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

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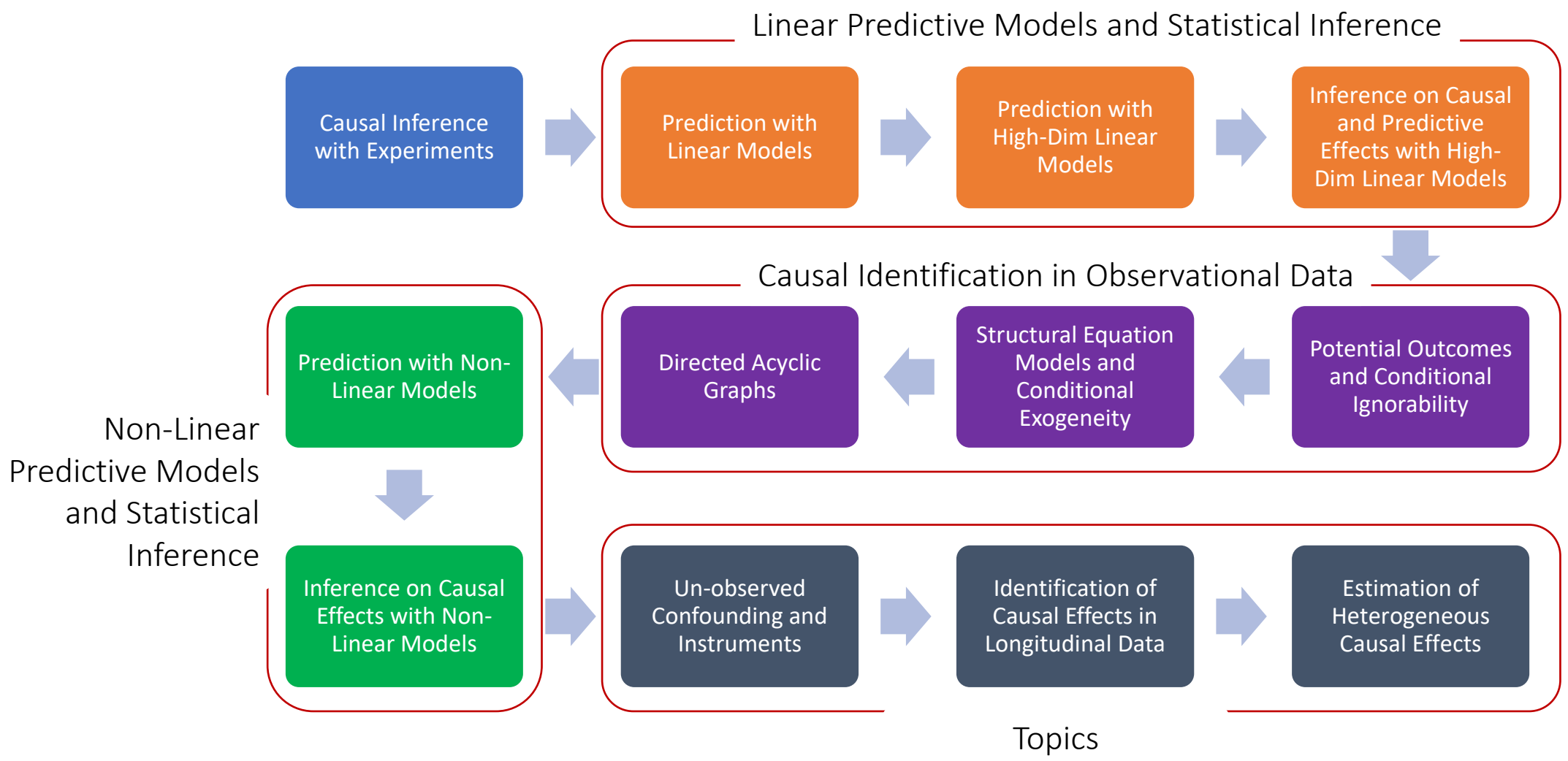
Linear Predictive Models and Statistical Inference
Causal Inference with Experiments
Prediction with Linear Models
Prediction with High-Dim Linear Models
Inference on Causal and Predictive Effects with High-Dim Linear Models
Causal Identification in Observational Data
Potential Outcomes and Conditional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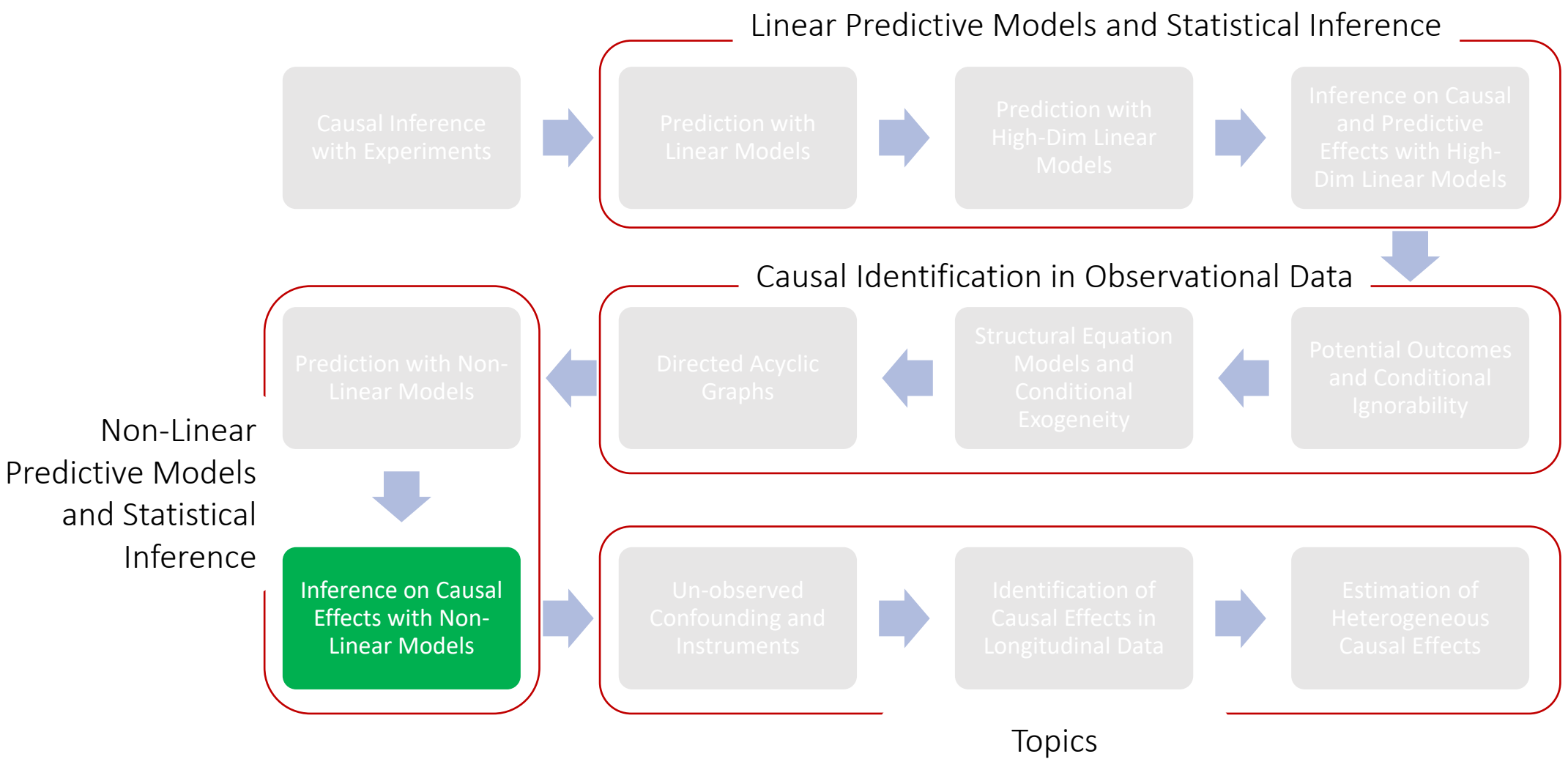
Inference on Causal Effects with Non-Linear Models
Un-observed Confounding and Instruments
Identification of Causal Effects in Longitudinal Data
Estimation of Heterogeneous Causal Effects
Topics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Goals for Today

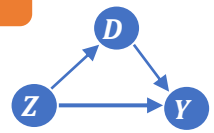
- Revisiting and expanding on theory from last time
- Sample-splitting and cross-fitting
- Example application

Recap of Last Lecture

Causal Inference Pipeline

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

There is no way to validate my causal estimate $\hat{\alpha}_d$, given the data that I have! I cannot observe counterfactuals. The best alternative is to **quantify uncertainty of my estimate** to see how confident I should be in the result.

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

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

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

- $\theta_0 \in R^d$ finite dimensional target parameter of interest
- $g_0 \in G$ potentially infinite dimensional (an un-known function) 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
- On first half, estimate $\hat{g}$ of g_0
- On second half, solution w.r.t. $\hat{\theta}$ of empirical plug-in moment equation:

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

Natural Estimation Algorithm (cross-fitting)

- Split data in K parts, $S_1, \ldots, S_K$
- For each part k, estimate $\hat{g}_k$ using data from all parts except S_k
- Return solution $\hat{\theta}$ to cross-fitted empirical moment equation:

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

Formal Definition

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

$$D_g M(\theta_0, g_0)[\nu] := \frac{\partial}{\partial t} M(\theta_0, g_0 + t\,\nu)\Big|_{t=0} = 0$$

Main Theorem

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

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

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

*plug regularity conditions

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*

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

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

influence function

- Consequently, it is *asymptotically normal*

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

Covariance of the influence function

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

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

Empirical variance of approximate influence

Approximate influence function

Empirical average of jacobian

Python Pseudocode

```
# General DML pseudocode
def general_dml(Z, ell, nfolds, moment, jacobian, nuisance_estimator):
    # construct out-of-fold predictions from the nuisance estimator
    ghat = cross_val_predict(nuisance_estimator, Z, cv=nfolds)
    # use these predictions to define the empirical moment equation
    # 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 parameters
    point = ell @ thetahat
    stderr_ell = np.sqrt(ell.T @ var @ ell / phihat.shape[0])
    return point, stderr_ell
```

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*

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

- 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

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

Python Pseudocode

```
# General DML pseudocode for linear moments: m(Z; theta, g) = nu(Z;g) - alpha(Z;g) theta
def general_dml_linear_moment(Z, ell, nfolds, alpha, nu, jacobian, nuisance_estimator):
    # construct out-of-fold predictions from the nuisance estimator
    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 parameters
    point = ell @ thetahat
    stderr_ell = np.sqrt(ell.T @ var @ ell / phihat.shape[0])
    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:

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

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

- 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

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

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 $\hat{\theta}$ is *asymptotically linear*

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

- Consequently, it is *asymptotically normal*

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

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

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

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: $E[\, Y \mid D, X \,] = \theta_0 D + f_0(X)$

$$Y = \theta_0 D + f_0(X) + \epsilon, \qquad E[\epsilon | D, X] = 0$$

- Parameter of interest θ_0 is constant marginal effect of treatment
- Orthogonal moment are normal equations after residualization

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

Orthogonal Method: Double ML

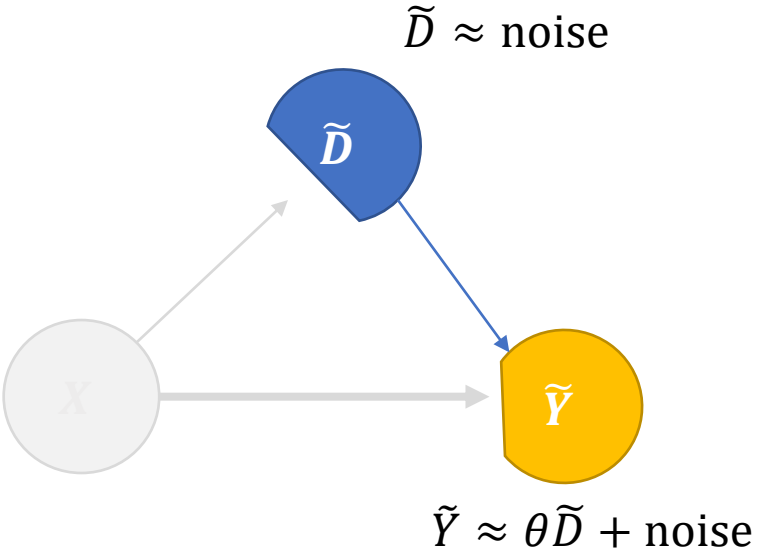
- Double ML. Split samples in half
  - Regress $Y \sim X$ with ML on first half, to get estimate $\hat{h}(S)$ of $E[Y|X]$
  - Regress $D \sim X$ with ML on first half, to get estimate $\hat{p}(S)$ of $E[D|X]$
  - Construct residuals on other half, $\widehat{D} \coloneqq D - \hat{p}(X)$ and $\hat{Y} \coloneqq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

- OLS equivalent to solving moment condition:

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

- Orthogonal Moment condition:

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



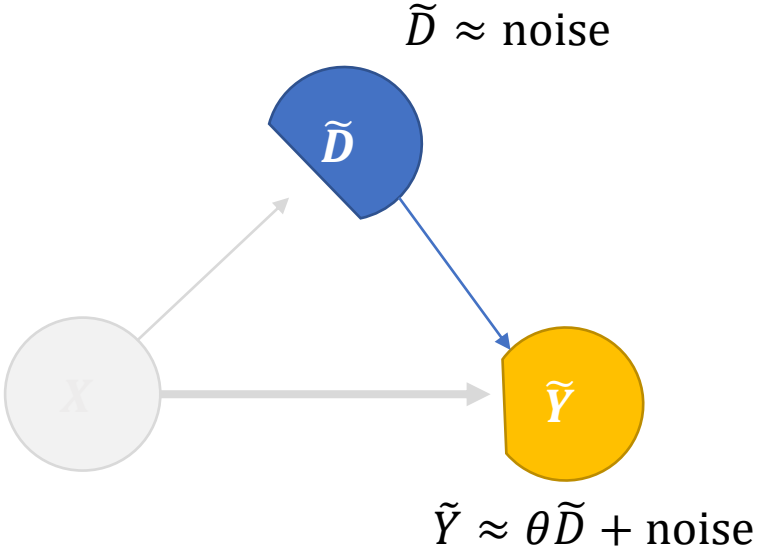
Orthogonal Method: Double ML

- OLS equivalent to solving moment condition:

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

- 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

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

- Directional derivative with respect to p

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

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

- 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

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

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 $\hat{\theta}$ is *asymptotically linear*

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

- Consequently, it is *asymptotically normal*

$$\sqrt{n}\left(\hat{\theta} - \theta_0\right) \sim_a N(0, V), \qquad V \coloneqq \frac{E\left[\left(\tilde{Y} - \theta_0 \tilde{D}\right)^2 \tilde{D}^2\right]}{E\left[\tilde{D}^2\right]^2}$$

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

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

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

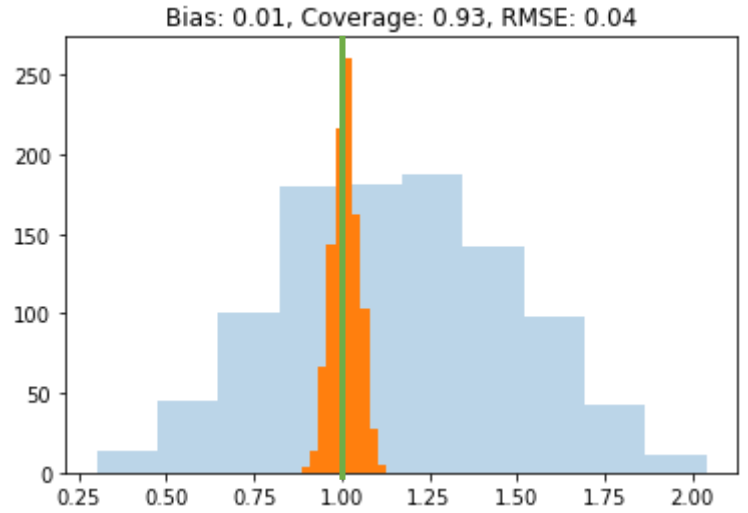
- Split the data in half
- On first half, estimate $\hat{g}_1$ of g_0 and predict on second half
- On second half, estimate $\hat{g}_2$ of g_0 and predict on first half
- On all data, solution $\hat{\theta}$ to empirical plug-in moment equation:

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

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

Natural Algorithm (Draft 3) Gone Right

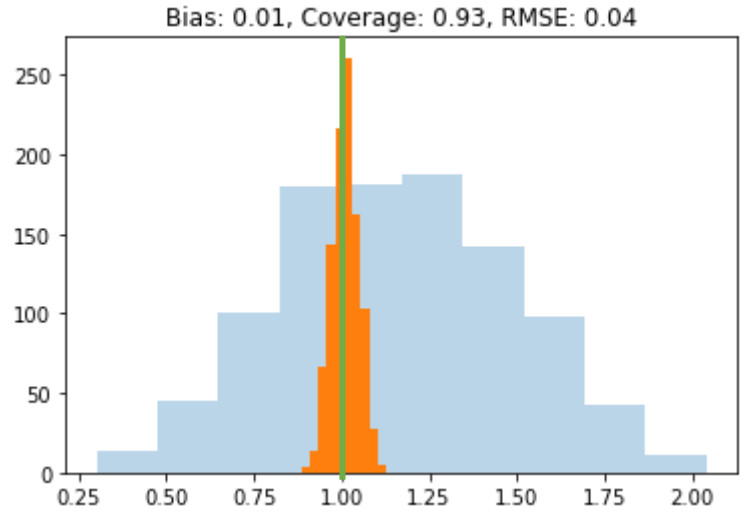
```
def dml2(X, D, y): # orthogonal dml with sample-splitting
    est_y = RandomForestRegressor(min_samples_leaf=20)
    yres = y - cross_val_predict(est_y, X, y, cv=3)
    est_t = RandomForestRegressor(min_samples_leaf=20)
    Dres = D - cross_val_predict(est_t, X, D, cv=3)
    theta = np.mean(yres * 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

```
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()
```



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)*
- 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
- Choose the model $\ell \in \{1, \ldots, L\}$ that optimizes out-of-sample RMSE
- On all data, solution $\hat{\theta}$ to empirical plug-in moment equation:

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

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

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

Semi-Cross-fitting 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 $\alpha_1, \ldots, \alpha_\ell$ on the models using all the data (stacking)

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

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

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

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

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

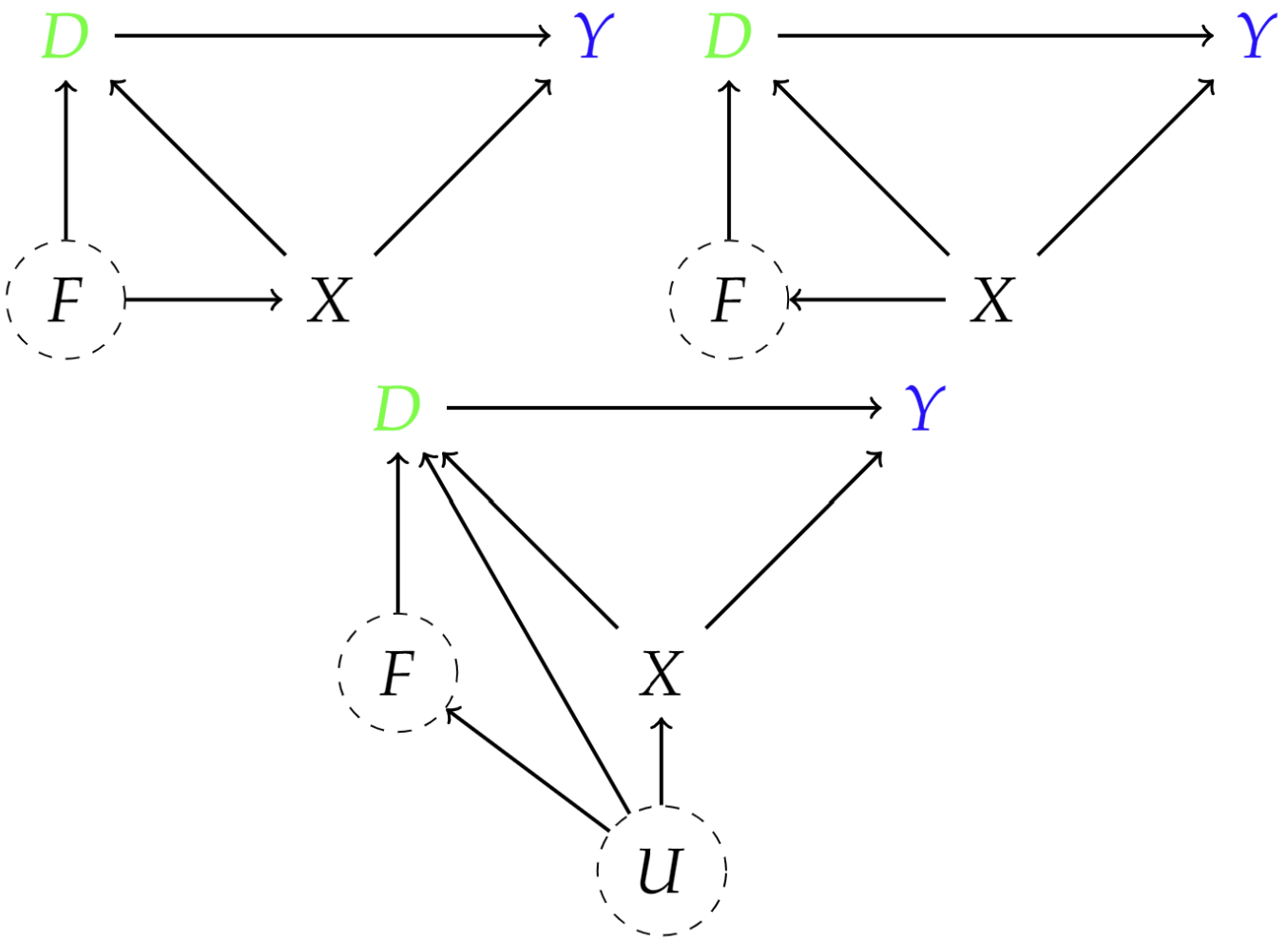
Application: Effect of 401k

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



Let's try it out!

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