Comprehensive Causal Machine Learning

Berlin, September 2024

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Trend 1: Methods were developed to credibly estimate causal effects empirically

Trend 2: Effective prediction of newly developed Machine Learning methods

Causal **M**achine **L**earning

- ML inspired estimators applied to *well-identified* causal questions with **rich** data
- Promise: 'Better' estimation for causal effects at various aggregation level
  - Population effects, group effects, individualized effects
- Most work based on experiments & selection-on-observables (unconfoundedness)

Many fields active in methodological developments

- Universities: Statistics, Computer science, econometrics, epidemiology, marketing, …
- Private: Tech industry & beyond

Applications in diverse empirical studies

General approaches to effect estimation

Parameter specific estimation methods

- Use ‘best’ method for each aggregation level (levels of granularity)
  - May work better for specific aggregation levels
  - Difficult to understand & monitor performance of different estimators
    - Many tuning parameters, …
  - Internal consistency not guaranteed: Aggregates of heterogeneous effects may differ from average effects

Comprehensive Causal Machine Learning (CCML)

- Unified approach for estimating of all parameters of interest
- CCML estimators for different effects share important components (estimated by machine learning)

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Comprehensive **C**ausal **M**achine **L**earning | Econometrics

Double/debiased **M**achine **L**earning

- Common element: **D**oubly **R**obust **S**core

Generalized **R**andom **F**orest

- Common element: Generalized Random Forest structure

Modified **C**ausal **F**orest

- Common element: Causal Forest
- Aggregate effects obtained by aggregation of finer-grained effects

The Econometrics Journal

Econometrics Journal (2018), volume **21**, pp. C1–C68.
doi: 10.1111/ectj.12097

Double/debiased machine learning for treatment and structural parameters

VICTOR CHERNOZHUKOV[†], DENIS CHETVERIKOV[‡], MERT DEMIRER[†], ESTHER DUFLO[†], CHRISTIAN HANSEN[§], WHITNEY NEWEY[†] AND JAMES ROBINS[‖]

The Annals of Statistics
2019, Vol. 47, No. 2, 1148–1178
https://doi.org/10.1214/18-AOS1709

GENERALIZED RANDOM FORESTS

BY SUSAN ATHEY*, JULIE TIBSHIRANI[†] AND STEFAN WAGER*

IZA DP No. 12040

Modified Causal Forests for Estimating Heterogeneous Causal Effects

Michael Lechner

DECEMBER 2018

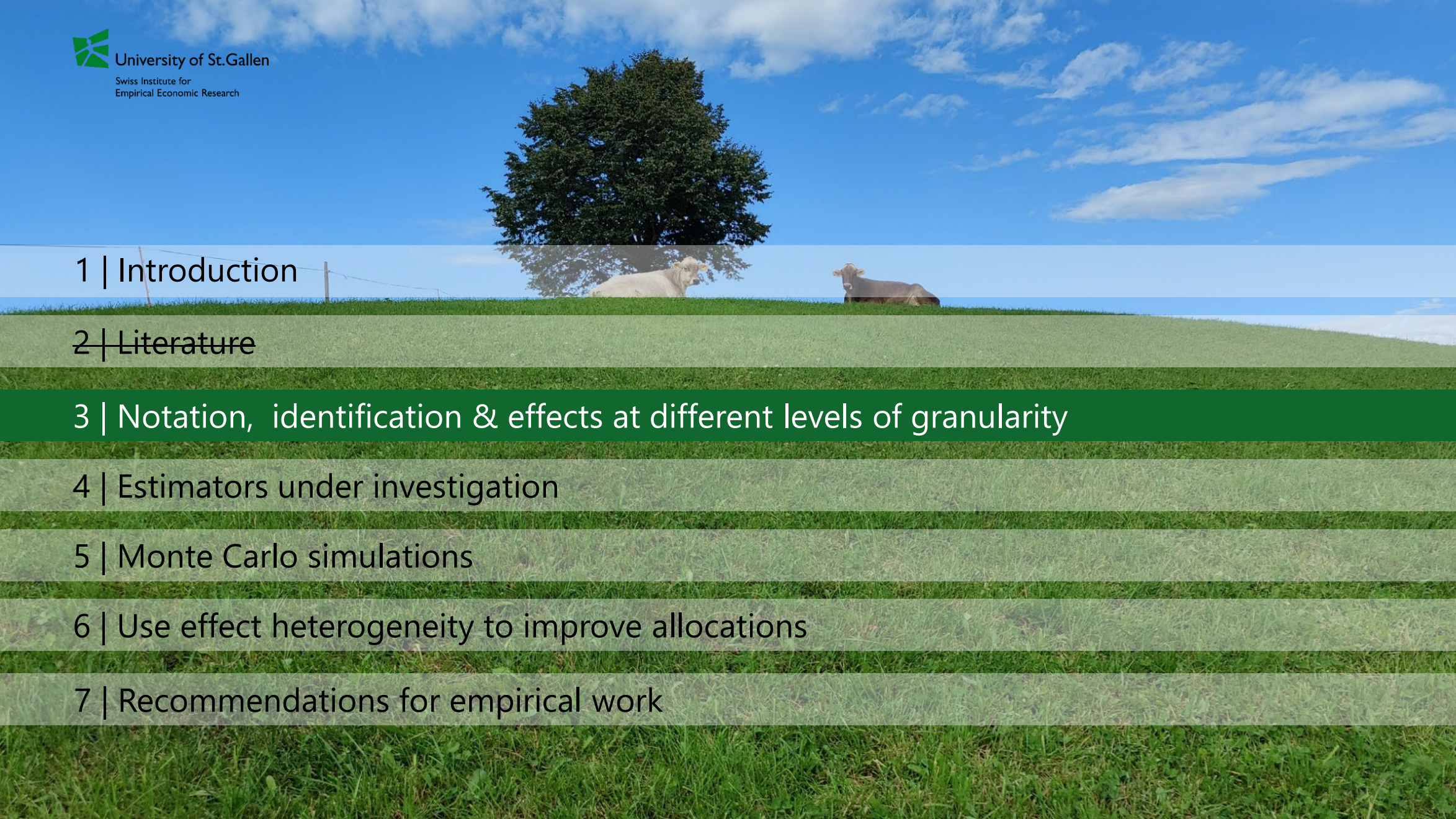
Contribution of this paper

Compare point estimators & inference of *dml*, *grf*, *mcf* in a ***selection-on-observable (unconfoundedness)*** setting with respect to …

- statistical guarantees (asymptotic properties)
  - Add some new statistical guarantees for the *mcf* (& *grf*)
- finite sample performance (Monte Carlo study)

Most important findings

- Efficiency – robustness trade-off for aggregate effects
  - Strength of selection into treatment is important for finite sample ranking of estimators
- Causal Forests superior (to DR-learner) for fine-grained heterogeneity



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1 | Introduction

~~2 | Literature~~

3 | Notation, identification & effects at different levels of granularity

4 | Estimators under investigation

5 | Monte Carlo simulations

6 | Use effect heterogeneity to improve allocations

7 | Recommendations for empirical work

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Here: Binary treatment (multiple treatments in paper)

Notation | Binary treatment

D Treatment

Y^0 Potential outcome for $D=0$

Y^1 Potential outcome for $D=1$

$Y = D\,Y^1 + (1-D)\,Y^0$

Propensity score: $p(x) = P(D=1 \mid X=x)$

Outcome regression: $\mu(d,x) = E(Y \mid D=d, X=x)$

X All confounders & heterogeneity variables

Z Specific heterogeneity variables (low dimensional; included in X)

Sample contains i.i.d. realisations of D, Y, X

Identification | Selection-on-observables | Unconfoundedness | CIA

Identifying assumptions

- *D* independent of Y^0, Y^1 given *X*
- Common support, no interactions between units, exogeneity of *X*

If assumptions are …

- fulfilled ➔ causal effects
- not fulfilled ➔ associations adjusted for distributional differences in *X*

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D: Treatment (0 or 1) | X: Confounder & heterogeneity variables
Y^1: Outcome when $D=1$ | Z: Specific heterogeneity variables (low dim.)
Y^0: Outcome when $D=0$ | Observable: $D, Y, X;\ Z \subset X$

Estimands of mean causal effects at different aggregation levels | 1

Individualized (**C**onditional) **A**verage **T**reatment **E**ffect (*IATE(x)*, *CATE(x)*)

$$IATE(x) = E(Y^1 - Y^0 \mid X = x) = \mu(1,x) - \mu(0,x)$$

$$\mu(d,x) = E(Y \mid D = d, X = x)$$

Group **A**verage **T**reatment **E**ffect (*GATE(z),CATE(z)*)

$$GATE(z) = E_{X|Z=z} IATE(X)$$

Average **T**reatment **E**ffect (*ATE*)

$$ATE = E_X IATE(X)$$

GATEs & ATEs on the treated / non-treated

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$$\mu(d,x) = E(Y \mid D = d, X = x)$$
$$p(x) = P(D = 1 \mid X = x)$$

The Econometrics Journal

Econometrics Journal (2022), volume **00**, pp. 1–26.
https://doi.org/10.1093/ectj/utac015

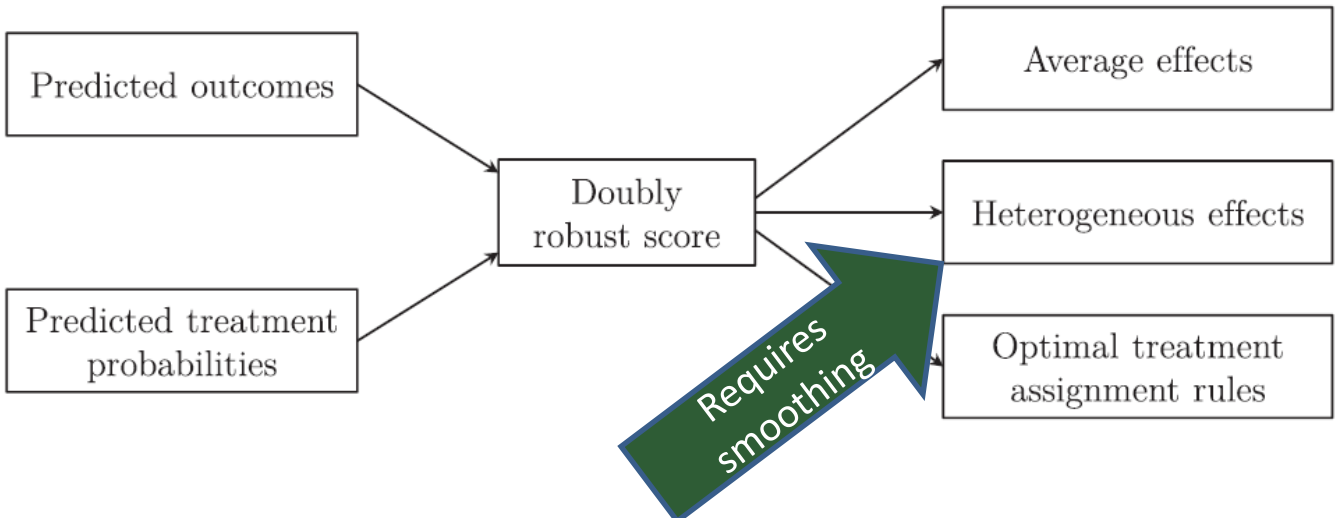
Double machine learning-based programme evaluation under unconfoundedness

MICHAEL C. KNAUS

DML for binary treatment

The central role of the (cross-fitted) **D**oubly **R**obust **S**core

$$DRS(y_i, d_i, x_i, \hat{\mu}_{-i}(\cdot), \hat{p}_{-i}(\cdot)) =$$
$$\hat{\mu}_{-i}(1, x_i) - \hat{\mu}_{-i}(0, x_i) + \frac{[y_i - \hat{\mu}_{-i}(1, x_i)]d_i}{\hat{p}_{-i}(x_i)} - \frac{[y_i - \hat{\mu}_{-i}(0, x_i)](1 - d_i)}{1 - \hat{p}_{-i}(x_i)}$$



DML for binary treatment | Averages of DR score

ATE $$\hat{ATE}_N^{dml} = \frac{1}{N}\sum_{i=1}^{N} DRS(y_i, d_i, x_i, \hat{\mu}_{-i}(\cdot), \hat{p}_{-i}(\cdot))$$

GATE(z) (z-discrete) $$\hat{GATE}(z)_N^{dml} = \frac{1}{N_z}\sum_{i=1}^{N} 1(z_i = z) DRS(y_i, d_i, x_i, \hat{\mu}_{-i}(\cdot), \hat{p}_{-i}(\cdot)) \qquad N_z = \sum_{i=1}^{N} 1(z_i = z)$$

IATE(x) (DR-Learner)

- If *f(x)* parametrically specified & estimation by OLS

$$\hat{IATE}(x)_N^{dml} = \arg\min_{f(x)} \frac{1}{N}\sum_{i=1}^{N} [DRS(y_i, d_i, x_i, \hat{\mu}_{-i}(\cdot), \hat{p}_{-i}(\cdot)) - f(x_i)]^2$$

  - Drawback: Not robust to misspecification of *f(x)*
- If *f(x)* is nonparametrically estimated, or by ML
  - Estimator is conjectured to be consistent

Basic principles of *Causal Forests* | 1

Homogeneous-in-X strata → no-selection-bias → difference of *Y* between treated & controls is 'good' estimator

Use Random-Forest-like splitting algorithm with adapted splitting rule

- Different Causal Forests use different splitting rules that try to approximate the MSE of the IATE
  - Maximise treatment effect heterogeneity: CF (Wager, Athey, 2018), ***grf*** (Athey, Tibshirani, Wager, 2019)
  - Approximate estimation errors directly: *mcf* (Lechner, 2018)

Honest estimation to avoid bias & getting inference

- Different data to build forest & to populate the final leaves with y_i

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Generalized Random Forests | 1 | Estimation of IATE

Extension of Random Forest to nonparametric local GMM

Local moment conditions: $E(\psi^{grf}(Y,X,D;\theta^0(X),\eta^{grf,0}(X))|X=x)=0;$ $\theta^0(x)$: True value of parameter of interest

$\eta^{grf,0}(x)$: True value of nuisance parameters

$$\hat{I}ATE_N^{grf}(x)=\hat{\theta}_N^{grf}(x)=\left(\sum_{i=1}^N w_i^{grf}(x)\left(d_i-\bar{d}_w\right)\left(d_i-\bar{d}_w\right)'\right)^{-1}\sum_{i=1}^N w_i^{grf}(x)\left(d_i-\bar{d}_w\right)\left(y_i-\bar{y}_w\right),$$

$$\bar{d}_w=\sum_{i=1}^N w_i^{grf}(x)d_i$$

$$\bar{y}_w=\sum_{i=1}^N w_i^{grf}(x)y_i$$

- Weights obtained from gradient-based splitting rule → maximise treatment effect heterogeneity
- Honesty (instead of cross-fitting)

Generalized Random Forests | 2 | Estimation ATE & GATE

ATEs & GATEs are estimated through additional regressions using *grf* score function

- *dml*-like score function:

$$\hat{\Gamma}^{grf}(o_i;\hat{\eta}) = \hat{\theta}(x_i) + \frac{d_i(y_i - \hat{\mu}(1;x_i))}{\hat{p}(x_i)} + \frac{(1-d_i)(y_i - \hat{\mu}(0;x_i))}{1-\hat{p}(x_i)} = \ldots < forest >$$

- ATE:

$$\hat{ATE}_N^{grf} = \hat{\theta}_N^{grf} = \frac{1}{N}\sum_{i=1}^{N}\hat{\Gamma}^{grf}(o_i;\hat{\eta})$$

$$\hat{Var}(\hat{ATE}_N^{grf}) = \frac{1}{N}\sum_{i=1}^{N}\hat{\Gamma}^{grf}(o_i;\hat{\eta})^2$$

- GATEs
  - Regress score on Z
  - Heteroscedasticity-robust standard errors of OLS regression

Modified Causal Forest | Main ideas

The *mcf* is a modification of the Causal Forest by Wager & Athey (2018)

Important modification

- Splitting rule based on alternative proxy for MSE & penalty function
- Representation of causal effect as weighted mean of y_i's is used for inference
  - Requires different implementation of sample splitting
- *ATE* & *GATE(z)* are obtained by aggregating *IATE(x)*'s

Summary of theoretical properties

ATE

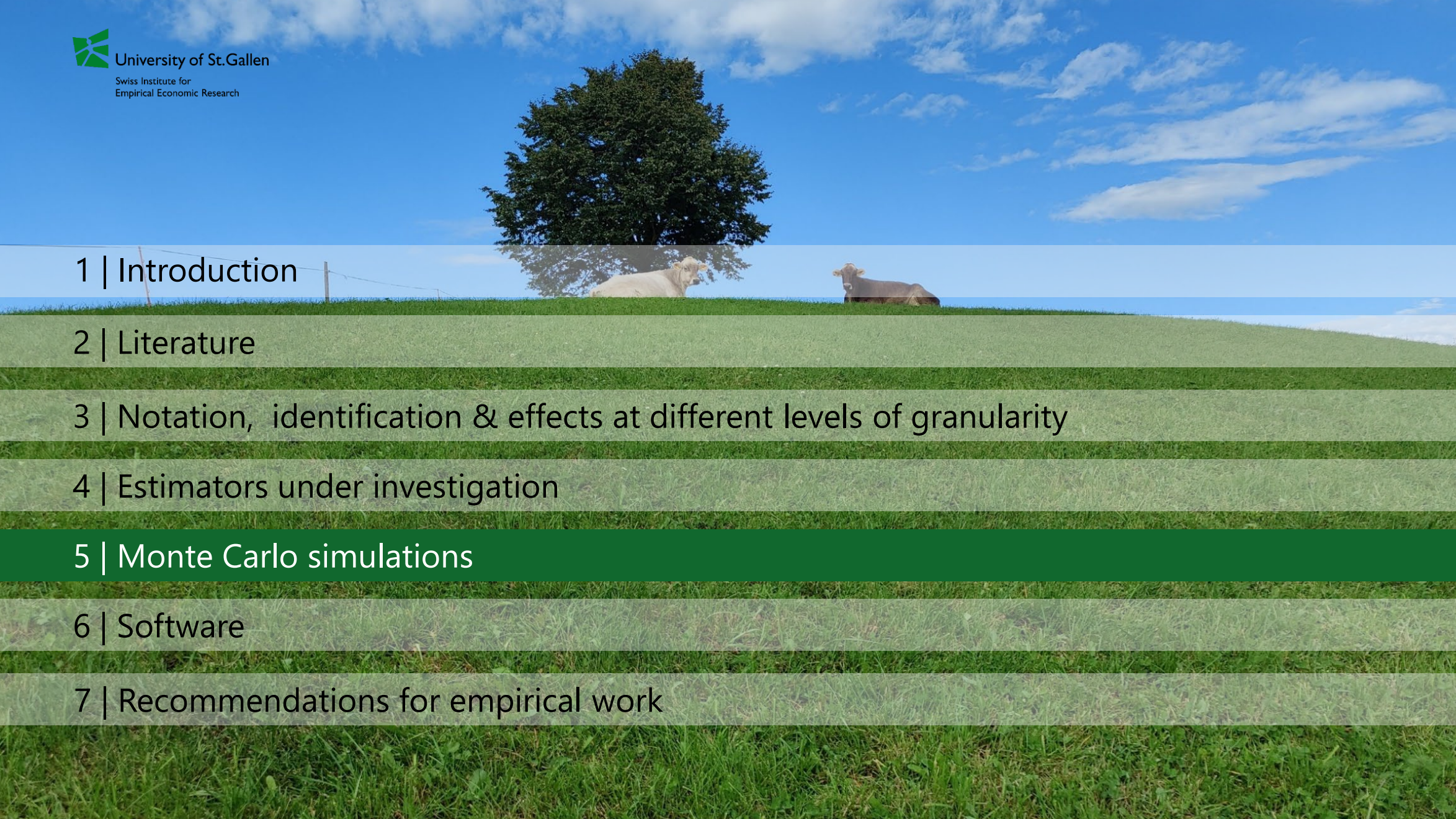
- All estimators are consistent, asymptotically normal
- *dml* & *grf* are efficient
- *mcf*: ATE is sum of IATEs

GATE

- All estimators are consistent, asymptotically normal (*Z* discrete)
- *mcf*: GATE is sum of IATEs in subsamples defined by values of *Z*

IATEs (finite dimensional *X*)

- *mcf* & *grf* are consistent, asymptotically normal
- *dml (DR-learner)* is consistent, asymptotically normal for parametric approximations (e.g., best linear predictors)



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Goal | 1

Compare finite sample behaviour of *dml*, *grf*, *mcf*

- Quality of point estimates **&** inference procedures (out-of-training sample)

Synthetic Monte Carlo study with different data generating processes

- **Sample size**: N=2'500 & 10'000
- **Covariates**
  - # of covariates in data: p = 10, 20, 50
  - # of covariates in DGP (sparsity): k = 0.2 p, 0.5 p, 0.8 p
  - Type of covariates: Normal, uniform, dummy (pure & mixtures of different types)
  - Z: Continuous covariate split into 5, 10, 20, 40 groups
- **Treatment**
  - # of treatments: 2, 4
  - Strength of selection (R^2 = 0, 10%, 42%)
  - Treatment shares: 25%, 50%
- **Potential outcomes**
  - Y^0: Sine function of linear index, R^2 = 0, 10%, 45%
  - Y^1: Y^0 + IATE + noise
  - IATE: 0, Linear, quadratic, logistic, step functions

Summary | 1

dml

- Dominates when # of groups is small & selectivity is not too large
- Performance may drastically deteriorate for a larger # of groups or stronger selectivity
- Is dominated by CFs for IATEs (bias)

grf (pre-centred)

- Similarly good as *dml* when # of groups is small & selectivity is not too large
- Performance drastically deteriorates for a larger # of groups (& stronger selectivity)
- Good performance for IATEs

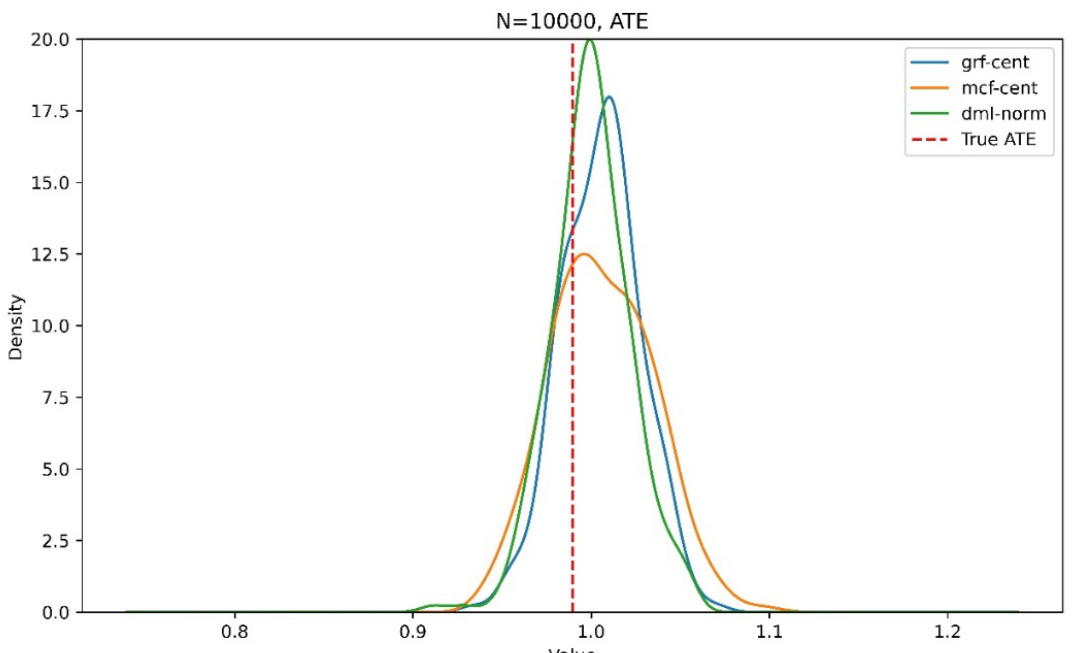
Summary | 2

mcf (pre-centred)

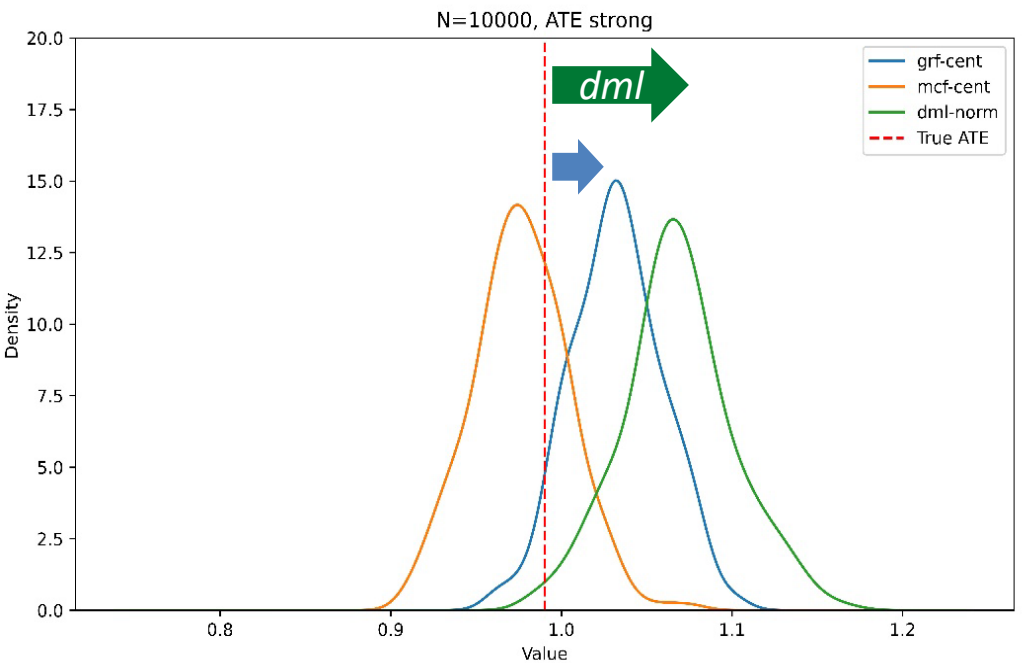
- Less efficient when # of groups is small & selectivity is not too large
- Much less affected by larger # of groups & stronger selectivity
- Overall robust (& competitive) behaviour

ATE estimator may be sensitive to different levels of selectivity

Medium selectivity (R^2=10%)



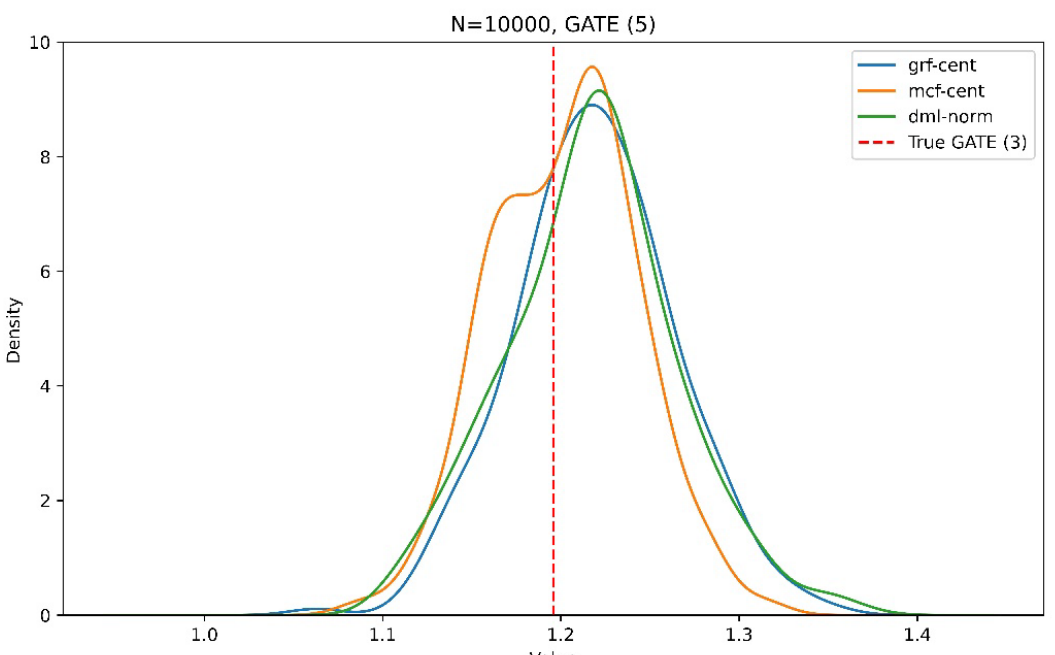
Strong selectivity (R^2=42%)



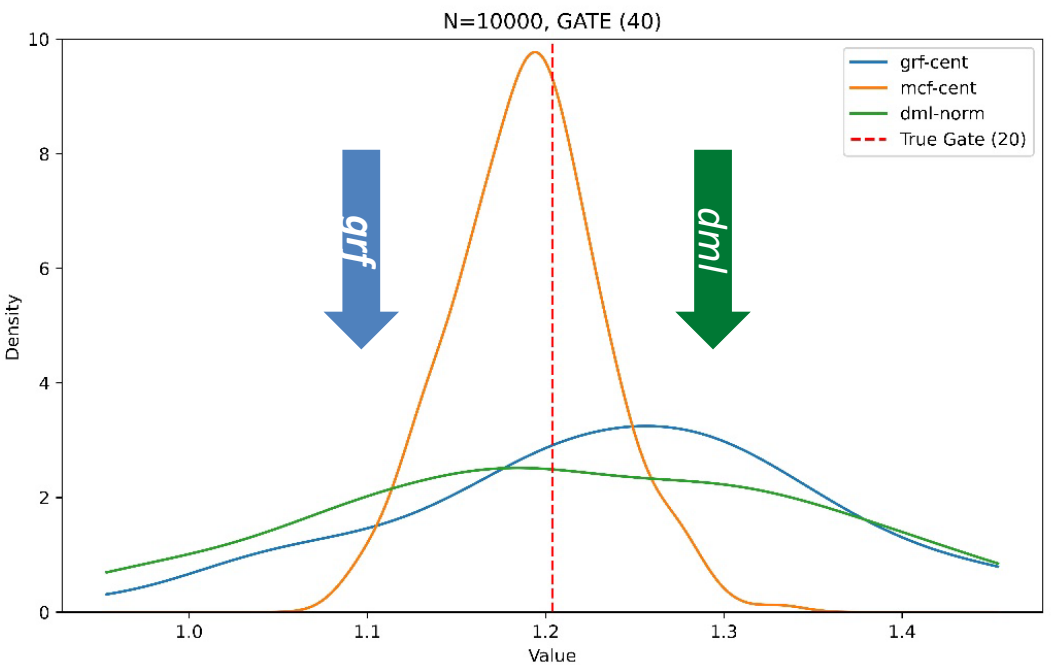
Bias (& MSE) is even larger for smaller sample

GATE estimator may be sensitive w.r.t. different # of groups

GATE with 5 groups



GATE with 40 groups



Variance (MSE) is even larger for smaller sample

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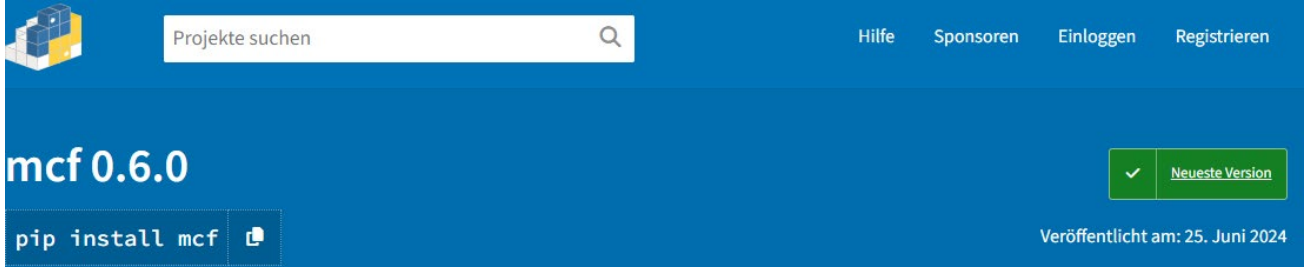
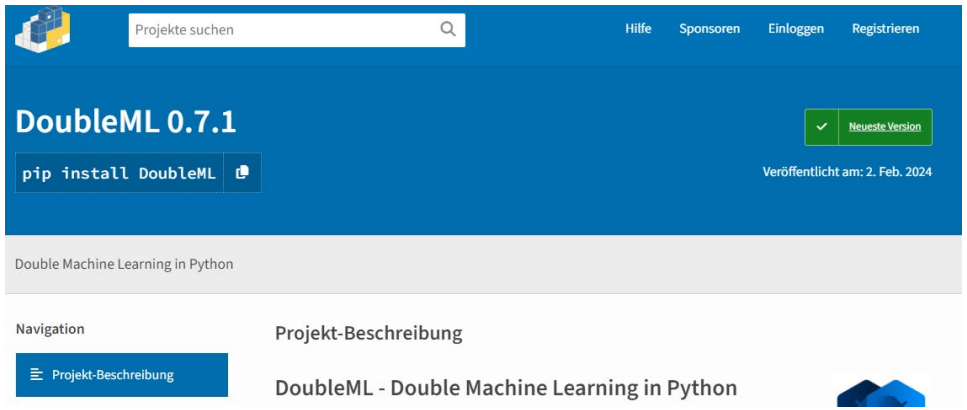
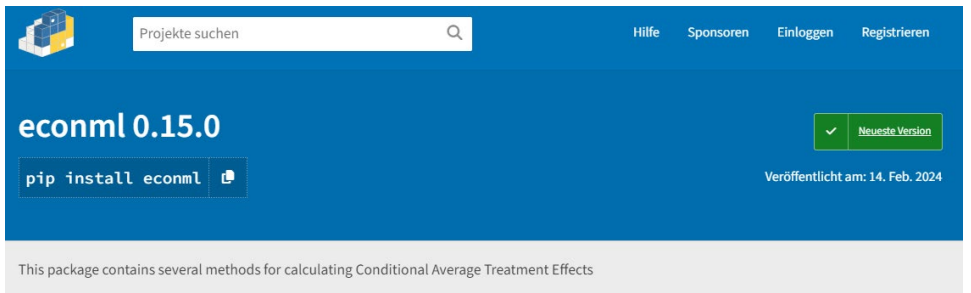
Some packages







DoubleML: Double Machine Learning in R

Implementation of the double/debiased machine learning framework of Chernozhukov et a
regression models. 'DoubleML' allows estimation of the nuisance parts in these models by
based on the 'R6' package is very flexible. More information available in the publication ir

Version:	1.0.0
Depends:	R (≥ 3.5.0)
Imports:	R6 (≥ 2.4.1), data.table (≥ 1.12.8), stats, checkmate, mlr3 (≥ 0.5.0), m
Suggests:	knitr, rmarkdown, testthat, covr, patrick (≥ 0.1.0), paradox (≥ 0.4.0), d
Published:	2024-02-15
Author:	Philipp Bach [aut, cre], Victor Chernozhukov [aut], Malte S. Kurz [au

grf: Generalized Random Forests

Forest-based statistical estimation and inference. GRF provides non-parametric methods for heterogeneous tre
regression, and survival regression, all with support for missing covariates.

Version:	2.3.2
Depends:	R (≥ 3.5.0)
Imports:	DiceKriging, lmtest, Matrix, methods, Rcpp (≥ 0.12.15), sandwich (≥ 2.4-0)
LinkingTo:	Rcpp, RcppEigen
Suggests:	DiagrammeR, MASS, rdd, survival (≥ 3.2-8), testthat (≥ 3.0.4)
Published:	2024-02-25
Author:	Julie Tibshirani [aut], Susan Athey [aut], Rina Friedberg [ctb], Vitor Hadad [ctb], Davi
Maintainer:	Erik Sverdrup <erik.sverdrup at monash.edu>

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1 | Introduction

2 | Literature

3 | Effects at different levels of granularity

4 | Comprehensive CML estimators

5 | Monte Carlo simulations

6 | Software

7 | Recommendations for empirical work

Recommendations for empirical work

Large sample available (standard error reduction not a major concern)

- *mcf*

Smaller sample (standard error reduction is important)

- ATE, GATE (few groups): *dml* or *grf* (robustness check with more robust mcf)
- GATE (many groups): *mcf*
- IATEs: *grf* or *mcf*

A note on computation

- User friendly packages available in *Python* & *R* (& Stata for *dml*)

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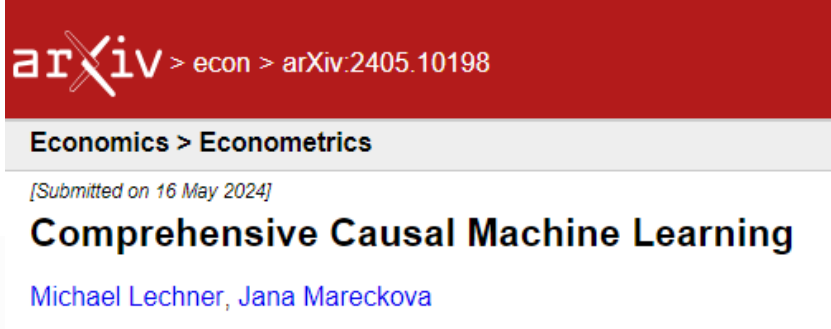

The end. Thanks.

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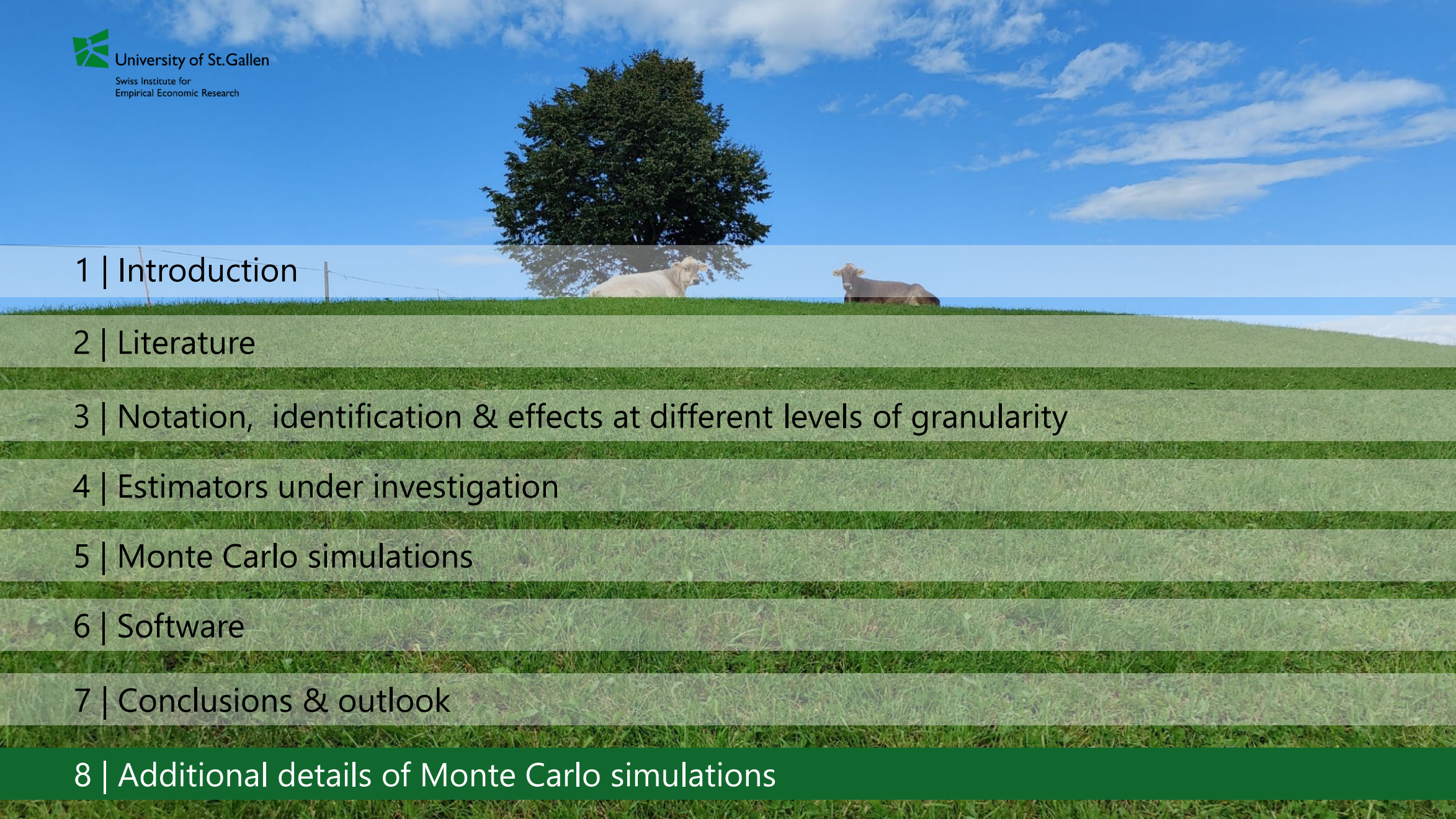

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Implementation details of estimators in Monte Carlo study | *dml*

Nuisance parameter

- Regression Forests
- 5-fold cross-fitting

Normalized *dml*

- Normalise sum of (implied) weights to 1
- Truncate normalized weights if larger than 0.05 → renormalize

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Implementation details of estimators in Monte Carlo study | *mcf*

Software

- Python package *mcf* (available on PyPI), most simulations based on version 0.3.3, some on 0.4.3

Tuning parameters

- Minimum leaf size of 5, 1000 trees, 50% subsamples

Other decisions

- Local centring ($E(Y|X=x)$) by Random Forest (scikit-learn) by 5-fold cross-fitting (in sample used to build Causal Forest)
- Nearest Neighbour Matching based on 1 (or 3 when 4 treatments) prognostic scores for MCE (weighting by Mahalanobis distance when 3 scores)
- Nonparametric estimations for weight-based inference use k-NN estimator (k=2 $\sqrt{N}$)

Implementation details of estimators in Monte Carlo study | *grf*

Software

- R package *grf* (2.3.1)

Tuning parameters

- 2000 trees
- Minimum node size = 5
- Number of variables used for splitting drawn from $Poisson(min(p, (p+20)^{0.5}))$
- Explicit centring with k-fold cross-fitting

Goal | 1

Comprehensive analysis of behaviour of *grf*, *dml*, *mcf* (& in different versions, OLS) in finite (but larger) samples

- Quality of point estimates **&** inference procedures

Computationally very demanding

- Many scenarios needed to see if some method breaks down in certain situations

General considerations | 1

Simulations (Econometrics) vs. *benchmark studies* (Machine learning)

- Difficult to use for inference (requires replications) ➔ *simulations*

Empirical Monte Carlo Study (EMCS) vs. *synthetic* design

- EMCS somewhat more realistic for special case
- We want to vary very many characteristics → *synthetic design*
  - Type & quantity of covariates, # of treatments , effect heterogeneity, degree of selectivity, sample size, functional forms, influence of covariates on outcomes & heterogeneity, share of treated

Fixed or *random* features (*X*)

- Only fixed-*X* design allows to analyse distributions of *IATEs(x)* for given *x*
- Random-*X* design better reflects distribution theory ➔ *fixed X*

Simulation design | 1

Repeat R times

- Draw 2 data sets of size *N*
  - Data set 1 (to train forest): contains *D*, Y, X
  - Data set 2 (to predict effects): contains *IATE(x)*, X
- Estimate effects & standard errors
- Save results

Compute performance measures

- 1st to 4th moments, bias, MSE, absolute error, bias of standard error, coverage probability

Data generating process (DGPs) | 1

Sample size: N=2'500 (R=1'000), 10'000 (R=250)

- About constant simulation errors for ATE & GATE

Covariates

- # of covariates in data: p = 10, 20, 50
- # of covariates in DGP (sparsity): k = 0.2 p, 0.5 p, 0.8 p
- Type of covariates: Normal, uniform, dummy (pure & mixtures of different types)
- Z: Continuous covariate split into 5, 10, 20, 40 groups of equal size

Treatment

- # of treatments: 2, 4
- Selection follows linear index model (R^2 = 0, 10%, 42%)
- Treatment shares: 25%, 50%

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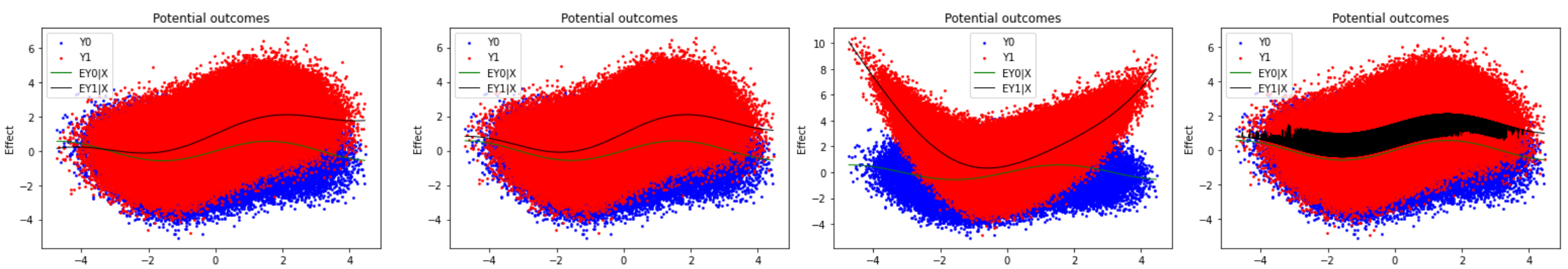
Data generating process (DGPs) | 2

Potential outcomes

- Y^0: Sine function of linear index, R^2 = 0, 10%, 45%
- Y^1: Y^0 + IATE + noise
- IATE: 0, linear & non-linear functions
  - Linear, quadratic, logistic function of linear index
  - Specification of Wager & Athey (2018): Complicated step-function



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Estimators

dml (own Python code)

- Nuisances estimated by Regression Random Forests (*scikit-learn*)
- With and w/o normalized weights (robustness against extreme propensity scores)

grf (R package)

- Outcomes centred (k-fold cross-fitting) before start of estimation // no external centring
- *Not competitive without explicit centring of Y*

mcf (Python package)

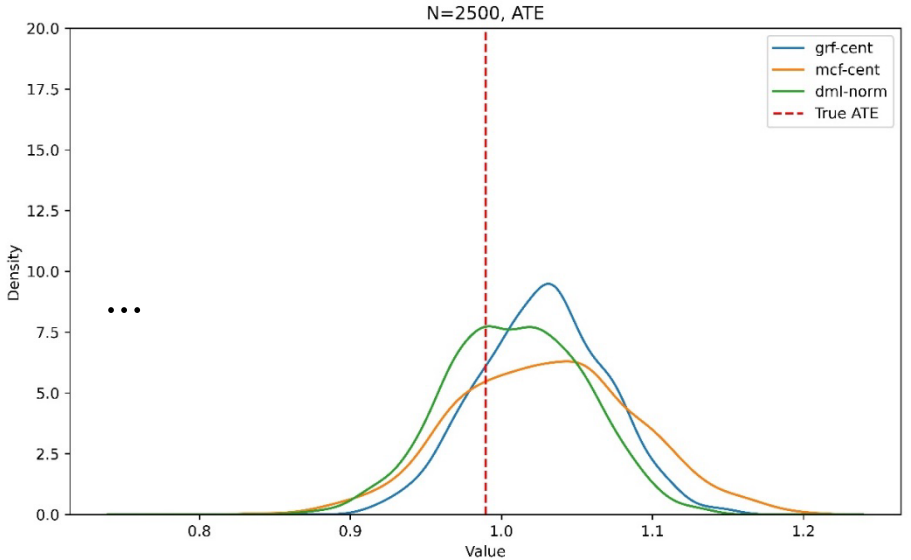
- Outcomes centred (k-fold cross-fitting) before start of estimation // no external centring
- More efficient version without inference (IATEs only)
- *Not competitive without explicit centring of Y, D*

OLS

- *Not competitive*

Important note
All ML & CML estimators use defaults (no explicit tuning)

Results | ATE in main scenario (main scenario)



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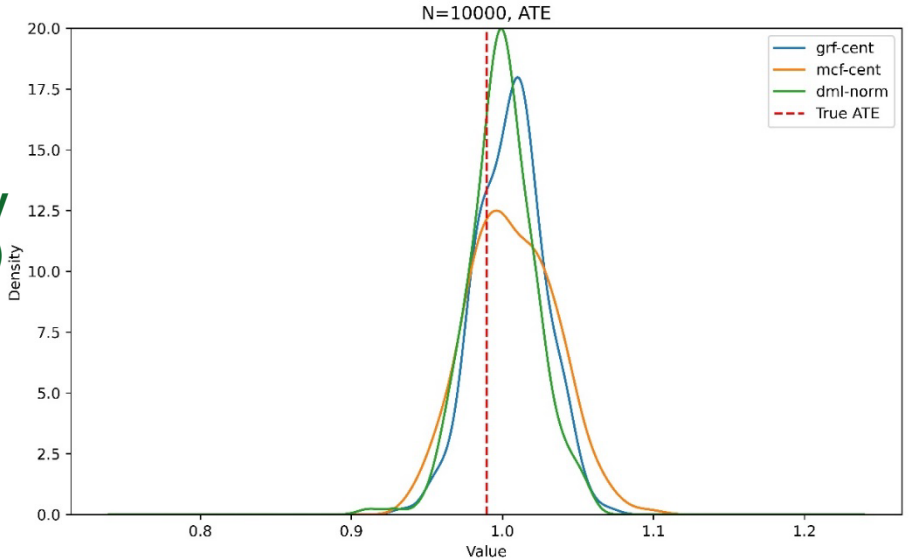
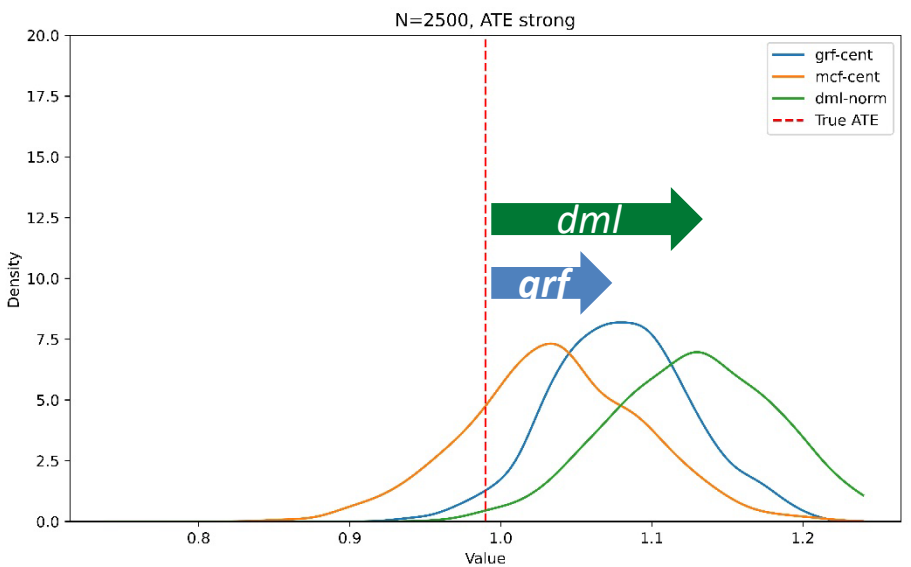
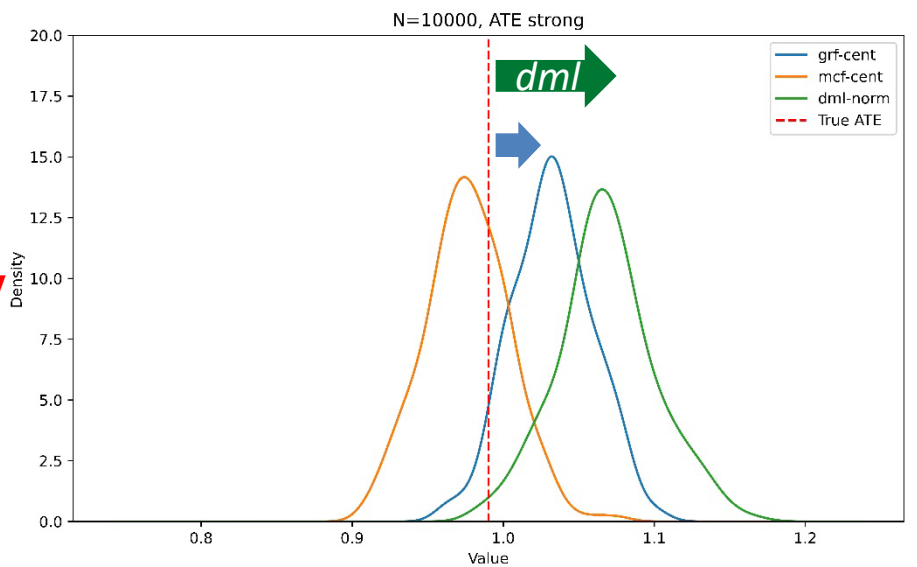
Medium selectivity (R^2=10%)





Strong selectivity (R^2=42%)



ATE

Selectivity

- General: Bias increases with increasing selectivity for all estimators (leading to worsening coverage)
- No & medium selectivity: *dml & grf* best, *mcf* ok, coverage ok for N=10'000
- Strong selectivity: *dml* collapses, *grf* deteriorates, *mcf* ok'ish
  - Conjecture: DR scores getting too extreme because of extreme propensity scores (more trimming needed?)

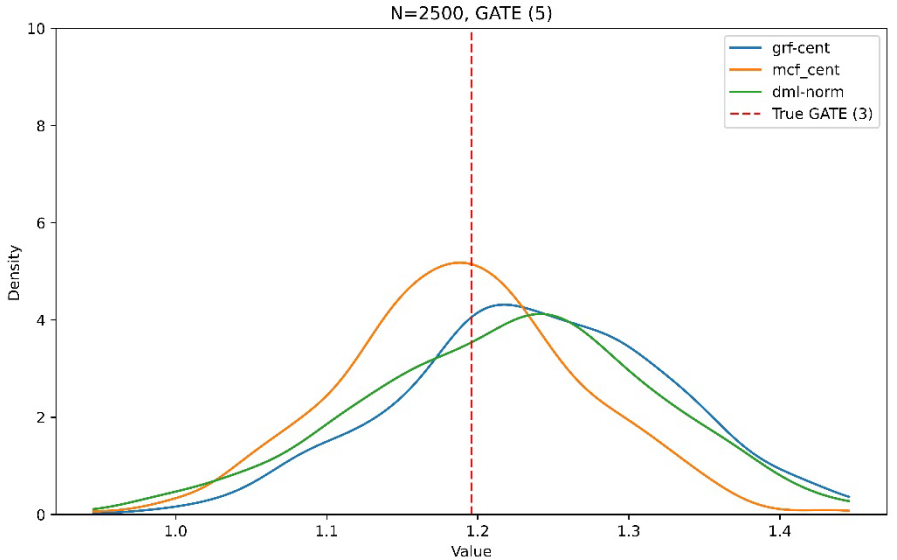
Sample size

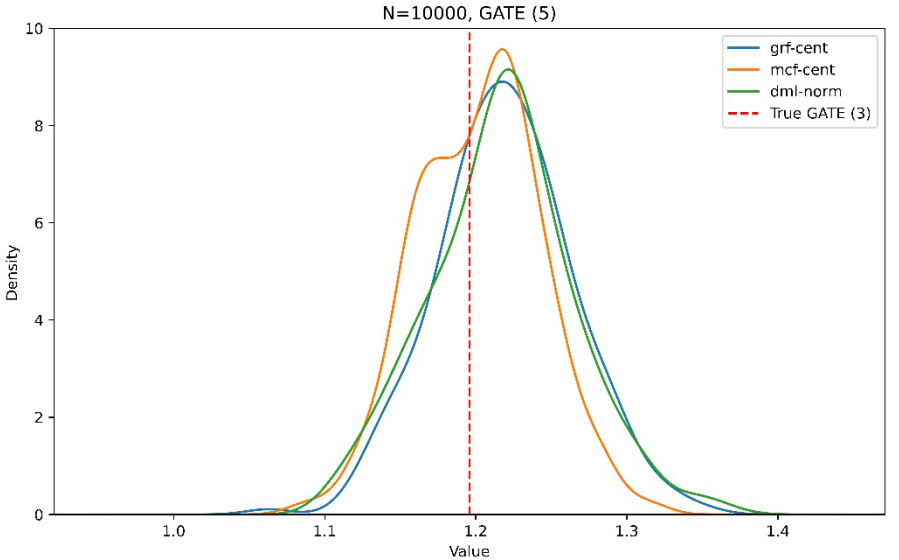
- Speed of reduction of SE suggestive of $\sqrt{N}$-convergence

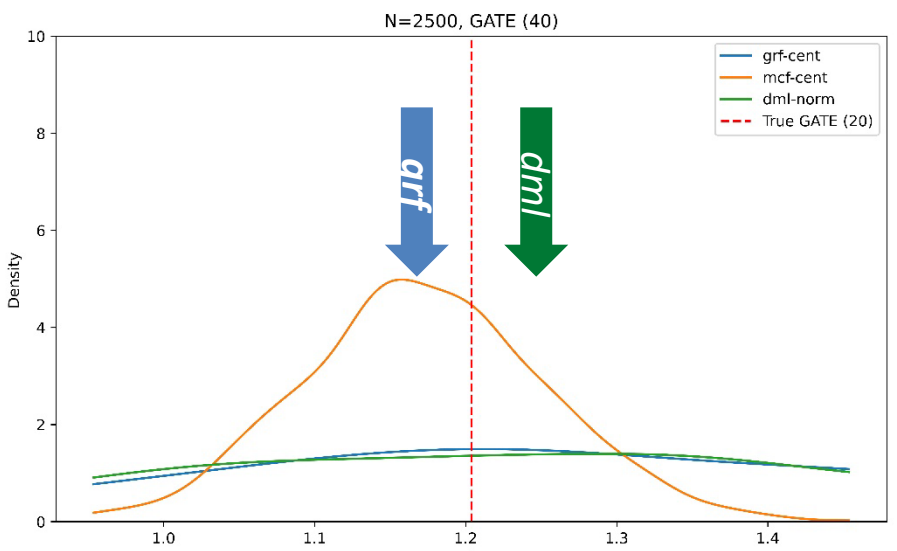
Further observations

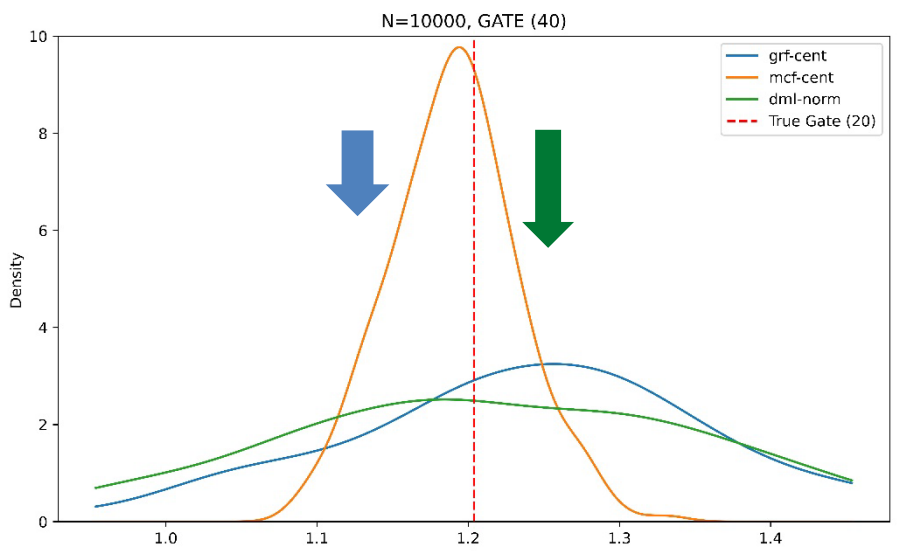
- All estimators deteriorate when R^2 of Y^0 is large

Results | GATE in main scenario for 5 & 40 groups









GATEs

5 groups: Generally same findings than for ATE

- *grf* almost always best estimator
- Coverage of *mcf* deteriorates (due to bias by cross-cell-of-Z smoothing)
- Strong selectivity: Relative performance loss of *dml* & *grf* less pronounced than for ATE

More groups: Performance of *dml* & *grf* deteriorates dramatically

- *dml & grf:* DR-scores regressed on up to 5, 10, 20, 40 dummies
  - Information from other values of *Z* only used in nuisance functions (no smoothing across z-values)
    ➔ # of observation for each value of z crucially important
- *mcf*: Aggregates of IATE(x) in cells by z-value
  - IATEs smooths across z-values ➔ # of observations for each value of z less relevant

IATEs

grf & *mcf* **clearly** outperform *dml* (OLS & Random Forest based)

- Even true when IATE(*x*) is 0, or a linear function of *x* (when there is selectivity)
- Only exception: No selectivity together with not much nonlinearity in IATE

Coverage is bad for all methods (worst for *dml*)

- If inference is not needed, *grf* & *mcf* can be improved
  - Problem seems to come from too much bias in point estimates

Summary | 1

dml

- Dominates when # of groups is small & selectivity is not too large
- Performance may drastically deteriorate for a larger # of groups or stronger selectivity
- Not useful for IATEs

grf (pre-centred)

- Similar good than *dml* when # of groups is small & selectivity is not too large
- Performance may drastically deteriorate for a larger # of groups (& to a lesser extend for strong selectivity)
- Good performance for IATE

Summary | 2

mcf (pre-centred)

- Less efficient when # of groups is small & selectivity is not too large
- Much less affected by larger # of groups & stronger selectivity
- Overall robust (& competitive) behaviour