MS&E 228: Inference with Modern Non-Linear Prediction

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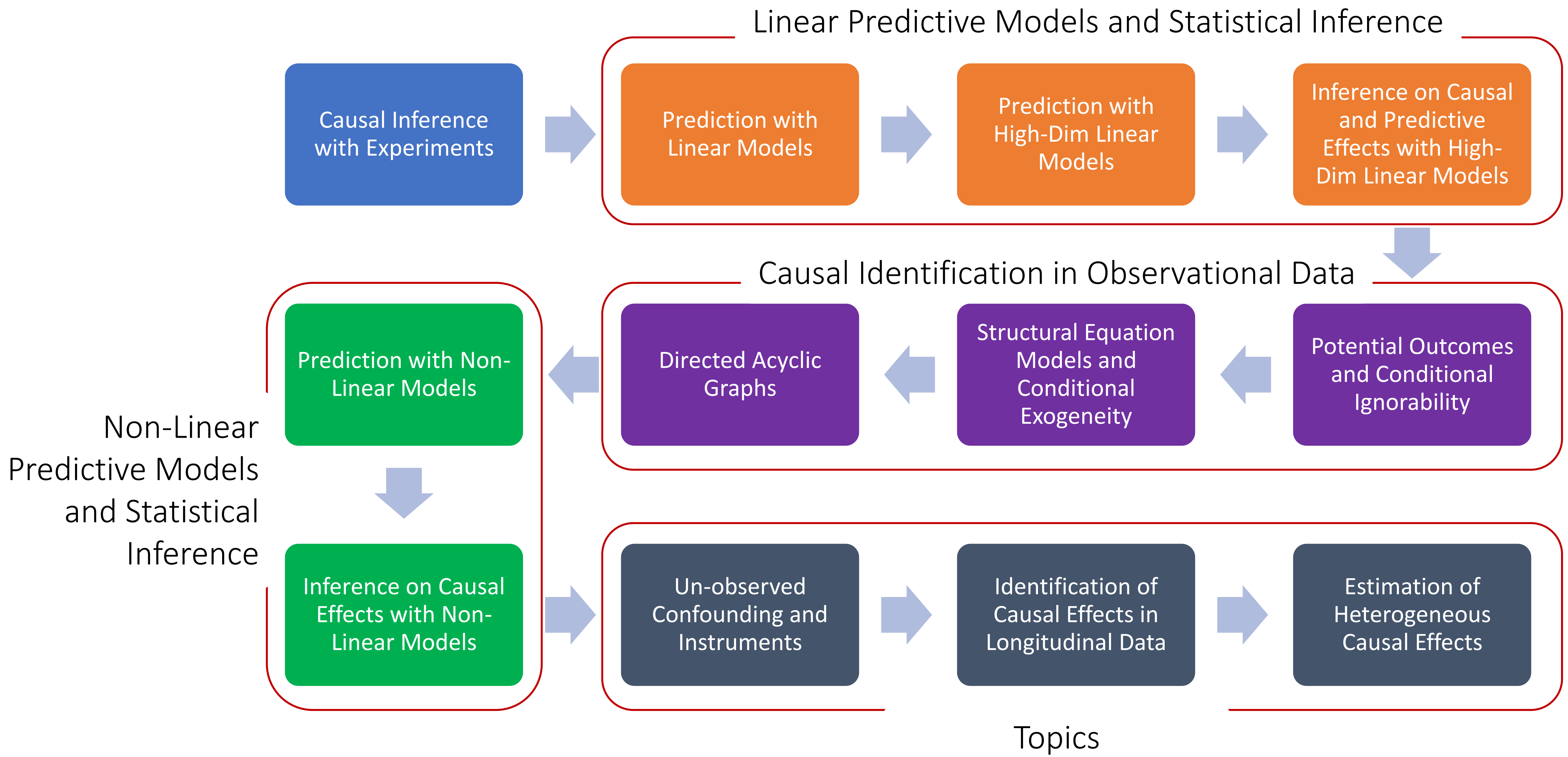
Linear Predictive Models and Statistical Inference
Causal Inference with Experiments
Prediction with Linear Models
Prediction with High-Dim Linear Models
Inference on Causal and Predictive Effects with High-Dim Linear Models
Causal Identification in Observational Data
Potential Outcomes and Conditional Ignorability
Structural Equation Models and Conditional Exogeneity
Directed Acyclic Graphs
Non-Linear Predictive Models and Statistical Inference
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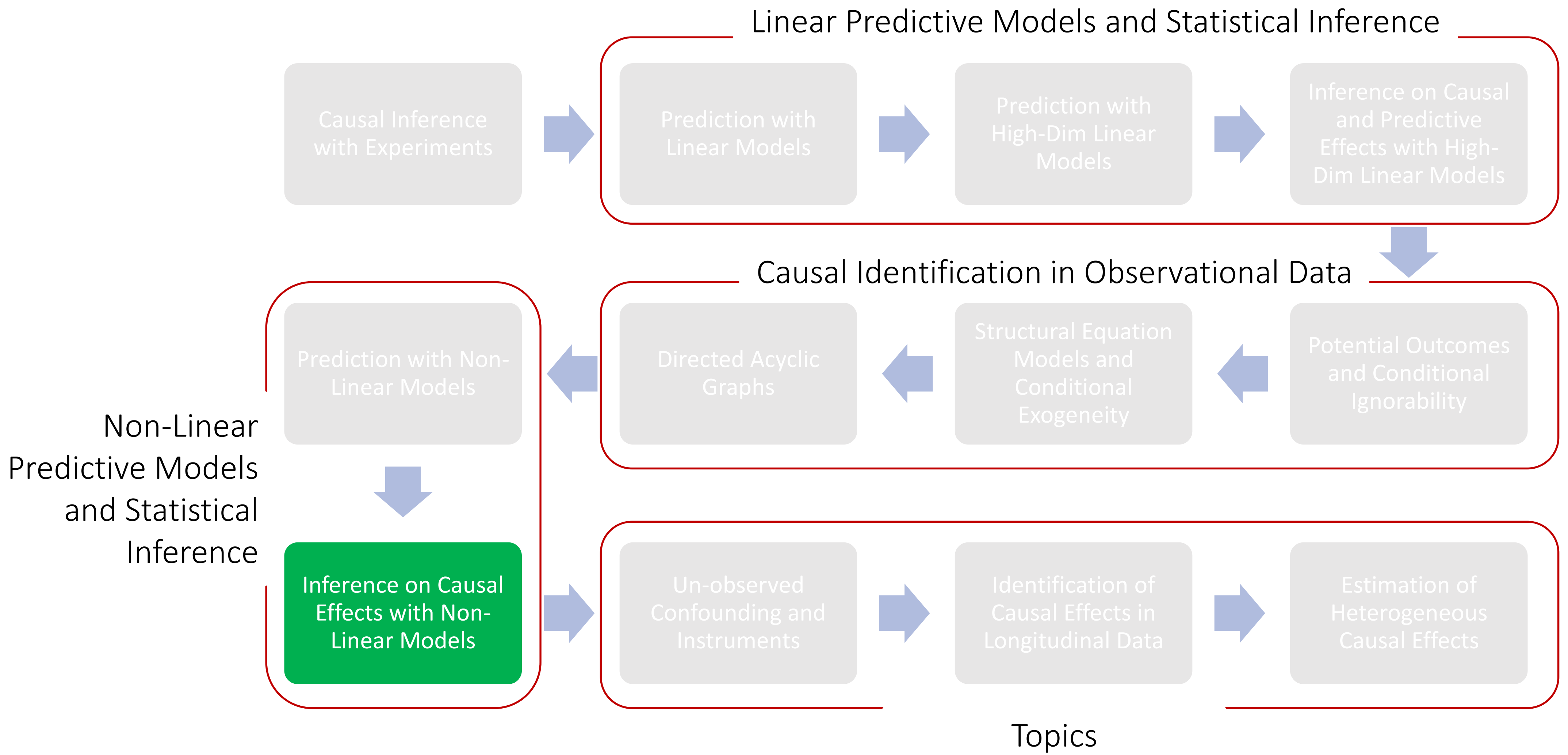
Inference on Causal Effects with Non-Linear Models
Un-observed Confounding and Instruments
Identification of Causal Effects in Longitudinal Data
Estimation of Heterogeneous Causal Effects
Topics



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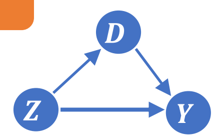
Recap of Last Lecture

Causal Inference Pipeline

Theory

DAGs/ASEMs



$$a_d = E[E[Y|D=d,Z]]$$

Construct estimate $\hat{g}(d,z)$ of predictive model

$$E[\,Y \mid D=d, Z=z\,]$$

Estimate mean counterfactual

$$\hat{a}_d = E_n[\hat{g}(d,Z)]$$

$a_d \in \hat{a}_d \pm 2\hat{\sigma}$

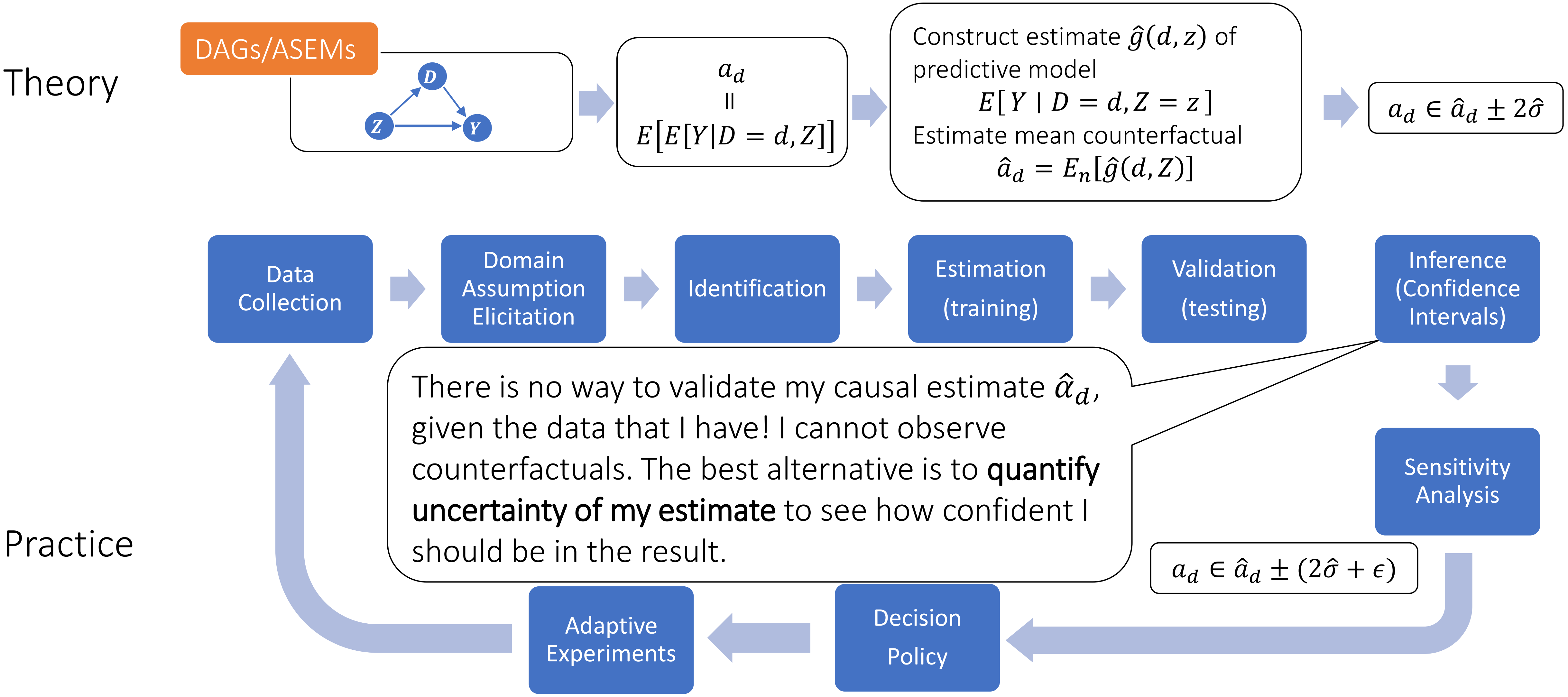
Practice

Data Collection → Domain Assumption Elicitation → Identification → Estimation (training) → Validation (testing) → Inference (Confidence Intervals) → Sensitivity Analysis → Decision Policy → Adaptive Experiments → Data Collection

So I need to estimate this **bigger predictive model, predicting the outcome from the treatment $\boldsymbol{D}$ and the controls $\boldsymbol{S}$**, in some manner. Then average the predictive values over S fixing $d = 1$.

$a_d \in \hat{a}_d \pm (2\hat{\sigma} + \epsilon)$

Causal Inference Pipeline



Goals for Today

- Methods for Confidence Intervals for ATE with non-linear models
- General Neyman Orthogonality Framework (Double/Debiased ML)
- Methods for Confidence Intervals for ATE in a partially-linear model
- Sample-splitting and cross-fitting

- Proof sketch of main theorem*

The Example Problem

Identification under Conditional Ignorability

- Once we condition on enough variables X that affect treatment assignment, remnant variation in D is exogenous (as-if trial)

$$Y^{(d)} \perp\!\!\!\perp D \mid X \quad \text{(conditional ignorability)}$$

- Why useful:

$$\begin{aligned} E[\, Y \mid D = d, X\,] &= E\left[\, Y^{(D)} \mid D = d, X\,\right] \\ &= E\left[\, Y^{(d)} \mid D = d, X\,\right] = E\left[\, Y^{(d)} \mid X\,\right] \end{aligned}$$

- Average treatment effect is "identified" as (g-formula):

$$\theta_0 = E\left[Y^{(1)} - Y^{(0)}\right] = E\left[E\left[\, Y^{(1)} - Y^{(0)} \mid X\,\right]\right]$$

$$= E\left[E[Y|D = 1, X] - E[\, Y \mid D = 0, X\,]\right]$$

Let's take it to data

- We observe n samples $Z_1, \ldots, Z_n$ where $Z_i = (X_i, D_i, Y_i)$

- Want to estimate average effect θ_0, which satisfies:

$$\theta_0 = E[g_0(1, X) - g_0(0, X)]$$

- Where:

$$g_0(D, X) \coloneqq E[\, Y \mid D, X \,]$$

- We want to be able to use ML to learn regression function g_0!

What do we want from $\hat{\theta}$?

- Ideally parametric rates for θ_0 even when we have slower rates for g_0
- Ideally construction of confidence intervals for θ_0

- One approach. Asymptotic normality

$$\sqrt{n}\left(\hat{\theta} - \theta_0\right) \to_d N\left(0, \sigma^2\right)$$

- Implies construction of approximately correct confidence intervals

with prob. $\approx$ 95%: $\theta_0 \in \left[\hat{\theta} \pm 1.96\hat{\sigma}/\sqrt{n}\right]$

Natural Estimation Algorithm

- Estimate $\hat{g}$ of g_0 from data
- Calculate empirical plug-in average:

$$\hat{\theta} \coloneqq \frac{1}{n}\sum_{i=1}^{n} \hat{g}(1, X) - \hat{g}(0, X)$$

Natural Algorithm Gone Wrong

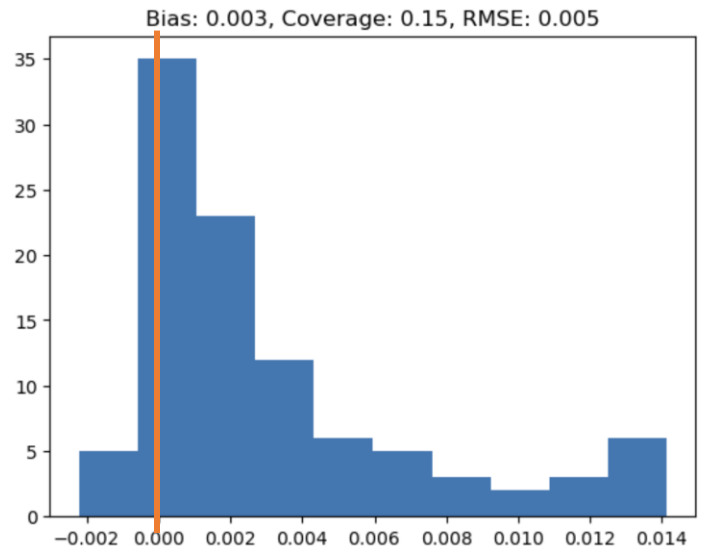
```
def est(X, D, y): # direct non-orthogonal estimator of average effect
    est = RandomForestRegressor(min_samples_leaf=20)
    est.fit(np.hstack([D.reshape(-1, 1), X]), y)
    ones = np.hstack([np.ones((X.shape[0], 1)), X])
    zeros = np.hstack([np.zeros((X.shape[0], 1)), X])
    preds = est.predict(ones) - est.predict(zeros)
    return np.mean(preds), np.std(preds)/np.sqrt(X.shape[0])
```

Simple Example

$X \sim N(0, I_{20})$

$D \sim \text{Binomial}\big(0.5 + \text{clip}(X_0, -0.4, 0.4)\big)$

$y \sim \theta_0 D + X_0 + X_1 + N(0,1)$



Natural Estimation Algorithm (Draft 2)

- Split the data in half S_1, S_2
- On first half S_1, estimate $\hat{g}$ of g_0
- Calculate empirical plug-in average on second half S_2:

$$\hat{\theta} := \frac{1}{|S_2|} \sum_{i \in S_2} \hat{g}(1, X) - \hat{g}(0, X)$$

Natural Estimation Algorithm (Draft 3)

- Split data in K parts, $S_1, \dots, S_K$
- For each part k, estimate $\hat{g}_k$ using data from all parts except S_k
- Calculate average over all data:

$$\hat{\theta} = \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in S_k} \hat{g}_k(1, X) - \hat{g}_k(0, X)$$

Natural Algorithm (Draft 3) Gone Wrong

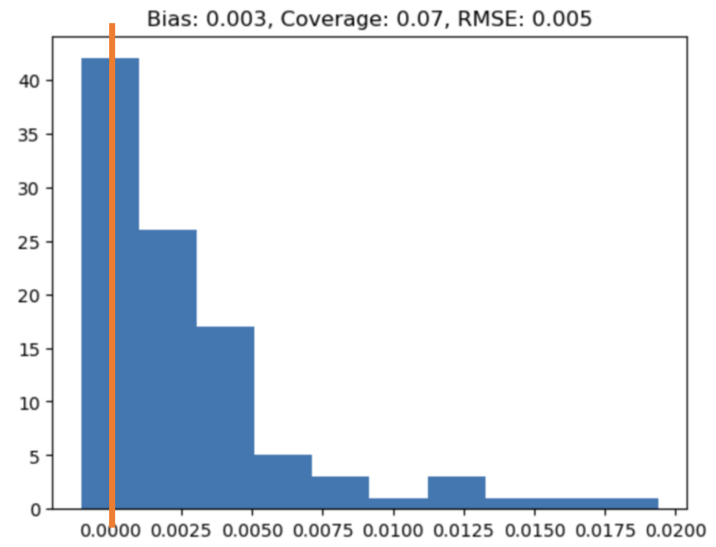
```
def est2(X, D, y): # direct non-orthogonal estimator with sample splitting
    effects = np.zeros(X.shape[0])
    for train, test in KFold(n_splits=3).split(X):
        est = RandomForestRegressor(min_samples_leaf=20)
        est.fit(np.hstack([D[train].reshape(-1, 1), X[train]]), y[train])
        ones = np.hstack([np.ones((X[test].shape[0], 1)), X[test]])
        zeros = np.hstack([np.zeros((X[test].shape[0], 1)), X[test]])
        effects[test] = est.predict(ones) - est.predict(zeros)
    return np.mean(effects), np.std(effects)/np.sqrt(X.shape[0])
```

Simple Example

$X \sim N(0, I_{20})$

$D \sim \text{Binomial}\big(0.5 + \text{clip}(X_0, -0.4, 0.4)\big)$

$y \sim \theta_0 D + X_0 + X_1 + N(0,1)$



When is estimate $\hat{\theta}$ $\sqrt{n}$-asymptotically normal?

When is estimate $\hat{\theta}$ $\sqrt{n}$-asymptotically normal?
We need to change the moment we use

Debiased Machine Learning

Average Causal Effect Example

- We observe n samples $Z_1, \ldots, Z_n$ where $Z_i = (X_i, D_i, Y_i)$
- Want to estimate average effect θ_0, which satisfies:

$$\theta_0 \coloneqq E[g_0(1, X) - g_0(0, X)]$$

- Where:

$$g_0(D, X) \coloneqq E[\, Y \mid D, X \,]$$

- The identification formula for θ_0 is sensitive to variations in g
- Any bias or error in g propagates to bias or error in moment and $\hat{\theta}$
- Can we add a correction that corrects the biases of $\hat{g}$

Better Formula for ATE

Regression residual is a proxy that g is biased

- Key Idea. Add a debiasing correction

$$M(g, a) = E[g(1, X) - g(0, X)] + E\left[a(D, X)\, \boxed{\left(Y - g(D, X)\right)}\right]$$

- What is a_0?
- Insensitivity: Take derivative with respect to g at θ_0, g_0, a_0 in any direction $\nu \in G$

$$\left.\frac{\partial}{\partial t} M(g_0 + t\,\nu, a_0)\right|_{t=0} = E[\nu(1, X) - \nu(0, X)] - E[a(D, X)\,\nu(D, X)] = 0$$

- If this holds then if g is very wrong but a is correct:

$$\theta = E[a_0(D, X) Y] = E\left[a_0(D, X) E[Y \mid D, X]\right]$$
$$= E[a_0(D, X) g(D, X)] = E[g(1, X) - g(0, X)]$$

Inverse Propensity Weighting (IPW)

- The following works: inverse propensity scoring

$$a_0(D, X) = \frac{D}{\Pr[D = 1|X]} - \frac{1 - D}{\Pr[D = 0|X]}$$

- Sketch:

$$\begin{aligned} E\left[\frac{D}{\Pr[D = 1|X]} g(D, X)\right] &= E\left[\frac{D}{\Pr[D = 1|X]} g(1, X)\right] \\ &= E\left[\frac{E[D|X]}{\Pr[D = 1|X]} g(1, X)\right] \\ &= E[g(1, X)] \end{aligned}$$

New Formula is Insensitive

$$M(g, a) = E[g(1, X) - g(0, X)] + E\big[a(D, X)\,\big(Y\ - g(D, X)\big)\big]$$

- Take derivative with respect to g at g_0, a_0 in any direction $\nu \in G$

$$\frac{\partial}{\partial t} M(g_0 + t\,\nu, a_0)\Big|_{t=0} = E[\nu(1, X) -\ \nu(0, X)] - E[a(D, X)\,\nu(D, X)] = 0$$

Take derivative with respect to a at g_0, a_0 in any direction $\nu \in A$

$$\frac{\partial}{\partial t} M(g_0, a_0 + t\nu)\Big|_{t=0} = E\big[\nu(D, X)\,\big(Y - g_0(D, X)\big)\,\big] = 0$$

Asymptotic Normality of De-biased Estimate

$$\hat{\theta} \coloneqq E_n\big[\hat{g}(1,X) - \hat{g}(0,X) + \hat{a}(D,X) \cdot \big(Y \ - \ \hat{g}(D,X)\big)\big]$$

- *Assume* that propensities are bounded away from 0 and 1 (strict overlap)
- *Assume* $\hat{g}, \hat{a}$ estimated on separate sample (or cross-fitting), are consistent and:

$$\sqrt{n}\, E\big[\big(a_0(D,X) - \hat{a}(D,X)\big)\big(\hat{g}(D,X) - g_0(D,X)\big)\big] \rightarrow_p 0$$

- *Assume* random variables $Y, a(D,X), g(D,X)$ have bounded fourth moments
- Then:

$$\sqrt{n}\big(\hat{\theta} - \theta_0\big) \rightarrow_d N\big(0, \sigma^2\big), \qquad \hat{\sigma}^2 = Var_n\Big(\hat{g}(1,X) - \hat{g}(0,X) + \hat{a}(X) \cdot \big(Y - \hat{g}(X)\big)\Big)$$

Python Pseudocode

```
cv = KFold(n_splits=nfolds, shuffle=True, random_state=123)
yhat0, yhat1 = np.zeros(y.shape), np.zeros(y.shape)
# we will fit a model E[Y| D, X] by fitting a separate model for D==0
# and a separate model for D==1.
for train, test in cv.split(X, y):
    # train a model on training data that received zero and predict on all test data
    yhat0[test] = modely.fit(X[train][D[train]==0], y[train][D[train]==0]).predict(X[test])
    # train a model on training data that received one and predict on all test data
    yhat1[test] = modely.fit(X[train][D[train]==1], y[train][D[train]==1]).predict(X[test])
# prediction for observed treatment
yhat = yhat0 * (1 - D) + yhat1 * D
# propensity scores
Dhat = cross_val_predict(modeld, X, D, cv=cv, method='predict_proba', n_jobs=-1)[:, 1]
Dhat = np.clip(Dhat, trimming, 1 - trimming)
# doubly robust quantity for every sample
drhat = yhat1 - yhat0 + (y - yhat) * (D/Dhat - (1 - D)/(1 - Dhat))
point = np.mean(drhat)
var = np.var(drhat)
stderr = np.sqrt(var / X.shape[0])
return point, stderr, yhat, Dhat, y - yhat, D - Dhat, drhat
```

Continuous Treatments under Partial Linearity

Partially Linear Model

- Relevant in many applications: dose-response curve in healthcare, effect of price on demand, return-on-investment
- Assume conditional exogeneity
$$Y^{(d)} \perp\!\!\!\perp D \mid X$$
- Assume partially linear response
$$Y = \theta_0 D + f_0(X) + \epsilon, \qquad E[\,\epsilon \mid D, X\,] = 0$$
- Equivalently, a partial linearity condition on the conditional expectation function
$$g_0(D, X) = E[\,Y \mid D, X\,] = \theta_0 D + f_0(X)$$
- Parameter of interest θ_0 is constant marginal effect of treatment

Generalization of FWL Theorem

- Let's define a slight variant of residualization

$$\tilde{V} = V - E[V|X]$$

- Generalization of FWL theorem to partially linear models

$$\tilde{Y} = \theta_0 \tilde{D} + \epsilon, \qquad E\left[\epsilon \middle| \tilde{D}\right] = 0$$

- Let's consider the residual outcome

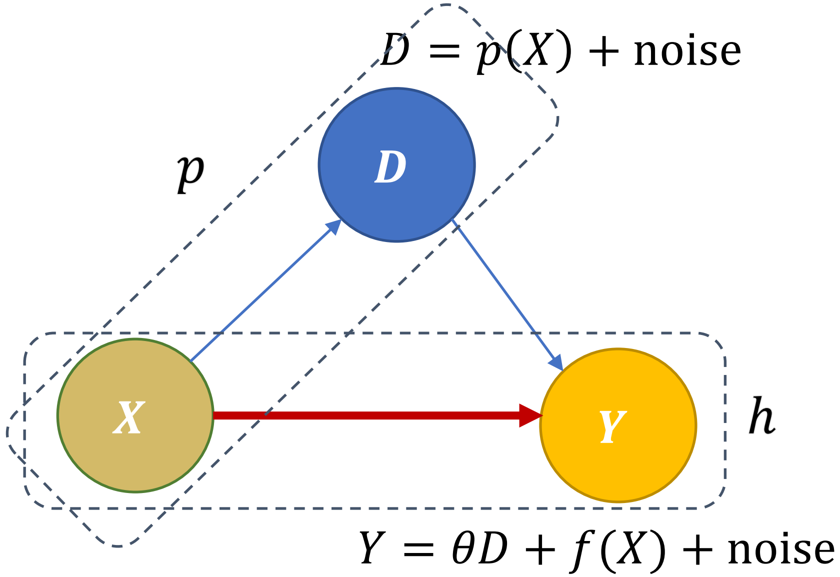
Regression model $h_0(X)$ predicting the outcome from the controls

$$\begin{aligned}\tilde{Y} &= Y - \boxed{E[Y|X]} \\ &= \theta_0 D + f_0(X) + \epsilon - E[\theta_0 D + f_0(X) + \epsilon|X] \\ &= \theta_0 D + f_0(X) + \epsilon - \theta_0 E[D|X] - f_0(X) \\ &= \theta_0(D - \boxed{E[D|X]}) + \epsilon\end{aligned}$$

Regression model $p_0(X)$ predicting the treatment from the controls

Orthogonal Method: Double ML

- **Double ML.** Split samples in half
  - Regress $Y \sim X$ with ML on first half, to get estimate $\hat{h}(S)$ of $E[Y|X]$
  - Regress $D \sim X$ with ML on first half, to get estimate $\hat{p}(S)$ of $E[D|X]$



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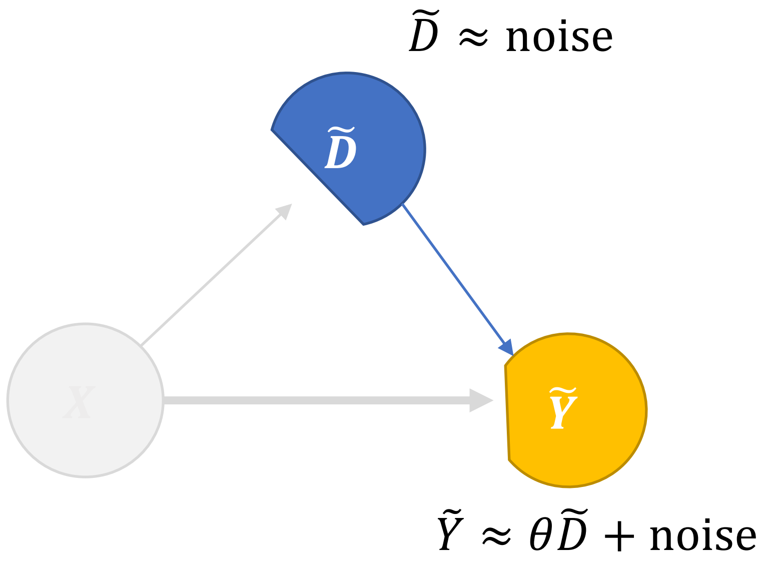
  - Regress $D \sim X$ with ML on first half, to get estimate $\hat{p}(S)$ of $E[D|X]$
  - Construct residuals on other half, $\widehat{D} \coloneqq D - \hat{p}(X)$ and $\hat{Y} \coloneqq Y - \hat{h}(X)$
  - Run OLS on residuals: $\hat{Y} \sim \widehat{D}$ to get $\hat{\theta}$

- Final OLS, *in population limit*, equivalent to solving normal equation:
$$E\left[\left(\tilde{Y} - \theta\widetilde{D}\right)\widetilde{D}\right] = 0$$
- Define the *formula*:
$$M(\theta;\ h, p) = E\left[\left(Y - h(X) - \theta\left(D - p(X)\right)\right)\ \left(D - p(X)\right)\right]$$
- Final OLS, *in population limit*, equivalent to solving for θ:
$$M(\theta; h_0, p_0) = 0$$



Insensitivity of Double ML Method

- The *formula* M is insensitive to the nuisance functions h, p

$$M(\theta, h, p) = E\left[\left(Y - h(X) - \theta\left(D - p(X)\right)\right)\ \left(D - p(X)\right)\right]$$

- Directional derivative with respect to h

$$\left.\frac{\partial}{\partial t} M(\theta_0; h_0, p_0 + t\,\nu)\right|_{t=0} = -E\left[\nu(X)\left(D - p_0(X)\right)\right] = E\left[\nu(X) E[\,D - p_0(X) \mid X\,]\right] = 0$$

- Directional derivative with respect to p

$$\left.\frac{\partial}{\partial t} M(\theta_0;\ h_0, p_0 + t\,\nu)\right|_{t=0} = E\left[\nu(X)\left(D - p_0(X)\right)\right] - E\left[\left(Y - h_0(X) - \theta_0\left(D - p_0(X)\right)\right)\nu(X)\right] = 0$$

Asymptotic Normality of DoubleML Estimate

$$E_n\left[\left(\hat{Y} - \theta\widehat{D}\right)\widehat{D}\right] = 0 \Leftrightarrow \hat{\theta} = \frac{E_n\left[\hat{Y}\widehat{D}\right]}{E_n\left[\widehat{D}^2\right]}$$

- *Assume* that $E\left[\widetilde{D}^2\right] = E[Var(\,D \mid X\,)] > 0$ (average overlap)
- *Assume* $\hat{h}, \hat{p}$ estimated on separate sample (or cross-fitting), are consistent and:

$$\sqrt{n}\,\left(\mathrm{RMSE}\left(\hat{h}\right) \cdot \mathrm{RMSE}(\hat{p}) + \mathrm{RMSE}(\hat{p})^2\right) \to_p 0$$

- *Assume* random variables Y, D, X have bounded fourth moments

$$\sqrt{n}\left(\hat{\theta} - \theta_0\right) \to_d N\left(0, \sigma^2\right),$$

Estimate asymptotically normal

$$\sigma^2 := \frac{E\left[\left(\tilde{Y} - \theta_0\widetilde{D}\right)^2\widetilde{D}^2\right]}{E\left[\widetilde{D}^2\right]^2},$$

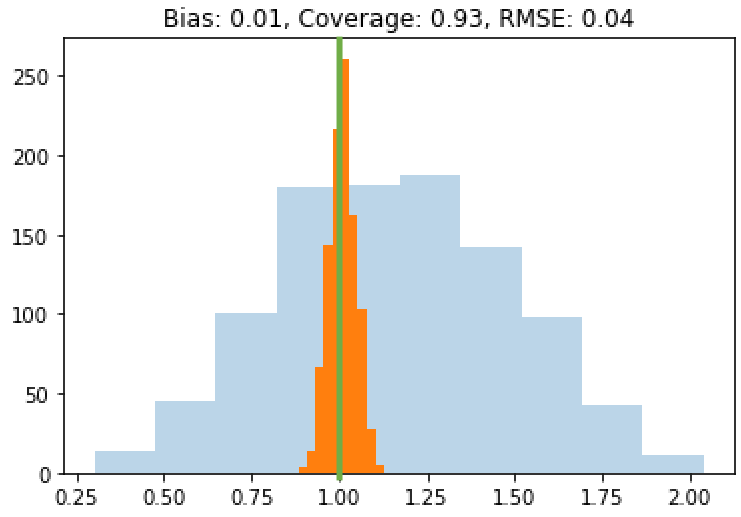
Asymptotic variance

$$\hat{\sigma}^2 = \frac{E_n\left[\left(\hat{Y} - \hat{\theta}\,\widehat{D}\right)^2\widehat{D}^2\right]}{E_n\left[\widehat{D}^2\right]^2}$$

Estimate of variance $\Rightarrow$ 95% CI $\left[\theta \pm 1.96\frac{\hat{\sigma}}{\sqrt{n}}\right]$

Natural Algorithm (Draft 3) Gone Right

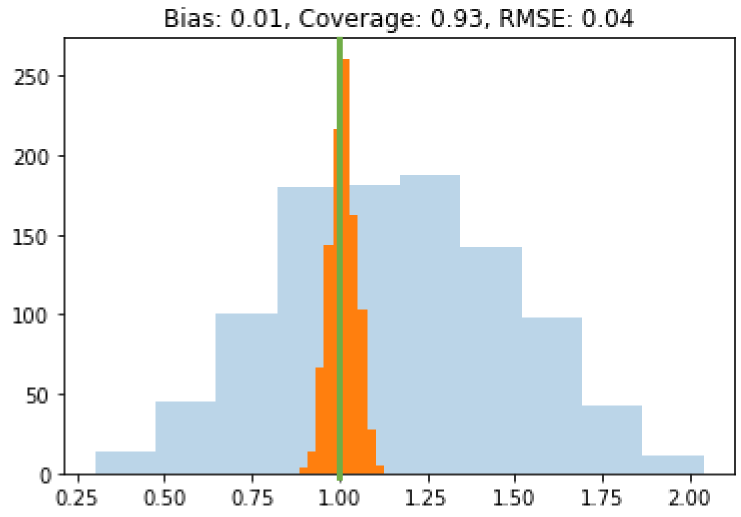
```
def dml2(X, D, y): # orthogonal dml with sample-splitting
    est_y = RandomForestRegressor(min_samples_leaf=20)
    yres = y - cross_val_predict(est_y, X, y, cv=3)
    est_t = RandomForestRegressor(min_samples_leaf=20)
    Dres = D - cross_val_predict(est_t, X, D, cv=3)
    theta = np.mean(yres * Dres) / np.mean(Dres**2)
    var = np.mean((Dres**2) * (yres - theta*Dres)**2) / np.mean(Dres**2)
    stderr = np.sqrt(var / X.shape[0])
    return theta, stderr
```



Natural Algorithm (Draft 3) Gone Right

```
from econml.dml import LinearDML

dml = LinearDML(model_y=RandomForestRegressor(min_samples_leaf=20),
                model_t=RandomForestRegressor(min_samples_leaf=20))
est.fit(y, D, W=X).effect_inference()
```



Proof sketch

$$\sqrt{n}(\hat{\theta} - \theta_0) = \sqrt{n}\left(\frac{E_n[\hat{Y}\widehat{D}]}{E_n[\widehat{D}^2]} - \theta_0\right)$$

$$\boxed{\approx \sqrt{n}\left(\frac{E_n[\tilde{Y}\widetilde{D}]}{E_n[\widetilde{D}^2]} - \theta_0\right)}$$

Due to insensitivity of the formula and fast enough rates of the nuisance models, we can ignore the error in the residuals

$$= \sqrt{n}\left(\frac{E_n[\tilde{Y}\widetilde{D}]}{E_n[\widetilde{D}^2]} - \frac{E_n[\widetilde{D}^2]}{E_n[\widetilde{D}^2]}\theta_0\right)$$

$$= \sqrt{n}\left(\frac{E_n[(\tilde{Y} - \theta_0\widetilde{D})\widetilde{D}]}{E_n[\widetilde{D}^2]}\right)$$

$$\boxed{\approx \sqrt{n}\left(\frac{E_n[(\tilde{Y} - \theta_0\widetilde{D})\widetilde{D}]}{E[\widetilde{D}^2]}\right)} = \sqrt{n}E_n\left[\frac{(\tilde{Y} - \theta_0\widetilde{D})\widetilde{D}}{E[\widetilde{D}^2]}\right] \boxed{\to_d N\left(0, Var\left(\frac{(\tilde{Y} - \theta_0\widetilde{D})\widetilde{D}}{E[\widetilde{D}^2]}\right)\right)}$$

By law of large numbers, the denominator can be replaced by the expectation, $E_n[\widetilde{D}^2] \approx E[\widetilde{D}^2]$

Central Limit Theorem

(Extended) Partially Linear Model

- Relevant in many applications: dose-response curve in healthcare, effect of price on demand, return-on-investment
- Assume conditional exogeneity

$$Y^{(d)} \perp\!\!\!\perp D \mid X$$

- Assume partially linear response, for a known feature map ϕ

$$Y = \theta_0{}'\phi(D, X) + f_0(X) + \epsilon, \qquad E[\,\epsilon \mid D, X\,] = 0$$

- Parameter of interest θ_0
- **Example:** in pricing applications $\phi(D, X) = \left(D, D^2, X \cdot D, X \cdot D^2\right)$

Orthogonal Method: (Extended) Double ML

- **Double ML.** Split samples in half
  - Regress $Y \sim X$ with ML on first half, to get estimate $\hat{h}(S)$ of $E[Y|X]$
  - Regress $\phi(D,X) \sim X$ with ML on first half, to get estimate $\hat{p}(S)$ of $E[\phi(D,X)|X]$
  - Construct residuals on other half, $\widetilde{D} \coloneqq \phi(D,X) - \hat{p}(X)$ and $\tilde{Y} \coloneqq Y - \hat{h}(X)$
  - Run OLS on residuals: $\tilde{Y} \sim \widetilde{D}$ to get $\hat{\theta}$

- Final OLS, in population limit, equivalent to solving normal equation:

$$E\left[\left(\tilde{Y} - \theta'\widetilde{D}\right)\widetilde{D}\right] = 0$$

- Define the *formula*:

$$M(\theta, h, p) = E\left[\left(Y - h(X) - \theta'\left(\phi(D,X) - p(X)\right)\right)\ \left(\phi(D,X) - p(X)\right)\right]$$

- OLS is equivalent to solving with respect to θ:

$$M(\theta, h_0, p_0) = 0$$

Asymptotic Normality of DoubleML Estimate

$$E_n\left[\left(\hat{Y} - \theta\widehat{D}\right)\widehat{D}\right] = 0 \Leftrightarrow \hat{\theta} = E_n\left[\widehat{D}\widehat{D}'\right]^{-1} E_n\left[\widehat{D}\hat{Y}\right]$$

- *Assume* that $E\left[\widetilde{D}\widetilde{D}'\right] \succcurlyeq 0$ (minimum eigenvalue bounded away)
- *Assume* $\hat{h}, \hat{p}$ estimated on separate sample (or cross-fitting), are consistent and:

$$\sqrt{n}\left(\mathrm{RMSE}\left(\hat{h}\right) \cdot \mathrm{RMSE}(\hat{p}) + \mathrm{RMSE}(\hat{p})^2\right) \to_p 0$$

- *Assume* random variables Y, D, X have bounded fourth moments

$$\sqrt{n}\left(\hat{\theta} - \theta_0\right) \to_d N(0, V), \qquad \hat{V} \coloneqq \boxed{E_n\left[\widehat{D}\widehat{D}'\right]^{-1} E_n\left[\left(\hat{Y} - \hat{\theta}\widehat{D}\right)^2 \widehat{D}\widehat{D}'\right] E_n\left[\widehat{D}\widehat{D}'\right]^{-1}}$$

Sandwich formula for heteroskedasticity-robust standard errors in OLS packages (HC0)

General Theory

Estimation from Moment Restrictions

- Observe samples $Z_1, \ldots, Z_n$ i.i.d. from data distribution D
- Parameter of interest $\theta_0 \in \mathbb{R}^d$ is identified as the solution to a set of *population formulas*

$$\boxed{M(\theta_0; g_0) := E_{Z\sim D}[m(Z; \theta_0, g_0)] = 0}$$

Vector of moment restrictions that distribution D needs to satisfy and which have a unique solution with respect to θ

- $g_0 \in G$ a function we don't care (*nuisance function*) but need to estimate from data

Examples.

$$m(Z; \theta, g, a) = g(1, X) - g(0, X) - a(D, X)\big(Y - g(D, X)\big) - \theta$$ *(ATE for binary treatment)*

$$m(Z; \theta, h, p) = \Big(Y - h(X) - \theta\big(D - p(X)\big)\Big) \cdot \big(D - p(X)\big)$$ *(ATE under PLR model)*

Cross-fitting Estimation Algorithm

Split the data in half

- On first half, estimate $\hat{g}_1$ of g_0 and predict on second half
- On second half, estimate $\hat{g}_2$ of g_0 and predict on first half

On all data, solution $\hat{\theta}$ to empirical plug-in moment equation:

$$M_n(\hat{\theta}, \hat{g}) := \frac{1}{n} \sum_{i \in S_1} m(Z_i; \hat{\theta}, \hat{g}_2) + \frac{1}{n} \sum_{i \in S_2} m(Z_i; \hat{\theta}, \hat{g}_1) = 0$$

In practice use $K \approx 3 \text{ to } 5$ folds: for each fold, train on all other folds and predict on that fold

Neyman Orthogonality (Insensitivity)

Moment $M(\theta, g)$ is Neyman orthogonal if for any $\nu \in G - g_0$:

$$\frac{\partial}{\partial t} M(\theta_0, g_0 + t\,\nu)\bigg|_{t=0} = 0$$

Main Theorem

If moment is Neyman orthogonal and RMSE of $\hat{g}$ is $o_p\left(n^{-1/4}\right)$, plus regularity conditions

$$\sqrt{n}\left(\hat{\theta} - \theta_0\right) \rightarrow N\left(0, J_0^{-1}\Sigma\left(\mathrm{J}_0^{-1}\right)^{\top}\right)$$

where $J_0 \coloneqq \nabla_\theta M(\theta_0, g_0)$ and $\Sigma \coloneqq E\left[m(Z;\theta_0, g_0)\, m(Z;\theta_0, g_0)^{\top}\right]$

Practical Variants of Cross-Fitting

Stacking and Model Selection

- If we want to choose among many models or perform stacking, we can just use a stacked or automl model in place of each ML model

Stacking ML Models

```
def dml2(X, D, y): # orthogonal dml with sample-splitting
    est_y = StackingRegressor([rf, nnet, gbf, lasso])
    yres = y - cross_val_predict(est_y, X, y, cv=3)
    est_t = StackingRegressor([rf, nnet, gbf, lasso])
    Dres = D - cross_val_predict(est_t, X, D, cv=3)
    theta = np.mean(yres * Dres) / np.mean(Dres**2)
    var = np.mean((Dres**2) * (yres - theta*Dres)**2) / np.mean(Dres**2)
    stderr = np.sqrt(var / X.shape[0])
    return theta, stderr
```

AutoML Models

```
from flaml import AutoML

def dml2(X, D, y): # orthogonal dml with sample-splitting
    est_y = AutoML()
    yres = y - cross_val_predict(est_y, X, y, cv=3)
    est_t = AutoML()
    Dres = D - cross_val_predict(est_t, X, D, cv=3)
    theta = np.mean(yres * Dres) / np.mean(Dres**2)
    var = np.mean((Dres**2) * (yres - theta*Dres)**2) / np.mean(Dres**2)
    stderr = np.sqrt(var / X.shape[0])
    return theta, stderr
```

Stacking and Model Selection

- If we want to choose among many models or perform stacking, we can just use a stacked or automl model in place of each ML model
- Model selection or stacking done many times within each training fold
- Computationally expensive and statistically lossy

- Can we use all the data to at least select among models?

Semi-Crossfitting Estimation Algorithm

Split the data in half *(in practice K folds)*

- On first half, estimate $\hat{g}_1^{(1)}, \dots, \hat{g}_1^{(\mathrm{L})}$ of g_0 and predict on second half
- On second half, estimate $\hat{g}_2^{(1)}, \dots, \hat{g}_2^{(\mathrm{L})}$ of g_0 and predict on first half

- Choose the model $\ell \in \{1, \dots, L\}$ that optimizes out-of-sample RMSE

- On all data, solution $\hat{\theta}$ to empirical plug-in moment equation:

$$M_n(\hat{\theta}, \hat{g}) := \frac{1}{n}\sum_{i \in S_1} m\left(Z_i; \hat{\theta}, \hat{g}_2^{(\ell)}\right) + \frac{1}{n}\sum_{i \in S_2} m\left(Z_i; \hat{\theta}, \hat{g}_1^{(\ell)}\right) = 0$$

Semi-Crossfitting

```python
def dml2(X, D, y): # orthogonal dml with semi-crossfitting
    # cross val predict with many models
    est_y = [rf, gbf, lasso]
    yres = np.array([y - cross_val_predict(est, X, y, cv=3) for est in est_y])
    est_d = [rf, gbf, lasso]
    Dres = np.array([D - cross_val_predict(est, X, D, cv=3) for est in est_d])
    # select models with best out of fold performance
    best_y = np.argmin(np.mean(yres**2, axis=1))
    best_d = np.argmin(np.mean(Dres**2, axis=1))
    yres = yres[best_y]
    Dres = Dres[best_d]
    # go with their corresponding residuals
    theta = np.mean(yres * Dres) / np.mean(Dres**2)
    var = np.mean((Dres**2) * (yres - theta*Dres)**2) / np.mean(Dres**2)
    stderr = np.sqrt(var / X.shape[0])
    return theta, stderr
```

Semi-Crossfitting

- If the number of models L is small, then "spillover" is ok and approach still works. For practical purposes L should be thought as constant.
- Under further regularity, provably asymptotic normality holds if

$$\sqrt{\log(L)} = \mathrm{o}\left(\mathrm{n}^{1/4}\right)$$

Semi-Crossfitting with Stacking

Split the data in half *(in practice K folds)*

- On first half, estimate $\hat{g}_1^{(1)}, \ldots, \hat{g}_1^{(\mathrm{L})}$ of g_0 and predict on second half
- On second half, estimate $\hat{g}_2^{(1)}, \ldots, \hat{g}_2^{(\mathrm{L})}$ of g_0 and predict on first half

- Construct weights $\alpha = (\alpha_1, \ldots, \alpha_L)$ on the models using all the data (stacking)
- Define stacked models $\hat{g}_k^{(\alpha)} = \sum_{j=1}^{L} a_j \cdot \hat{g}_k^{(j)}$

- On all data, solution $\hat{\theta}$ to empirical plug-in moment equation:

$$M_n(\hat{\theta}, \hat{g}) := \frac{1}{n} \sum_{i \in S_1} m\left(Z_i; \hat{\theta}, \hat{g}_2^{(\alpha)}\right) + \frac{1}{n} \sum_{i \in S_2} m\left(Z_i; \hat{\theta}, \hat{g}_1^{(\alpha)}\right) = 0$$

Semi-Crossfitting with Stacking

```
def dml2(X, D, y): # orthogonal dml with semi-crossfitting and stacking
    # cross val predict with many models
    est_y = [rf, gbf, lasso]
    ypreds = np.array([cross_val_predict(est, X, y, cv=3) for est in est_y]).T
    est_d = [rf, gbf, lasso]
    Dpreds = np.array([cross_val_predict(est, X, D, cv=3) for est in est_d]).T
    # calculate stacked residuals by finding optimal coefficients
    # and weigthing out-of-sample predictions by these coefficients
    yres = y - LinearRegression().fit(ypreds, y).predict(ypreds)
    Dres = D - LinearRegression().fit(Dpreds, D).predict(Dpreds)
    # go with the stacked residuals
    theta = np.mean(yres * Dres) / np.mean(Dres**2)
    var = np.mean((Dres**2) * (yres - theta*Dres)**2) / np.mean(Dres**2)
    stderr = np.sqrt(var / X.shape[0])
    return theta, stderr
```

Semi-Crossfitting

- If the number of models L is small, then "spillover" is ok and approach still works. For practical purposes L should be thought as constant.
- Under further regularity, provably asymptotic normality holds if

$$\sqrt{L} = \mathrm{o}\left(\mathrm{n}^{1/4}\right)$$

Equivalent view of cross-fitting with stacking (lens of FWL theorem)

- Construct out of fold predictions based on many ML models
- Use these predictions as engineered features X in a simple OLS regression on D, X
- Use the coefficient and standard error of D from this final OLS

Appendix:
General Theory (Expanded)

Main Theorem (expanded)

Define RMSE: $\|h\|_{L^2} = \sqrt{E[h(X)^2]}$

- If moment is Neyman orthogonal and RMSE of $\hat{g}$ goes down at rate $n^{1/4}$, plus regularity conditions

$$n^{1/4}\|\hat{g} - g_0\|_{L^2} \approx 0$$

- Then the estimate $\hat{\theta}$ is *asymptotically linear*

$$\sqrt{n}\left(\hat{\theta} - \theta_0\right) \approx \sqrt{n}\, E_n[\phi_0(Z)], \qquad \phi_0(Z) = -J_0^{-1}\, m(Z;\theta_0, g_0), \qquad J_0 := \partial_\theta E[m(Z;\theta_0, g_0)]$$

Jacobian of moments with respect to parameter; relates to identification strength

influence function

influence is a linear transformation of the moment; transforming from "moment space" to "parameter space"

- Consequently, it is *asymptotically normal*

$$\sqrt{n}\left(\hat{\theta} - \theta_0\right) \sim_a N(0, V), \qquad V := E[\phi_0(Z)\phi_0(Z)']$$

Covariance of the influence function

- *Confidence intervals* for any projection based on estimate of variance are asymptotically valid

$$\ell'\theta \in \left[\ell'\hat{\theta} \pm c\sqrt{\frac{\ell'\hat{V}\ell}{n}}\right], \qquad \hat{V} = \mathrm{Var}_n\left(\hat{\phi}(Z)\right), \qquad \hat{\phi}(Z) := -\hat{J}^{-1} m\left(Z;\hat{\theta},\hat{g}\right), \qquad \hat{J} = \partial_\theta E_n\left[m\left(Z;\hat{\theta},\hat{g}\right)\right]$$

Empirical variance of approximate influence

Approximate influence function

Empirical average of jacobian

Python Pseudocode

```python
# General DML pseudocode
def general_dml(Z, ell, nfolds, moment, jacobian, nuisance
    # construct out-of-fold predictions from the nuisan
    ghat = cross_val_predict(nuisance_estimator, Z, cv=nfol
     use these predictions to define the empirical moment
     with respect to theta
    avg_moment = lambda theta: np.mean(moment(Z, theta, ghat), axis=0)
    # solve for the empirical moment equation equals zero
    thetahat = fsolve(avg_moment)
    # calculate empirical jacobian with respect to theta, evaluated
    # at the estimates thetahat and ghat
    Jhat = np.mean(jacobian(Z, thetahat, ghat), axis=0)
    # construct approximate influence function for each sample
    phihat = - moment(Z, thetahat, ghat) @ np.linalg.pinv(Jhat).T
    # variance estimate
    var = phihat.T @ phihat / phihat.shape[0]
    # estimate and standard error for any projection ell of the pa
    point = ell @ thetahat
    stderr_ell = np.sqrt(ell.T @ var @ ell / phihat.shape[0])
    return point, stderr_ell
```

Estimate $\hat{g}$ out of fold and predict

Construct cross-fitted moment function
$\theta \to E_n[m(Z;\theta,\hat{g})]$

Solve that moment = 0 wrt θ

Calculate
$\hat{J} := \partial_\theta E_n[m(Z;\hat{\theta},\hat{g})]$

Approximate influence function
$Z \to \hat{\phi}(Z) := \hat{J}^{-1} m(Z;\hat{\theta},\hat{g})$

Empirical covariance of estimate
$\hat{V} = E_n[\hat{\phi}(Z)\hat{\phi}(Z)']$

Main Theorem (linear moments)

- If moments are linear
$$m(Z;\theta,g)=\nu(Z;g)-a(Z;g)\theta$$
- Estimate is closed form:
$$\hat\theta=\hat J^{-1}E_n[\nu(Z;g)],\qquad \hat J=E_n[a(Z;g)]$$
- Then the estimate $\hat\theta$ is *asymptotically linear*
$$\sqrt{n}\left(\hat\theta-\theta_0\right)\approx\sqrt{n}\,E_n[\phi_0(Z)],\qquad \phi_0(Z)=-J_0^{-1}\,m(Z;\theta_0,g_0),\qquad J_0:=E[a(Z;\ g_0)]$$
- Consequently, it is *asymptotically normal*
$$\sqrt{n}\left(\hat\theta-\theta_0\right)\sim_a N(0,V),\qquad V:=E[\phi_0(Z)\phi_0(Z)']$$
- *Confidence intervals* for any projection based on estimate of variance are asymptotically valid
$$\ell'\theta\in\left[\ell'\hat\theta\pm c\sqrt{\frac{\ell'\hat V\ell}{n}}\right],\qquad \widehat{\mathrm{V}}=\mathrm{Var_n}\left(\hat\phi(Z)\right),\qquad \hat\phi(Z):=-\hat J^{-1}m\left(Z;\hat\theta,\hat g\right),\qquad \hat J=E_n[a(Z;\hat g)]$$

Python Pseudocode

```
# General DML pseudocode for linear moments: m(Z; theta, g)
def general_dml_linear_moment(Z, ell, nfolds, alpha, nu, ja
    # construct out-of-fold predictions from the nuisance
    ghat = cross_val_predict(nuisance_estimator, Z, cv=nfolds)
    # use these predictions to define the empirical moment equation
    # and solve explicitly with respect to theta
    Jhat = np.mean(alpha(Z, ghat), axis=0)
    avg_nu = np.mean(nu(Z, ghat), axis=0)
    # solve for the empirical moment equation equals zero
    invJhat = np.linalg.pinv(Jhat)
    thetahat = invJhat @ avg_nu
    # construct approximate influence function for each sample
    phihat = - (nu(Z, ghat) - alpha(Z, ghat) @ thetahat) @ invJhat.T
    # variance estimate
    var = phihat.T @ phihat / phihat.shape[0]
    # estimate and standard error for any projection ell of the param
    point = ell @ thetahat
    stderr_ell = np.sqrt(ell.T @ var @ ell / phihat.shape[0])
    return point, stderr_ell
```

Estimate $\hat{g}$ out of fold and predict

cross-fitted jacobian $\hat{J} \coloneqq E_n[a(Z;\hat{g})]$

cross-fitted offset $E_n[\nu(Z;\hat{g})]$

Closed form solution: $\theta = \hat{J}^{-1} E_n[\nu(Z;\hat{g})]$

Approximate influence function

$Z \to \hat{\phi}(Z) \coloneqq \hat{J}^{-1} m(Z;\hat{\theta},\hat{g})$

Empirical covariance of estimate

$\hat{V} = E_n[\hat{\phi}(Z)\hat{\phi}(Z)']$

Proving the Main Theorem

Linear in θ Moments

- We will restrict attention to a broad class that simplifies proof
- Moment is linear in target parameter

$$m(Z;\theta,g) = a(Z;g)'\theta + \nu(Z;g)$$

- Expected moment also linear in θ

$$M(\theta,g) = A(g)'\theta + V(g)$$

Proof Ingredients: Linear in θ Moments

- Since $M_n\left(\hat{\theta}, \hat{g}\right) = 0$ we expect by concentration and sample splitting $M\left(\hat{\theta}, \hat{g}\right) \approx n^{-1/2}$
- Since $M(\theta_0, g_0) = 0$ we expect by Neyman orthogonality $M(\theta_0, \hat{g}) \approx RMSE(\hat{g})^2 = o\left(n^{-1/2}\right)$
- Since moment is linear in θ: $A(\hat{g})\left(\hat{\theta} - \theta_0\right) = M\left(\hat{\theta}, \hat{g}\right) - M(\theta_0, \hat{g})$
- Since A is Lipschitz and $\hat{g} \to g_0$: $A(g_0)\left(\hat{\theta} - \theta_0\right) = M\left(\hat{\theta}, \hat{g}\right) - M(\theta_0, \hat{g}) + \mathrm{o_p}\left(\left\|\hat{\theta} - \theta_0\right\|\right)$
- Since $A(g_0)$ is invertible: $\left\|\hat{\theta} - \theta_0\right\| = \mathrm{O}\left(\left\|M\left(\hat{\theta}, \hat{g}\right)\right\| + \|M(\theta_0, \hat{g})\|\right) = O_p\left(n^{-1/2}\right)$

- More fine-grained analysis of $M\left(\hat{\theta}, \hat{g}\right)$ term, shows: $\sqrt{n}M\left(\hat{\theta}, \hat{g}\right) \to \mathrm{N}(0, \mathrm{V})$

Proof of Main Theorem (visually)

CLT
+
sample-splitting
+
concentration
+
$\hat{g} \to g_0$

$M_n(\hat{\theta}, \hat{g}) = 0$

$N(0, V) \leftarrow$

2nd order Taylor
+
orthogonality
+
$\|\hat{g} - g_0\| = o_p(n^{-1/4})$

$$A(\hat{g})\left(\hat{\theta} - \theta_0\right) = M(\hat{\theta}, \hat{g}) - M(\theta_0, \hat{g})$$

$= o_p(n^{-1/2})$

$o_p(\|\hat{\theta} - \theta_0\|) =$

$M(\theta_0, g_0) = 0$

$A(g_0)\left(\hat{\theta} - \theta_0\right)$

Lipschitz $A(g)$
+
$\hat{g} \to g_0$

Proof of Main Theorem (algebraically)

- Since moment $M(\theta, g)$ is linear in θ and $M_n(\hat{\theta}, \hat{g}) = 0$ and $M(\theta_0, g_0) = 0$

$$A(\hat{g})\left(\hat{\theta} - \theta_0\right) = M\left(\hat{\theta}, \hat{g}\right) - M(\theta_0, \hat{g})$$
$$= M\left(\hat{\theta}, \hat{g}\right) - M_n\left(\hat{\theta}, \hat{g}\right) + M(\theta_0, g_0) - M(\theta_0, \hat{g})$$

- Since $\mathrm{RMSE}(\hat{g}) = \|\hat{g} - g_0\| = o_p(1)$

$$A(g_0)\left(\hat{\theta} - \theta_0\right) = A(\hat{g})\left(\hat{\theta} - \theta_0\right) + \mathrm{o_p}\left(\left\|\hat{\theta} - \theta_0\right\|\right)$$

- Thus

$$A(g_0)\left(\hat{\theta} - \theta_0\right) = \underbrace{M\left(\hat{\theta}, \hat{g}\right) - M_n\left(\hat{\theta}, \hat{g}\right)}_{\to N(0,V)} + \underbrace{M(\theta_0, g_0) - M(\theta_0, \hat{g})}_{= o_p\left(n^{-1/2}\right)} + \mathrm{o_p}\left(\left\|\hat{\theta} - \theta_0\right\|\right)$$

$\to N(0, V)$
via CLT
+ sample-splitting
+ concentration
+ $\hat{g} \to g_0$

$= o_p\left(n^{-1/2}\right)$
via orthogonality
+ $\|\hat{g} - g_0\| = o_p\left(n^{-1/4}\right)$

Proof of Main Theorem: Orthogonality

- By Neyman orthogonality and bounded second derivative of $M(\theta_0, g)$ w.r.t. g
  $$M(\theta_0, g_0) - M(\theta_0, \hat{g}) = D_g M(\theta_0, g_0)[g_0 - g] + O(\|\hat{g} - g_0\|^2) = o_p(n^{-1/2})$$

- Thus
  $$A(g_0)\,(\hat{\theta} - \theta_0) = \underbrace{M(\hat{\theta}, \hat{g}) - M_n(\hat{\theta}, \hat{g})}_{G_n(\hat{\theta}, \hat{g})} + \mathrm{o_p}\left(n^{-1/2} + \|\hat{\theta} - \theta_0\|\right)$$

Proof of Main Theorem: Sample-Splitting (1)

- Let $G_n(\theta, g) = M(\theta, g) - M_n(\theta, g)$
$$G_n(\hat{\theta}, \hat{g}) = G_n(\theta_0, g_0) + G_n(\hat{\theta}, \hat{g}) - G_n(\theta_0, \hat{g}) + G_n(\theta_0, \hat{g}) - G_n(\theta_0, g_0)$$

- Linearity of moment + (sample-splitting and concentration ⇒ $\|A(\hat{g}) - A_n(\hat{g})\| = o_p(1)$):
$$G_n(\hat{\theta}, \hat{g}) - G_n(\theta_0, \hat{g}) = \left(A(\hat{g}) - A_n(\hat{g})\right)\left(\hat{\theta} - \theta_0\right) = o_p\left(\|\hat{\theta} - \theta_0\|\right)$$

- Thus
$$A(g_0)\left(\hat{\theta} - \theta_0\right) = G_n(\theta_0, g_0) + G_n(\theta_0, \hat{g}) - G_n(\theta_0, g_0) + \mathrm{o_p}\left(n^{-1/2} + \|\hat{\theta} - \theta_0\|\right)$$

Proof of Main Theorem: Sample-Splitting (2)

- Note for $X_i = m(Z_i; \theta_0, \hat{g}) - m(Z_i; \theta_0, \hat{g}) - E[m(Z_i; \theta_0, \hat{g}) - m(Z_i; \theta_0, \hat{g})]$

$$G_n(\theta_0, \hat{g}) - G_n(\theta_0, g_0) = \frac{1}{n_2} \sum_{i \in S_2} X_i$$

- By sample splitting, X_i are i.i.d. with $E[X_i] = 0$. By variance decomposition (concentration)

$$\left\| \frac{1}{n_2} \sum_{i \in S_2} X_i \right\|_{L_2} \leq \sqrt{\frac{E\left[X_i^2\right]}{n}}$$

- Thus

$$\|G_n(\theta_0, \hat{g}) - G_n(\theta_0, g_0)\|_{L_2} \leq \frac{1}{\sqrt{n}} \sqrt{E\left[\left(m(Z_i; \theta_0, \hat{g}) - m(Z_i; \theta_0, \hat{g})\right)^2\right]} = O\left(\frac{\|\hat{g} - g_0\|}{\sqrt{n}}\right) = o_p\left(n^{-1/2}\right)$$

Concluding

- So far

$$A(g_0)\left(\hat{\theta}-\theta_0\right) = G_n(\theta_0, g_0) + \mathrm{o_p}\left(n^{-1/2} + \left\|\hat{\theta}-\theta_0\right\|\right)$$

- Since $A(g_0)$ is invertible and $G_n(\theta_0, g_0) = O_p\left(n^{-1/2}\right)$ by concentration

$$\left\|\hat{\theta}-\theta_0\right\| = O_p\left(n^{-1/2}\right)$$

- Thus, we have asymptotic linearity

$$\sqrt{n}\left(\hat{\theta}-\theta_0\right) = \sqrt{n}A(g_0)^{-1}G_n(\theta_0, g_0) + \mathrm{o_p}(1) = \frac{1}{\sqrt{n_2}}\sum_{i\in S_2} A(g_0)^{-1}m(Z_i; \theta_0, g_0) + o_p(1)$$

- By CLT we get the theorem

Main Theorem

- If moment is Neyman orthogonal and RMSE of $\hat{g}$ is $o_p\left(n^{-1/4}\right)*$

$$\sqrt{n}\left(\hat{\theta}-\theta_0\right) \rightarrow N\left(0, A^{-1}\Sigma\left(\mathrm{A}^{-1}\right)^{\top}\right)$$

- $A = \nabla_\theta M(\theta_0, g_0)$ and $\Sigma = E\left[m(Z;\theta_0, g_0)\, m(Z;\theta_0, g_0)^{\top}\right]$

*plus regularity conditions