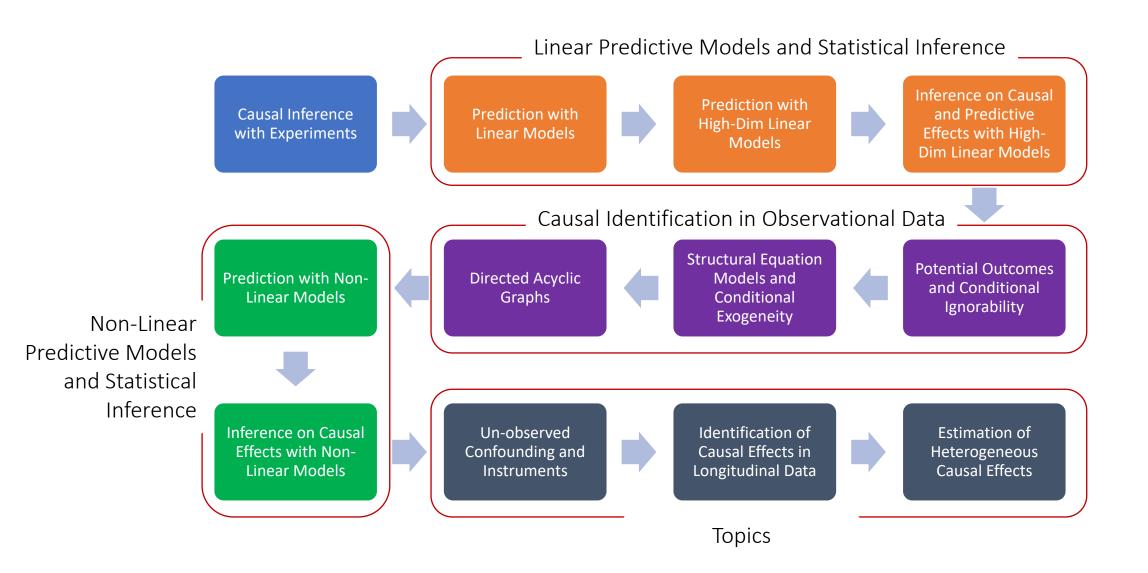
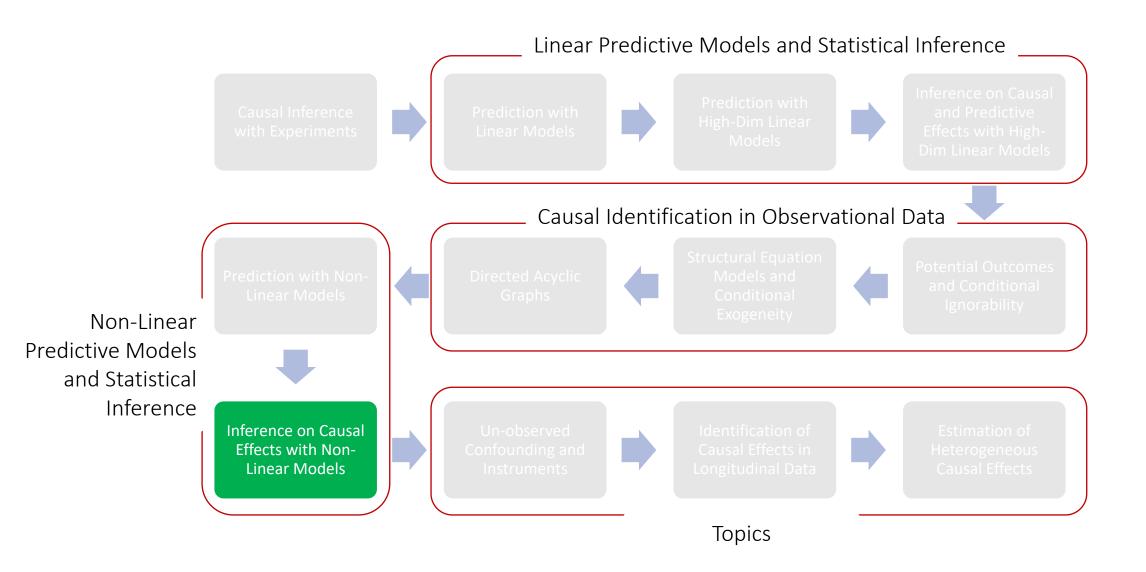
MS&E 228: Inference with Modern Non-Linear Prediction

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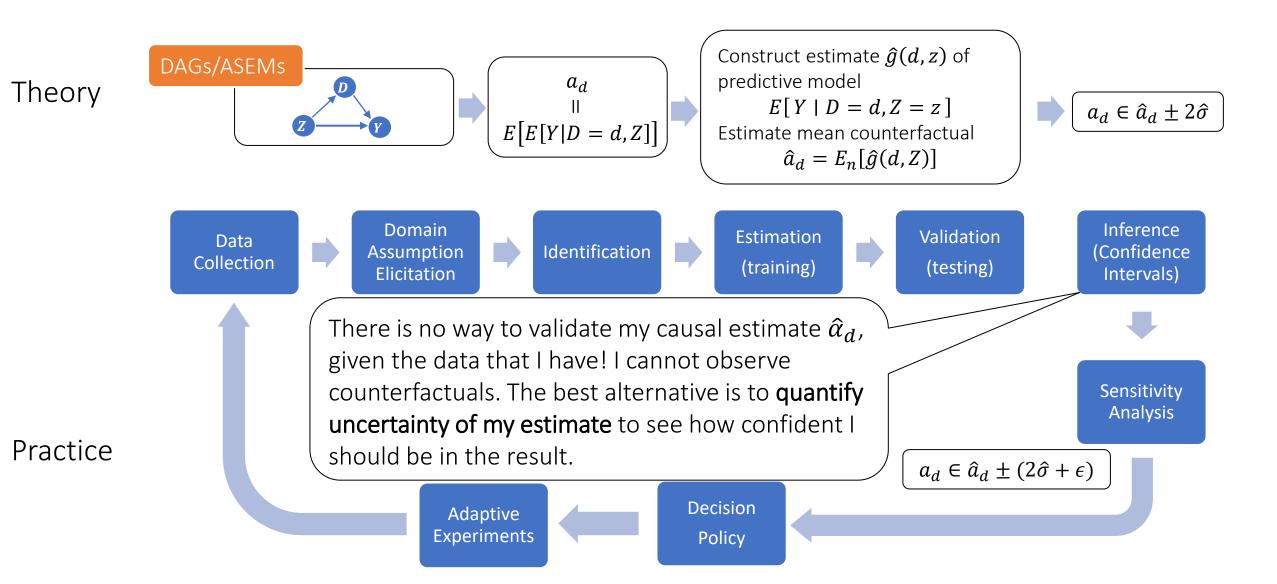


Goals for Today

- Revisiting and expanding on theory from last time
- Sample-splitting and cross-fitting
- Example application

Recap of Last Lecture

Causal Inference Pipeline



Semi-Parametric Moment Restrictions

- Observe samples Z_1, \ldots, Z_n i.i.d. from data distribution D
- Distribution D satisfies vector of moment restrictions $M(\theta_0, g_0) \coloneqq E_{Z \sim D}[m(Z; \theta_0, g_0)] = 0$
- $\theta_0 \in \mathbb{R}^d$ finite dimensional target parameter of interest
- $g_0 \in G$ potentially infinite dimensional parameter we don't care (nuisance)
- g_0 is un-known and needs to be estimated from data

Natural Estimation Algorithm (sample-splitting)

Split the data in half (S_1, S_2)

- ullet On first half S_1 , estimate \widehat{g} of g_0
- On second half S_2 , $\hat{\theta}$ is solution w.r.t. θ of empirical plug-in moment equation:

$$M_n(\theta, \hat{g}) \coloneqq \frac{1}{n_2} \sum_{i \in S_2} m(Z_i; \theta, \hat{g}) = 0$$

Natural Estimation Algorithm (cross-fitting)

- Split data in K parts, S_1, \dots, S_K
- ullet For each part k, estimate \widehat{g}_k using data from all parts except S_k
- $\hat{\theta}$ is solution w.r.t. θ of cross-fitted empirical moment equation:

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

Neyman Orthogonality

Moment $M(\theta,g)$ is Neyman orthogonal if for any $v \in G - g_0$: $D_g M(\theta_0,g_0)[v] \coloneqq \frac{\partial}{\partial t} M(\theta_0,g_0+t \ v) \bigg|_{t=0} = 0$

Main Theorem

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

$$\sqrt{n}\left(\widehat{\theta}-\theta_0\right)\to N\left(0,J_0^{-1}\Sigma\left(J_0^{-1}\right)^{\mathsf{T}}\right)$$

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

Two Main Applications

- Average Treatment Effect in identification by conditioning and a binary treatment
- Doubly robust moment which combines identification by regression and identification via propensity scores

- Average Treatment Effect in identification by conditioning under a partially linear model; response linear in treatment
- Residual-on-residual moment which generalizes the partialling out approach (FWL) to non-linear models

Expanding More on Theory

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 $\hat{ heta}$ is asymptotically linear

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

$$\phi_0(Z) = -J_0^{-1} m(Z; \theta_0, g_0)$$

$$J_0 \coloneqq \partial_\theta E[m(Z; \theta_0, g_0)]$$

influence function

influence is a linear transformation of the moment; transforming from

Consequently, it is asymptotically normal

 $\sqrt{n} \left(\hat{\theta} - \theta_0 \right) \sim n \sqrt{n} e^{n} e^{n} \sqrt{n} e^{n} e^{n}$

Covariance of the influence function

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

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

$$\widehat{V} = \operatorname{Var}_{n} \left(\widehat{\phi}(Z) \right)$$

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

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

Empirical variance of approximate influence

Approximate influence function Empirical average of jacobian

Python Pseudocode

```
# General DML pseudocode
     def general_dml(Z, ell, nfolds, moment, jacobian, nuisance
                                                                            Estimate \hat{g} out of fold and predict
         # construct out-of-fold predictions from the nuisar
          ghat = cross_val_predict(nuisance_estimator, Z, cv=nfo]
                                                                            Construct cross-fitted moment function
          use these predictions to define the empirical moment
Solve that
                                                                                     \theta \to E_n[m(Z;\theta,\hat{g})]
moment = 0 with respect to theta
          moment = lambda theta: np.mean(moment(Z, theta, ghat), axis=0)
  wrt 	heta
         # solve for the empirical moment equation equals zero
          thetahat = fsolve(avg moment)
         # calculate empirical jacobian with respect to theta, evaluated
                                                                                                Calculate
         # at the estimates thetahat and ghat
                                                                                          \hat{J} := \partial_{\theta} E_n[m(Z; \hat{\theta}, \hat{g})]
          Jhat = np.mean(jacobian(Z, thetahat, ghat), axis=8)
         # construct approximate influence function for each sample
                                                                                        Approximate influence
          phihat = - moment(Z, thetahat, ghat) @ np.linalg.pinv(Jhat).T
                                                                                              function
         # variance estimate
                                                                                     Z \to \widehat{\phi}(Z) \coloneqq \widehat{J}^{-1}m(Z; \widehat{\theta}, \widehat{g})
         var = phihat.T @ phihat / phihat.shape[0]
         # estimate and standard error for any projection ex
                                                                                        Empirical covariance of
          point = ell @ thetahat
                                                                                              estimate
          stderr_ell = np.sqrt(ell.T @ var @ ell / phihat.shape[0])
                                                                                         \hat{V} = E_n [\hat{\phi}(Z)\hat{\phi}(Z)']
         return point, stderr_ell
```

Main Theorem (linear moments)

If moments are linear

$$m(Z; \theta, g) = \nu(Z; g) - \alpha(Z; g)\theta$$

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

Consequently, it is asymptotically normal

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

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

$$\ell'\theta \in \left[\ell'\hat{\theta} \pm c\sqrt{\frac{\ell'\hat{V}\ell}{n}}\right], \qquad \widehat{V} = \operatorname{Var}_{n}\left(\widehat{\phi}(Z)\right), \qquad \widehat{\phi}(Z) \coloneqq -\widehat{J}^{-1}m(Z; \widehat{\theta}, \widehat{g}), \qquad \widehat{J} = E_{n}[a(Z; \widehat{g})]$$

Python Pseudocode

```
# General DML pseudocode for linear moments: m(Z; theta, g)
def general_dml_linear_moment(Z, ell, nfolds, alpha, nu, jac
                                                                        Estimate \hat{q} out of fold and predict
    # 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
                                                             cross-fitted jacobian \hat{J} := E_n[a(Z; \hat{g})]
    Jhat = np.mean(alpha(Z, ghat), axis=0)
                                                                 cross-fitted offset E_n[\nu(Z; \hat{g})]
    avg_nu = np.mean(nu(Z, ghat), axis=0)_
    # solve for the empirical moment equation equals zero
    invJhat = np.linalg.pinv(Jhat)
                                                    Closed form solution: \theta = \hat{J}^{-1}E_n[\nu(Z;\hat{g})]
    thetahat = invJhat @ avg_nu
    # construct approximate influence function for each sample
    phihat = - (nu(Z, ghat) - alpha(Z, ghat) @ thetahat) @ invJhat.T
                                                                                      Approximate influence
    # variance estimate
                                                                                            function
    var = phihat.T @ phihat / phihat.shape[0]
                                                                                   Z \to \widehat{\phi}(Z) \coloneqq \widehat{J}^{-1}m(Z; \widehat{\theta}, \widehat{g})
    # estimate and standard error for any projection
                                                                                     Empirical covariance of
    point = ell @ thetahat
    stderr_ell = np.sqrt(ell.T @ var @ ell / phihat.shape[0])
                                                                                            estimate
                                                                                      \hat{V} = E_n [\hat{\phi}(Z)\hat{\phi}(Z)']
    return point, stderr_ell
```

ATE under Conditional Exogeneity

• 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:

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

• Where:

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

• We want to be able to use ML to learn regression function g!

Better Moment for ATE

Add a "debiasing" correction:

$$\widetilde{M}(\theta, g, a) = M(\theta, g) + E[a(D, X)(Y - g(D, X))]$$

• What is a_0 ? Should be such that

$$E[a_0(D, X) g(D, X)] = E[g(1, X) - g(0, X)]$$

• The following works: inverse propensity scoring

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

Doubly robust estimation algorithm

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 $\sqrt{n}(\hat{\theta}-\theta_0) \approx \sqrt{n} \, E_n[\phi_0(Z)], \qquad \phi_0(Z) = -J_0^{-1} \, m(Z;\theta_0,g_0), \qquad J_0 \coloneqq \partial_\theta E[m(Z;\theta_0,g_0)]$
- Consequently, it is asymptotically normal $\sqrt{n} \left(\hat{\theta} \theta_0 \right) \sim_a N(0, V), \qquad V \coloneqq E[\phi_0(Z)\phi_0(Z)']$
- Confidence intervals for any projection based on estimate of variance are asymptotically valid

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

Inference with Doubly Robust Algorithm

• Moment is Neyman orthogonal

$$m(Z;\theta,g) \coloneqq g(1,X) - g(0,X) - a(D,X) \left(Y - g(D,X) \right) - \theta$$

- If RMSE of propensity and regression model goes down at rate $n^{1/4}$, plus regularity conditions
- Then the estimate $\hat{ heta}$ is asymptotically linear

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

Consequently, it is asymptotically normal

$$\sqrt{n}\left(\hat{\theta} - \theta_0\right) \sim_a N(0, V), \qquad V \coloneqq E[m(Z; \theta_0, g_0)^2]$$

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

$$\ell'\theta \in \left| \ell'\hat{\theta} \pm c \sqrt{\frac{\ell'\hat{V}\ell}{n}} \right|, \qquad \hat{V} = \operatorname{Var}_{n}\left(\hat{\phi}(Z)\right), \qquad \hat{\phi}(Z) \coloneqq -m(Z;\hat{\theta},\hat{g}), \qquad \hat{J} = 1$$

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
```

Partially Linear Model

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

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

- Assume partially linear response: $E[Y \mid D, X] = \theta_0 D + f_0(X)$ $Y = \theta_0 D + f_0(X) + \epsilon, \qquad E[\epsilon \mid D, X] = 0$
- Parameter of interest θ_0 is constant marginal effect of treatment
- Orthogonal moment are normal equations after residualization

$$\widetilde{Y} = \theta_0 \widetilde{D} + \epsilon, \qquad E[\epsilon | \widetilde{D}] = 0 \Rightarrow E[(\widetilde{Y} - \theta_0 \widetilde{D})\widetilde{D}] = 0$$

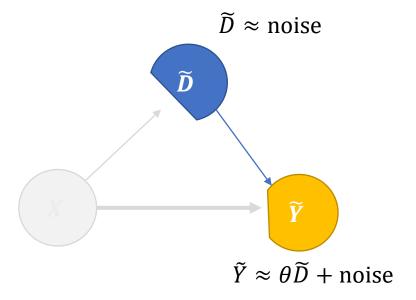
Orthogonal Method: Double ML

- 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]
 - Construct residuals on other half, $\widehat{D}\coloneqq D-\widehat{p}(X)$ and $\widehat{Y}\coloneqq Y-\widehat{h}(X)$
 - Run OLS on residuals: $\widehat{Y} \sim \widehat{D}$ to get $\widehat{\theta}$
- OLS equivalent to solving moment condition:

$$E_n[(\hat{Y} - \theta \hat{D})\hat{D}] = 0$$

Orthogonal Moment condition:

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



Orthogonal Method: Double ML

• OLS equivalent to solving moment condition:

$$E\big[\big(\widetilde{Y} - \theta \widetilde{D}\big)\widetilde{D}\big] = 0$$

Orthogonal Moment condition:

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

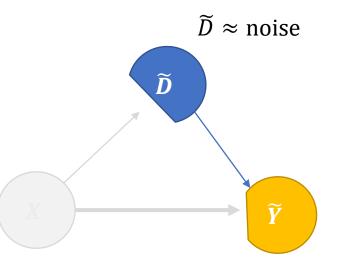
Verifying orthogonality

Directional derivative with respect to h

$$\partial_t E \left[\left(Y - h_0(X) - t \, \nu(X) - \theta_0 \left(D - p_0(X) \right) \right) \, \left(D - p_0(X) \right) \right] \bigg|_{t=0} = 0$$

• Directional derivative with respect to p

$$\partial_t E[(Y - h_0(X) - \theta_0 (D - p_0(X) - t \nu(X))) (D - p_0(X) - t \nu(X))]\Big|_{t=0} = 0$$



 $\widetilde{Y} \approx \theta \widetilde{D} + \text{noise}$

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 $\sqrt{n}(\hat{\theta}-\theta_0) \approx \sqrt{n} \, E_n[\phi_0(Z)], \qquad \phi_0(Z) = -J_0^{-1} \, m(Z;\theta_0,g_0), \qquad J_0 \coloneqq \partial_\theta E[m(Z;\theta_0,g_0)]$
- Consequently, it is asymptotically normal $\sqrt{n} \left(\hat{\theta} \theta_0 \right) \sim_a N(0, V), \qquad V \coloneqq E[\phi_0(Z)\phi_0(Z)']$
- Confidence intervals for any projection based on estimate of variance are asymptotically valid

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

Inference with DML in PLR Setting

- If RMSE of propensity model and outcome model goes down at rate $n^{1/4}$, plus regularity conditions
- Then the estimate $\hat{ heta}$ is asymptotically linear

$$\sqrt{n}(\hat{\theta} - \theta_0) \approx \sqrt{n} E_n[\phi_0(Z)], \qquad \phi_0(Z) = -J_0^{-1} (\widetilde{Y} - \theta_0 \widetilde{D}) \widetilde{D}, \qquad J_0 := E[\widetilde{D}^2]$$

Consequently, it is asymptotically normal

$$\sqrt{n}\left(\hat{\theta}-\theta_{0}\right)\sim_{a}N(0,V), \qquad V\coloneqq\frac{E\left[\left(\widetilde{Y}-\theta_{0}\widetilde{D}\right)^{2}\widetilde{D}^{2}\right]}{E\left[\widetilde{D}^{2}\right]^{2}} \qquad \text{respect to parameter; related} \\ to identification strength} \\ E\left[\widetilde{D}^{2}\right]=E\left[Var(D|X)\right]$$

Jacobian of moments with respect to parameter; relates

Confidence_intervals for any projection based on estimate of variance are asymptotically valid

$$\ell'\theta \in \left| \ell'\hat{\theta} \pm c \sqrt{\frac{\ell'\hat{V}\ell}{n}} \right|, \qquad \hat{V} = \operatorname{Var}_{\mathbf{n}} \left(\hat{\phi}(Z) \right), \qquad \hat{\phi}(Z) \coloneqq -\hat{J}^{-1} \left(\hat{Y} - \hat{\theta} \widehat{D} \right) \widehat{D}, \qquad \hat{J} = E_n \left[\widehat{D}^2 \right]$$

Python Pseudocode

```
cv = KFold(n splits=nfolds, shuffle=True, random state=123)
# out-of-fold predictions for y
yhat = cross_val_predict(modely, X, y, cv=cv, n_jobs=-1)
# out-of-fold predictions for D
Dhat = cross val predict(modeld, X, D, cv=cv, n jobs=-1)
# calculate outcome and treatment residuals
resy = y - yhat
resD = D - Dhat
# final stage ols based point estimate and standard error
point = np.mean(resy * resD) / np.mean(resD**2)
epsilon = resy - point * resD
var = np.mean(epsilon**2 * D**2) / np.mean(D**2)**2
stderr = np.sqrt(var / X.shape[0])
return point, stderr
```

Practical Variants of Sample-Splitting

Cross-fitting and semi-cross-fitting

Cross-fitting

Sample splitting is statistically lossy

- Only half of the data are used for the final parameter estimation
- Can we utilize all the data?

- Cross-fitting: analogous to cross-validation
- Use the second half to train g and predict on first half
- Then calculate parameter using all the data

Cross-fitting Estimation Algorithm

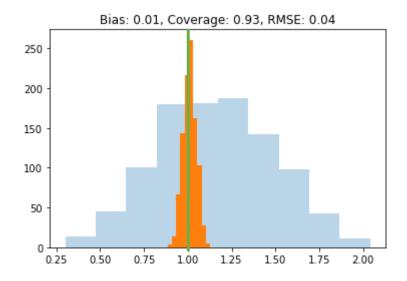
- Split the data in half
- ullet On first half, estimate \hat{g}_1 of g_0 and predict on second half
- ullet On second half, estimate \hat{g}_2 of g_0 and predict on first half
- On all data, solution $\hat{ heta}$ to empirical plug-in moment equation:

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

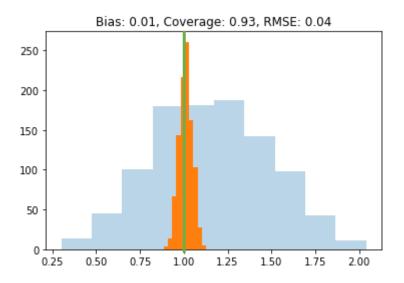
• In practice do this with $K \approx 3$ to 5 folds: for each fold k train on all other folds and predict on fold k

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



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-Cross-fitting Estimation Algorithm

- Split the data in half (in practice K folds)
- ullet On first half, estimate $\widehat{g}_1^{(1)}$, ..., $\widehat{g}_1^{(\mathrm{L})}$ of g_0 and predict on second half
- ullet On second half, estimate $\hat{g}_2^{(1)}$, ... , $\hat{g}_2^{(\mathrm{L})}$ of g_0 and predict on first half
- Choose the model $\ell \in \{1, ..., L\}$ that optimizes out-of-sample RMSE
- ullet On all data, solution $\hat{ heta}$ to empirical plug-in moment equation:

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

Semi-Crossfitting

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

Semi-Cross-fitting with Stacking

- Split the data in half (in practice K folds)
- ullet On first half, estimate $\hat{g}_1^{(1)}$, ..., $\hat{g}_1^{(L)}$ of g_0 and predict on second half
- On second half, estimate $\hat{g}_2^{(1)}$, ..., $\hat{g}_2^{(L)}$ of g_0 and predict on first half
- Construct weights $\alpha_1, \dots, \alpha_\ell$ on the models using all the data (stacking)
- On all data, solution $\hat{\theta}$ to empirical plug-in moment equation:

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

Semi-Crossfitting 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 $\sqrt{L} = \mathrm{o}(\mathrm{n}^{1/4})$

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

- Construct out of fold predictions based on many ML models
- ullet 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

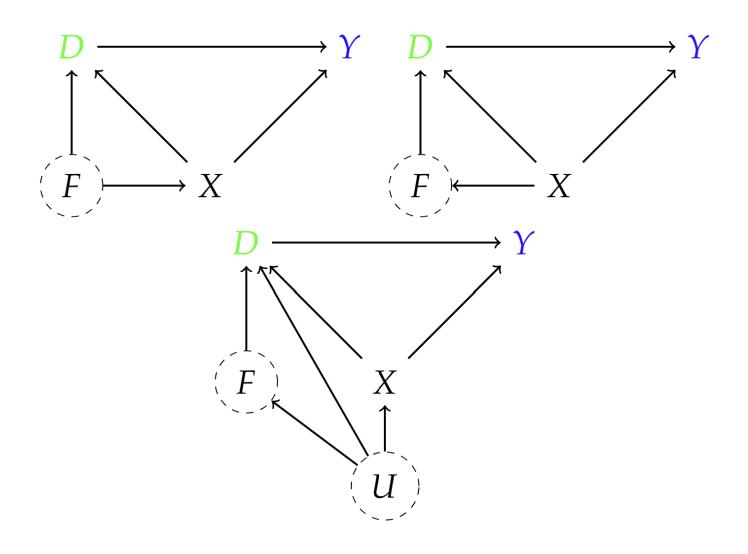
Application: Effect of 401k

Problem

- Impact of 401k eligibility on financial assets
- Working for a firm that offers access to 401k eligibility not randomly assigned
- After conditioning on important characteristics of the worker and job, assignment can be thought as exogenous
- Most important: income
- At least around 1991 (early in 401k deployment), workers would not really base their employment decision on 401k eligibility

Causal Diagrams

- F: firm characteristics
- D: eligibility for 401k
- Y: net financial assets
- X: age, income, family size, years of education, a married indicator, a two-earner status indicator, a defined benefit pension status indicator, an IRA participation indicator, and a home ownership indicator



Possible Violations

- F: firm characteristics
- D: eligibility for 401k
- Y: net financial assets
- X: age, income, family size, years of education, a married indicator, a two-earner status indicator, a defined benefit pension status indicator, an IRA participation indicator, and a home ownership indicator
- M: match amount

