.0002	0.1137 0.0001 0.0000 0.0000	0.1104 0.0002 0.2106 0.2179	0.1159 0.0001 0.0000 0.0000
supportstudy	5	798	mean st.dev. t-test wilcox-test	0.1872 0.0011 0.0000 0.0000	0.1849 0.0010 0.0000 0.0000	0.1834 0.0009 0.0052 0.0073	0.1800 0.0008 1.0000 1.0000	0.1823 0.0008	0.1931 0.0003 0.0000 0.0000	0.1857 0.0007 0.0000 0.0000	0.1944 0.0004 0.0000 0.0000
vlbw	9	218	mean st.dev. t-test wilcox-test	0.1595 0.0011 1.0000 1.0000	0.1713 0.0026 0.0100 0.0116	0.1724 0.0030 0.0023 0.0010	0.1603 0.0014 1.0000 1.0000	0.1686 0.0021	0.1623 0.0005 1.0000 1.0000	0.1685 0.0020 0.5143 0.5733	0.1642 0.0003 1.0000 1.0000
winequality	6	4893	mean st.dev. t-test wilcox-test	0.0756 0.0000 0.0000 0.0000	0.0501 0.0003 1.0000 0.9999	0.0503 0.0002 0.9992 0.9986	0.0596 0.0001 0.0000 0.0000	0.0507 0.0002	0.0673 0.0001 0.0000 0.0000	0.0504 0.0002 0.9971 0.9966	0.0683 0.0000 0.0000 0.0000

Table 2.B.23: Empirical Results: Accuracy Measure = ARPS

Notes: Table reports the average measures of the RPS based on 10 repetitions of 10-fold cross-validation. The fourth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, *t-test* and *wilcox-test* contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods.

	Dataset Summary							Comparison of Methods			
Data	Class	Size	Statistic	Ologit	Naive	Ordinal	Cond.	Ordered	$Ordered*$	Multi	$Multi*$
mammography	3	412	mean st.dev. t-test wilcox-test	0.1754 0.0007 0.9923 0.9943	0.2593 0.0025 0.0000 0.0000	0.2222 0.0031 0.0000 0.0000	0.1720 0.0008 1.0000 1.0000	0.1766 0.0012	0.1726 0.0004 1.0000 1.0000	0.1770 0.0013 0.2467 0.2179	0.1726 0.0004 1.0000 1.0000
nhanes	5	1914	mean st.dev. t-test wilcox-test	0.1310 0.0003 1.0000 1.0000	0.1309 0.0003 1.0000 1.0000	0.1332 0.0003 0.7067 0.6579	0.1304 0.0002 1.0000 1.0000	0.1332 0.0003	0.1329 0.0001 0.9936 0.9955	0.1319 0.0003 1.0000 1.0000	0.1343 0.0001 0.0000 0.0000
supportstudy	5	798	mean st.dev. t-test wilcox-test	0.1124 0.0005 0.0000 0.0000	0.1110 0.0004 0.0000 0.0000	0.1094 0.0004 0.0020 0.0008	0.1078 0.0004 1.0000 0.9999	0.1088 0.0004	0.1129 0.0002 0.0000 0.0000	0.1101 0.0003 0.0000 0.0000	0.1135 0.0002 0.0000 0.0000
vlbw	9	218	mean st.dev. t-test wilcox-test	0.0944 0.0002 1.0000 1.0000	0.0986 0.0008 1.0000 1.0000	0.0990 0.0009 0.9999 0.9999	0.0956 0.0004 1.0000 1.0000	0.1008 0.0008	0.0958 0.0003 1.0000 1.0000	0.1006 0.0009 0.7224 0.7821	0.0956 0.0002 1.0000 1.0000
winequality	6	4893	mean st.dev. t-test wilcox-test	0.1001 0.0000 0.0000 0.0000	0.0692 0.0003 1.0000 1.0000	0.0698 0.0003 0.9960 0.9974	0.0831 0.0001 0.0000 0.0000	0.0702 0.0003	0.0906 0.0001 0.0000 0.0000	0.0693 0.0003 1.0000 1.0000	0.0913 0.0001 0.0000 0.0000

Table 2.B.24: Empirical Results: Accuracy Measure = AMSE

Notes: Table reports the average measures of the MSE based on 10 repetitions of 10-fold cross-validation. The fourth column Statistic shows the mean and the standard deviation of the accuracy measure for all methods. Additionally, t-test and wilcox-test contain the p-values of the parametric t-test as well as the nonparametric Wilcoxon test for the equality of means between the results of the Ordered Forest and all the other methods.

2.B.4 Software Implementation

The Monte Carlo study has been conducted using the R statistical software (R Core Team, [2018\)](#page-109-0) in version 3.5.2 (Eggshell Igloo) and the respective packages implementing the estimators used. With regards to the forest-based estimators the main tuning parameters, namely the number of trees, the number of randomly chosen covariates and the minimum leaf size have been specifed according to the values in Table [2.5.1](#page-92-1) in the main text.

	Software Implementation and Tuning Parameters											
method	Ologit	Naive	Ordinal	Conditional	Ordered	$Ordered*$	Multi	$Multi*$				
package	rms	ordinalForest	ordinalForest	party	ranger	grf	ranger	grf				
function	Irm	ordfor	ordfor	cforest	ranger	regression_forest	ranger	regression_forest				
max. iterations	25											
trees		1000	1000	1000	1000	1000	1000	1000				
random subset		\sqrt{p}	\sqrt{p}	\sqrt{p}	\sqrt{p}	\sqrt{p}	\sqrt{p}	\sqrt{p}				
leaf size		5		0	5	Ð	Ð	5.				
B_{sets}		0	1000									
B_{prior}		0	100									
performance		equal	equal									
S_{best}		0	10									

Table 2.B.25: Overview of Software Packages and Tuning Parameters

In terms of the particular R packages used the ordered logistic regression has been implemented using the rms package (version 5.1-3) written by Harrell [\(2019\)](#page-108-3). The respective lrm function for ftting the ordered logit has been used with the default parameters, except setting the maximum number of iterations, maxit=25 as for some of the DGPs the ordered logit has experienced convergence issues. Next, the naive and the ordinal forest have been applied based on the ordinalForest package in version 2.3 (Hornung, [2019b\)](#page-108-4) with the ordfor function. As described in Appendix [2.A.3](#page-113-0) the ordinal forest introduces additional tuning parameters for which we use the default parameters as suggested in the package manual. Further, the conditional forest has been estimated with the package party in version 1.3-1 (Hothorn, B¨uhlmann, Dudoit, Molinaro, & Van Der Laan, [2006a;](#page-108-5) Strobl, Boulesteix, Zeileis, & Hothorn, [2007;](#page-110-1) Strobl, Boulesteix, Kneib, Augustin, & Zeileis, [2008\)](#page-110-2). Regarding the choice of the tuning parameters, we rely on the default parameters of the cforest function. A particularity of the conditional forest is, due to the conceptual diferences to standard regression forest in terms of the splitting criterion, the choice of the stopping rule. This is controlled by the significance level α (see Appendix [2.A.2](#page-112-2) for details). However, in order to grow deep trees we follow the suggestion in the package manual to set mincriterion= 0 , which has been also used in the simulation study conducted in Janitza et al. [\(2016\)](#page-108-1). Lastly, the Ordered Forest as well as the multinomial forest algorithms are implemented using the package ranger in version 0.11.1 (Wright & Ziegler, [2017\)](#page-110-3) with the default hyperparameters. The honest versions of the above two estimators rely on the grf package in version 0.10.2 (Tibshirani et al., [2018\)](#page-110-4) with the default hyperparameters as well. A detailed overview of packages with the corresponding tuning parameters is provided in Table [2.B.25.](#page-140-0)

Furthermore, Tables [2.B.26](#page-141-0) and [2.B.27](#page-142-0) compare the absolute and relative computation time of the respective methods. For comparison purposes, we measure the computation time for the four main DGPs presented in Section [2.5.3](#page-94-0) of the main text, namely the simple DGP in the low- and high-dimensional case as well as the complex DGP in the low- and high-dimensional case, for both the small sample size $(N = 200)$ and the big sample size $(N = 800)$ for all considered number of outcome classes. We estimate the model based on the training set and predict the class probabilities for a test set of size $N = 10'000$ as in the main simulation. We repeat this procedure 10 times and report the average computation time. The tuning parameters and the software implementations are chosen as defned in Table [2.5.1](#page-92-1) in the main text and Table [2.B.25](#page-140-0) herein, respectively. All simulations are computed on a 64-Bit Windows machine

		Simulation Design						Comparison of Methods			
Class	Dim.	DGP	Size	Ologit	Naive	Ordinal	Cond.	Ordered	$Ordered*$	Multi	Multi*
3	Low	Simple	200	0.01	1.22	10.33	46.61	0.62	1.24	0.91	1.86
3	Low	Simple	800	0.02	1.58	40.83	150.84	1.03	1.96	1.61	2.98
3	Low	Complex	200	0.02	1.19	11.93	47.43	0.63	1.26	0.98	1.92
3	Low	Complex	800	0.03	1.71	52.45	150.59	1.08	1.94	1.73	3.06
3	High	Simple	200		3.50	61.89	64.28	4.05	5.08	6.06	7.27
3	High	Simple	800		13.91	332.60	175.76	7.19	7.10	12.19	11.02
3	High	Complex	200		3.46	60.25	59.98	4.02	4.96	6.02	7.10
3	High	Complex	800		13.83	325.65	173.63	6.83	6.61	11.50	10.66
66	Low	Simple	200	0.02	1.88	12.79	46.80	1.47	3.00	1.74	3.52
6	Low	Simple	800	0.03	2.28	48.98	151.58	2.45	4.75	3.10	5.82
6	Low	Complex	200	0.03	1.85	14.75	46.97	1.56	3.12	1.85	3.66
6	Low	Complex	800	0.04	2.54	64.44	151.84	2.68	4.82	3.30	6.02
6	High	Simple	200		4.21	69.80	64.14	10.24	11.74	12.01	13.63
6	High	Simple	800		15.86	386.02	176.27	19.34	17.43	26.24	19.97
6	High	Complex	200		4.11	70.51	60.85	9.98	11.52	11.95	13.61
6	High	Complex	800		15.85	371.69	174.17	18.11	17.18	24.43	19.52
9	Low	Simple	200	0.03	2.32	20.53	46.70	2.27	4.71	2.44	5.03
9	Low	Simple	800	0.04	2.69	57.22	145.21	3.82	7.29	4.61	7.99
9	Low	Complex	200	0.03	2.29	22.86	47.36	2.40	4.83	2.65	5.28
9	Low	Complex	800	0.05	3.07	79.15	151.36	4.27	$7.75\,$	5.81	8.68
9	High	Simple	200		4.85	80.76	63.25	16.05	17.84	17.69	19.56
9	High	Simple	800		16.91	413.74	169.91	31.34	26.91	38.95	27.38
9	High	Complex	200		4.62	78.86	57.68	15.79	17.78	17.57	19.59
9	High	Complex	800		18.10	437.04	175.07	31.12	27.33	37.59	28.16

Table 2.B.26: Absolute Computation Time in Seconds

Notes: Table reports the average absolute computation time in seconds based on 10 simulation replications of training and prediction. The frst column denotes the number of outcome classes. Columns 2 and 3 specify the dimension and the DGP, respectively. The fourth column contains the number of observations in the training set. The prediction set consists of 10 000 observations.

The results reveal the expected pattern for the *Ordered Forest*. The more outcome classes the longer the computation time as by defnition of the algorithm more forests have to be estimated. Furthermore, we also observe a longer computation time if the number of observation and/or the number of considered splitting covariates increases which is also an expected behaviour. However, the computation time is not sensitive to the particular DGP which it should not be either. The latter two patterns are true for all considered methods. In comparison to the other forest-based methods, the computational advantage of the *Ordered Forest* becomes apparent. The *Ordered Forest* outperforms the ordinal and the conditional forest in all cases. In some cases the Ordered Forest is even more than 100 times faster and even in the closest cases it is more than 3 times faster than the two. In absolute terms this translates to computation time of around 1 second for the *Ordered Forest* and around 50 seconds for the ordinal and around 150 seconds for the conditional forest in the most extreme case. Contrarily, in the closest case, the computation time for the Ordered Forest is around 15 seconds, while for the ordinal forest this is around 80 seconds and around 60 seconds for the conditional forest. This points to the additional computation burden of the ordinal and the conditional forest due to the optimization procedure and the permutation tests, respectively. The only exception is the naive forest which does not include the optimization step. Furthermore, we observe a slightly longer computation time for the multinomial forest in comparison to the Ordered Forest, which is due to one extra forest being estimated. The honest versions of the two forests take a bit longer in general, but this seems to reverse once bigger samples are considered (in terms

of both number of observations as well as number of considered covariates).

		Simulation Design						Comparison of Methods			
Class	Dim.	DGP	Size	Ologit	Naive	Ordinal	Cond.	Ordered	$Ordered*$	Multi	$Multi*$
3	Low	Simple	200	0.02	1.98	16.76	75.66	$\mathbf{1}$	2.02	1.48	3.02
3	Low	Simple	800	0.02	1.53	39.68	146.59	1	1.91	1.56	2.90
3	Low	Complex	$200\,$	0.03	1.87	18.79	74.70	$\mathbf{1}$	1.99	1.55	3.03
3	Low	Complex	800	0.03	1.59	48.79	140.09	1	1.81	1.61	2.84
$\sqrt{3}$	High	Simple	200		0.86	15.27	15.86	$\mathbf{1}$	1.25	1.50	1.79
3	High	Simple	800		1.94	46.28	24.46	1	0.99	1.70	1.53
3	High	Complex	200		0.86	14.99	14.92	$\mathbf 1$	1.23	1.50	1.77
3	High	Complex	800		2.02	47.68	25.42	1	0.97	1.68	1.56
6	Low	Simple	200	0.02	1.28	8.73	31.95	$\mathbf{1}$	2.05	1.19	2.40
6	Low	Simple	800	0.01	0.93	19.95	61.74	$\mathbf{1}$	1.94	1.26	2.37
6	Low	Complex	200	0.02	1.18	9.45	30.09	1	2.00	1.19	2.34
6	Low	Complex	800	0.02	0.94	24.02	56.59	$\mathbf 1$	1.80	1.23	2.24
6	High	Simple	200		0.41	6.81	6.26	$\mathbf{1}$	1.15	1.17	1.33
6	High	Simple	800		0.82	19.96	9.11	1	0.90	1.36	1.03
6	High	Complex	200		0.41	7.07	6.10	$\mathbf{1}$	1.16	1.20	1.36
6	High	Complex	800		0.88	20.52	9.62	$\mathbf{1}$	0.95	1.35	1.08
9	Low	Simple	200	0.01	1.02	9.03	20.54	$\mathbf{1}$	2.07	1.07	2.21
9	Low	Simple	800	0.01	0.70	14.98	38.01	$\mathbf 1$	1.91	1.21	2.09
9	Low	Complex	200	0.01	0.95	9.51	19.69	$\mathbf{1}$	2.01	1.10	2.19
9	Low	Complex	800	0.01	0.72	18.55	35.48	$\mathbf 1$	1.82	1.36	2.03
9	High	Simple	200		0.30	5.03	3.94	$\mathbf{1}$	1.11	1.10	1.22
9	High	Simple	800		0.54	13.20	5.42	$\mathbf 1$	0.86	1.24	0.87
9	High	Complex	200		0.29	5.00	3.65	$\mathbf 1$	1.13	1.11	1.24
9	High	Complex	800		0.58	14.04	5.63	$\mathbf{1}$	0.88	1.21	0.90

Table 2.B.27: Relative Computation Time

Notes: Table reports the average relative computation time with regards to the Ordered Forest estimator based on 10 simulation replications of training and prediction. The frst column denotes the number of outcome classes. Columns 2 and 3 specify the dimension and the DGP, respectively. The fourth column contains the number of observations in the training set. The prediction set consists of 10 000 observations.

Generally, the sensitivity with regards to the computation time appears to be very diferent for the considered methods. For the Ordered Forest as well as the multinomial forest, including their honest versions, the most important aspect is clearly the number of outcome classes. For the naive and the ordinal forest the number of observations seems to be most decisive and for the conditional forest paradoxically the size of the prediction set is most relevant. Overall, the above result support the theoretical argument of the Ordered Forest being computationally advantageous in comparison to the ordinal and the conditional forest.

2.C Empirical Application

In this appendix we provide the descriptive statistics for the dataset used in the empirical application of the main text as well as supplementary results containing the estimation of marginal efects.

2.C.1 Descriptive Statistics

NHIS Dataset									
variable	type	mean	sd	median	min	max			
Health Status*	Categorical	3.93	0.95	4.00	1.00	5.00			
Health Insurance [*]	Categorical	0.84	0.37	1.00	0.00	1.00			
$Female*$	Categorical	0.50	0.50	0.50	0.00	1.00			
Non White*	Categorical	0.20	0.40	0.00	0.00	1.00			
Age	Numeric	42.72	8.70	43.00	26.00	59.00			
Education	Numeric	13.74	2.99	14.00	0.00	18.00			
Family Size	Numeric	3.63	1.37	4.00	2.00	18.00			
$Employd*$	Categorical	0.82	0.39	1.00	0.00	1.00			
$Income*$	Categorical	94178.04	56738.46	85985.78	19282.93	167844.53			

Table 2.C.1: Descriptive Statistics: NHIS Dataset

Table 2.C.2: Descriptive Statistics by Class: NHIS Dataset

NHIS Dataset										
Health Status										
variable	poor	fair	good	very good	excellent					
Health Status	1.14	5.66	25.14	34.92	33.13					
Health Insurance	79.07	71.50	77.88	87.52	87.76					
Female	49.77	51.08	49.28	50.43	49.92					
Non White	31.63	23.89	22.84	18.18	18.21					
Age	47.65	45.37	43.75	42.73	41.30					
Education	12.11	12.20	12.89	13.97	14.46					
Family Size	3.33	3.68	3.68	3.59	3.64					
Employed	28.84	65.57	80.99	84.35	84.21					
Income	53409.03	62473.99	78957.11	99685.45	106743.21					
N	215	1063	4724	6562	6226					
share in $%$	1.14	5.66	25.14	34.92	33.13					

Note: Means of variables for respective outcome class displayed. Shares for dummy variables are indicated in %.
2.C.2 Marginal Efects

In what follows, the results for the marginal efects at mean are presented for the considered NHIS dataset. Similarly as in the main text, the efects are computed for each outcome class of the dependent variable both for the Ordered Forest as well as for the ordered logit. The estimations are done in R version 3.6.1 using the orf package (Lechner & Okasa, [2019\)](#page-109-0) in version 0.1.3 for the Ordered Forest and the oglmx package (Carroll, [2018\)](#page-107-0) in version 3.0.0.0 for the ordered logit.

Dataset				Ordered Forest			Ordered Logit					
Variable	Class		Effect Std.Error t -Value p-Value				Effect Std.Error t-Value p-Value					
Age	$\mathbf{1}$	0.01	0.01	0.69	48.80	0.04	0.00	12.77	0.00	$***$		
	$\overline{2}$	$0.31\,$	$0.20\,$	1.55	12.07	0.18	$0.01\,$	20.08	0.00	***		
	$\sqrt{3}$	-3.76	$3.10\,$	-1.21	22.49	0.62	$0.03\,$	22.63	$0.00\,$	$***$		
	$\overline{4}$	-1.31	4.67	-0.28	77.93	0.00	$0.01\,$	0.15	87.78			
	$\bf 5$	4.75	5.63	0.84	39.88	-0.83	0.04	-23.38	0.00	$***$		
Education	$\overline{1}$	0.00	0.00	0.00	100.00	-0.09	0.01	-11.83	0.00	***		
	$\,2$	$0.00\,$	$0.00\,$	0.00	100.00	-0.46	$0.03\,$	-16.90	0.00	***		
	$\sqrt{3}$	0.00	0.00	0.00	100.00	-1.60	$0.09\,$	-18.19	0.00	***		
	$\,4\,$	$0.00\,$	0.00	0.00	100.00	-0.00	$\rm 0.02$	-0.15	87.78			
	$\overline{5}$	0.00	$0.00\,$	0.00	100.00	$2.16\,$	$0.12\,$	18.63	0.00	***		
Employed	$\overline{1}$	-2.07	0.56	-3.73	0.02	*** -0.35	0.05	-7.22	0.00	***		
	$\,2$	-1.79	1.39	-1.28	19.89	-1.69	$\rm 0.21$	-8.08	0.00	***		
	$\sqrt{3}$	-6.76	11.87	-0.57	56.88	-5.49	$\,0.61\,$	-8.94	0.00	***		
	$\,4\,$	4.13	9.18	0.45	65.29	$0.57\,$	$0.15\,$	$3.86\,$	$\rm 0.01$	***		
	$\overline{5}$	6.49	16.14	0.40	68.74	6.96	0.73	9.52	0.00	$***$		
FamilySize	$\overline{1}$	0.08	0.09	0.95	34.06	-0.01	0.01	-0.81	42.00			
	$\sqrt{2}$	-5.07	4.12	-1.23	$21.81\,$	-0.04	$0.05\,$	-0.81	41.95			
	$\sqrt{3}$	3.81	15.41	0.25	80.45	-0.13	0.16	-0.81	41.94			
	$\overline{4}$	2.96	33.98	$0.09\,$	93.07	-0.00	$0.00\,$	-0.15	87.99			
	$\bf 5$	-1.78	39.79	-0.04	96.43	0.18	0.22	0.81	41.94			
Female	$\overline{1}$	-0.01	0.01	-0.58	56.51	0.02	0.03	0.68	49.85			
	$\,2$	$0.21\,$	0.79	0.27	78.66	$0.09\,$	0.13	0.68	49.81			
	$\sqrt{3}$	-2.61	$5.01\,$	-0.52	60.28	$0.30\,$	0.45	0.68	49.80			
	$\,4\,$	-3.07	$10.21\,$	-0.30	76.38	0.00	$0.00\,$	$0.15\,$	88.10			
	5	5.47	11.73	0.47	64.10	-0.41	0.60	-0.68	49.80			
HealthInsurance	$\overline{1}$	-0.00	0.02	-0.01	98.90	-0.09	$0.04\,$	-2.17	2.97	$\overline{**}$		
	$\,2$	-1.15	$1.26\,$	-0.91	36.12	-0.44	$0.20\,$	-2.20	2.77	$***$		
	$\sqrt{3}$	$2.96\,$	6.17	0.48	63.14	-1.52	$0.68\,$	-2.25	$2.43\,$	$***$		
	$\overline{4}$	-9.14	16.51	-0.55	57.96	0.05	$0.05\,$	0.98	32.83			
	$\bf 5$	7.34	17.48	0.42	67.48	$2.01\,$	$0.87\,$	$2.30\,$	$2.16\,$	$***$		
Income	$\overline{1}$	0.02	0.01	1.46	14.45	-0.00	0.00	-12.16	0.00	$***$		
	$\sqrt{2}$	-0.36	0.92	-0.39	69.70	-0.00	0.00	-18.01	0.00	$***$		
	$\sqrt{3}$	1.87	10.11	0.18	85.36	-0.00	0.00	-19.87	0.00	***		
	$\,4\,$	-4.32	10.98	-0.39	69.37	-0.00	$0.00\,$	-0.15	87.78			
	$\bf 5$	$2.80\,$	16.54	0.17	86.56	0.00	$0.00\,$	20.36	0.00	$***$		
NonWhite	$\mathbf{1}$	0.03	0.03	0.92	35.56	0.30	0.04	6.99	0.00	***		
	$\,2$	$\rm 0.96$	$1.59\,$	0.60	54.76	1.45	0.19	7.81	0.00	$***$		
	$\sqrt{3}$	1.98	$6.55\,$	$0.30\,$	76.22	4.76	$0.56\,$	8.48	0.00	***		
	$\overline{4}$	$0.37\,$	10.52	0.04	97.18	-0.41	0.12	-3.52	0.04	$***$		
	5	-3.34	12.61	-0.27	79.10	-6.09	0.68	-8.94	0.00	***		

Table 2.C.3: Marginal Efects at Mean: NHIS Dataset

Significance levels correspond to: $***$, < 0.01 , $**$, < 0.05 , $*$, < 0.1 .

Notes: Table shows the comparison of the marginal effects at mean in % points between the Ordered Forest and the ordered logit. The efects are estimated for all classes, together with the corresponding standard errors, t-values and p-values. The standard errors for the Ordered Forest are estimated using the weight-based inference and for the ordered logit are obtained via the delta method.

Chapter 3

The Effect of Sport in Online Dating: Evidence from Causal Machine Learning

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Abstract

Online dating emerged as a key platform for human mating. Previous research focused on sociodemographic characteristics to explain human mating in online dating environments, neglecting the commonly recognized relevance of sport. This research investigates the efect of sport activity on human mating by exploiting a unique data set from an online dating platform. Thereby, we leverage recent advances in the causal machine learning literature to estimate the causal efect of sport frequency on the contact chances. We fnd that for male users, doing sport on a weekly basis increases the probability to receive a frst message from a woman by 50%, relatively to not doing sport at all. For female users, we do not fnd evidence for such an efect. In addition, for male users the efect increases with higher income.

Keywords: Online dating, sports economics, big data, causal machine learning, efect heterogeneity, Modifed Causal Forest.

JEL classifcation: J12, Z29, C21, C45.

3.1 Introduction

Human interactions that have traditionally taken place in physical reality have increasingly shifted to the online world and the Covid-19 pandemic has substantially accelerated this trend. Human mating is also afected by this development, resulting in numerous novel formats of online dating. Indeed, online dating emerged as pivotal instrument for human mating. Rosenfeld, Thomas, and Hausen [\(2019\)](#page-172-0), for instance, showed, that online dating represents the most common way for heterosexual couples to meet in the US. Cacioppo, Cacioppo, Gonzaga, Ogburn, and Vanderweele [\(2013\)](#page-170-0) furthermore showed, that more than one-third of marriages in the US (2005-2012) are attributed to an initial contact via online dating.

Understanding the mechanisms that explain human mating in online dating environments is, in turn, decisive to elucidate the structure of societal evolution and to derive algorithms increasing the efficiency of the matching of potential partners. Explaining human mating in online dating environments relies essentially on the information that users share online, including socio-demographic, psychological, and physical traits. Indeed, previous research referred to socio-demographic (e.g., age; Hitsch, Hortaçsu, & Ariely, [2010a\)](#page-171-0) and psychological (e.g., extroversion; Cuperman & Ickes, [2009\)](#page-170-1) traits to explain human mating in online dating environments (for a detailed review, see Eastwick, Luchies, Finkel, & Hunt, [2014\)](#page-170-2). Research considering physical traits, commonly interpreted as sport activity (Schulte-Hostedde, Eys, Emond, & Buzdon, [2012\)](#page-172-1), to explain human mating in online dating environments, however, remains sparse even though few research provides indications that sport activity has substantial efects on human mating (Schulte-Hostedde et al., [2012\)](#page-172-1). However, the efect of sport activity on human mating has not yet been fully understood. This paper attempts to fll this gap. In particular, this paper is, to the best of our knowledge, the frst to investigate the causal efect of sport activity on human mating in online dating environments. It is also the frst paper to analyze the heterogeneity of this causal efect using the novel causal machine learning methods.

Following this notion, we leverage unique data of more than 16'000 users, forming altogether almost 180'000 interactions. The data allows us not only to map interactions among users on a second-by-second basis, including visiting a user profle and contacting a user via private message, but also to observe more than 600 user characteristics describing the socio-demographic, psychological, and importantly, physical traits, including the frequency of the sport activity. This setting allows us to create a credible research design that eliminates potential sources of endogeneity by focusing on the frst, one-way interactions between users, and by observing essentially the very same information, and even beyond, as an actual user. Hence, we can reliably identify the efect of sport activity on contact chances by relying on the conditional independence, i.e. the unconfoundedness research design. Moreover, we exploit recent advances in causal machine learning to estimate the causal efect of sport activity on contact chances in our large-dimensional setting in a very fexible way, while considering potential efect heterogeneities. In particular, we apply the Modifed Causal Forest (Lechner, [2018\)](#page-171-1), an estimator that reams the concept of Causal Trees and Forests, by allowing for multiple treatments, as applicable to our measure of sport activity. Furthermore, the Modifed Causal Forest improves the splitting rule to account for selection bias and the mean correlated error. Additionally, it allows for estimation and inference on diferent aggregation levels in one estimation step. All of these aspects are crucial and benefcial for our research. Specifcally, we can relax on the functional form assumptions, unlike classical parametric approaches, which is particularly important in large-dimensional settings as ours. Moreover, we can go beyond average efects and can fexibly investigate efect heterogeneities on various aggregation levels.

Leveraging the benefts of the Modifed Causal Forest, we fnd diferent patterns for males and females. Particularly, for male users, we observe uniformly increasing contact chances by a potential female partner, for increasing levels of sport activity. Specifcally, the contact chances increase by more than 50% if male users practice sport on a weekly basis, relative to no sport at all. However, for female users, we do not fnd evidence for such an efect. Beyond the average efects, we uncover interesting efect heterogeneities both for males and females. In particular, for male users, we fnd that the efect of sport frequency on contact chances increases with higher income. This holds true for the income levels of the male users themselves, as well as for the income levels of the potential female partners. This implies that higher income male users enjoy a higher efect of a weekly sport activity, and that higher income female users value the regular sport activity of the potential male partners more. These heterogeneous efects are both statistically precise, as well as substantially relevant. In addition, for female users, we fnd indications that the efect of sport activity on contact chances increases with a higher sport frequency of the potential male partner. Furthermore, analysing the individualized efects provides additional descriptive evidence for these heterogeneous efects. It reveals further insights for potential heterogeneity mechanisms driven by education level or relationship preferences, among others. Lastly, a placebo test shows the robustness of our results.

This study contributes to research and practice as well as to the society. First, this paper provides new insights for the literature on human mating by demonstrating that sport activity, a key behavioral trait, afects human mating. Second, this paper supports social science research in assessing causal efects in large-dimensional data environments by showcasing an empirical approach, which allows for a very fexible estimation of average efects as well as a systematic assessment of underlying heterogeneities. Third, this paper helps individuals to increase their dating success by exhibiting how sport activities can contribute to the likelihood to be recognized by potential partners, fnally highlighting the relevance of sport activity not only from a health but also from a human mating perspective. Finally, this paper serves product developers to improve the architecture of online dating platforms by highlighting the relevance of sport activity, while considering efect heterogeneities (e.g., demographic characteristics) at the same time.

This paper is structured as follows. Section [3.2](#page-148-0) provides a short overview on prior work related to our research. Section [3.3](#page-150-0) describes the online dating platform and the respective data. Section [3.4](#page-155-0) explains the empirical approach, including the identifcation strategy and the estimation method. Following this, Section [3.5](#page-159-0) presents the results, comprising the average and disaggregated efects. Section [3.6](#page-167-0) discusses the results and the implications for research, practice, and society.

3.2 Literature

In this section we briefy describe prior work related to our research, comprising literature on sport activity in general as well as literature on sport activity and human mating.

3.2.1 Sport Activity

Sport activity has been ascribed relevant efects on human life, including physical and mental health as well as social outcomes, some of which are summarized next.

First, sport activity was shown to afect health outcomes. For instance Warburton, Nicol, and Bredin [\(2006\)](#page-172-2) confrmed, based on an extensive review of the literature, that sport activity facilitates the prevention of several chronic diseases (e.g., cardiovascular disease and diabetes). In a similar vein, Humphreys, McLeod, and Ruseski [\(2014\)](#page-171-2) found, that sport activity reduces self-reported incidences of diabetes, high blood pressure, heart disease, asthma, and arthritis (for a review, see Penedo & Dahn,

[2005,](#page-171-3) and; Eime, Young, Harvey, Charity, & Payne, [2013\)](#page-170-3).

Second, sport activity was demonstrated to enfold efects on mental health. Hillman, Erickson, and Kramer [\(2008\)](#page-171-4), for instance, showed that sport activity enhances cognition and brain functions (for a review, see Strong et al., [2005,](#page-172-3) and; Janssen & LeBlanc, [2010\)](#page-171-5). Moreover, sport activity was shown to increase self-reported life satisfaction and happiness (Huang & Humphreys, [2012;](#page-171-6) Ruseski, Humphreys, Hallman, Wicker, & Breuer, [2014\)](#page-172-4).

Third, sport activity was proven to afect social outcomes. For instance, Caruso [\(2011\)](#page-170-4) showed that sport activity decreases property and juvenile crime among young adults. Moreover, sport activity was found to enfold positive efects on economic outcomes such as wages and earnings (e.g. Lechner, [2009;](#page-171-7) Rooth, [2011\)](#page-172-5), human capital (Steckenleiter & Lechner, [2020\)](#page-172-6), and quality of work performance (Pronk et al., [2004\)](#page-172-7). Finally, sport activity has been confrmed to lead to higher academic achievements (Fox, Barr-Anderson, Neumark-Sztainer, & Wall, [2010;](#page-171-8) Pfeifer & Cornelißen, [2010;](#page-172-8) Felfe, Lechner, & Steinmayr, [2016;](#page-170-5) Lechner, [2017;](#page-171-9) Fricke, Lechner, & Steinmayr, [2018\)](#page-171-10), to positively afect concentration, memory and classroom behavior (Trudeau & Shephard, [2008\)](#page-172-9), and to improve social relations (Stempel, [2005\)](#page-172-10).

The efects of sport activity are, thus, explored in various spheres of human life. The efect of sport activity on human mating, however, is almost unexplored, as discussed next.

3.2.2 Sport Activity and Human Mating

Research on human mating has established in sociology, psychology, economics, and, more recently, computer science, mostly attributable to the range of potential explanatory factors that determine human mating (Eastwick et al., [2014\)](#page-170-2) and novel data opportunities due to computer-mediated approaches for human mating (i.e., online dating). In addition to various studies referring to socio-demographic and psychological characteristics to explain human mating (for a detailed review, see Eastwick et al., [2014\)](#page-170-2), a few studies also consider sport activity as potentially relevant factor in explaining human mating.

Schulte-Hostedde, Eys, and Johnson [\(2008\)](#page-172-11) studied the efect of males' practiced sport discipline on females' willingness to engage in a relationship, applying an experimental setting. The authors showed that $'[\ldots]$ team sport athletes were perceived as being more desirable as potential mates than individual sport athletes and non-athletes' (p. 114). Moreover, the authors argued that 'team sport athletes may have traits associated with good parenting such as cooperation, likeability, and role acceptance' (p. 114) to explain the positive efect of team sport participation on desirability. However, the authors restrict sport activities to a particular type of sport, namely team vs. individual sport, which, in turn, impedes a valid assessment of the general efect of sport activity on human mating. In a similar vein, Farthing [\(2005\)](#page-170-6) showed, also applying an experimental setting, that $\langle \ldots \rangle$ females and males preferred heroic sport risk takers as mates, with the preference being stronger for females' (p. 171) , while interpreting (non-) heroic sport risk as, for example, engaging in (non-) risky sport activities. However, the previously raised concerns apply in the same way to the fndings by Farthing [\(2005\)](#page-170-6).

Further research provides insights on potential indirect efects of sport activity on human mating. In particular, previous research indicated that sport activity improves, inter alia, attractiveness (Park, Buunk, & Wieling, [2007\)](#page-171-11), health (Warburton et al., [2006\)](#page-172-2), and income generation (Lechner, [2009\)](#page-171-7), all of which have been shown to affect human mating (e.g. Hitsch et al., [2010a;](#page-171-0) Hitsch, Hortacsu, $\&$ Ariely, [2010b;](#page-171-12) Eastwick et al., [2014\)](#page-170-2). However, these studies remain inconclusive with respect to human mating, given the missing integration of relevant context-factors (i.e., further relevant personal/sport characteristics) afecting human mating.

Taken together, sport activity seems relevant for explaining human mating. However, a conclusive, finally valid, assessment on the effect of sport activity on human mating is missing, given that previous research assessed the efect of sport activity on human mating either in the absence of potentially relevant socio-demographic characteristics or by utilizing a narrowed interpretation, respectively representation, of sport activity. These limitations surprise given that information on sport activity are one of the most articulated and visible features on online dating platforms. Furthermore, as discussed previously, sport activity is ascribed relevant efects on various spheres of human life, including physical and mental health as well as social and economic conditions. Following the above mentioned limitations, we focus on the analysis of the efect of sport activity on human mating.

3.3 Setup and Data

In the course of this research, we collaborated with a German online dating platform operator. The operator provided us both with information on the functionality as well as with data from the online dating platform.

3.3.1 Online Dating

The online dating platform allows a user to virtually meet and communicate with other users. The user has to pay a monthly fxed subscription fee to register and to utilize the online dating platform. The registration at the online dating platform is subdivided into three major sections. First, the user is requested to provide socio-demographic information (e.g., sex, age, education, and income). Second, the user is requested to specify search criteria for potential partners (e.g., sex, age, education, and income). Third, the user is requested to answer a personality test that relates to the users' life style, personality, attitudes and views (79 categories in total). Moreover, the user articulates the language preferences and may include one or more photos on the personal profle page. However, these photos remain fully blurred until the user decides to release the photo for the potential partner.^{[1](#page-150-1)} Most importantly, with specifc regard to the intended analysis, a user articulates her/his sport preferences and actual sport activities within a total of 27 disciplines, how often she/he actively practices sport, and, fnally, which recreational activities dominate in her/his leisure time. A detailed description of the survey questions and the corresponding variables together with descriptive statistics can be found in Appendix [3.D.](#page-183-0)

Following the registration at the online dating platform, the user can defne a query, indicating the preferred sex, age, and geographic location to explore potential partners. The search query returns a shortlist of potential partners, who correspond to the previously defned qualifcations. The shortlist includes the potential partners' username, age, a blurred version of the photo, and a matching score, which is computed by the online dating platform operator in order to support users in fnding a potentially ftting partner.[2](#page-150-2) The user can investigate the potential partner in detail by browsing on the potential partners' profle page, which displays a blurred version of the photo as well as information on the previously described survey. The user can then choose from multiple possible actions. As such, the user can either send a private text message, a 'Smile' icon, or a 'Smile Back' icon (if initially received a 'Smile' icon) to a potential partner. Additionally, a user may leave a 'like' or a text note on a potential partners' profle page. Moreover, the user can initiate a friendship with a potential partner by initiating a profle release

¹In our analysis we restrict the user interactions by excluding the actions involving the release of the blurred photo. We discuss this point in Detail in Section [3.4.2.](#page-156-0)

²The online dating platform operator does not provide the formula to calculate the matching score. However, it provided us with all data required for its calculation. We elaborate more on this point in Section [3.4.2.](#page-156-0)

or accepting an initial profle release by a potential partner. Furthermore, a user may request an 'Applet' (game with questions) to a potential partner, which works out similarities/diferences between the user and the potential partner. Finally, a user may prevent unwanted users from contacting in any form.

3.3.2 Data

The acquired data consists of two samples. The frst, user sample, contains personal information about the registered users on the platform. The second, interaction sample, contains information about the users' interactions on the platform.

The user sample includes 18'036 newly registered users who joined the platform between January 1st, 2016 and April 30th, 2016.[3](#page-151-0) For each registered user, we observe the full information flled upon the registration, which comprises 667 variables in total. For our intended analysis with regard to the sport activity, we exclude the users with daily sport frequency, as these comprise only around 3% of all users, which would prevent a meaningful analysis for this group. Furthermore, we restrict ourselves to the sample of users, whose residency is located in Germany, as only for these users we observe full location information, including the ZIP codes. This restriction afects only about 2% of the observations as the platform provider operates on the German market. Lastly, we exclude users with incomplete information (around 1% of the sample) and those with implausible and inconsistent values (less than 1% of the sample).[4](#page-151-1) This leaves us with an available sample consisting of 16'864 users for our analysis. A descriptive summary of selected variables for the user sample is presented in Appendix [3.A.](#page-173-0)

The interaction sample includes 1'415'645 user actions among the population of newly registered users over the same time period. For each action, we observe the IDs of both users involved in the action, as well as the precise time stamp and the type of action. Each interaction between users must begin with a visit action (invisible to a user), upon which further types of actions are possible, such as a message, like or smile (visible to a user). We refer to the user who initiates an interaction as a sender of an action, and the user who gets involved in an interaction as a *recipient* of an action. For the purposes of our analysis, we flter the interactions such that we consider only one-way interactions initiated by a visit action, with either no further action at all, or immediately followed by any visible action from the sender, without considering any visible recipient's response to the initial action from the sender. Thus, we select only unique interactions in the sense that the sender was visibly or invisibly active, while the recipient stayed visibly passive. Thereby, we restrict the interactions between the users until the point of a possible reciprocal interaction taking place.^{[5](#page-151-2)} This selection of the sample will be later important for the validity of our identifcation strategy (see Section [3.4.2](#page-156-0) for details). We further shape our sample such that each observation represents a valid interaction accompanied by indicators of visible sender actions that have taken place within the particular interaction as well as the sender and recipient user IDs. This leaves us with an available sample consisting of 178'372 valid unique interactions for our analysis.

Lastly, to construct our fnal estimation sample, we merge the interaction sample with the user sample. As a result, each observation in our estimation sample represents a valid interaction between two users and consists of sender and recipient user IDs together with sender's actions from the interaction sample, and both the sender's as well as recipient's characteristics obtained from the user sample. Furthermore, as the data contains only heterosexual users based on a binary measure for gender, i.e. we never observe a sender and recipient of the same sex in our sample, we split the sample based on gender for a clearer interpretation of the results. Hence, we refer to the sample with only female recipients as

 3 Other empirical studies using online dating data focused on observation periods of similar length (see Hitsch et al., [2010a,](#page-171-0) and; Hitsch et al., [2010b\)](#page-171-12).

 4 This includes, for example, users with more than one single value for a mutually exclusive answer selection, among others. 5 For a more detailed definition of valid user interactions with practical examples, see Appendix [3.B.](#page-176-0)

the female sample, as here the females are in the role of an approached user upon receiving a visit action, and possibly further actions, by a male sender of an action. Analogously, we refer to the sample with only male recipients as the male sample, as in this case the males are in the role of an approached user upon receiving a visit action, and possibly further actions, by a female sender of an action.

Thus, we are left with 108'456 observations for the female sample and with 69'916 observations for the male sample. The corresponding descriptive statistics of selected variables for the two samples are listed in Appendix [3.A.](#page-173-0)

3.3.2.1 Sport Activity

In order to investigate the efect of sport in online dating, we leverage the rich information set regarding the sport activities on the user profle. In particular, each profle includes a detailed statement of the user's sport frequency. This information stems from the initial questionnaire flled by the user upon registration. First, the user is asked about the sport types done actively, namely: 'What sports do you do actively?', with multiple options (mutually inclusive) such as basketball, fitness, hiking, soccer, tennis, etc., or specifying the option 'none'. Second, only if the user has not specifed the option 'none', a further question regarding the particular sport frequency is asked: 'How often do you practice sport?'. The possible values (mutually exclusive) include the following answers: 'every day', 'several times a week', 'several times a month', or 'less common'. Thus, we not only observe the user's binary indication of practicing sport or not, i.e. the extensive margin, but also the particular sport frequency, i.e. the intensive margin. This provides us with a much fner measure of the actual sport activity. Accordingly, we define the sport activity measure to be multi-valued with sport frequencies of weekly, monthly, rarely and never. We omit the daily frequency for lack of data within this category, as previously mentioned. Furthermore, we leave the sport types out of consideration too, as these include many diferent and not mutually exclusive values, which prevents a clear separation of the categories.

Table [3.3.1](#page-153-0) shows the descriptive statistics for the sport frequency shares in the samples of males and females, respectively as well as the corresponding shares from the innovation sample of the German socioeconomic panel (SOEP-IS; Richter, Schupp, et al., [2015\)](#page-172-12) for a comparison with a representative population sample.[6](#page-152-0) First, we see that the sport frequency is unevenly distributed in both samples. Second, we can also observe that the shares are very similar in both samples. Nonetheless, the *never* category is more represented in the female sample, while the weekly category is more represented in the male sample. Additionally, we also observe that the subjective sport frequency of the users from the online dating platform is in general much higher than the one of the representative individuals from Germany.[7](#page-152-1) Third, with respect to the number of observations in the corresponding samples, we immediately see that even though we have a balanced user sample in terms of gender,^{[8](#page-152-2)} females get visited more often than males do.

⁶Similar values for the sport frequency statistics for Germany are documented also in the Eurobarometer Survey (Eurobarometer, [2014\)](#page-170-7), as pointed out by Steckenleiter and Lechner [\(2020\)](#page-172-6).

⁷Note, that this might be both due to truly higher sport frequency of the registered users as well as due to an overestimation of own actual sport frequency of the users, or the combination of both. Also note, that our sample consists only of singles, which is in contrast to the representative population sample.

⁸The user sample consists of 48% of females and 52% of males. For more descriptive statistics with regard to the user sample, see Appendix [3.A.](#page-173-0)

	<i>Never</i>	Rarely	Monthly	Weekly	Observations
Males	0.07	0.08	0.29	0.56	69'916
Females	0.12	0.09	0.29	0.49	108'456
SOEP-IS	0.33	0.23	0.10	0.34	25'544

Table 3.3.1: Shares of Sport Frequency for Male and Female Sample

Note: Color intensity represents the corresponding share sizes for males and females.

Finally, given our defnition, the impact of sport activity can be illustrated as follows. The user, here the sender, visits a profle of another user, here the recipient, and gets exposed to an information revealed on the profle. Among other indicators, the sender observes the recipient's indication of the sport frequency, i.e. the variable of interest. Based on the available information, the sender then decides to perform or not to perform a further action.

3.3.2.2 The Interaction between Users

We are interested in the one-way actions of a sender upon visiting a recipient's profle on the website. Even though there are multiple actions a sender can initiate, we focus explicitly on the action of sending a text message for several reasons. First, a text message is the most evident action of showing a serious interest, as in order to compose a text message, the sender has to exhibit a substantial efort, in comparison to other available options, such as simply sending a smile or like. Second, unlike the other generic options, by sending a text message, the sender directly approaches the recipient in an individualized manner. Third, an outcome measure of sending a text message or an email has been previously used in the online dating literature under the assumption that users send a message if and only if the potential utility of the match exceeds some minimum threshold value (compare e.g. Hitsch et al., [2010a;](#page-171-0) or Bruch, Feinberg, & Lee, [2016\)](#page-170-8). Hence, we defne our action of interest as a binary measure of sending (1) or not sending (0) a text message upon a profle visit. Given the binary scale, the natural interpretation as contact chances in terms of message probabilities arises.

Figure 3.3.1: Average Contact Chances according to Sport Activity for Males and Females

Figure [3.3.1](#page-153-1) shows the average message probability in percentages for males and females according to

the sport frequency. First, we see that the levels of females are substantially higher than those of males, i.e. women have unconditionally a higher probability to get messaged than men do. This is in line with previous evidence from studies based on online dating data (Bruch et al., [2016\)](#page-170-8). Second, we observe a slightly increasing message probability with higher sport frequency for males, while for females no clear pattern can be identifed.

3.3.2.3 Information about Users

In our sample, we have access to complete information flled by the user upon registration. Hence, we not only observe the condensed information displayed on the main user profle page, but also the expanded information stored in the background of the user profle. Thus, we efectively observe the very same information that a real user observes upon a profle visit of a potential partner, and even beyond. The full information observable to us includes the following components. First, we observe the user's demographic information such as gender, age, height, etc., the socio-demographic information such as education and income level, type of occupation, etc., as well as personal information such as place of residence, smoking habits, or even (self-judged) appearance. Second, in addition to the user specifc information, we observe the user's preferences for a potential partner in terms of the search criteria related to the above mentioned socio-demographic information as well. Third, we furthermore observe the user's information stemming from the detailed personality test, which refects on the user's life style, personality, attitudes and preferences. This includes an extensive information on topics like religion, political views, music and travel preferences, or even partner requirements. The aforementioned user information comprises of an exhaustive list of 663 variables in total. However, given the structure of our data, we include the user information both for the recipient as well as for the sender, resulting in efectively more than thousand variables. Apart from the information coming directly from the platform, we additionally generate a variable measuring the distance between the recipient and the sender, based on the available ZIP codes.^{[9](#page-154-0)}

We consider all the aforementioned variables as controls in the sense of potential confounders, i.e. as variables jointly infuencing both the recipient's sport activity as well as the recipient's potential outcome of receiving or not receiving a text message, and thus, de facto the sender's action to contact or not to contact the recipient. Conditioning on such a large-dimensional covariate space is a challenging estimation task. However, we refrain ourselves from an arbitrary selection of the confounding variables in order to reduce the dimension of the estimation problem. Rather, we apply a novel causal machine learning estimator, which can efectively deal with such large-dimensional setting, performing implicit variable selection in a fexible and data-driven way. The only variable deselection we perform manually is related to endogenous variables.^{[10](#page-154-1)} Thus, we remove all variables that could be potentially influenced by the sport frequency. These include mainly variables indicating the specifc sport type, but also variables describing sport-related choices such as holiday and leisure time preferences, as well as variables regarding the body type and clothing style. In total, we dismiss 38 endogenous variables. Lastly, we leave out 2 variables without any variation. As a result, we are left with 1247 covariates in total (1229 ordered, including dummies and 18 unordered), refecting the recipient and sender characteristics.

Apart from the confounding role, the covariates are useful for analysing the efect heterogeneity, too. For this purpose, we pre-specify a small subset of heterogeneity variables, consisting of age, income and education level on both recipient as well as sender side, together with the corresponding distance between the recipient and the sender. We focus on these heterogeneity variables for two main reasons. First, these

⁹The average distance between the recipient and the sender in our sample is 67.32 km. A detailed plot of the distribution of the distance between the users can be found in Appendix [3.A.](#page-173-0)

 10 We elaborate on this issue more closely when discussing the identifying assumptions in Section [3.4.2.](#page-156-0)

socio-demographic information are widely recognized in the literature as being the main determinants of the partner choice (for a review of the importance of selected socio-demographic characteristics see Hitsch et al., [2010a;](#page-171-0) and Eastwick et al., [2014\)](#page-170-2). Second, these are also the main variables that are most visible to the user on the profle summary and thus can potentially impact the shape of the efect. Additionally, we analyze the heterogeneous efects also along the sport frequency for the recipient as well as for the sender. Complementary to the pre-specifed subset of heterogeneity variables, the remaining variables might serve for a supplementary descriptive analysis of the efects.

3.4 Empirical Approach

To analyze the efect of sport activity on human mating, we leverage the recent advances in the causal machine learning literature. Below, we outline the parameters of interest together with the identifcation and estimation thereof.

3.4.1 Parameters of Interest

In order to defne the parameters of interest, we rely on the Rubin's [\(1974\)](#page-172-13) potential outcome framework. We denote the treatment variable of a user i by D_i , which in our case can take on four different integer values, i.e. $D_i \in \{0, 1, 2, 3\}$, corresponding to sport frequencies of never, rarely, monthly, and weekly, respectively. According to the treatment status, d , we define the potential outcomes for the user i by Y_i^d , which in this case is the action of receiving or not receiving a text message. However, we only observe the potential outcome under the treatment which the user i is associated with (see Holland, [1986,](#page-171-13) for a discussion of the fundamental problem of causal inference). Thus, the realized outcome can be defined through the observational rule as follows: $Y_i = \sum_{d=0}^{3} \mathbb{I}(D_i = d) \cdot Y_i^d$, which implies that we observe the action of receiving the text message only under a particular sport frequency of the recipient. Further, we denote the observed vector of covariates by X_i , which contains the recipient and sender characteristics, together with a subset of pre-specified heterogeneity variables Z_i , such that $Z_i \subset X_i$.

To analyze the efect of sport frequency on the message probability, we are interested in the following causal parameters. First, the Average Treatment Effect (ATE) of treatment $D_i = m$ compared to treatment $D_i = l$ is defined as

$$
ATE = \theta = \mathbb{E}[Y_i^m - Y_i^l]
$$

and constitutes the classical parameter of interest in microeconometrics, which provides us with an aggregated efect measure (compare e.g. Imbens & Wooldridge, [2009\)](#page-171-14). Second, the Group Average Treatment $Effect (GATE)$ is characterized as

$$
GATE = \theta(z) = \mathbb{E}[Y_i^m - Y_i^l \mid Z_i = z]
$$

and measures the differential effects along the heterogeneity variables Z_i . Thus, it provides us with a disaggregated efect measure according to the specifc variables of interest, as in our case is the age, income and education level, distance as well as the sport frequency itself. In the latter case, the GATE corresponds to the Average Treatment Efect on the Treated (ATET). Third, the Individualized Average Treatment Effect (IATE) is denoted as

$$
IATE = \theta(x) = \mathbb{E}[Y_i^m - Y_i^l \mid X_i = x]
$$

and describes the heterogeneous effects based on the full set of observed covariates X_i . As such, the

IATEs present the disaggregated efects on the fnest level of granularity and thus provide us with usertype specifc efects.

Notice, that both the treatment variable, i.e. the sport frequency, as well as the outcome variable, i.e. receiving a text message, are measured on the recipient side, and hence, also the above defned causal efects refer to the recipient.

3.4.2 Identifcation Strategy

Given our observational study design, it is not possible to only compare the unconditional message probabilities for diferent sport frequencies, as displayed in Figure [3.3.1,](#page-153-1) to infer the causal efects, since the user decision regarding the sport activity is not random. The level of sport frequency might be infuenced by other variables representing socio-demographic information, which might also infuence the potential outcome of receiving or not receiving a text message. For example, recipients with a higher level of education might have a higher probability of doing sport on a weekly basis, as well as a higher probability of getting messaged. This phenomenon is known as selection bias (Imbens & Wooldridge, [2009\)](#page-171-14). In order to disentangle the causal efect from the selection efect, we need to eliminate such confounding via credible identifcation strategy.

For the identifcation of the aforementioned parameters of interest in a multiple treatment case, we rely on the so-called *selection-on-observables* strategy (see Imbens, [2000;](#page-171-15) or Lechner, [2001\)](#page-171-16). Such identifcation approach assumes that all confounding variables jointly infuencing both the treatment as well as the potential outcomes are observed, and thus, can be conditioned on. Given our rich data on user characteristics and the unique research design, we argue to capture all possible confounding efects for two main reasons. First, for both the recipient and the sender, we observe socio-demographic (e.g., age, education, income) and personal (e.g., family status, smoking habits, place of residence) characteristics, together with the preferences for a potential partner as well as the answers given in a detailed personality test. Thereby we have access to even richer personal information than the actual users when browsing the profles, and as such, we are able to control for confounding efects stemming from the user's characteristics. Second, given our research design, focusing only on the very frst one-way interactions between the recipient and the sender, we efectively eliminate any possible unobserved efects coming from the reciprocal interaction between the users such as sympathy or kindness. By doing so, we explicitly focus only on situations, in which the recipient's profle gets visited by a sender, upon which the recipient does receive or does not receive the very frst text message from the sender, without any visible encouragement to do so from the recipient her/him-self. In such a situation, the sender decides solely based on the information visible on the recipient's profle to send or not to send the message. Within our research design, we observe exactly the same information, and even beyond, as the actual sender when facing the decision of sending the frst text message. For this reason, we are also able to control for confounding efects stemming from the user's interaction.

Taken together, combining the highly-detailed user information, which exceeds the information directly observable by the actual users, with the unique research design, which eliminates any possible unobservable information, we are confdent to capture all confounding efects. In particular, our selectionon-observables strategy relies on the following set of identifcation assumptions.

First, the so-called conditional independence assumption (CIA), states that the potential outcomes and the treatment are independent once conditioned on the covariates. This hinges on the availability of all covariates that jointly infuence the potential outcome and the treatment. As we argue, we observe sufficiently rich information on both the recipient as well as the sender side to ensure the plausibility

of the CIA. In addition, our research design eliminates any further infuence from a possible reciprocal interaction between the users. Thus, we are confdent about the validity of the CIA in this particular case. There are only two potential sources of vulnerability of the CIA in this case. First, it could be caused by the availability of the blurred photo of the user. Even though the photo remains blurred, as we do not allow interactions between the users which would include the action to release the photo, we cannot rule out that information such as the shape of the face or the hair and skin colour could be, nonetheless, inferred. However, despite the information inferred from the blurred photo might possibly afect the outcome, i.e. the message probability of the recipient, we argue that this information should not have an efect on the treatment itself, i.e. the recipient's sport frequency. Thus, it arguably does not qualify as a potential confounder. Nevertheless, limitations in the availability of profle pictures, respectively opportunities to represent the information in profle pictures, are common in the literature on online dating (Fiore, Taylor, Mendelsohn, & Hearst, [2008\)](#page-170-9). Second, it could be caused by the availability of the matching score. However, despite the fact, that we do not observe the score directly, we know that we observe, and indeed condition on, all information which serves for its calculation. Moreover, even though we do not know the exact formula, by using a very fexible estimation approach, we are able to reproduce any arbitrary functional form of the matching score. Nonetheless, if the matching score would consist of the user's sport frequency, the treatment would be indirectly observed as a part of the shortlist of potential partners even before actually visiting the user profle. However, this would not violate the CIA as such, it could rather potentially reduce the size of our efect estimates. For this reason, we conduct a placebo test to provide evidence that this is indeed not the case. We discuss the placebo test in more detail in Section [3.5.3.](#page-165-0)

Second, the *common support* assumption, ensures that for each value in the support of the covariates, there is a possibility to observe all treatments. This means that we fnd users with the same age, education, income, etc., for all sport frequency levels. Thus, we are able to check the validity of the common support assumption in the data directly, but do not fnd any violations thereof (see Lechner & Strittmatter, [2019,](#page-171-17) for a discussion of common support issues).

Third, the *stable unit treatment value* assumption (see e.g. Rubin, [1991\)](#page-172-14), implies that for each user we observe only one of the potential outcomes based on the treatment status. It further implies that there is no interference among users, hence ruling out any general equilibrium or spillover efects. This means that the sport frequency of one particular user does not afect the message probability of other users. We argue that the SUTVA is plausible in this case, as we analyze only a short time period after the user registration such that general equilibrium or learning efects would not yet emerge.

Fourth, the *exogeneity of confounders* assumptions, indicates that the values of the covariates are not infuenced by the treatment. In other words, the user characteristics should not be impacted by the sport frequency. For this reason, we discard all potentially endogenous variables such as indicators of particular sport type, sporty clothing style, preferences for sport holidays or sport club memberships. Therefore, we are confdent that the exogeneity assumption holds.

Under the aforementioned assumptions, it can be shown that the above parameters of interest are identifed. For technical details, see Lechner [\(2018\)](#page-171-1).

3.4.3 Estimation Method

In our analysis, we face two major challenges with regard to the estimation of the causal efects of interest. First, we need to deal with a very large conditioning set with an unknown functional form of the covariates. Second, we want to investigate potential efect heterogeneity. In order to overcome these

challenges, we take advantage of the newly developing causal machine learning literature (see Athey, [2018;](#page-170-10) Athey & Imbens, [2019;](#page-170-11) or Knaus, Lechner, & Strittmatter, [2021,](#page-171-18) for overviews). It combines the fexibility and prediction power of machine learning (Hastie, Tibshirani, & Friedman, [2009\)](#page-171-19) with the causal inference from econometrics (Imbens & Wooldridge, [2009\)](#page-171-14). One of the most popular machine learning methods are the so-called regression trees (Breiman, Friedman, Olshen, & Stone, [1984\)](#page-170-12) and random forests (Breiman, [2001\)](#page-170-13). The trees and forests are highly fexible, local nonparametric prediction methods, which can efectively deal with large-dimensional settings (Biau & Scornet, [2016\)](#page-170-14). Adapting these prediction algorithms towards causal inference has lead to developments of Causal Trees (Athey & Imbens, [2016\)](#page-170-15) and Causal Forests (Wager & Athey, [2018\)](#page-172-15), respectively. These methods inherit the advantages of the prediction versions, while fexibly estimating the causal efects with systematically uncovering their heterogeneity. Furthermore, Lechner [\(2018\)](#page-171-1) extends the Causal Forest for the multiple treatment case, and additionally improves the splitting rule to account for selection bias and for the mean correlated error. The resulting Modifed Causal Forest also allows for estimation as well as inference for the parameters of interest at all aggregation levels in one estimation step. Since our application involves multiple treatments with potential confounding, while analyzing various heterogeneity levels of the causal efects, we opt for the latter approach.

In our analysis, we rely on estimating the so-called 'honest' forest, which has been shown to lower the bias of the causal efect estimates and to enable valid statistical inference (Wager & Athey, [2018,](#page-172-15) and; Lechner, [2018\)](#page-171-1). As such, we randomly split the estimation sample in two equally sized parts and use one sample, i.e. the *training* sample, to build the Modified Causal Forest and the other sample, i.e. the *honest* sample, to estimate the causal effects.^{[11](#page-158-0)} Then, the estimation procedure of the Modified Causal Forest can be described as follows. First, the estimator draws a random subsample s of the training sample and subsequently estimates a single causal tree. As such, the subsample gets recursively splitted into smaller subsets, the so-called 'leaves' of the tree $L(x)$. The partitioning follows a splitting rule which removes selection bias and reveals efect heterogeneity. As a result, the observations are homogeneous with regard to the covariate values within the leaf, while being heterogeneous *across* the leaves. Then, the treatment efect is estimated within each terminal leaf by simply subtracting the mean outcomes of the respective treatment levels $D_i = m$ and $D_i = l$ from the honest sample as

$$
\hat{\theta}_s(x) = \frac{1}{\{i : D_i = m, X_i \in L(x)\}} \sum_{\{i : D_i = m, X_i \in L(x)\}} Y_i - \frac{1}{\{i : D_i = l, X_i \in L(x)\}} \sum_{\{i : D_i = l, X_i \in L(x)\}} Y_i.
$$

Second, as a single tree might be quite unstable due to its path-dependent nature, the forest estimates many such trees by drawing S random subsamples in total. The Causal Forest estimate is then given by the ensemble of many causal trees as

$$
\widehat{IATE} = \hat{\theta}(x) = \frac{1}{S} \sum_{s=1}^{S} \hat{\theta}_s(x).
$$

The additional averaging of the trees helps to reduce the variance and to smooth the edges of the leaves (Bühlmann & Yu, [2002\)](#page-170-16). Conceptionally, the Causal Forest can be thought of as a nearest neighbor matching estimator with an adaptive neighbor choice and can be thus described using a weighted representation, too (Wager & Athey, [2018;](#page-172-15) Athey, Tibshirani, & Wager, [2019\)](#page-170-17).

Third, the Modifed Causal Forest estimates the GATEs by averaging the IATEs in the corresponding

 11 Lechner [\(2018\)](#page-171-1) shows in a simulation study that the efficiency loss of the 'honest' forest due to sample-splitting is minimal in comparison to the case of 'honest' trees as in Wager and Athey [\(2018\)](#page-172-15).

subsets defined by the heterogeneity variables Z_i and the ATE by averaging the IATEs in the whole sample as follows

$$
\widehat{GATE} = \hat{\theta}(z) = \frac{1}{\{i: Z_i = z\}} \sum_{\{i: Z_i = z\}} \hat{\theta}(X_i)
$$

and

$$
\widehat{ATE} = \widehat{\theta} = \frac{1}{N} \sum_{i=1}^{N} \widehat{\theta}(X_i).
$$

Thus, it provides a computationally attractive option to estimate the efects of interest on all desired levels of heterogeneity without the need for re-estimating the whole forest for each single aggregation $level.¹²$ $level.¹²$ $level.¹²$

Fourth, the Modifed Causal Forest then explicitly uses the weighted representation of the estimated efects for inference. The weight-based inference can be then conveniently applied to all aggregation levels as well.[13](#page-159-2) For an in-depth discussion of the Modifed Causal Forest, see Lechner [\(2018\)](#page-171-1) as well as Cockx, Lechner, and Bollens [\(2019\)](#page-170-18) and Hodler, Lechner, and Raschky [\(2020\)](#page-171-20) for empirical applications.

Estimating the efects of sport frequency on the message probability by applying causal machine learning allows us to improve on previous empirical studies in an online dating setting in several dimensions. First of all, we do not have to specify the exact functional relationship between outcome, treatment and covariates, as in the case of using parametric approaches such as the logistic regression (see e.g. Hitsch et al., [2010a;](#page-171-0) Hitsch et al., [2010b;](#page-171-12) or Bruch et al., [2016\)](#page-170-8). This is particularly important when dealing with a large-dimensional covariate space, including the characteristics of both the recipient and the sender, as the functional form of the interactions thereof is not a priori clear. Furthermore, using causal machine learning also advances the semiparametric approaches used in online dating studies (see e.g. Lee, [2016,](#page-171-21) for a matching estimation), thanks to more fexible adaptive estimation and its implicit variable selection properties. Lastly, causal machine learning allows us to go beyond the average efects and systematically investigate the efect heterogeneity on various aggregation levels, without the need to specify interactions or to build subsets of data in an *ad-hoc* fashion.

3.5 Results

Below, we present the results for the average and heterogeneous efects of sport activity on contact chances, based on the Modifed Causal Forest estimation.

3.5.1 Average Efects

The results for the average efects of the sport activity on the contact chances are summarized in Table [3.5.1.](#page-160-0) The diagonal presents the potential outcomes, while the corresponding efects are depicted in the lower triangle.

In case of the male sample, for increasing sport frequency, the results show a clear and increasing pattern of the potential outcomes, i.e. of the potential message probability. While the potential message

 12 In our setting, we additionally apply treatment sampling probability weights for the ATE and GATEs aggregation of the IATEs to account for the unbalanced treatment shares.

 13 Athey et al. [\(2019\)](#page-170-17) further suggest usage of the forest weights for solving many different econometric estimation problems.

probability for users who never practice sport is on average only 2.50%, for users doing sport on a weekly basis, the chances to get messaged increase by more than 50% and amount to 3.82%. Comparing the respective potential outcomes across the sport frequency levels yields the corresponding causal efects measured in percentage points. Accordingly, all efects for all sport frequency comparisons are positive. The most sizeable and the most precise efects are estimated for the most distinct sport frequencies, as one would intuitively expect. Thus, the average efect of a weekly sport activity versus no sport activity at all, is equal to an 1.32 percentage points increase. Similarly, the average efect of a weekly in comparison to only rare sport activity amounts to an 1.20 percentage point increase. Moreover, these efects are both substantively as well as statistically relevant. As such, a male user increasing his sport activity from no sport or only rare sport activity to doing sport on a weekly basis signifcantly increases the probability of getting messaged by 52.80% and 45.80%, respectively. In practice, this implies receiving 13, respectively, 12 extra messages out of 1000 profle visits. Hence, the contact chances of a male user can be substantially increased solely by becoming more sporty. The remaining efects comparing less distinct sport frequencies lack the statistical relevance, which stems mainly from the substantially lower number of observations for these categories (see Table [3.3.1\)](#page-153-0).

Regarding the female sample, the results do not suggest increasing contact chances with increasing frequency of sport activity, as in the case of the male sample. The potential outcomes thus do not indicate any clear pattern as the message probability frstly drops, when switching from no sport to rare sport activity, and then increases steadily throughout the monthly and weekly sport frequencies, reaching comparable levels with the category of never doing sport. Accordingly, the estimated average efects do not show any explicit structure and lack statistical relevance. The only exception is the precise estimate of the efect of the weekly vs. rare sport activity, with a sizeable increase of an 1.61 percentage points, yet this represents only a minor relative increase of 17.18% in comparison to the efects seen in the male sample. Taken together, based on the overall results, no substantial conclusions can be drawn.

Table 3.5.1: Average Efects of Sport Activity on the Contact Chances for Males and Females

Note: Effects in % points. Potential outcomes on the diagonal. Standard errors in parentheses. Significance levels refer to: ∗∗∗ < 0.01, ∗∗ < 0.05, [∗] < 0.1. Color intensity represents the corresponding level sizes.

In general, based on the results of the average efects, we fnd sizeable and signifcant positive efects of a more frequent sport activity, when analyzing the male users, while we fnd only weak evidence for such efects for the case of female users. It means that for men a higher sport frequency substantially increases the probability of getting messaged by a woman, on average. However, higher sport frequency for women does not seem to consistently lead on average to considerably higher chances of getting messaged by a man.

3.5.2 Heterogeneous Efects

While the average effects provide a general measure for the causal effects of sport activity, a more detailed description of the efect heterogeneity beyond gender, remains unknown. Therefore, we study the heterogeneous efects in respect to the pre-defned set of variables of interest, i.e. the group average treatment efects (GATEs), to uncover possibly diferential efects of the sport activity on the contact chances. For the sake of clarity, we focus on the efects comparing the most distinct cases, namely the weekly sport frequency with no sport activity. In this regard, we analyze the efect heterogeneity along age, education and income of the users, on both the recipient as well as the sender side, together with the mutual user distance, based on the following considerations. First, these variables have been previously identifed as the main determinants of the partner choice (Hitsch et al., [2010a;](#page-171-0) Eastwick et al., [2014\)](#page-170-2) and second, these are also the variables which appear on the main profle summary. Thus, we expect these variables to have a higher potential to infuence the shape of the efect of the sport activity. Lastly, we investigate the efect heterogeneity based on the particular recipient's as well as sender's sport frequency, which is a natural choice as it corresponds to the efect on the treated, a classical microeconometric parameter of interest (compare e.g. Abadie & Cattaneo, [2018\)](#page-170-19). Essentially, the heterogeneity analysis enables us to investigate if the benefts of the regular sport activity in terms of higher contact chances vary among specifc groups of users. Thus, we shed light on the open questions such as if potentially the users with higher age, or with lower education and income level enjoy higher benefts of weekly sport activity than those with lower age, or with higher education and income level, or vice versa.

In order to test for the presence of heterogeneity along the variables of interest, we conduct the Wald test of equality of the estimated GATEs. Additionally, we conduct t -tests for differences of the estimated GATEs from the average efect. Rejection of both tests thus gives support for the existence of heterogeneity with respect to the particular variable.^{[14](#page-161-0)}

The results of the Wald test suggest heterogeneous efects with regard to the income level for males, both for the recipient as well as the corresponding sender, however, no evidence of heterogeneity in case of females. Furthermore, the heterogeneous efects for males are statistically diferent from the average efect as well, indicating an explicit pattern, while none of this is the case for females. The respective income level GATE estimates are depicted in Figure [3.5.1](#page-162-0) for the recipient and the sender in the male sample. The corresponding results for the female sample are presented in Figure [3.C.1](#page-179-0) in Appendix [3.C.](#page-176-1)

Concerning the male sample, we observe a clear increasing trend of the GATEs for increasing levels of income. As such, for a male recipient, the efect of weekly sport activity in contrast to no sport is greater, the higher the income level of the male recipient himself, and the higher the income level of the female sender, too. As a result, male users with a higher income level, beneft from a regular sport activity on a weekly basis in comparison to no sport, more than male users with a lower income level. This implies that particularly the wealthy males, who earn more than 100'000 EUR in a year, can increase their contact chances the most by practicing sport on a weekly basis. In a similar vein, male users having a potential female partner with high income level, beneft from the higher sport frequency more than the male users, which have a potential female partner with low income level. This pattern suggests also that more wealthy female users value the regular sport activity of a male user more. In addition, not only are these heterogeneous efects statistically relevant, the substantive relevance is documented, too, as the efect sizes are relatively large. As such, the magnitudes of the income level GATEs are ranging from 1.06% points to 1.46% points with respect to the income level of a male recipient, and similarly, from 1.15% points to 1.47% points with respect to the income level of a female sender, in reference to the

 14 Detailed results of the Wald test for equality of the GATEs as well as the tests for differences from the ATE are listed in Appendix [3.C.](#page-176-1)

average efect of 1.32% points. This implies an increase in the message probability of at least 42.40% for the low income users, up to an increase of 58.80% for the high income users, respectively. This results in a 16.40% diference in message probability solely due to the user's income. A simple back of the envelope calculation reveals this diference in income levels to amount to 4 extra messages out of 1000 profle visits.

Figure 3.5.1: Heterogeneous Efects of Sport Activity based on Income for Males

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.

As opposed to the male sample, we do not fnd such evidence of heterogeneity, if we switch the roles of the recipient and the sender (see Figure [3.C.1](#page-179-0) in Appendix [3.C\)](#page-176-1). As such, even though we observe a similar increasing pattern for female recipients associated with male senders, the estimated efects lack statistical relevance.

However, in contrast to the results for income heterogeneity, we fnd supportive evidence for heterogeneity for females in terms of the sport activity, while no such evidence is detected for males. As such, for females, both the Wald test of efect equality as well as the t-tests for diferences from the average efect suggest presence of heterogeneity with respect to the level of sport frequency of the male sender with a clear increasing pattern, whilst the heterogeneity with respect to the female recipient lacks the statistical precision. Contrarily, for the male sample, even though we observe a similar increasing pattern as for the female sample, the statistical relevance is, however, absent. The corresponding results for the female sample regarding the sport frequency GATE estimates are presented in Figure [3.5.2](#page-163-0) for both the female recipient and the male sender. The respective results for the male sample are depicted in Figure [3.C.2](#page-179-1) in Appendix [3.C.](#page-176-1)

The heterogeneity results with respect to the sport frequency suggest that for a female user, the efect of a weekly sport activity in contrast to no sport is greater, the higher the sport frequency of the potential male partner. Thus, females enjoy a higher efect of their own weekly sport activity, if the sport activity of a potential male partner is on a weekly basis as well. This further suggests that sporty male users appreciate sporty female users more. Nevertheless, despite the clear statistical pattern of the heterogeneity itself, in this case the overall substantive implications remain rather limited as the efect sizes are only moderate, ranging from 0.08% points to 0.41% points, given the average effect of 0.31% points. Additionally, neither for the average efect nor for the respective group efects the presence of an actual null efect can be ruled out.

Figure 3.5.2: Heterogeneous Efects of Sport Activity based on Sport for Females

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.

Further results of the Wald tests regarding the remaining heterogeneity variables do not indicate differential efects at conventional signifcance levels in terms of age or the mutual user distance, concerning both males as well as females. Neither do the diferences of the estimated GATEs from the ATE support the evidence for heterogeneous efects. Furthermore, although the Wald test of equality of GATEs based on the education level suggests presence of efect heterogeneity, the diferences from the average efect are not statistically relevant and lack an explicit pattern.^{[15](#page-163-1)}

Altogether, based on the GATEs analysis, we conclude to fnd a supporting evidence, both statistical as well as substantive, for heterogeneity in terms of the income level for males and statistical, however, not substantive evidence, in terms of the sport frequency for females, whereas, we fnd lack of evidence in general, for heterogeneous efects along the age, distance and education level for both males and females.

Additionally, in order to gain more insight for the efect heterogeneity, we analyze the efects on the fnest level possible and study the underlying individualized average treatment efects. Figure [3.5.3](#page-164-0) provides the distribution of the IATEs for the weekly vs. never comparison, for both the male as well as the female sample, respectively. In both cases, we observe that there is indeed substantial heterogeneity in the considered efects as the efect distributions are noticeably spread out around the mean, i.e. the realized ATE.[16](#page-163-2) Additionally, we see that for males, virtually all efects are positive, while for females, about half of the efects are positive and half are negative. This further substantiates the fndings on the aggregated levels in terms of the GATEs and the ATE.

 15 The exhaustive results for the effect heterogeneity analysis can be found in Appendix [3.C.](#page-176-1)

¹⁶Part of the observed variability is also due to estimation uncertainty: the average standard error for the IATEs is 0.61 for the male and 1.06 for the female sample, respectively.

Figure 3.5.3: Distribution of the Individualized Efects of Sport Activity for Males and Females

Note: Distribution of IATEs smoothed with the Epanechnikov kernel using the Silverman's bandwidth.

To understand these efect distributions more thoroughly, we apply the k-means++ clustering (Arthur & Vassilvitskii, [2007\)](#page-170-20) to provide further descriptive evidence of the dependence of the efects on the heterogeneity variables (see Cockx et al., [2019,](#page-170-18) for an analogous approach). For this purpose, we perform the clustering by using the IATEs for the weekly vs. never comparison to form distinct clusters, which we sort increasingly according to the mean efect size. We then describe the clusters by the means of the corresponding heterogeneity variables, which however, have not been used to form the clusters. Table [3.5.2](#page-165-1) presents the clusters for the IATEs of the male and female sample, respectively.

In general, the clustering reveals consistent patterns with the heterogeneity analysis based on the GATEs. For the male sample, the increasing efects of the sport frequency along the clusters are associated with an increasing level of income on both the recipient as well as the sender side. As such, the lowest efects of sport are clearly for the users with the lowest income level, and vice-versa, the highest efects are evidently for those users with the highest income level. Complementary to the GATEs analysis, the clustering additionally reveals similar increasing patterns in terms of education level and the sport frequency for males. This indicates a further positive relationship, which, however, lacks statistical relevance within the GATEs analysis. Nonetheless, the clustering does not fnd any particularly clear patterns in terms of age or mutual distance, which is consistent with the GATE estimates.

In case of the female sample, complementary to the GATEs, the clusters suggest an increasing efect for higher sport frequency as documented within the GATEs analysis. However, according to the cluster analysis, this holds true not only for the sender, but also for the recipient side, for which the statistical evidence in terms of the GATEs is missing. In a similar vein, the clusters also suggest a relevant heterogeneity with respect to the income level with an increasing pattern. Furthermore, as for the male clusters, also the female clusters suggest additionally a positive association of the IATEs with the education level, however, no apparent indication of heterogeneity for age or mutual distance.

In addition to the GATE analysis, the clusters further allow for a more detailed description of the IATEs based on the user characteristics, beyond the pre-specifed subset of heterogeneity variables. Notably, the cluster analysis reveals a particular relationship between the IATEs and the behavior and preferences of the users, both for males and females. As such, higher IATEs are associated with increasing preference to fnd the signifcant other and to have an intimate relationship, as well as with increasing satisfaction of own appearance. In contrast, lower IATEs are associated with increasing smoking frequency, as well as increasing preference for media consumption and comfortable dining. These insights provide not only a better understanding of the specifc individualized efects of sport activity on the contact chances, but might serve as a basis and guidance for a selection of relevant heterogeneity variables in future research. An overview of the relevant clusters with variable description is provided in Table [3.C.3](#page-182-0) in Appendix [3.C.](#page-176-1)

	Males					Females					
Clusters	1	$\boldsymbol{2}$	3	$\overline{4}$	5		$\mathbf{1}$	$\overline{2}$	3	$\overline{4}$	5
IATEs: Weekly vs. Never	0.41	0.88	1.22	1.52	1.85		-1.41	-0.52	0.12	0.71	1.38
Recipient Features											
Age	45.77	45.19	44.57	43.80	43.71		33.53	37.07	38.39	38.15	36.90
Education Level	3.51	3.86	4.24	4.58	4.76		3.65	3.74	3.80	3.93	4.05
Income Level	3.69	3.98	4.26	4.57	4.83		2.98	3.16	3.32	3.46	3.53
Sport Frequency	1.85	2.16	2.37	2.46	2.49		1.55	1.92	2.15	2.34	2.43
Sender Features											
Age	43.94	43.09	42.37	41.53	41.43		36.33	40.15	41.68	41.46	40.23
Education Level	3.46	3.69	3.96	4.16	4.34		3.74	3.82	3.93	4.06	4.25
Income Level	2.94	3.25	3.52	3.79	4.07		3.51	3.82	3.99	4.10	4.14
Sport Frequency	1.86	2.03	2.16	2.24	2.32		1.91	2.06	2.15	2.27	2.44
Shared Features											
Distance	70.39	71.65	70.23	70.16	64.91		64.43	66.22	67.10	66.36	62.97
<i>Observations</i>											
Share	0.07	0.18	0.29	0.31	0.15		0.07	0.20	0.29	0.29	0.15
Total	2288	6439	10153	10826	5252		3753	11048	15896	15484	8047

Table 3.5.2: Clusters of the Individualized Efects of Sport Activity for Males and Females

Note: Means of clustered efects sorted in an increasing order, matched with the heterogeneity variables. Color intensity represents the corresponding efect sizes and highlights the relevant GATEs.

Overall, the cluster analysis of the IATEs emphasizes the results from the GATEs, and as such provides additional evidence for the income heterogeneity for males, as well as the sport heterogeneity for females. Moreover, it reveals further descriptive evidence for increasing efects based on education level, albeit no particular heterogeneity patterns for age or mutual distance. Lastly, it provides valuable insights for additional heterogeneity channels such as relationship preferences.

3.5.3 Placebo Test

In our analysis of the efect of sport activity on contact chances, we assume that the treatment, i.e. the sport frequency is observed once a profle of a recipient has been visited by a sender. However, as discussed in Section [3.4.2,](#page-156-0) the sport frequency might potentially be entailed in the matching score, which is observable already before the actual profle visit as part of the shortlist of potential partners suggested by the online dating platform. If that would be the case, the sport frequency could potentially indirectly infuence already the decision to visit the profle, and not only the decision to send a text message after a profle visit. However, even under such circumstances, this would not violate the CIA per se, but rather reduce the size of the estimated efect, which could be then interpreted as a lower bound of the true underlying efect. In order to examine if such mechanism takes place in our setting, we conduct a placebo test inspired by Imbens and Wooldridge [\(2009\)](#page-171-14) to assess the validity of the CIA by testing for a zero efect

on an outcome variable assumed to be unafected by the treatment, here the decision to visit the user profle. Accordingly, we redo our main analysis, while swapping the message outcome for a visit outcome. Thus, we estimate the average treatment efects of sport frequency on the visit probability, given the same conditioning set. Therefore, if the sport frequency is, as assumed, not part of the matching score, its efect on the probability to visit a user profle should be equal to zero.

In order to implement such placebo test, we frst need to impute the 'potential' visits, as by construction, we only observe the realized visits. For a given user, we consider all registered user profles with opposite sex and within a specified distance radius as potential visits.^{[17](#page-166-0)} We end up with a sample consisting of 38'552'821 observations, out of which 178'372 represent the actual realized and the rest the imputed potential visits. Analogously as in the main analysis, we split the sample into a male and a female sample. Furthermore, due to the computational feasibility and general consistency of the analysis, we randomly draw an identically sized male and female sample as in the main estimation, such that we replicate the corresponding sport frequency shares, too.[18](#page-166-1) A similar approach to impute the potential visits has been used also in previous studies focusing on online dating platforms (Bruch et al., [2016\)](#page-170-8).

Table 3.5.3: Average Efects of Sport Activity on the Visit Chances for Males and Females

Note: Effects in % points. Potential outcomes on the diagonal. Standard errors in parentheses. Significance levels refer to: *** < 0.01 , ** < 0.05 , * < 0.1 . Color intensity represents the corresponding level sizes.

Table [3.5.3](#page-166-2) summarizes the ATE results of the Modifed Causal Forest estimation for the placebo test. First of all, we observe that the potential outcomes for both males and females do not exhibit any particular upward or downward trend as is the case for the main analysis. Furthermore, for neither the male nor the female sample, we fnd evidence for statistically relevant efects. Moreover, the efect sizes and the levels of potential outcomes are an order of magnitude lower than our main results, being efectively zero in terms of the substantive relevance. Even though the results of such placebo tests do not completely rule out the possibility of a presence of an efect on the visit probability, they provide a supportive evidence that this is, indeed, not the case. Hence, we conclude that our main analysis estimates the full causal efects of sport activity on the contact chances, rather than only lower bounds thereof.

 17 We restrict the potential visits to opposite sex as we observe only heterosexual users in our sample. Furthermore, we restrict the distance of potential users due to dimensionality concerns, as the share of the realized visits would otherwise be almost completely diminished, if unrestricted. Here, we remain rather conservative and set the potential distance to 95% of the maximum observed distance of an actual realized visit.

 18 We repeated the random draw several times, while the results remained qualitatively robust.

3.6 Discussion

The main objective of this paper was to analyze the efect of sport activity on human mating. Following this objective, we examined the efect of sport frequency on contact chances based on a unique dataset from an online dating platform and applying the Modifed Causal Forest estimator (Lechner, [2018\)](#page-171-1). We found that for male users, doing sport on a weekly basis increases the probability to receive a frst message by more than 50% relatively to not doing sport at all, while for female users, we do not fnd evidence for such an efect. In addition, we uncover important efect heterogeneities. In particular, the efect of sport frequency on contact chances increases with higher income for male, but not for female, users.

This paper ofers notable implications for research and practice. First, this study contributes to the literature on human mating. In particular, we demonstrate that sport activity, as an essential behavioral trait and pivotal information on online dating platforms, enfolds a causal efect on contact chances. In turn, this paper overcomes limitations of previous work that did not consider or comprehensively map the efect of sport activity on human mating. Moreover, this paper expands previous work on the efects of sport activity by demonstrating that sport activity does not only afect physical/mental health and social and economic conditions, as well-documented by prior research (Strong et al., [2005;](#page-172-3) Lechner, [2009\)](#page-171-7), but also one of the most decisive spheres of human existence, that is human mating.

Second, this paper advances empirical approaches for assessing causal efects in large-dimensional data environments, as applicable, for example, to remote-sensing data. In particular, this research applies a very fexible estimation procedure, which ofers not only greater fexibility in considering (interrelated efects of) covariates, but also a systematic analysis of the underlying heterogeneities of the efects on diferent levels of aggregation (Lechner, [2018\)](#page-171-1). Thus, this paper may support future research in analyzing human behavior in large-dimensional data environments. However, even though the causal machine learning approach is capable of detecting statistically relevant heterogeneities, it is crucial to assess also its substantive relevance. Following this notion, the efect heterogeneities in this research provide diferent perspectives on practical implications. In particular, the increasing efect of sport activity on contact chances with higher income for male users is both statistically justifed as well as substantially relevant, leading to the above mentioned implication. Contrarily, potential implications, resulting from the observation that the efect of sport frequency on contact chances increases with higher sport frequency for females, are limited as the particular evidence in our setting is not substantially relevant, even though it is statistical justifed. In addition to the main heterogeneity analysis, the post-estimation descriptive cluster analysis of the most disaggregated efects provides additional insights for possible heterogeneity channels, such as the education level or relationship preferences of the users.

Third, this study may support individuals to increase their chances of fnding a mate on online dating platforms by demonstrating if and to what extent sport activity contributes to the likelihood to be recognized. In particular, men may beneft from the insights of this research by being aware that sport on a weekly basis relative to no sport can increase their probability to receive a first message by more than 50%, or even up to 60% in case of higher income individuals, while for women the efect of sport activity on the contact chances is not entirely evident. Thus, this study may incentivise individuals to increase the level of sport activity, not only because of the well-documented efects on, for example, health (Penedo & Dahn, [2005\)](#page-171-3), but also for their chances of finding a mate.

Moreover, from a public health perspective, this paper provides empirical reasoning for justifying and evaluating incentives for public health promotion due to the impact of sport activities for human partnering, family planning, and reproduction.

Finally, this paper may serve practitioners, namely product developers and software engineers, as a foundation to improve the architecture of online dating platforms, including interface designs and matching algorithms. In particular, this study points out the relevance of sport activity for mate evaluation and selection patterns, while considering efect heterogeneities based on established socio-demographic characteristics at the same time. In turn, this research may help practitioners to assess humans' mate evaluation and selection in much more detail and, correspondingly, to evaluate improvements of the architecture of online dating platforms (e.g., customized weighting of sport activity in matching algorithms or specifc placement of information on sport activity on individual profle pages). In a similar vein, the insights of this research are applicable to engineer architectures of other platforms with a likewise high degree of interpersonal computer-mediated interaction, for example, social networks.

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Appendix

3.A Descriptive Statistics

	Mean	SD	Min	Max
Sport Frequency				
Never	0.13	0.34	0.00	1.00
Rarely	0.10	0.31	0.00	1.00
Monthly	0.29	0.45	0.00	1.00
Weekly	0.48	0.50	0.00	1.00
Demographic Features				
Gender $(=1$ if female)	0.48	0.50	0.00	1.00
Age (in years)	40.05	11.41	18.00	82.00
Income Level				
Lowest	0.12	0.32	0.00	1.00
Low	0.16	0.37	0.00	1.00
Medium	0.20	0.40	0.00	1.00
High	0.24	0.43	0.00	1.00
Highest	0.22	0.42	0.00	1.00
$Highest+$	0.06	0.24	0.00	1.00
Education Level				
Lowest	0.00	0.06	0.00	1.00
Low	0.08	0.27	0.00	1.00
Medium	0.37	0.48	0.00	1.00
High	0.16	0.37	0.00	1.00
Highest	0.39	0.49	0.00	1.00

Table 3.A.1: Descriptive Statistics for the User Sample

Note: Main variables describing the population displayed.

Figure 3.A.1: Distribution of the Distance between Users

	Never	Rarely	Monthly	Weekly	Total
Outcome					
First Message	0.11	0.10	0.10	0.11	0.11
Recipient Features					
Age	35.49	37.65	37.84	37.83	37.53
Income Level					
Lowest	0.20	0.20	0.10	0.07	0.10
Low	0.28	0.23	0.19	0.14	0.18
Medium	0.28	0.25	0.23	0.22	0.23
High	0.17	0.21	0.27	0.33	0.28
Highest	0.05	0.11	0.18	0.21	0.18
Highest+	0.01	0.01	0.03	0.04	0.03
Education Level					
Lowest	0.00	0.00	0.00	0.00	0.00
Low	0.08	0.06	0.02	0.02	0.03
Medium	0.61	0.52	0.41	0.36	0.42
High	0.20	0.21	0.21	0.22	0.21
Highest	0.11	0.21	0.35	0.41	0.33
Sender Features					
Age	38.57	40.80	41.11	41.07	40.75
Income Level					
Lowest	0.09	0.07	0.05	0.04	0.05
Low	0.16	0.13	0.09	0.07	0.09
Medium	0.23	0.21	0.17	0.16	0.18
High	0.26	0.26	0.27	0.27	0.27
Highest	0.21	0.26	0.32	0.35	0.32
Highest+	0.04	0.07	0.10	0.11	0.09
Education Level					
Lowest	0.00	0.00	0.00	0.00	0.00
Low	0.11	0.10	0.07	0.05	0.06
Medium	0.47	0.41	$\rm 0.32$	0.28	0.33
High Highest	0.14 0.28	0.14 0.35	0.16 0.45	0.17 0.50	0.16 0.44
Sport Frequency					
Never	0.16	0.14	$0.11\,$	0.09	0.11
Rarely	0.13	0.12	0.10	0.09	0.10
Monthly	0.29	0.30	0.31	0.28	0.29
Weekly	0.42	0.44	0.49	0.55	0.50
<i>Observations</i>					
Total Share	0.12	0.09	0.29	0.49	1.00
Total Observations	13'408	98'33	$31^\circ\hspace{-3pt}.801$	53'414	108'456

Table 3.A.2: Descriptive Statistics by Sport Frequency for Female Sample

Note: Means of variables displayed in all columns.

	Never	Rarely	Monthly	Weekly	Total
Outcome					
First Message	0.02	0.03	0.03	0.04	0.04
Recipient Features					
Age	44.88	46.21	45.56	43.43	44.37
Income Level					
Lowest	0.06	0.03	0.02	0.02	0.02
Low	0.15	0.08	0.05	0.04	0.05
Medium	0.21	0.19	0.14	0.12	0.14
High	0.22	0.32	0.27	0.25	0.26
Highest	0.30	0.30	0.41	0.42	0.40
$Highest+$	0.05	0.07	0.11	0.15	0.13
Education Level					
Lowest	0.00	0.01	0.00	0.00	0.00
Low	0.11	0.07	0.03	0.02	0.03
Medium	0.37	0.36	0.24	0.17	0.22
High	0.15	0.20	0.15	0.15	0.16
Highest	0.37	0.37	0.58	0.66	0.59
Sender Features					
Age	43.15	44.20	43.37	41.19	42.19
Income Level					
Lowest	0.13	0.09	0.07	0.06	0.07
Low	0.20	0.18	0.13	0.11	0.13
Medium	0.25	0.25	0.23	0.22	0.23
High	0.26	0.29	0.31	0.33	0.32
Highest	0.14	0.16	0.21	0.23	0.21
Highest+	0.03	0.03	0.04	0.04	0.04
Education Level					
Lowest	0.00	0.00	0.00	0.00	0.00
Low	$_{0.05}$	0.04	0.03	0.02	0.02
Medium	0.48	0.47	0.39	0.33	$0.37\,$
High	0.18	0.20	0.19	0.18	0.19
Highest	0.28	0.29	0.40	0.47	0.42
Sport Frequency					
Never	0.18	0.16	0.12	0.10	0.12
Rarely	0.12	0.11	0.10	0.09	0.09
Monthly	0.30	0.30	0.31	0.30	0.30
Weekly	0.40	0.44	0.47	0.52	0.49
Observations					
Total Share	0.07	0.08	0.29	0.56	1.00
Total Observations	4'690	5'827	19'970	39'429	69'916

Table 3.A.3: Descriptive Statistics by Sport Frequency for Male Sample

Note: Means of variables displayed in all columns.

3.B Online Dating Platform

3.B.1 Valid User Interactions

In our analysis, we restrict ourselves to *one-way* user interactions. These interactions are always initiated by a visit from the sender, which is invisible to the recipient. The visit is then immediately followed by either a visible action from the sender, or possibly no further action at all. However, in both cases a visible reply of the recipient to this initial action by the sender is not permitted. In that sense, we retain only one-way interactions such that the sender was visibly or invisibly active, while the recipient stayed visibly passive. Hence, we do not allow for any visible reciprocal interaction between the sender and the recipient.

For instance, a sender visit followed by a sender message is a valid interaction. Also, two successive sender visits followed by a message is a valid interaction. A single sender visit is valid interaction, too. Further notice, that a sender visit followed by a recipient visit and afterwards a sender message is a valid interaction as well, as the sender has not seen the recipient's visit. However, a sender visit and sender like followed by a recipient visit and like back inducing a sender message is not a valid interaction anymore as the sender message has already been provoked by the recipient. Hence, we always restrict the interactions until the point a possible reciprocal interaction taking place.

3.C Additional Results

3.C.1 Heterogeneous Efects

GATEs: Weekly vs. Never		Males	Females		
Wald Test	χ^2	p -Value	χ^2	p -Value	
Recipient Features					
Age	23.56	37.08	13.17	96.32	
Education Level	14.03	0.72	7.63	10.62	
Income Level	22.67	0.04	1.79	87.72	
Sport Frequency	9.15	2.74	3.43	32.94	
Sender Features					
Age	32.18	7.45	24.18	50.90	
Education Level	20.40	0.04	9.75	4.49	
Income Level	17.33	0.39	6.49	26.13	
Sport Frequency	6.55	8.76	4.41	0.24	
Shared Features					
Distance	23.01	40.12	13.59	96.84	

Table 3.C.1: Wald Tests for Equality of Group Efects for Males and Females

Note: Wald tests of Equality of the GATEs. p-Values in %.

GATEs: Weekly vs. Never		Males			Females			
t - $Test$	Group	Δ	SE	p -Value	Group	Δ	SE	p -Value
Recipient Features								
Age	23.50	-0.02	0.08	80.04	21.00	-0.09	0.27	75.02
	30.00	0.02	0.07	83.72	25.00	-0.12	0.23	59.96
	31.50	0.06	0.07	40.97	26.50	0.01	0.21	95.03
	33.00	0.04	0.07	56.74	27.50	-0.10	0.14	48.40
	34.50	0.05	0.06	45.19	28.50	-0.09	0.13	49.29
	35.50	0.03	0.09	76.92	29.50	-0.07	0.09	47.27
	36.50 37.50	0.06 -0.01	0.08 0.04	49.74 83.13	30.50 31.50	-0.04 0.14	0.10 0.12	66.35 22.45
	39.00	0.04	0.05	40.91	32.50	-0.01	0.09	88.68
	40.50	0.03	0.06	60.45	33.50	0.13	0.10	17.17
	42.50	-0.02	0.03	40.11	34.50	0.06	0.06	36.87
	45.00	-0.05	0.04	14.49	35.50	0.07	0.09	45.64
	46.50	-0.01	0.05	76.75	36.50	0.07	0.06	26.29
	48.00	-0.00	0.05	91.87	37.50	0.12	0.07	9.96
	49.50	0.02	0.05	74.89	38.50	0.03	0.08	69.35
	50.50	0.01	0.06	82.71	40.00	0.01	0.08	93.72
	51.50	0.00	0.06	94.83	42.00	-0.05	0.11	67.89
	52.50 54.00	-0.05	0.07	44.77	43.50	-0.09	0.13	48.02
		0.02	0.07 0.07	72.17 41.80	45.00 46.50	0.07 0.06	0.11 0.12	51.04 62.45
	55.50 57.00	-0.06 -0.02	0.10	84.60	48.00	0.03	0.12	80.54
	59.50	-0.07	0.12	54.40	49.50	0.02	0.14	89.29
	71.50	-0.09	0.13	52.15	51.00	-0.02	0.14	88.52
					53.50	-0.05	0.15	75.73
					67.00	-0.03	0.16	87.07
Education Level	Lowest	-0.15	0.11	17.30	Lowest	0.11	0.29	70.80
	Low	-0.42	0.19	2.36	Low	-0.22	0.20	27.04
	Medium	-0.27	0.15	7.51	Medium	-0.10	0.07	19.95
	High Highest	0.03 0.09	0.02 0.05	15.84 9.19	High	0.04 0.09	0.04 0.10	30.37 35.32
					Highest			
Income Level	Lowest	-0.19	0.09	3.62	Lowest	-0.15	0.26	56.30
	Low	-0.26	0.09	0.47	Low	-0.11	0.12	33.82
	Medium	-0.16	0.07	1.83	Medium	-0.00	0.04	95.63
	High	-0.03	0.02	13.33	High	0.04	0.06	51.80
	Highest	0.06	0.03	3.07	Highest	0.08	0.10	41.01
	$Highest+$	0.14	0.08	6.43	$Highest+$	0.09	0.13	51.46
Sport Frequency	Never	-0.24	0.12	5.62	Never	-0.42	0.39	28.34
	Rarely	-0.16	0.10	14.20	Rarely	-0.30	0.27	26.33
	Monthly	-0.05	0.05	34.31	Monthly	-0.16	0.16	33.56
	Weekly	0.03	0.02	26.99	Weekly	0.09	0.09	30.43
Sender Features								
Age	22.50	-0.03	0.09	76.98	22.00	-0.16	0.29	58.20
	28.00	0.02	0.07	75.51	27.00	-0.08	0.22	71.84
	29.50	0.05	0.08	55.52	28.50	-0.14	0.17	40.21
	30.50	0.06	0.08	43.37	$29.50\,$	-0.14	0.15	36.84
	32.00	0.05	0.08	50.57	30.50	-0.01	0.11	$\boldsymbol{90.90}$
	33.50	0.02	0.08	78.09	31.50	-0.04	0.12	72.55
	34.50 35.50	0.06 0.00	0.07 0.05	43.61 94.99	32.50 33.50	-0.03 0.03	0.09 0.08	73.61 66.48
	36.50	0.04	0.06	48.48	34.50	0.02	0.07	82.77
	38.00	0.03	0.03	34.29	35.50	0.09	0.07	17.47
	40.00	-0.02	0.03	36.95	36.50	0.16	0.08	4.37
	42.00	-0.00	0.03	96.81	37.50	0.06	0.05	28.04
	44.00	-0.07	0.05	12.42	38.50	0.06	0.06	34.36
	45.50	-0.00	0.04	89.46	40.00	0.10	0.06	8.29
	47.00	-0.01	0.05	77.00	41.50	0.01	0.07	$87.26\,$
	48.50	-0.00	0.05	98.54	43.00	0.05	0.07	52.76
	49.50	0.03	0.06	63.18	44.50	0.00	0.08	95.30

Table 3.C.2: Tests for Diferences of GATEs to ATE for Males and Females

continued on next page

Note: t-tests for Differences of the GATEs from the ATE. Δ in % points. *p*-Values in %.

Figure 3.C.1: Heterogeneous Efects of Sport Activity based on Income for Females

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.

Figure 3.C.2: Heterogeneous Efects of Sport Activity based on Sport for Males

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.
Figure 3.C.3: Heterogeneous Efects of Sport Activity based on Age for Males

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.

Figure 3.C.4: Heterogeneous Efects of Sport Activity based on Age for Females

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.

Figure 3.C.5: Heterogeneous Efects of Sport Activity based on Education for Males

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.

Figure 3.C.6: Heterogeneous Efects of Sport Activity based on Education for Females

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.

Figure 3.C.7: Heterogeneous Efects of Sport Activity based on Distance

Note: Efects in % points as GATE deviations from the ATE (zero dotted line) with 90% confdence intervals.

3.C.2 Clustering Analysis

Code				Males					Females		
	Clusters	$\mathbf{1}$	$\overline{2}$	3	$\overline{4}$	5	$\mathbf{1}$	$\overline{2}$	3	$\overline{4}$	5
	IATEs: Weekly vs. Never	0.41	0.88	1.22	1.52	1.85	-1.41	-0.52	0.12	0.71	1.38
	Recipient Features										
$\overline{5}$	Smoking Frequency	1.30	0.85	0.32	0.10	0.03	0.50	0.47	0.45	0.37	0.29
14	Relevance of Sexuality	0.38	0.44	0.47	0.49	0.52	0.21	0.27	0.31	0.32	0.31
108	TV in Leisure Time	0.27	0.26	0.25	0.25	0.28	0.32	0.27	0.21	0.15	0.11
223	Radio/TV at Home	0.62	0.62	0.60	0.59	0.60	0.73	0.68	0.65	0.64	0.67
284	Appearance Satisfaction	0.18	0.19	0.20	0.21	0.22	0.11	0.16	0.18	0.20	0.21
292	Importance of Sexuality	0.29	0.33	0.36	0.38	0.40	0.21	0.24	0.28	0.29	0.30
303	Comfortable Dining	0.67	0.63	0.57	0.55	0.55	0.73	0.66	0.60	0.57	0.58
324	Wish Significant Other	0.27	0.28	0.29	0.32	0.33	0.26	0.26	0.26	0.27	0.30
	Sender Features										
5	Smoking Frequency	0.69	0.52	0.36	0.31	0.27	0.48	0.50	0.49	0.42	0.32
14	Relevance of Sexuality	0.24	0.28	0.29	0.33	0.40	0.35	0.40	0.44	0.45	0.46
108	TV in Leisure Time	0.23	0.21	0.20	0.19	0.17	0.29	0.30	0.29	0.27	0.24
223	Radio/TV at Home	0.65	0.61	0.60	0.58	0.55	0.67	0.66	0.64	0.63	0.61
284	Appearance Satisfaction	0.18	0.17	0.17	0.19	0.22	0.12	0.16	0.17	0.19	0.23
292	Importance of Sexuality	0.21	0.24	0.23	0.25	0.28	0.29	0.32	0.33	0.35	0.38
303	Comfortable Dining	0.68	0.65	0.60	0.56	0.54	0.63	0.62	0.60	0.58	0.54
324	Wish Significant Other	0.23	0.23	0.25	0.25	0.27	0.28	0.29	0.31	0.32	0.35
	<i>Observations</i>										
	Share	0.07	0.18	0.29	0.31	0.15	0.07	0.20	0.29	0.29	0.15
	Total	2288	6439	10153	10826	5252	3753	11048	15896	15484	8047

Table 3.C.3: Descriptive Clusters of IATEs based on the k-means++ Clustering

Note: Means of clustered efects sorted in an increasing order, matched with selected user characteristics. Variable codes refer to the exact questions from the registration questionnaire presented in Table [3.D.1.](#page-183-0)

3.D Supplementary Material

3.D.1 Registration Questionnaire and Descriptive Statistics

Table 3.D.1: Summary of the Registration Questionnaire and the Descriptive Statistics

\sim Code	Mean	\sim T ىلە	\mathbf{r} Mın	Max	Question	\sim oding	Answer
	0.01	U. LU	$0.00\,$	1.00		T I Unordereo	7ID. Ω - uu \mathbf{L} - 22

Note: First column lists a unique identifier for each variable. Second, third, fourth and fifth column report the corresponding mean, standard deviation, minimum and maximum values for the variable, respectively. Sixth column contains the specifc questions from the registration questionnaire. Seventh column indicates the variable encoding: dummy stands for a binary variable equal to 1 if the respective answer has been chosen (mutually inclusive); ordered stands for a numeric value with a clear inherent ordering (both continuous and categorical), directly filled by the user (mutually exclusive); unordered stands for a text value without an ordered structure (categorical), directly flled by the user (mutually exclusive). Last column lists the corresponding answers available in the registration questionnaire.

Curriculum Vitae

EDUCATION

EXPERIENCE

St.Gallen, November 9, 2021 Gabriel Okasa