(5) Double Machine Learning

Causal Data Science for Business Analytics

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Preliminaries

Observed Confounding

- We need these assumptions:

Assumption A1: "Conditional Exchangeability / Unconfoundedness / Ignorability / Independence".

$$Y_i(t) \perp\!\!\!\perp T_i \mid \mathbf{X_i} = \mathbf{x}, \forall t \in \{0, 1, \dots\}, \text{ and } \mathbf{x} \in \mathbb{X}.$$

Assumption A2: "Positivity / Overlap / Common Support".

$$0 < P(T_i = t | \mathbf{X_i} = \mathbf{x}), \forall t \in \{0, 1, \dots\}, \text{ and } \mathbf{x} \in \mathbb{X}.$$

Assumption A3: "Stable Unit Treatment Value Assumption (SUTVA)."

$$Y_i = Y(T_i)$$

- ... to achieve identification of the ATE:

Theorem: "Identification of the ATE":

$$\tau_{\text{ATE}} = \mathbb{E}[Y_i(1)] - \mathbb{E}[Y_i(0)] = \mathbb{E}_{\mathbb{X}}[\mathbb{E}[Y_i | T_i = 1, \mathbf{X_i} = \mathbf{x}] - \mathbb{E}[Y_i | T_i = 0, \mathbf{X_i} = \mathbf{x}]]$$

Types of Parameters

Causal Machine Learning methods force us to distinguish between two types of parameters:

- 1. Target parameter is motivated by the research question and defined under modelling assumption,
  - e.g. effect of a treatment on some outcome.
- 2. Nuisance parameters are inputs that are required to obtain the target parameter, but are not relevant for our research question.
  - e.g. propensity scores.
- Focus on the target parameter and do not get tempted to interpret every single coefficient from a regression.

Frisch–Waugh–Lovell (FWL) Theorem

- We can estimate β_T in a standard linear regression $Y_i = \beta_0 + \beta_T T_i + \beta_{\mathbf{X}}' \mathbf{X_i} + \epsilon_i$ in a three-stage procedure:

1. Run a regression of the form $Y_i = \beta_{Y0} + \beta_{\mathbf{Y}\sim\mathbf{X}}' \mathbf{X_i} + \epsilon_{Y_i \sim X_i}$ and extract the estimated residuals $\hat{\epsilon}_{Y_i \sim X_i}$.
2. Run a regression of the form $T_i = \beta_{T0} + \beta_{\mathbf{T}\sim\mathbf{X}}' \mathbf{X_i} + \epsilon_{T_i \sim X_i}$ and extract the estimated residuals $\hat{\epsilon}_{T_i \sim X_i}$.
3. Run a residual-on-residual regression of the form $\hat{\epsilon}_{Y_i \sim X_i} = \beta_T \hat{\epsilon}_{T_i \sim X_i} + \epsilon_i$ (no constant).

The resulting estimate $\hat{\beta}_T$ is numerically identical to the estimate we would get if we just run the full OLS model.

Target Parameters

- Average potential outcome (APO): $\mu_t := \mathbb{E}[Y_i(t)]$.
  - What is the expected outcome if everybody receives treatment t?
- Average Treatment Effect (ATE): $\tau_{\text{ATE}} := \mathbb{E}[Y_i(1)] - \mathbb{E}[Y_i(0)] = \mu_1 - \mu_0$.
  - What is the expected treatment effect in the population?

- Note that the target parameters are just different aggregations of the Conditional Average Potential Outcome (CAPO): $\mathbb{E}[Y_i(t) \mid \mathbf{X_i} = \mathbf{x}]$
  - $\mu_t := \mathbb{E}[Y_i(t)] \overset{LIE}{=} \mathbb{E}[\mathbb{E}[Y_i(t) \mid \mathbf{X_i} = \mathbf{x}]]$
  - $\tau_{\text{ATE}} := \mathbb{E}[Y_i(1)] - \mathbb{E}[Y_i(0)] \overset{LIE}{=} \mathbb{E}[\mathbb{E}[Y_i(1) \mid \mathbf{X_i} = \mathbf{x}]] - \mathbb{E}[\mathbb{E}[Y_i(0) \mid \mathbf{X_i} = \mathbf{x}]]$.
- It suffices to show that the CAPO is identified.

General Approach

- Causal Machine Learning methods are mostly about rewriting stuff such that we are allowed to leverage supervised ML to estimate the nuisance parameters.
- Importantly, the target parameters of interest remain the same although the rewritten form can look quite different to the original/familiar model.
- The methods usually boil down to running multiple supervised ML regressions and combining their predictions into a final OLS regression.
- Supervised ML holds the promise of data-driven model selection and complex non-linear relationships, and thus, getting (one of) the nuisance parameters right.
- The crucial point is that the statistical inference in this final OLS regression is valid if we follow a particular recipe.
  - Recipe of how to split the estimation of causal effects into prediction tasks.

Doubly Robust Methods

Doubly Robust Methods: Idea

- Given the three assumptions hold, we have seen two ways to identify the ATE: $\tau_{\text{ATE}} = \mathbb{E}[Y_i(1)] - \mathbb{E}[Y_i(0)] = \mu_1 - \mu_0$
- Conditional outcome regression:
  - $\tau_{\text{ATE}} = \mathbb{E}_{\mathbb{X}}[\mathbb{E}[Y_i|T_i = 1, \mathbf{X_i} = \mathbf{x}] - \mathbb{E}[Y_i|T_i = 0, \mathbf{X_i} = \mathbf{x}]]$
  - Simplified notation with nuisance parameter $\mu(t, \mathbf{x}) = \mathbb{E}[Y_i|T_i = t, \mathbf{X_i} = \mathbf{x}]$ as conditional average potential outcome:
  - $\tau_{\text{ATE}} = \mathbb{E}_{\mathbb{X}}[\mu(t = 1, \mathbf{x}) - \mu(t = 0, \mathbf{x})]$
- Inverse probability weighting:
  - $\tau_{\text{ATE}} = \mathbb{E}\left[\frac{T_i Y_i}{P(T_i=1|\mathbf{X_i}=\mathbf{x})}\right] - \mathbb{E}\left[\frac{(1-T_i)Y_i}{1-P(T_i=1|\mathbf{X_i})}\right]$
  - $\tau_{\text{ATE}} = \mathbb{E}\left[\frac{T_i Y_i}{PS(\mathbf{X_i})}\right] - \mathbb{E}\left[\frac{(1-T_i)Y_i}{1-PS(\mathbf{X_i})}\right]$
  - Simplified notation with nuisance parameter $e_t(\mathbf{x}) = P(T_i = t \mid \mathbf{X_i} = \mathbf{x})$ as propensity score:
  - $\tau_{\text{ATE}} = \mathbb{E}\left[\frac{\mathbb{1}(T_i=1)Y_i}{e_{t=1}(\mathbf{x})}\right] - \mathbb{E}\left[\frac{\mathbb{1}(T_i=0)Y_i}{e_{t=0}(\mathbf{x})}\right]$
- Idea of doubly robust methods:
  - Combine both approaches, such that the ATE estimator is consistent, even if only one of the two models is correctly specified.

Doubly Robust Estimator: Definition

- Doubly robust or Augmented Inverse Propensity Score Weighting (AIPW) estimator:
- Conditional average potential outcome (CAPO) given by:

$$\mu_t^{\text{AIPW}}(\mathbf{x}) := \mathbb{E}[Y_i(t)|\mathbf{X_i} = \mathbf{x}] \overset{(A1,A3)}{=} \mathbb{E}[Y_i|T_i = 0, \mathbf{X_i} = \mathbf{x}] := \mu(t, \mathbf{x})$$

(conditional outcome regression)

$$\overset{(2)}{=} \mathbb{E}\left[\frac{\mathbb{1}(T_i = t)Y_i}{e_t(x)}\middle|\mathbf{X_i} = \mathbf{x}\right]$$

(inverse probability weighting)

$$\overset{(3)}{=} \mathbb{E}\left[\mu(t, \mathbf{x}) + \frac{\mathbb{1}(T_i = t)(Y_i - \mu(t, \mathbf{x}))}{e_t(\mathbf{x})}\middle|\mathbf{X_i} = \mathbf{x}\right]$$

(augmenting outcome regression with IPW weights)

- Average potential outcome (APO) given by:

$$\mu_t^{\text{AIPW}} = \mathbb{E}_{\mathbb{X}}\left[\mathbb{E}\left[\mu(t, \mathbf{x}) + \frac{\mathbb{1}(T_i = t)(Y_i - \mu(t, \mathbf{x}))}{e_t(\mathbf{x})}\middle|\mathbf{X_i} = \mathbf{x}\right]\right] = \mathbb{E}\left[\mu(t, \mathbf{x}) + \frac{\mathbb{1}(T_i = t)(Y_i - \mu(t, \mathbf{x}))}{e_t(\mathbf{x})}\right]$$

Doubly Robust Estimator: Proof

- Proof for Equation (2):

$$
\begin{aligned}
\mu_t(\mathbf{x}) := \mathbb{E}[Y_i(t)|\mathbf{X_i} = \mathbf{x}] &= \mathbb{E}[Y_i|T_i = 0, \mathbf{X_i} = \mathbf{x}] \\
&= \mathbb{E}[\underbrace{\mathbb{1}(T_i = t)}_{=1} Y_i \mid T_i = t, \mathbf{X_i} = \mathbf{x}] \\
&= \mathbb{E}\left[\mathbb{1}(T_i = t)\frac{e_t(\mathbf{x})}{e_t(\mathbf{x})} \mid T_i = t, \mathbf{X_i} = \mathbf{x}\right] + (1 - e_t(\mathbf{x}))\mathbb{E}[\underbrace{\mathbb{1}(T_i = t)}_{=0} Y_i \mid T_i \neq t, \mathbf{X_i} = \mathbf{x}]/e_t(\mathbf{x}) \\
&= \frac{\overbrace{e_t(\mathbf{x})\mathbb{E}[\mathbb{1}(T_i = t)Y_i \mid T_i = t, \mathbf{X_i} = \mathbf{x}] + (1 - e_t(\mathbf{x}))\mathbb{E}[\mathbb{1}(T_i = t)Y_i \mid T_i \neq t, \mathbf{X_i} = \mathbf{x}]}^{\overset{LIE}{=}\mathbb{E}[\mathbb{1}(T_i=t)Y_i|\mathbf{X_i}=\mathbf{x}]}}{e_t(\mathbf{x})} \\
&= \frac{\mathbb{E}\left[\mathbb{1}(T_i = t)Y_i \mid \mathbf{X_i} = \mathbf{x}\right]}{e_t(\mathbf{x})} = \mathbb{E}\left[\frac{\mathbb{1}(T_i = t)Y_i}{e_t(\mathbf{x})}\middle| \mathbf{X_i} = \mathbf{x}\right]
\end{aligned}
$$

Doubly Robust Estimator: Proof

- Proof for Equation (3):

$$
\begin{aligned}
\mu_t(\mathbf{x}) := \mathbb{E}[Y_i(t)|\mathbf{X_i} = \mathbf{x}] &= \mathbb{E}\left[\mu(t,\mathbf{x}) + \frac{\mathbb{1}(T_i = t)(Y_i - \mu(t,\mathbf{x}))}{e_t(\mathbf{x})}\middle|\mathbf{X_i} = \mathbf{x}\right] \\
&= \mathbb{E}\left[Y_i(t) - Y_i(t) + \mu(t,\mathbf{x}) + \frac{\mathbb{1}(T_i = t)(Y_i - \mu(t,\mathbf{x}))}{e_t(\mathbf{x})}\middle|\mathbf{X_i} = \mathbf{x}\right] \\
&= \mathbb{E}\left[Y_i(t) - Y_i(t) + \mu(t,\mathbf{x}) + \frac{\mathbb{1}(T_i = t)(Y_i(t) - \mu(t,\mathbf{x}))}{e_t(\mathbf{x})}\middle|\mathbf{X_i} = \mathbf{x}\right] \\
&= \mathbb{E}[Y_i(t) \mid \mathbf{X_i} = \mathbf{x}] + \mathbb{E}\left[(Y_i(t) - \mu(t,\mathbf{x}))\left(\frac{\mathbb{1}(T_i = t) - e_t(\mathbf{x})}{e_t(\mathbf{x})}\right)\middle|\mathbf{X_i} = \mathbf{x}\right] \\
&\overset{(4)}{=} \mu_t(\mathbf{x}) + \underbrace{\mathbb{E}\left[(Y_i(t) - \mu(t,\mathbf{x}))\left(\frac{\mathbb{1}(T_i = t) - e_t(\mathbf{x})}{e_t(\mathbf{x})}\right)\middle|\mathbf{X_i} = \mathbf{x}\right]}_{\text{needs to be 0 for the conditional APO to be identified}}
\end{aligned}
$$

Doubly Robust Estimator: Proof

- Proof for Equation (4):
- Let $\tilde{\mu}(t, \mathbf{x})$ and $\tilde{e}_t(\mathbf{x})$ be some candidate functions for the conditional outcome regression and the propensity score, respectively.

$$\mathbb{E}\left[(Y_i(t) - \tilde{\mu}(t, \mathbf{x}))\left(\frac{\mathbb{1}(T_i = t) - \tilde{e}_t(\mathbf{x})}{\tilde{e}_t(\mathbf{x})}\right)\middle|\mathbf{X_i} = \mathbf{x}\right] = \mathbb{E}[(Y_i(t) - \tilde{\mu}(t, \mathbf{x})) \mid \mathbf{X_i} = \mathbf{x}]\mathbb{E}\left[\left(\frac{\mathbb{1}(T_i = t) - \tilde{e}_t(\mathbf{x})}{\tilde{e}_t(\mathbf{x})}\right)\middle|\mathbf{X_i} = \mathbf{x}\right]$$

(ignorability allows to separate expectations)

$$= (\mathbb{E}[Y_i(t) \mid \mathbf{X_i} = \mathbf{x}] - \tilde{\mu}(t, \mathbf{x}))\left(\frac{\mathbb{E}[\mathbb{1}(T_i = t \mid \mathbf{X_i} = \mathbf{x}] - \tilde{e}_t(\mathbf{x})}{\tilde{e}_t(\mathbf{x})}\right)$$

$$= (\mu_t(\mathbf{x}) - \tilde{\mu}(t, \mathbf{x}))\frac{(e_t(\mathbf{x}) - \tilde{e}_t(\mathbf{x}))}{\tilde{e}_t(\mathbf{x})}$$

- the last expression becomes 0 if either $\tilde{\mu}(t, \mathbf{x}) = \mu_t(\mathbf{x})$ or $\tilde{e}_t(\mathbf{x}) = e_t(\mathbf{x})$.

Doubly Robust Estimator: Theorem

- Augmentation leads to the following theoretical properties:

Theorem 4.3: "Doubly Robust Estimator".

Given $Y_i(t) \perp\!\!\!\perp T_i \mid \mathbf{X_i} = \mathbf{x}$ (conditional unconfoundedness) and given $0 < P(T_i = t|\mathbf{X_i} = \mathbf{x}), \forall t$ (positivity), then:

1. If either $\tilde{e}_t(\mathbf{x}) = e_t(\mathbf{x})$ or $\tilde{\mu}(t = 1, \mathbf{x}) = \mu_1(\mathbf{x})$, then $\mu_1 = \mathbb{E}[Y_i(1)]$
2. If either $\tilde{e}_t(\mathbf{x}) = e_t(\mathbf{x})$ or $\tilde{\mu}(t = 0, \mathbf{x}) = \mu_0(\mathbf{x})$, then $\mu_0 = \mathbb{E}[Y_i(0)]$
3. If either $\tilde{e}_t(\mathbf{x}) = e_t(\mathbf{x})$ or $\tilde{\mu}(t = 1, \mathbf{x}) = \mu_1(\mathbf{x}), \tilde{\mu}(t = 0, \mathbf{x}) = \mu_0(\mathbf{x})$, then $\mu_1 - \mu_0 = \tau_{\text{ATE}}$

- with $\tilde{\mu}(t, \mathbf{x})$ and $\tilde{e}_t(\mathbf{x})$ being some candidate functions for the conditional outcome regression and the propensity score, respectively.

Doubly Robust Estimator: Theorem

- Proof showing that $\mu_t = \mathbb{E}[Y_i(t)]$:

$$
\begin{aligned}
\tilde{\mu}_t - \mathbb{E}[Y_i(t)] &= \mathbb{E}\left[\tilde{\mu}(t,\mathbf{x}) + \frac{\mathbb{1}(T_i = t)(Y_i - \tilde{\mu}(t,\mathbf{x}))}{\tilde{e}_t(\mathbf{x})}\right] - \mathbb{E}[Y_i(t)] && \text{(by defintion)} \\
&= \mathbb{E}\left[\frac{\mathbb{1}(T_i = t)(Y_i - \tilde{\mu}(t,\mathbf{x}))}{\tilde{e}_t(\mathbf{x})} - (Y_i(t) - \tilde{\mu}(t,\mathbf{x}))\right] && \text{(linearity of expectations)} \\
&= \mathbb{E}\left[\frac{\mathbb{1}(T_i = t) - \tilde{e}_t(\mathbf{x})}{\tilde{e}_t(\mathbf{x})}(Y_i(t) - \tilde{\mu}(t,\mathbf{x}))\right] && \text{(combining terms)} \\
&= \mathbb{E}\left(\mathbb{E}\left[\frac{\mathbb{1}(T_i = t) - \tilde{e}_t(\mathbf{x})}{\tilde{e}_t(\mathbf{x})}(Y_i(t) - \tilde{\mu}(t,\mathbf{x}))\middle|\mathbf{X_i}\right]\right) && \text{(law of iterated expectations)} \\
&= \mathbb{E}\left(\mathbb{E}\left[\frac{\mathbb{1}(T_i = t) - \tilde{e}_t(\mathbf{x})}{\tilde{e}_t(\mathbf{x})}\middle|\mathbf{X_i}\right] \cdot \mathbb{E}\left[Y_i(t) - \tilde{\mu}(t,\mathbf{x})\middle|\mathbf{X_i}\right]\right) && \text{(ignorability allows to separate expectations)} \\
&= \mathbb{E}\left(\frac{(e_t(\mathbf{x}) - \tilde{e}_t(\mathbf{x}))}{\tilde{e}_t(\mathbf{x})}(\mu_t(\mathbf{x}) - \tilde{\mu}(t,\mathbf{x}))\right)
\end{aligned}
$$

Doubly Robust Estimator: Sample Version

- Step 1: obtain the fitted values of the propensity scores:
  - $\hat{e}_t(\mathbf{X_i})$
- Step 2: obtain the fitted values of the outcome regressions:
  - $\hat{\mu}(t, \mathbf{X_i})$.
- Step 3: construct the doubly robust estimator:
  - $\hat{\tau}_{\text{ATE}} = \hat{\mu}_1 - \hat{\mu}_0$ with
  - $\hat{\mu}_1 = \frac{1}{n} \sum_{i=1}^{n} \left[\hat{\mu}(t = 1, \mathbf{X_i}) + \frac{\mathbb{1}(T_i{=}1)(Y_i - \hat{\mu}(t{=}1, \mathbf{X_i})}{\hat{e}_1(\mathbf{X_i})} \right]$
  - $\hat{\mu}_0 = \frac{1}{n} \sum_{i=1}^{n} \left[\hat{\mu}(t = 0, \mathbf{X_i}) + \frac{\mathbb{1}(T_i{=}0)(Y_i - \hat{\mu}(t{=}0, \mathbf{X_i})}{\hat{e}_0(\mathbf{X_i})} \right]$

Doubly Robust Estimator: Example

- Assess the impact of participating in the U.S. National Supported Work (NSW) training program targeted to 445 individuals with social and economic problems on their real earnings.

```
library(Matching)                          # load Matching package
data(lalonde)                              # load lalonde data
attach(lalonde)                            # store all variables in own objects
library(drgee)                             # load drgee package
T = treat                                 # define treatment (training)
Y = re78                                   # define outcome
X = cbind(age,educ,nodegr,married,black,hisp,re74,re75,u74,u75) # covariates
dr = drgee(oformula = formula(Y ~ X), eformula = formula(T ~ X), elink="logit") # DR reg
summary(dr)                                # show results
```

```
Call:  drgee(oformula = formula(Y ~ X), eformula = formula(T ~ X), elink = "logit")

Outcome:  Y

Exposure:  T

Covariates:  Xage,Xeduc,Xnodegr,Xmarried,Xblack,Xhisp,Xre74,Xre75,Xu74,Xu75

Main model:  Y ~ T

Outcome nuisance model:  Y ~ Xage + Xeduc + Xnodegr + Xmarried + Xblack + Xhisp + Xre74 + Xre75 + Xu74 + Xu75

Outcome link function:  identity

Exposure nuisance model:  T ~ Xage + Xeduc + Xnodegr + Xmarried + Xblack + Xhisp + Xre74 + Xre75 + Xu74 + Xu75

Exposure link function:  logit

  Estimate Std. Error z value Pr(>|z|)
T   1674.1      672.4    2.49   0.0128 *
---
```

Double Machine Learning with Partially Linear Regression

Partially Linear Regression Model

- Observed Y_i and T_i are a partially linear function of confounding variables X_i:

$$Y_i = \tau T_i + g(\mathbf{X_i}) + \epsilon_{Y_i}, \qquad \mathbb{E}(\epsilon_{Y_i}|T_i, \mathbf{X_i}) = 0$$
$$T_i = m(\mathbf{X_i}) + \epsilon_{T_i}, \qquad \mathbb{E}(\epsilon_{T_i}|\mathbf{X_i}) = 0$$

- Conditional average potential outcome:
  - $\mathbb{E}[Y_i(t)|\mathbf{X_i}] \overset{(A1,A3)}{=} \mathbb{E}[Y_i|T_i = t, \mathbf{X_i}] = \tau t + g(\mathbf{X_i})$

- Target parameters:
  - $\tau_{\text{CATE}} = \mathbb{E}[Y_i|T_i = 1, \mathbf{X_i}] - \mathbb{E}[Y_i|T_i = 0, \mathbf{X_i}]$
  - $\tau_{\text{CATE}} = (\tau 1 + g(\mathbf{X_i})) - (\tau 0 + g(\mathbf{X_i})) = \tau$
  - $\tau_{\text{ATE}} = \mathbb{E}_{\mathbb{X}}[\beta_T] = \tau$
  - => homogeneous treatment effects

Identification under Partial Linearity

- Following Robinson (1988), we can write the partially linear regression model as a generalization of the Frisch-Waugh-Lovell theorem:
  - $\underbrace{Y_i - \overbrace{\mathbb{E}[Y_i \mid \mathbf{X_i}]}^{\mu(\mathbf{X_i})}}_{\text{outcome residual}} = \tau \underbrace{(T_i - \overbrace{\mathbb{E}[T_i \mid \mathbf{X_i}]}^{e(\mathbf{X_i})})}_{\text{treatment residual}} + \epsilon_{Y_i}$
- τ_{ATE} is identified by a residual-on-residual regression without constant:
  - Population estimand:
    - $\tau_{\text{ATE}} = \arg\min_{\tilde{\tau}} \mathbb{E}[(\underbrace{Y_i - \mu(\mathbf{X_i})}_{\text{pseudo outcome}} - \tilde{\tau}\underbrace{(T_i - e(\mathbf{X_i}))}_{\text{single regressor}})^2] = \frac{\text{Cov}[(Y_i - \mu(\mathbf{X_i}))(T_i - e(\mathbf{X_i}))]}{\text{Var}[T_i - e(\mathbf{X_i})]}$
  - Sample estimator:
    - $\hat{\tau}_{\text{ATE}} = \arg\min_{\tilde{\tau}} \frac{1}{N} \sum_{i=1}^{n} (\underbrace{Y_i - \mu(\mathbf{X_i})}_{\text{pseudo outcome}} - \tilde{\tau}\underbrace{(T_i - e(\mathbf{X_i}))}_{\text{single regressor}})^2 = \frac{\sum_{i=1}^{n}(Y_i - \mu(\mathbf{X_i}))(T_i - e(\mathbf{X_i}))}{\sum_{i=1}^{n}(T_i - e(\mathbf{X_i}))^2}$
- However, regression not feasible because nuisance parameters unknown: ML toolbox might be useful.

Double Machine Learning under Partial Linearity

- Chernozhukov et al. (2018) propose a three step procedure:
  1. Form prediction model for the treatment: $\hat{e}(\mathbf{X_i})$
  2. Form prediction model for the outcome: $\hat{\mu}(\mathbf{X_i})$
  3. Run feasible residual-on-residual regression:
     - $\hat{\tau}_{\text{ATE}} = \arg\min_{\tilde{\tau}} \frac{1}{N} \sum_{i=1}^{n} (Y_i - \hat{\mu}(\mathbf{X_i}) - \tilde{\tau}(T_i - \hat{e}(\mathbf{X_i})))^2 = \frac{\sum_{i=1}^{n} (Y_i - \hat{\mu}(\mathbf{X_i}))(T_i - \hat{e}(\mathbf{X_i}))}{\sum_{i=1}^{n} (T_i - \hat{e}(\mathbf{X_i}))^2}$

- Predictions of nuisance parameters $\hat{e}(\mathbf{X_i})$ and $\hat{\mu}(\mathbf{X_i})$ have to fulfill two conditions:
  1. High-quality: consistency and convergence rates faster than $N^{\frac{1}{4}}$.
  2. Out-of-sample: individual predictions formed without the observation itself.

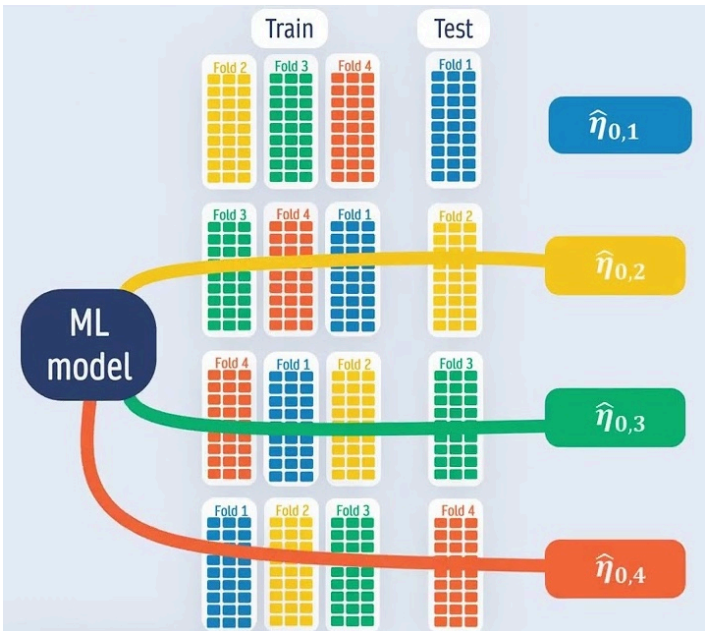
  => standard (robust) OLS inference is valid (see Chernozhukov et al. (2018)).

High Quality Predictions in DML

- Consistency: ML methods converge to the true nuisance parameters as $N \to \infty$.
- Convergence rate:
  - Parametric models like OLS converge at the rate $N^{\frac{1}{2}}$:
    - RMSE ($\mathbb{E}[\sqrt{(\hat{\mu}(\mathbf{X_i}) - \mu(\mathbf{X_i}))^2}]$) expected to halve if sample increases by factor four
  - ML methods usually do not converge as quickly because they can not leverage the structural information of a parametric model.
  - For Double ML to work, it suffices that the RMSE more than halves if we increase sample size by factor 16 (convergence rate: $N^{\frac{1}{4}}$).
  - Achievable with popular ML methods like (Post-) LASSO, Random Forests, or Neural Networks .

Out-of-Sample Predictions in DML

- K-fold Cross-Fitting:
  - Split the sample into K folds.
  - For each fold k, train a prediction model for the nuisance parameters on the remaining $K-1$ folds.
  - Predict the nuisance parameters for fold k using the model trained on the remaining $K-1$ folds.
  - Repeat for all K folds to obtain predictions for each individual observation in each fold.
  - Use combined predictions for the residual-on-residual regression.



=> Predictions are formed without the observation itself, still no waste of information.

=> Nuisance parameters induce no bias by overfitting (Chernozhukov et al. (2018)).

Neyman-orthogonal Score Functions

- Predicted nuisance parameters have to be used in a Neyman-orthogonal score function (score) ψ!
- ψ has to satisfy moment condition $\mathbb{E}[\psi(Y_i, T_i, \hat{\tau}, \hat{\mu}(\mathbf{X_i}), \hat{e}(\mathbf{X_i}))] = 0$ to identify the target parameter τ_{ATE}.
- In PLR, ψ is the solution to the minimization problem of the residual-on-residual regression - derivative w.r.t. $\hat{\tau}$:

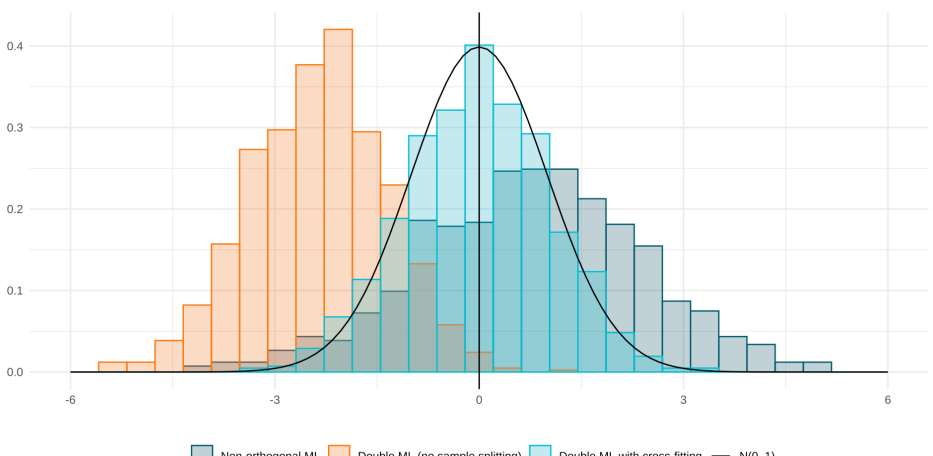
$$\frac{1}{N} \sum_{i=1}^{N} \underbrace{(Y_i - \hat{\mu}(\mathbf{X_i}) - \hat{\tau}(T_i - \hat{e}(\mathbf{X_i})))(T_i - \hat{e}(X_i))}_{\psi(Y_i, T_i, \hat{\tau}, \hat{\mu}(\mathbf{X_i}), \hat{e}(\mathbf{X_i}))} = 0$$

$$\Rightarrow \hat{\tau}_{\text{ATE}} = \frac{\sum_{i=1}^{n} (Y_i - \hat{\mu}(\mathbf{X_i}))(T_i - \hat{e}(\mathbf{X_i}))}{\sum_{i=1}^{n} (T_i - \hat{e}(\mathbf{X_i}))^2}$$

- Neyman-orthogonality of score $\psi(Y_i, T_i, \hat{\tau}, \hat{\mu}(\mathbf{X_i}), \hat{e}(\mathbf{X_i}))$:
  - (Gateaux) derivative of the score function with respect to the nuisance parameters is zero in expectation at the true value of the nuisance parameters:
    - $\partial_r \mathbb{E}[\psi(Y_i, T_i, \hat{\tau}, \mu(\mathbf{X_i}) + r(\mu(\mathbf{X_i}) - \hat{\mu}(\mathbf{X_i})), e(\mathbf{X_i}) + r(e(\mathbf{X_i}) - \hat{e}(\mathbf{X_i})))] \mid_{r=0} = 0$
  - Ensures that the $\hat{\tau}$ is robust against biases in the prediction of nuisance parameters (e.g. by regularization).
  - Note (without proof): residual-on-residual regression fulfills this requirement!

Overcoming Regularization & Overfitting Bias

- Compare a non-orthogonal score function, e.g. $\hat{\tau}_{\text{ATE}} = \frac{\sum_{i=1}^{n} T_i(Y_i - \hat{\mu}(\mathbf{X_i}))}{\sum_{i=1}^{n} T_i^2}$ to orthogonal one: $\hat{\tau}_{\text{ATE}} = \frac{\sum_{i=1}^{n} (Y_i - \hat{\mu}(\mathbf{X_i}))(T_i - \hat{e}(\mathbf{X_i}))}{\sum_{i=1}^{n} (T_i - \hat{e}(\mathbf{X_i}))^2}$.
- Compare with and without K-fold Cross-Fitting.




```r
# simulating the data
library(DoubleML)
set.seed(1234)
n_rep = 1000 # number samples
n_obs = 500 # number of observations
n_vars = 20 # number of covariates
alpha = 0.5 # true treatment effect


data = list()
for (i_rep in seq_len(n_rep)) {
# command to simulate Y_i and T_i based on true non-linear nuisance func
  data[[i_rep]] = make_plr_CCDDHNR2018(alpha=alpha, n_obs=n_obs, dim_x=n
                                       return_type="data.frame")
}

# define custom (non-othogonal) score function
non_orth_score = function(y, d, l_hat, m_hat, g_hat, smpls) {
  u_hat = y - g_hat
  psi_a = -1*d*d
  psi_b = d*u_hat
  psis = list(psi_a = psi_a, psi_b = psi_b)
  return(psis)
}

library(mlr3)
```

Double Machine Learning with Augmented Inverse Probability Weighting

Interactive Regression Model

- More general model that relaxes the homogeneous treatment assumption (binary T_i is not additively separable anymore):

$$Y_i = g(T_i, \mathbf{X_i}) + \epsilon_{Y_i}, \qquad \mathbb{E}(\epsilon_{Y_i}|T_i, \mathbf{X_i}) = 0$$
$$T_i = m(\mathbf{X_i}) + \epsilon_{T_i}, \qquad \mathbb{E}(\epsilon_{T_i}|\mathbf{X_i}) = 0$$

- We can use the identification results from the Doubly Robust / AIPW estimator:
  - Average potential outcome (APO):
    - $\mu_t^{\text{AIPW}} = \mathbb{E}[Y_i(t)] = \mathbb{E}\left[\mu(t, \mathbf{X_i}) + \frac{\mathbb{1}(T_i=t)(Y_i-\mu(t,\mathbf{X_i}))}{e_t(\mathbf{X_i})}\right]$
  - Average treatment effect (ATE):
    - $\tau_{\text{ATE}}^{\text{AIPW}} = \mathbb{E}[Y_i(1) - Y_i(0)] = \mathbb{E}\left[\mu(1, \mathbf{X_i}) - \mu(0, \mathbf{X_i}) + \frac{T_i(Y_i-\mu(1,\mathbf{X_i}))}{e_1(\mathbf{X_i})} - \frac{(1-T_i)(Y_i-\mu(0,\mathbf{X_i})}{e_0(\mathbf{X_i}))}\right]$

Double Machine Learning under AIPW

- Chernozhukov et al. (2018) propose a three step procedure:
  1. Form prediction model for the treatment: $\hat{e}(\mathbf{X_i})$
  2. Form prediction model for the outcome: $\hat{\mu}(T_i, \mathbf{X_i})$
  3. a. Estimate the APO:
     - $\mu_t^{\text{AIPW}} = \frac{1}{N} \sum_{i=1}^{n} \left(\hat{\mu}(t, \mathbf{X_i}) + \frac{\mathbb{1}(T_i=t)(Y_i - \hat{\mu}(t, \mathbf{X_i}))}{\hat{e}_t(\mathbf{X_i})} \right)$
  3. b. Estimate the ATE:
     - $\tau_{\text{ATE}}^{\text{AIPW}} = \frac{1}{N} \sum_{i=1}^{n} \left(\hat{\mu}(1, \mathbf{X_i}) - \hat{\mu}(0, \mathbf{X_i}) + \frac{T_i(Y_i - \hat{\mu}(1, \mathbf{X_i}))}{\hat{e}_1(\mathbf{X_i})} - \frac{(1-T_i)(Y_i - \hat{\mu}(0, \mathbf{X_i})}{\hat{e}_0(\mathbf{X_i}))} \right)$
- To obtain a consistent, asymptotically normal and semi-parametrically efficient estimator that allows standard (robust) inference, we need the same three key ingredients:
  1. High-quality machine learning methods
  2. K-fold cross-validation
  3. Neyman-orthogonal score function: let's proof this!

DML-AIPW Score Function (1)

- As the score defining the ATE is just the difference between APOs, it inherits ist Neyman orthogonality. Hence let's focus on the AIPW score of the APO, which is:

$$\mathbb{E}\Big[\underbrace{\mu(t,\mathbf{X_i}) + \frac{\mathbb{1}(T_i = t)(Y_i - \mu(t,\mathbf{X_i}))}{e_t(\mathbf{X_i})} - \mu_t^{\text{AIPW}}}_{\psi(Y_i,T_i,\mu(t,\mathbf{X_i}),e(\mathbf{X_i}))}\Big] = 0$$

$$\Rightarrow \mu_t^{\text{AIPW}} = \mathbb{E}\left[\mu(t,\mathbf{X_i}) + \frac{\mathbb{1}(T_i = t)(Y_i - \mu(t,\mathbf{X_i}))}{e_t(\mathbf{X_i})}\right]$$

- Neyman-orthogonality of a score ψ means that the Gateaux derivative with respect to the nuisance parameters is zero in expectation at the true nuisance parameters (NP). This means:

$$\partial_r \mathbb{E}\left[\psi(Y_i, T_i, \mu + r(\tilde{\mu} - \mu), e + r(\tilde{e} - e)) \mid \mathbf{X_i} = \mathbf{x}\right]|_{r=0} = 0$$

- where we suppress the dependencies of NPs and denote by, e.g., $\tilde{\mu}$ a value of the outcome nuisance that is different to the true value μ. We can show this equation holds with the following four steps.

DML-AIPW Score Function (2)

- 1. Add perturbations to the true nuisance parameters in the score:

$$\begin{aligned}&\psi(Y_i, T_i, \mu + r(\tilde{\mu} - \mu), e + r(\tilde{e} - e)) \\ &= (\mu + r(\tilde{\mu} - \mu)) + \frac{\mathbb{1}(T_i = t)Y_i}{e + r(\tilde{e} - e)} - \frac{\mathbb{1}(T_i = t)(\mu + r(\tilde{\mu} - \mu))}{e + r(\tilde{e} - e)} - \mu_t^{\text{AIPW}}\end{aligned}$$

- 2. Take the conditional expectation:

$$\begin{aligned}&\mathbb{E}\left[\psi(Y_i, T_i, \mu + r(\tilde{\mu} - \mu), e + r(\tilde{e} - e)) \mid \mathbf{X_i} = \mathbf{x}\right] \\ &= \mathbb{E}\left[(\mu + r(\tilde{\mu} - \mu)) + \frac{\mathbb{1}(T_i = t)Y_i}{e + r(\tilde{e} - e)} - \frac{\mathbb{1}(T_i = t)(\mu + r(\tilde{\mu} - \mu))}{e + r(\tilde{e} - e)} - \mu_t^{\text{AIPW}} \middle| \mathbf{X_i} = \mathbf{x}\right] \\ &= (\mu + r(\tilde{\mu} - \mu)) + \frac{e\mu}{e + r(\tilde{e} - e)} - \frac{e(\mu + r(\tilde{\mu} - \mu))}{e + r(\tilde{e} - e)} - \mu_t^{\text{AIPW}}\end{aligned}$$

- where we use that $\mathbb{E}[\mathbb{1}(T_i = t)Y_i \mid \mathbf{X_i} = \mathbf{x}] \overset{(A3)}{=} \mathbb{E}[\mathbb{1}(T_i = t)Y_i(t) \mid \mathbf{X_i} = \mathbf{x}] \overset{(A1)}{=} e\mu$ and $\mathbb{E}[\mathbb{1}(T_i = t) \mid \mathbf{X_i} = \mathbf{x}] = e$.

DML-AIPW Score Function (3)

- 3. Take the derivative with respect to r:

$$\begin{aligned}
&\frac{\partial}{\partial r}\mathbb{E}[\psi(Y_i, T_i, \mu + r(\tilde{\mu} - \mu), e + r(\tilde{e} - e)) \mid X_i = x] \\
&\quad = (\tilde{\mu} - \mu) - \frac{e\mu(\tilde{e} - e)}{(e + r(\tilde{e} - e))^2} - \frac{e(\tilde{\mu} - \mu)(e + r(\tilde{e} - e)) - e(\mu + r(\tilde{\mu} - \mu))(\tilde{e} - e)}{(e + r(\tilde{e} - e))^2}
\end{aligned}$$

- 4. Evaluate at the true nuisance values, i.e. set $r = 0$:

$$\begin{aligned}
&\frac{\partial}{\partial r}\mathbb{E}[\psi(Y_i, T_i, \mu + r(\tilde{\mu} - \mu), e + r(\tilde{e} - e)) \mid X_i = x]|_{r=0} \\
&\quad = (\tilde{\mu} - \mu) - \frac{e\mu(\tilde{e} - e)}{(e + 0(\tilde{e} - e))^2} - \frac{e(\tilde{\mu} - \mu)(e + r(\tilde{e} - e)) - e(\mu + 0(\tilde{\mu} - \mu))(\tilde{e} - e)}{(e + 0(\tilde{e} - e))^2} \\
&\quad = (\tilde{\mu} - \mu) - \frac{e\mu(\tilde{e} - e)}{e^2} - \frac{e(\tilde{\mu} - \mu)e - e\mu(\tilde{e} - e)}{e^2} \\
&\quad = (\tilde{\mu} - \mu) - \frac{e\mu(\tilde{e} - e)}{e^2} - \frac{e^2}{e^2}(\tilde{\mu} - \mu) + \frac{e\mu(\tilde{e} - e)}{e^2} \\
&\quad = 0
\end{aligned}$$

DML-AIPW: Example

- Assess the effect of 401(k) program participation on net financial assets of 9,915 households in the US in 1991.

```r
# Load required packages
library(DoubleML)
library(mlr3)
library(mlr3learners)
library(data.table)

# suppress messages during fitting
lgr::get_logger("mlr3")$set_threshold("warn")

# load data as a data.table
data = fetch_401k(return_type = "data.table", instrument = TRUE)

# Set up basic model: Specify variables for data-backend
features_base = c("age", "inc", "educ", "fsize","marr", "twoearn", "db", "pira", "hown")

# Initialize DoubleMLData (data-backend of DoubleML)
data_dml_base = DoubleMLData$new(data,
                                 y_col = "net_tfa", # outcome variable
                                 d_cols = "e401", # treatment variable
                                 x_cols = features_base) # covariates

# Initialize Random Forrest Learner
randomForest = lrn("regr.ranger")
randomForest_class = lrn("classif.ranger")

# Random Forest
```

```
Estimates and significance testing of the effect of target variables
     Estimate. Std. Error t value Pr(>|t|)
e401      8206       1106   7.421 1.16e-13 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

General Recipe

Definitions

- Data and parameters;
  - W is a set of observed variables; e.g., $W = \{Y, T, X\}$.
  - θ is the target parameter.
  - η is a set of nuisance parameters; e.g., $\eta = \{\mu(X), e(X)\}$.
- Score functions $\psi(W, \tilde{\theta}, \tilde{\eta})$ must satisfy two properties in Double ML:
  - $\mathbb{E}[\psi(W, \theta, \eta)] = 0$: i.e. moment condition with expectation zero if evaluated at true parameters.
  - $\partial_r \mathbb{E}[\psi(W, \theta, \eta + r(\hat{\eta} - \eta))]|_{r=0} = 0$: i.e. Neyman-orthogonality.

Examples

- Moment condition of the residual-on-residual regression:
  - $\mathbb{E}\left[(Y - \mu(X) - \tau(T - e(X)))(T - e(X))\right] = 0$
  - $W = (T, X, Y), \quad \theta = \tau, \quad \eta = (\mu(X), e(X))$
  - with $\mu(X) := \mathbb{E}[Y \mid X]$ and $e(X) := \mathbb{E}[T \mid X]$
- Moment condition of the AIPW-ATE:
  - $\mathbb{E}\left[\mu(1, X) - \mu(0, X) + \frac{T(Y-\mu(1,X))}{e(X)} - \frac{(1-T)(Y-\mu(0,X))}{1-e(X)} - \tau_{ATE}\right] = 0$
  - $W = (T, X, Y), \quad \theta = \tau_{\text{ATE}}, \quad \eta = (\mu(1, X), \mu(0, X), e(X))$
  - with $\mu(t, X) := \mathbb{E}[Y \mid T = t, X]$ and $e(X) := \mathbb{E}[T = 1 \mid X]$

Linear Score Functions

- We will focus on linear score functions that can be represented as follows:
  - $\psi(W, \tilde{\theta}, \tilde{\eta}) = \tilde{\theta}\psi_a(W, \tilde{\eta}) + \psi_b(W, \tilde{\eta})$
- such that the moment condition can be written as:
  - $\mathbb{E}[\psi(W, \theta, \eta)] = \theta\mathbb{E}[\psi_a(W, \eta)] + \mathbb{E}[\psi_b(W, \eta)] = 0$
- and the solution is:
  - $\theta = -\frac{\mathbb{E}[\psi_b(W,\eta)]}{\mathbb{E}[\psi_a(W,\eta)]}$

Example Residual-on-residual Regression

- Moment condition:

$$\mathbb{E}\left[(Y - \mu(X) - \tau(T - e(X)))(T - e(X))\right] = 0$$

$$\mathbb{E}\left[(Y - \mu(X))(T - e(X)) - \tau(T - e(X))(T - e(X))\right] = 0$$

$$\tau \underbrace{\mathbb{E}[-1(T - e(X))^2]}_{\psi_a} + \underbrace{\mathbb{E}[(Y - \mu(X))(T - e(X))]}_{\psi_b} = 0$$

$$\Rightarrow \tau = -\frac{\mathbb{E}[\psi_b(W;\eta)]}{\mathbb{E}[\psi_a(W;\eta)]} = \frac{\mathbb{E}[(Y - \mu(X))(T - e(X))]}{\mathbb{E}[(T - e(X))^2]}$$

Example AIPW-ATE

- Moment condition:

$$\mathbb{E}\left[\mu(1,X) - \mu(0,X) + \frac{T(Y-\mu(1,X))}{e(X)} - \frac{(1-T)(Y-\mu(0,X))}{1-e(X)} - \tau_{\text{ATE}}\right] = 0$$

$$\tau_{\text{ATE}}\underbrace{(-1)}_{\psi_a} + \mathbb{E}\Bigg[\underbrace{\mu(1,X) - \mu(0,X) + \frac{T(Y-\mu(1,X))}{e(X)} - \frac{(1-T)(Y-\mu(0,X))}{1-e(X)}}_{\psi_b}\Bigg] = 0$$

$$\Rightarrow \tau_{\text{ATE}} = -\frac{\mathbb{E}[\psi_b(W;\eta)]}{\mathbb{E}[\psi_a(W;\eta)]} = \mathbb{E}\left[\mu(1,X) - \mu(0,X) + \frac{T(Y-\mu(1,X))}{e(X)} - \frac{(1-T)(Y-\mu(0,X))}{1-e(X)}\right]$$

Double ML Recipe

1. Find Neyman-orthogonal score for your target parameter:
   - can be constructed (see Chernozhukov et al. (2018), Section 2)
2. Predict nuisance parameters $\hat{\eta}$ with cross-fitted high-quality ML.
3. Solve empirical moment condition to estimate the target parameter:
   - $\theta = -\frac{\mathbb{E}[\psi_b(W,\eta)]}{\mathbb{E}[\psi_a(W,\eta)]}$
4. Calculate standard error:
   - $\hat{\sigma}^2 = \frac{N^{-1}\sum_i \psi(W_i;\hat{\theta},\hat{\eta}_i)^2}{[N^{-1}\sum_i \psi_a(W_i;\hat{\eta}_i)]^2} \quad \Rightarrow \quad \text{se}(\hat{\theta}) = \sqrt{\frac{\hat{\sigma}^2}{N}}$
   - To calculate t-values, confidence intervals, etc.
   - Can be motivated by the concept of influence functions.

Standard Errors in DML

- Influence functions:
  - $\Psi(W;\theta,\eta) := -\mathbb{E}\left[\frac{\partial\psi}{\partial\theta}\right]^{-1}\psi(W;\theta,\eta) = -\mathbb{E}[\psi_a(W;\eta)]^{-1}\psi(W;\theta,\eta)$
  - Scaled version of the score with important characteristics:
    - $\Psi(W_i;\theta,\eta_i)$ measures the influence of an estimator θ to infinitesimal changes in the distribution, i.e. of each observation W_i
    - $\mathbb{E}[\Psi(W;\theta,\eta)] = \mathbb{E}[-\mathbb{E}[\psi_a(W;\eta)]^{-1}\psi(W;\theta,\eta)] = -\mathbb{E}[\psi_a(W;\eta)]^{-1}\underbrace{\mathbb{E}[\psi(W;\theta,\eta)]}_{=0} = 0$
- Estimator distribution and influence function are closely linked:
  - $\sqrt{N}(\hat{\theta}-\theta) = \frac{1}{\sqrt{N}}\sum_i \psi(W_i;\theta,\eta_i) + o_p(1) \xrightarrow{d} N(0, \underbrace{\mathrm{Var}[\psi(W;\theta,\eta)]}_{\sigma^2})$
- Estimator variance (suppressing arguments for brevity):
  - $\sigma^2 = \mathrm{Var}[\psi] = \mathbb{E}[\psi^2] - \underbrace{\mathbb{E}[\psi]^2}_{=0} = \mathbb{E}[\psi^2] = \mathbb{E}[(\mathbb{E}[\psi_a]^{-1}\psi)^2] = \mathbb{E}[\psi_a]^{-2}\mathbb{E}[\psi^2] = \frac{\mathbb{E}[\psi^2]}{\mathbb{E}[\psi_a]^2}$

Thank you for your attention!

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