

EGAL, IHR WISST SCHON ...
SCHÖNEN NIKOLAUSTAG!

# **Web-Mining Agents**

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### Structural Causal Models

Slides prepared by Özgür Özçep

Part III: Causality in Linear SCMs and Instrumental Variables



#### Literature

 J.Pearl, M. Glymour, N. P. Jewell: Causal inference in statistics – A primer, Wiley, 2016.

(Main Reference)

- J. Pearl: Causality, CUP, 2000.
- B. Chen & Pearl: Graphical Tools for Linear Structural Equation Modeling, Technical Report R-432, July 2015

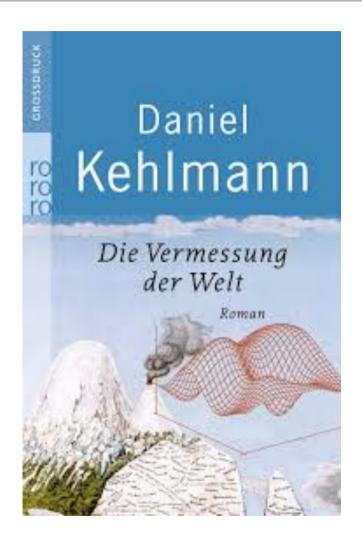


#### Causal Inference in Linear SCMs

- All techniques and notions developed so far applicable for any SCM
- Of importance are linear SCMs
  - Equations of form  $Y = a_0 + a_1X_1 + a_2X_2 + ... a_nX_n$
  - In focus of traditional causal analysis (in economics)
- Assumption for the following
  - All variables depending linearly on others (if at all)
  - Error variables (exogenous variables) have
     Gaussian/Normal distribution



### Want to learn something about Gauss?





## Why Gaussian?

 Andrew Moore: "Gaussians are as natural as Orange Juice and Sunshine"

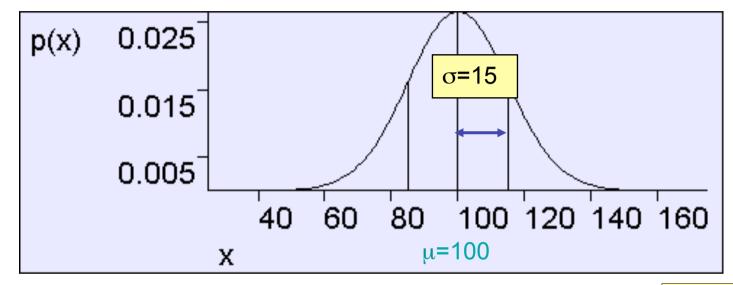
(http://www.cs.cmu.edu/~awm/tutorials)

(Used in the following slides on Gaussians)

- Proves useful to model RVs that are combinations of many (non)-measured influences
- Makes life easy because
  - 1. Efficient representation
  - 2. Substitute probabilities by expectations
  - 3. Linearity of expectations
  - 4. Invariance of regression coefficients



### **General Gaussian**



$$E[X] = \mu$$

$$Var[X] = \sigma^2$$

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Also known as the normal distribution or Bell-shaped curve

Shorthand: We say X ~ N( $\mu$ , $\sigma^2$ ) to mean "X is distributed as a Gaussian with parameters  $\mu$  and  $\sigma^2$ ".

In the above figure,  $X \sim N(100,15^2)$ 

ÖÖ: So need only specify  $\mu$ , $\sigma^2$ 



### **Bivariate Gaussians**

Write r.v. 
$$\mathbf{X} = \begin{pmatrix} X \\ Y \end{pmatrix}$$
 Then define  $X \sim N(\boldsymbol{\mu}, \boldsymbol{\Sigma})$  to mean

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$$p(\mathbf{X}) = \frac{1}{2\pi \|\mathbf{\Sigma}\|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{X} - \mathbf{\mu})^T \mathbf{\Sigma}^{-1}(\mathbf{X} - \mathbf{\mu})\right)$$

Where the Gaussian's parameters are...

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix} \quad \boldsymbol{\Sigma} = \begin{pmatrix} \boldsymbol{\sigma}^2_x & \boldsymbol{\sigma}_{xy} \\ \boldsymbol{\sigma}_{xy} & \boldsymbol{\sigma}^2_y \end{pmatrix}$$

 $\mu = \begin{pmatrix} \mu_x \\ \mu_y \end{pmatrix} \quad \Sigma = \begin{pmatrix} \sigma^2_x & \sigma_{xy} \\ \sigma_{xy} & \sigma^2_y \end{pmatrix}$  ÖÖ: Covariance matrix in 2 dimesions  $\sigma_{XY} = E[(X-E(X))(Y-E(Y))]$ 

Where we insist that  $\Sigma$  is symmetric non-negative definite

It turns out that  $E[X] = \mu$  and  $Cov[X] = \Sigma$ . (Note that this is a resulting property of Gaussians, not a definition)\*

\*This note rates 7.4 on the pedanticness scale



ÖÖ: So need only specify 5= 2\*2 + 2(2-1)/2 paramters

### Multivariate Gaussians

Write r.v. 
$$\mathbf{X} = \begin{pmatrix} X_1 \\ X_2 \\ \vdots \\ X_m \end{pmatrix}$$
 Then define  $X \sim N(\mathbf{\mu}, \mathbf{\Sigma})$  to mean

ÖÖ: So, it is enough to consider pairwise correlation Of Xi, Xj (next to their expectations and variances) 2\*N + N(N-1)/2 => efficient representation of joint

$$p(\mathbf{x}) = \frac{1}{(2\pi)^{\frac{m}{2}} \|\mathbf{\Sigma}\|^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\mathbf{x} - \boldsymbol{\mu})^T \mathbf{\Sigma}^{-1}(\mathbf{x} - \boldsymbol{\mu})\right)$$

Where the Gaussian's parameters have...

$$\boldsymbol{\mu} = \begin{pmatrix} \mu_1 \\ \mu_2 \\ \vdots \\ \mu_m \end{pmatrix} \quad \boldsymbol{\Sigma} = \begin{pmatrix} \sigma^2_1 & \sigma_{12} & \cdots & \sigma_{1m} \\ \sigma_{12} & \sigma^2_2 & \cdots & \sigma_{2m} \\ \vdots & \vdots & \ddots & \vdots \\ \sigma_{1m} & \sigma_{2m} & \cdots & \sigma^2_m \end{pmatrix}$$

Where we insist that  $\Sigma$  is symmetric non-negative definite

Again, E[X] =  $\mu$  and Cov[X] =  $\Sigma$ . (Note that this is a resulting property of Gaussians, not a definition) IM FOCUS DAS LEBEN

## Why Gaussian?

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(Used in the following slides on Gaussians)

- Proves useful to model RVs that are combinations of many (non)-measured influences
- Makes life easy because
  - 1. Efficient representation
  - 2. Substitute probabilities by expectations



### Substitute Probabilities by Expectations

- P(X) becomes E[X]
- P(Y|X) becomes E[Y|X]

(Conditional expectation defined as expected

$$E[Y|X=x] = \sum_{y} y P(Y=y|X=x)$$

- → Can use regression to determine causal relations
  - E[Y|X] defines a function f(X,Y)
  - By regression we circumvent the problem of calculating the probabilities required for E[Y|X]

So, we will be guessing the deep/hidden structure (linear SCMs equations) as far as needed for our tasks – instead of working on probabilities level



## Why Gaussian?

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(Used in the following slides on Gaussians)

- Proves useful to model RVs that are combinations of many (non)-measured influences
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  - 2. Substitute probabilities by expectations
  - 3. Linearity of expectations
  - 4. Invariance of regression coefficients



## Linearity of Expectations

Expectations can be written as linear combinations

$$- E[Y|X_1=x_1,X_2=x_2, ..., X_n=x_n] = r_0 + r_1x_1 + ... + r_nx_n$$

- Each of the slopes r<sub>i</sub> are partial regression coefficients
- Example and Notation

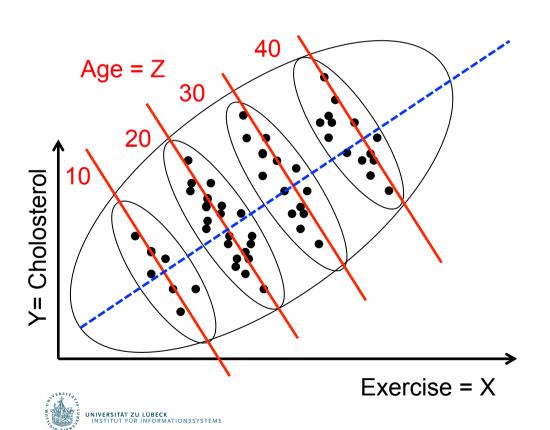
```
r_i = R_{Y \times i \times X_1 \dots X_{i-1}, X_{i+1}, \dots X_n}
= slope of Y on X_i when fixing all other X_i (j \neq i)
```

- r<sub>i</sub> does not depend on the values of the X<sub>i</sub> but only which set of Xis (the set of regressors) was chosen
- This independency also part of a continuous version of the Simpson's paradox (next slides)



### Slope Constancy

Measure weakly exercise and cholesterol in different age groups

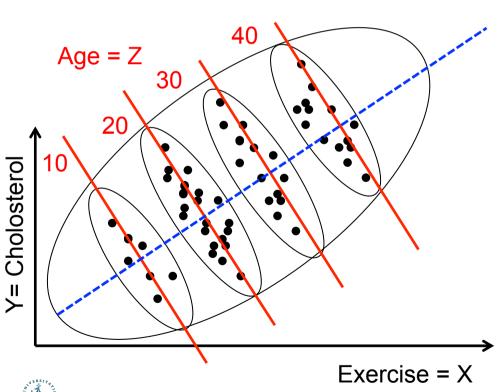


• 
$$Y = r_0 + r_1 X + r_2 Z$$

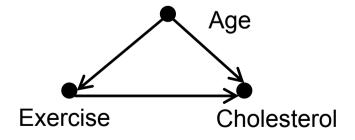
- $r_1 = R_{YX,Z} < 0$
- Z-fixed slope for Y,X independent of Z (and negative)
- Ignoring Z (regressing Y w.r.t X only) leads to combind positive slope R<sub>YX</sub>
- → Simpson's paradox

### Resolving the Paradox

Measure weakly exercise and cholesterol in different age groups



- Age a cofounder of Exercise and Cholosterol
- Need to condition on Age=Z to find correct P(Y|do(X))



### Regression coefficients and covariance

- Usually one finds (partial) regression coefficients by sampling
- But there exists formulae expressing connections to statistical measures such as covariance.
- $\sigma_{XY} = E[(X-E[Y])(Y-E[Y])]$  (covariance of X and Y)
- $\rho_{XY} = \sigma_{XY}/(\sigma_X \sigma_Y)$  (Correlation)
- Note:  $\sigma_{XY} = 0 = \rho_{XY}$  iff X and Y are independent



### **Theorem** (Orthogonality principle)

If 
$$Y = r_0 + r_1 X_1 + ... + r_k X_k + \varepsilon$$

then the best (least-square error minimizing) coefficients ri (for any distributions Xi) result when  $\sigma_{\epsilon Xi} = 0$  for all  $1 \le i \le k$ 



### Regression coefficients and covariance

- Assume w.l.og.  $E[\varepsilon] = 0$
- $Y = r_0 + r_1 X + \epsilon$  (\*)
- $E[Y] = r_0 + r_1 E[X]$
- $XY = Xr_0 + r_1X^2 + X\varepsilon$
- $E[XY] = r_0 E[X] + r_1 E[X^2] + E[X_{\epsilon}]$
- $E[X\epsilon] = 0$
- Solving for r<sub>0</sub> and r<sub>1</sub>

$$- r_0 = E[Y] - E[X](\sigma_{XY}/\sigma_{XX})$$

$$- r_1 = \sigma_{XY}/\sigma_{XX}$$

(by applying E)

(by multiyplying (\*) with X)

(by applying E)

(by orthogonality)

Similar derivations fore multiple regression

## Path Coefficients (Example)

### **Example**

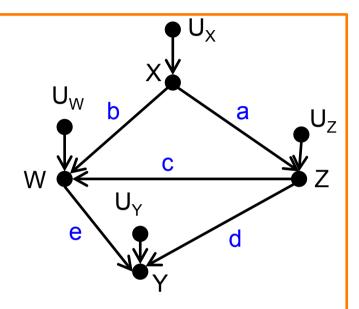
Linear SCM

$$-X = U_X$$

$$-Z = aX + U_Z$$

$$-W = bX + cZ + U_W$$

$$-Y = dZ + eW + U_Y$$



- Graph of SCM as usual
- But now additional information by edge labels:

**Path Coefficients** 

Linearity assumption makes association of coefficient to edge a well-formed operation

## Path Coefficients (Example)

### **Example**

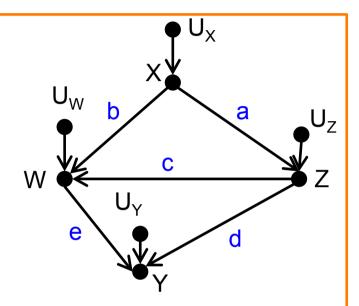
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- Graph of SCM as usual
- But now additional information by edge labels:

Path Coefficients

#### Warning from the beginning:

Path coeefficients (causal) ≠ regression coefficients (descriptive)



## Path Coefficients (Semantics)

Linear SCM

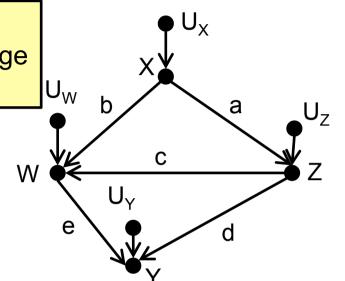
$$-X = U_{\times}$$

Note: CDE does not depend on the exact change  $-X = U_X$  of Z but only its rate Z=+1



$$-W = bX + cZ + U_{W}$$

$$-Y = dZ + eW + U_Y$$



- Q: What is the semantics of the path coefficients on edge Z-Y?
- A: Direct effect CDE on Y of change Z=+1

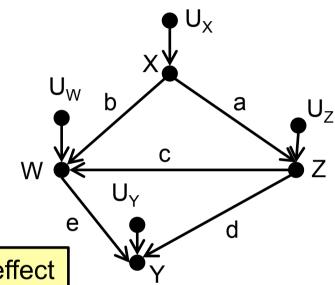
CDE = E[Y|do(Z=z+1), do(W=w)]- E[Y|do(Z = z), do(W=w)]  
= 
$$d(z+1)$$
 +ew +E[U<sub>Y</sub>]- (dz +ew+E[U<sub>Y</sub>])  
=  $d$  = label on Z-Y edge We used the linearity of E



We used the linearity of E E[aX + bY] = aE[X] + bE[Y]

## Total Effect in Linear Systems (Example)

- Linear SCM
  - $-X = U_X$
  - $Z = aX + U_7$
  - $-W = bX + cZ + U_{W}$
  - $-Y = dZ + eW + U_Y$

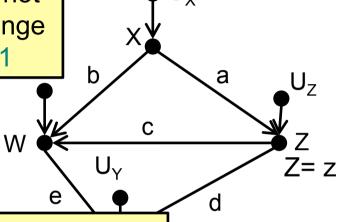


- Total effect = general causal effect
- Q: What is the total effect of Z on Y?
- A: Sum of coefficient products over each directed Z-Y path
  - Directed path 1: Z-d->Y; product = d
  - Directed path 2: Z-c->W-e->Y; product =ec
  - Total effect = d + ec

## Total Effect in Linear Systems (Intuition)

- Linear SCM
  - $-X = U_X$
  - $Z = aX + U_7$
  - $-W = bX + cZ + U_{W}$
  - $-Y = dZ + eW + U_Y$

Note 2: Total effect does not depend on the exact change of Z but only its rate Z=+1



Note 3: Holds for any linear SCM (U<sub>i</sub>s may be dependent)

- Q: What is the total effect of Z on Y?
- A: Sum of coefficient products over each directed
   Z-Y path
  - Total effect T: Intervene on Z and express Y by Z

$$- Y = dZ + eW + U_Y = dZ + e(bX + cZ + U_W) + U_Y$$
  
=  $(d+ec)Z + ebX + U_Y + eU_W = \tau Z + U$  Note1: X,U<sub>Y</sub>,U<sub>W</sub>



Note1: X,U<sub>Y</sub>,U<sub>W</sub>
do not depend on Z

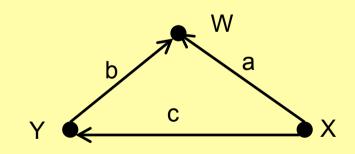
#### Note 4

- We followed (Bollen 1989)) and summed over directed paths
- In book of Pearl, Glymour & Jewell (p.82-83) summation over non-backdoor paths
  - Seems to be an error (due to wrongly applied Wright's path rule?)
  - Consider SCM

• 
$$W = bY + aX$$

• 
$$Y = cX$$

• ACE = c ( and not c + b\*a )



K. Bollen: Structural Equations with latent variables. New York, 1989.

#### Addendum and Historical Note to Note 4

- Earliest use of graphs in causal analysis in (Wright 1920)
- Wright path tracing for calculating covariances in linear SCMs

$$\sigma_{XY} = \sum_{p} product(p)$$

- where all p are X-Y paths not containing a collider and
- product(p) = product of all structural coeeficients and covariances of error terms



### Identifying Structural Coefficients

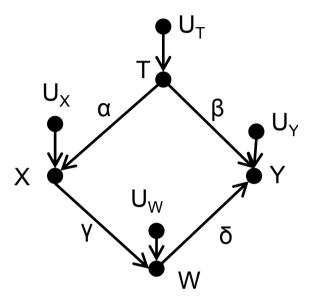
- What if path coefficients are not known apriori or are not testable?
- One has to identify only those relevant for the specific task, e.g., total effect of X to Y or direct effect of Z on X
- For those required for the task one can use linear regression on the data
  - 1. Identify relevant variables for linear regression
  - 2. Identify within linear equation coefficients for the specific task



## Total effect in Incomplete Linear Systems

- Q: Total effect (GCE) of X on Y?
- Now path coefficients not necessarily known (greek letters)
- Recall: With backdoor criterion identify Z to adjust for

GCE = 
$$P(y|do(x)) = \sum_{z} P(y \mid x,z)P(z)$$



- Use backdoor to identify variables to regress for
- Here  $Z = \{T\}$ , so do linear regression on X,T:

$$- Y(X,T) = r_X X + r_T T + \varepsilon$$

$$- r_X = total effect of X on Y$$

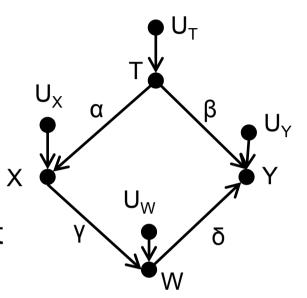
- linear regression equation ≠ structural equation
- Regression coefficients handmade
- Path coefficients nature made



## Direct Effect in Incomplete Linear Systems

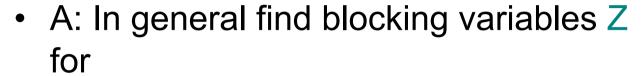
Q: Direct effect of X on Y?

- A: Here, direct effect = 0
  - There is no edge from X to Y
  - Which amounts to path coefficient for X-Y edge = 0



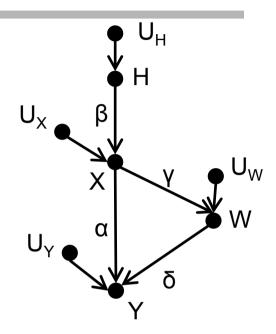
## Direct Effect in Incomplete Linear Systems

Q: Direct effect of X on Y?





2. Indirect X-Y paths



- This can be achieved as follows
  - $-G_{\alpha}$  = Graph G without edge  $X \alpha Y$
  - Z = variables d-separating X and Y

Here: 
$$Z = \{W\}$$

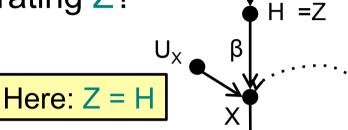
• 
$$Y = r_X X + r_Z Z + \varepsilon$$
 Here:  $Y = r_X X + r_W W + \varepsilon$ 

Direct effect of X on  $Y = r_X = :\alpha$ 



## Direct Effect in Incomplete Linear Systems

Q: What if there are no d-separating Z?



- A:
  - 1. Find instrumental variables Z
    - 1. Z is d-connected to X in G<sub>a</sub> and
    - 2. Z is d-separated from Y in G<sub>a</sub>
  - 2. Regress  $Y = r_1 Z + \varepsilon$

Dashed arrow denotes existence 3. Regress  $X = r_2 Z + \varepsilon$  of unobserved confounder

4.  $r_1/r_2 = \beta_{YZ}/\beta_{XZ} =: \alpha = \text{direct effect of X on Y}$ 

#### This is because

- Z = H emits no backdoors, so  $r_2 = \beta$
- $r_1$  = total effect of Z on Y =  $\beta\alpha$



## Instrumental Variables (IVs)

 Usage of IVs to trace causal effects starts already in 1925 (econometrics)

Wright. Corn and Hog correlations, Tech. Rep. 1300, US Department of Agriculture, 1925.

 Standard definitions in econometrics defined IVs w.r.t. single equation not parameter

Definition (classically according to economist's)

For an equation

$$Y = \alpha_1 X_1 + ... + \alpha_k X_k + U_Y$$
 (\*)

Z is instrumtenal variable for equation (\*) iff

- Z is correlated with X={X<sub>1</sub>, ... X<sub>k</sub>} and
- Z is not correlated with U<sub>Y</sub>



#### What's in a definition?

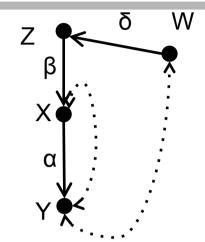
- The early economist's definition not (!) equivalent with our official definition
  - General question: What's a good definition?
  - Main problem with classical equation-: too global
    - Full equation may not be identifiable though some parameters are.
- The new definition is an example of a general interesting phenomen
  - Many simplifications (clarifications/disambiguations) of (IV) research in econometrics by considering associated graph structure for SCM



#### Conditional IVs

- Z no IV anymore for α, because
  - Z not d-separated from Y
- But conditioning on W helps

C. Brito & J.Pearl: Generalized instrumental variables. In *Uncertainty in Artificial Intelligence, Proceedings of the Eighteenth Conference*, 85–93, 2002.



Definition (Brito & Pearl, 02) A variable Z is a conditional instrumental variable given set W for coefficient α (from X to Y) iff

- Set of descendants of Y not intersecting with W
- W d-separates Z from Y in G<sub>α</sub>
- W does not d-separate Z from X in G<sub>α</sub>

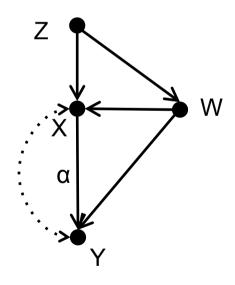
If conditions fulfilled, then  $\alpha = \beta_{YZ,W} / \beta_{XZ,W}$ 

## Conditional IVs (Examples)

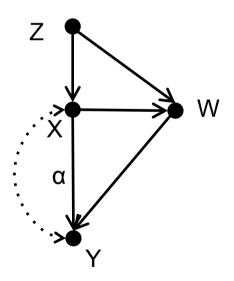
### Z instrument for $\alpha$ given W?

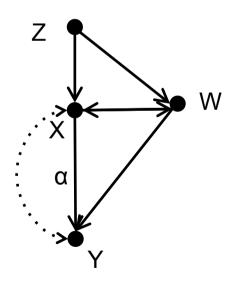
**Definition** Z is a conditional IV given set W for  $\alpha$  iff

- Set of descendants of Y not intersecting with W
- W d-separates Z from Y in G<sub>α</sub>
- W does not d-separate Z from X in G<sub>α</sub>



yes

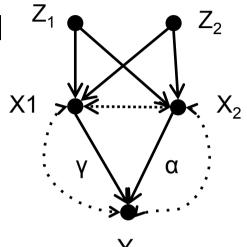




no

#### Sets of IVs

- Sometimes need sets of instrumental variables
- Neither Z<sub>1</sub> nor Z<sub>2</sub> (on their own) are instrumental variables (for the identification of α or γ)



- Using them both helps.
  - Definition not trivial due to possible path intersections of paths

Using Wright's path tracing and solving for γ and α

$$\sigma_{Z1Y} = \sigma_{Z1X1}\gamma + \sigma_{Z1X2}\alpha$$
$$\sigma_{Z2Y} = \sigma_{Z2X1}\gamma + \sigma_{Z2X2}\alpha$$

#### **Definition**

Set  $\{Z_1, ..., Z_k\}$  is an instrumental set for path coefficients  $\alpha_1, ..., \alpha_k$  with  $X_i$ - $\alpha_k$ ->Y iff

- 1. For each i, Z<sub>i</sub> is separated from Y in G' (= G with edges X<sub>1</sub>->Y, ..., X<sub>k</sub>->Y deleted)
- 2. There are paths  $p_i$ :  $Z_i$  to Y containing  $X_i$ ->Y (1 <= i <=k) s.t. for paths  $p_i$   $p_j$  (i  $\neq j$  in  $\{1,2,...k\}$ ) and any common RV V one of the following holds:
  - Both  $p_i[Z_i...V]$  and  $p_i[V...Y]$  point to V or
  - Both  $p_i[Z_i...V]$  and  $p_i[V...Y]$  point to V

 $p_i[W...H]$  = subpath of  $p_i$  from W to H



#### **Definition** (Instrumental Set)

### Condition 2. says:

Cannot merge two intersecting paths pi and pi to yield two unblocked paths: one must contain collider

- 2. There are unblocked paths  $p_i$ :  $Z_i$  to Y containing  $X_{i-1}$ >Y  $(1 \le i \le k)$  s.t. for paths  $p_i$   $p_i$  and any common RV V one of the following conditions holds:
  - Both  $p_i[Z_i...V]$  and  $p_i[V...Y]$  point to V or
  - Both  $p_i[Z_i...V]$  and  $p_i[V...Y]$  point to V  $(i \neq j \text{ in } \{1,2,...k\})$



#### **Theorem**

Let  $\{Z_1, ..., Z_k\}$  be an instrumental set for coefficients  $\alpha_1...\alpha_k$  with  $X_i$ - $\alpha_k$ ->Y.

Then: The equations below are linearly independent for almost all parameterizations of the model and can be solved to obtain expressions for  $\alpha_1...\alpha_k$  in terms of

the covariance matrix

$$\sigma_{Z1Y} = \sigma_{Z1X1}\alpha_1 + \sigma_{Z1X2}\alpha_2 + \dots + \sigma_{Z1Xk}\alpha_k$$
  
$$\sigma_{Z2Y} = \sigma_{Z2X1}\alpha_1 + \sigma_{Z2X2}\alpha_2 + \dots + \sigma_{Z2Xk}\alpha_k$$

Ensuring linear independence:

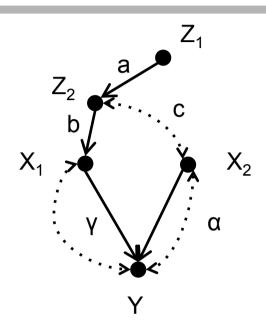
- The rank of the covriance matrix has its maximum
- -> no information loss
- ensuring identifiability of parameters α<sub>1</sub>...α<sub>k</sub>

. . .

$$\sigma_{ZkY} = \sigma_{ZkX1}\alpha_1 + \sigma_{ZkX2}\alpha_2 + ... + \sigma_{ZkXk}\alpha_k$$

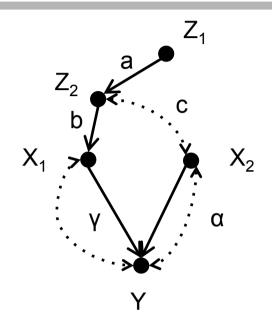
# Example: Instrument sets (positive case)

- $p_1 = Z_1 -> Z_2 -> X_1 -> Y$
- $p_2 = Z_2 < -> X_2 -> Y$
- $p_1$  and  $p_2$  satisfy condition 2 w.r.t. common variable  $V = Z_2$ 
  - $p_1[Z_1...V] = Z_1->Z_2$  points to  $Z_2$
  - $-p_2[V...Y] = p_2$  also points to  $Z_2$
  - Z<sub>2</sub> as a collider blocks possible path merges of p<sub>1</sub> and p<sub>2</sub>



# Example: Instrument sets (positive case)

- Algebraically
  - $\sigma_{Z1Y}$  lacks influence of path  $Z_2 <-> X_2 -> Y$  and hence does not contain term  $ac\alpha$
  - σ<sub>Z2Y</sub> contains term cα



Applying Wright's rule

$$\sigma_{Z1Y} = \sigma_{Z1X1}\gamma + \sigma_{Z1X2}\alpha = \sigma_{Z1X1}\gamma + 0\alpha = ab\gamma$$
  
$$\sigma_{Z2Y} = \sigma_{Z2X1}\gamma + \sigma_{Z2X2}\alpha = b\gamma + c\alpha$$

Solving linearly independent equations:

$$- \gamma = \sigma_{71Y} \sigma_{71X1}$$

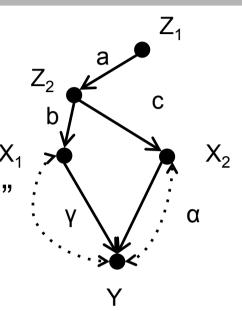


# Example: Instrument sets (negative case)

• 
$$p_1 = Z_1 -> Z_2 -> X_1 -> Y$$

• 
$$p_2 = Z_2 -> X_2 -> Y$$

Every path from Z<sub>2</sub> to Y is a "sub-path"
 of a path from Z<sub>1</sub> to Y



Applying Wright's rule

$$\sigma_{Z2Y} = b\gamma + c\alpha$$

$$\sigma_{Z1Y} = ab\gamma + ac\alpha = a(b\gamma + c\alpha) = a\sigma_{Z2Y}$$



### **Conditional Instrumental Sets**

See

C. Brito & J.Pearl: Generalized instrumental variables. In *Uncertainty in Artificial* Intelligence, Proceedings of the Eighteenth Conference, 85–93, 2002.



### Mediation in Linear Systems

- Direct effect (DE) of X on Y mediated by Z
  - Estimate path coefficient between X and Y as shown before
- Total effect (T) of X on Y mediated by Z
  - Estimate by regression as shown before
- Indirect effect of X on Y
  - IE =  $\tau$  DE

(For non-linear systems need approach with counterfactuals)

