

# Causal Inference with Graphical Models

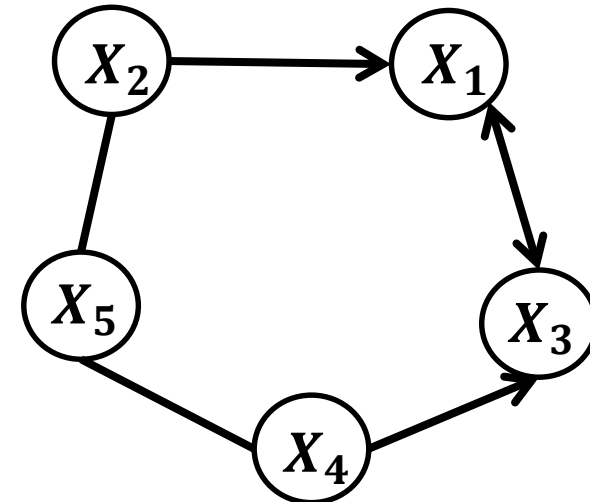
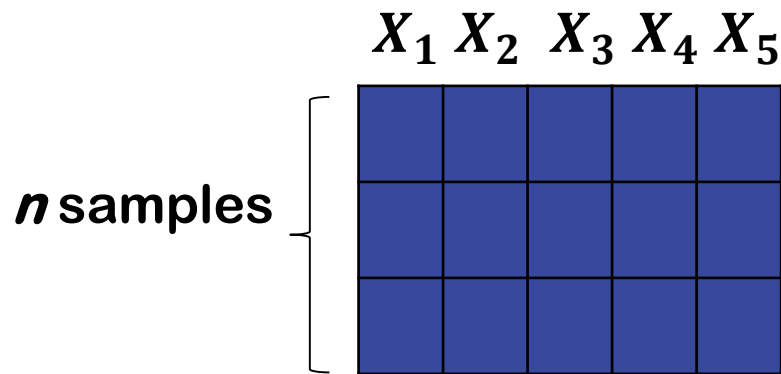
Definition, Correlation vs. Causality, Challenges, Constraint-based learning using PC algorithm, Additive Noise Model: LiNGAM, Recent developments in causal discovery

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Department of Computer Science  
North Carolina State University

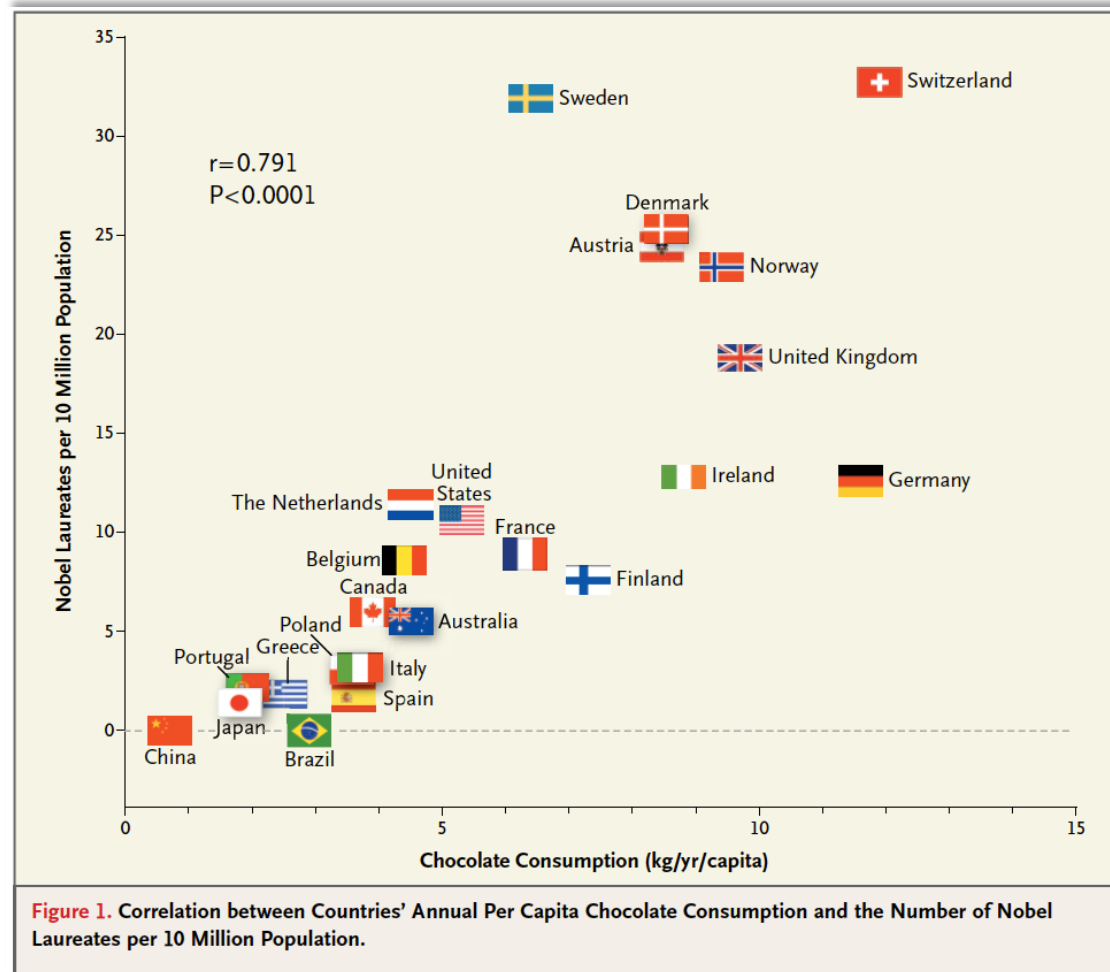
# What is Causal Inference?

- **Causal Inference** is the task of learning **cause-effect relationships** and estimating **causal effects** from the data.
- A **directed edge** represents a **potential causal relationship**, whereas an **undirected** or a **bidirected edge** represents an **ambiguous relationship**.
- For example, the directed edge  $X_2 \rightarrow X_1$  indicates  $X_2$  is a **potential cause (or parent)** and  $X_1$  is the **effect (or child)**.



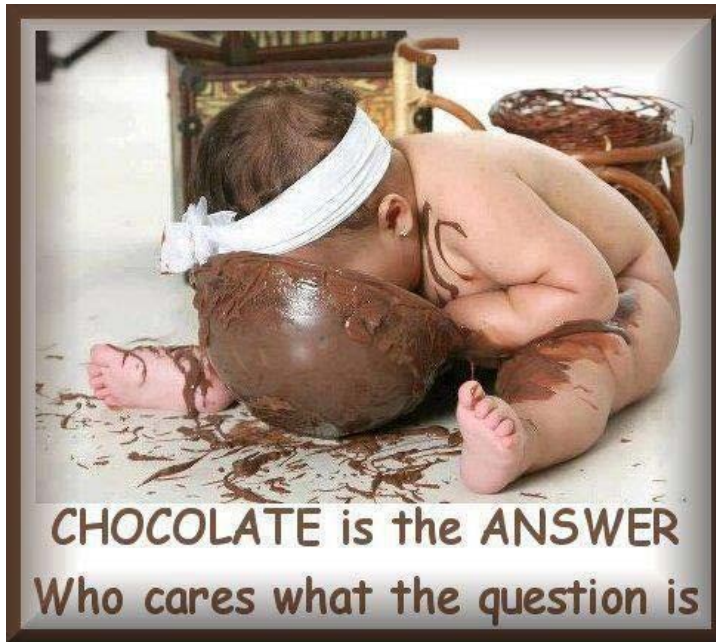
An estimated causal structure  
from the PC algorithm

# Correlation vs. Causality

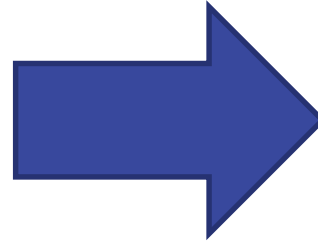


This research shows there is a strong correlation between chocolate consumption and winning Nobel prize!

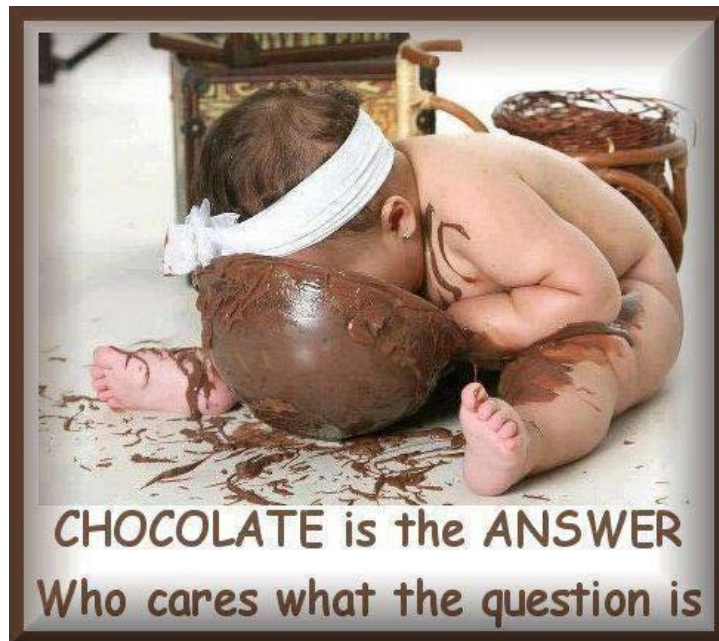
# If Correlation == Causality



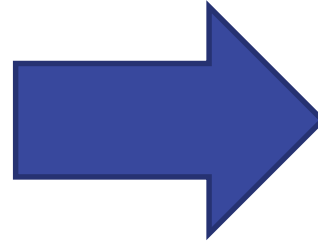
more awesome pictures at [THEMETAPICTURE.COM](http://THEMETAPICTURE.COM)



# But the reality is...

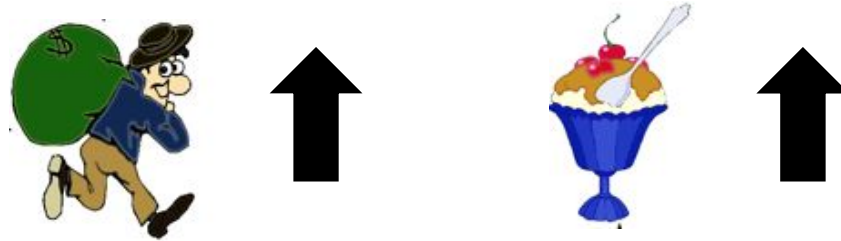


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# Example

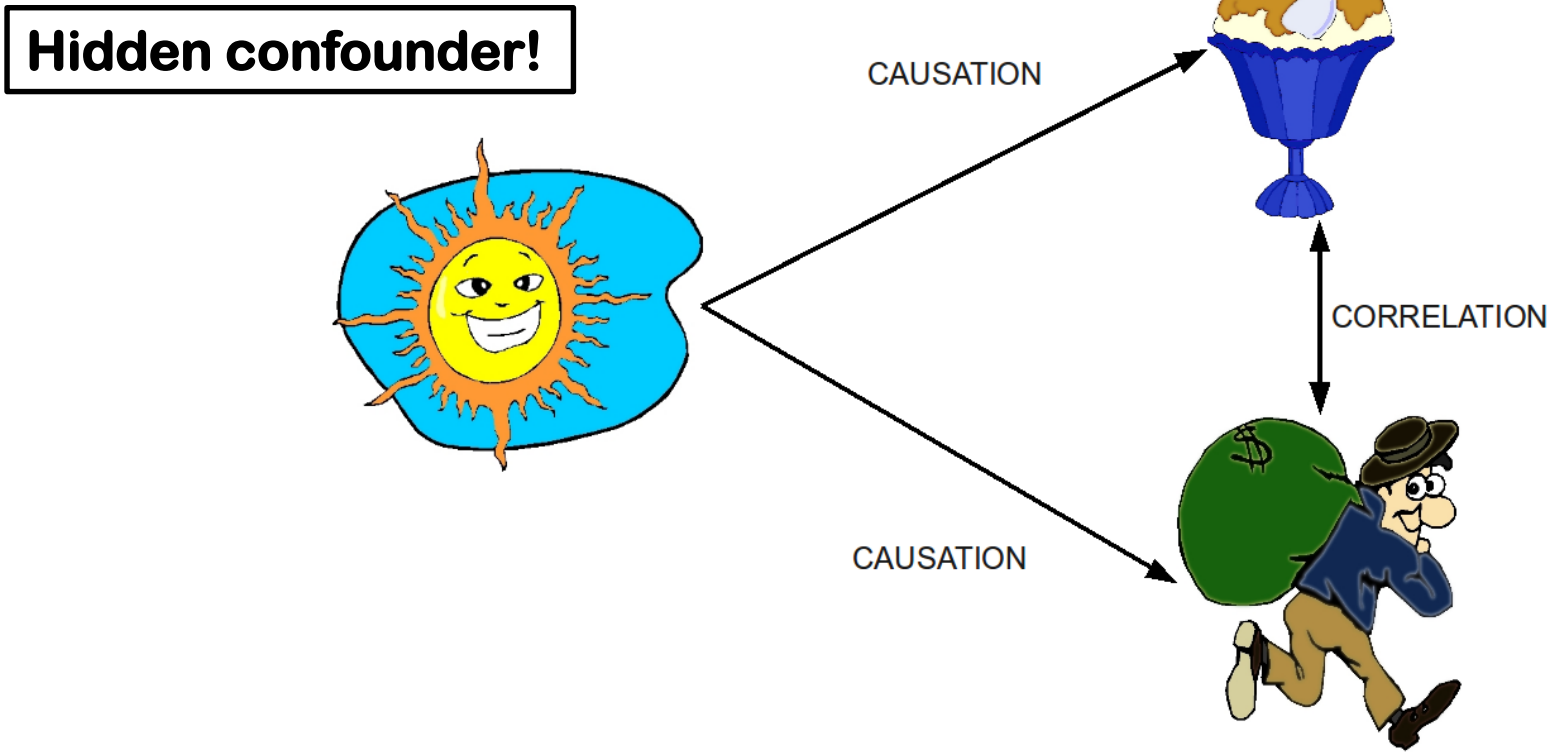
- During summer, there is an increase in ice-cream sales and the crimes committed.



- Does this mean?



# Example (cont.)



Courtesy: Google Images

# Challenges

- Identifying **accurate cause-effect relationships** is obscured by **spurious associations** in the data.
- Difficult to test causality in real-world applications:
  - it involves **performing randomized experiments** that might not be feasible
- **Underdetermined data sets**
  - with fewer than hundred samples and thousands of variables
  - make it even more difficult to estimate cause-effect relationships

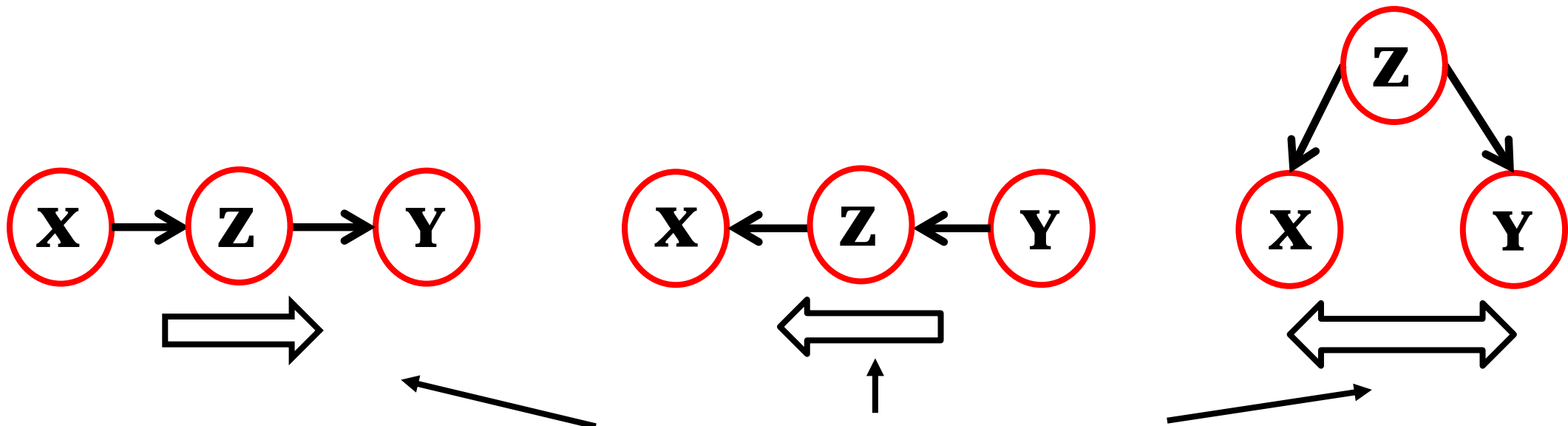


# Constraint-based method: PC Algorithm

- Goal: Test **every pair of adjacent variables** by performing **(un)conditional independence tests** to remove as many spurious associations as possible.

# Conditional Independence: $d$ -separation

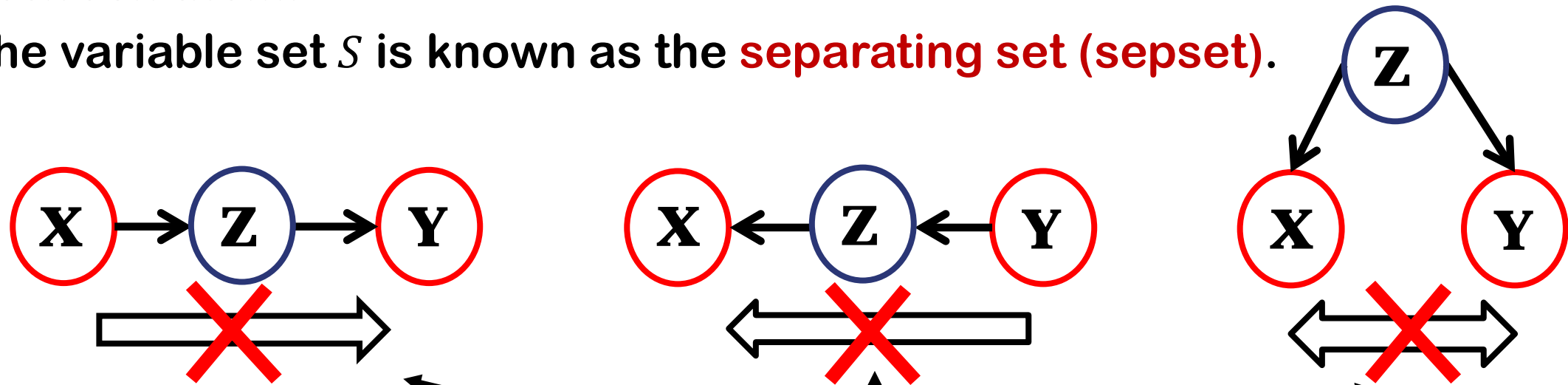
- Two variables  $X$  and  $Y$  are said to be  $d$ -separated by a set of variables  $S$  if  $X$  and  $Y$  are independent conditioned on  $S$ .
  - The idea is to **block the information flow** between  $X$  &  $Y$  using the set of variables in  $S$ .
- Consider the following three structures between  $X$  and  $Y$ , with  $S = \{Z\}$ :



The arrows indicate the flow of information between  $X$  and  $Y$ .

# Conditional Independence: $d$ -separation (cont.)

- Variable  $Z \in S$  :
  - $d$ -separates  $X$  and  $Y$  as it blocks the information flow between the two variables
- The variables in  $S$  should  **$d$ -separate**  $X$  and  $Y$  for **each path** that exists between them.
- The variable set  $S$  is known as the **separating set (sepset)**.

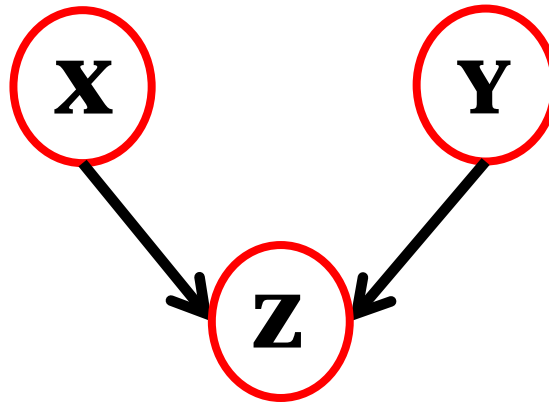


The information flow between  $X$  and  $Y$  is blocked by  $Z$ .

$$X \perp\!\!\!\perp Y \mid Z \quad \text{sepset}(X, Y) = Z$$

# Conditional Independence: $v$ -structure

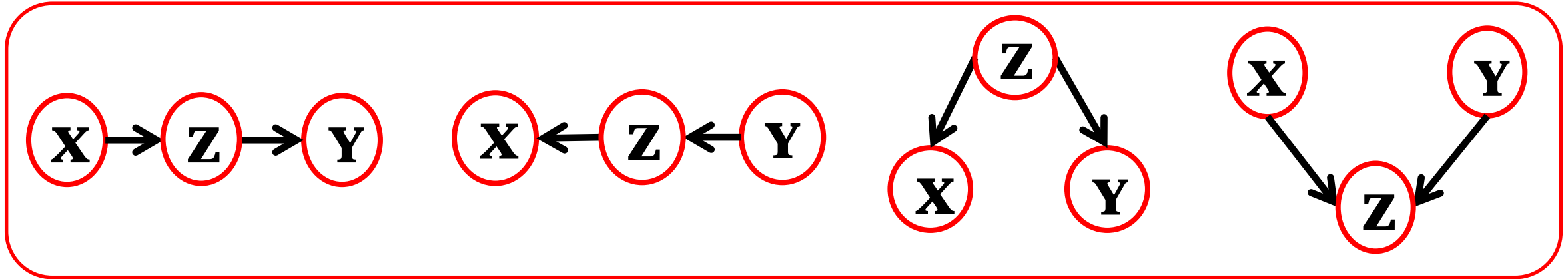
- A  $v$ -structure is a triple  $X \rightarrow Z \leftarrow Y$  such that  $X$  and  $Y$  are not adjacent.
- $X$  and  $Y$  are **unconditionally independent** but they are **conditionally dependent** given their child  $Z$ .



$$X \perp\!\!\!\perp Y$$

$$X \not\perp\!\!\!\perp Y | Z$$

# Conditional Independence: Statistical tests




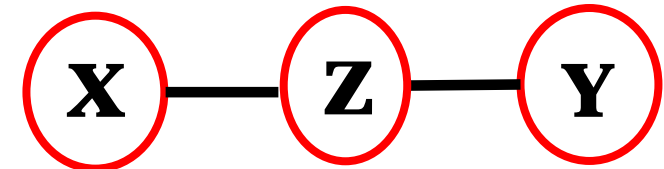
- In real-world the real causal structure is rarely known.
- To infer the structure we have a data set and statistical tests at our disposal.

X	Y	Z

+

Statistical tests  
for conditional  
independence

$$X \perp\!\!\!\perp Y | Z$$




There is a high chance that X and Y do not have a direct causal relationship.

# Conditional Independence: Stat test: **Continuous Variables**

- **Continuous variables: Fisher's Z test**

$$Z = \sqrt{N - |W| - 3} * \frac{1}{2} \log_e \left( \frac{1 + \tilde{\rho}_{X,Y|W}}{1 - \tilde{\rho}_{X,Y|W}} \right)$$

- where  $\tilde{\rho}_{X,Y|W}$  is the sample partial correlation between two variables  $X$  and  $Y$  given a set of variables  $W$ .
- The null hypothesis,  $H_0: \tilde{\rho}_{X,Y|W} = 0$  is rejected if,

$$Z > \Phi^{-1}\left(1 - \frac{\alpha}{2}\right)$$

- where  $\Phi$  is a cumulative distribution function of a Gaussian distribution with mean 0 and variance 1.

# Conditional Independence: Stat test: **Categorical Variables**

- **Binary or Discrete variables:  $G^2$  test**

$$G = 2 * \sum_i O_i \log \left( \frac{O_i}{E_i} \right)$$

- where  $O_i$ =observed frequencies and  $E_i$ =expected frequencies of the discrete variables.
- To test if  $X$  is independent of  $Y$  given  $Z$ , a contingency table is built for every level of  $Z$  and the  $G$ -statistic is the summation over all levels.

$O_i$		
$X \backslash Y$	0	1
0	$N_{00}$	$N_{01}$
1	$N_{10}$	$N_{11}$

$$N = N_{00} + N_{01} + N_{10} + N_{11}$$

$E_i$		
$X \backslash Y$	0	1
0	$(N_{+0} * N_{0+}) / N$	$(N_{+1} * N_{0+}) / N$
1	$(N_{+0} * N_{1+}) / N$	$(N_{+1} * N_{1+}) / N$

$$N_{+0} = N_{00} + N_{10}, N_{0+} = N_{00} + N_{01}$$
$$N_{+1} = N_{01} + N_{11}, N_{1+} = N_{10} + N_{11}$$

# Conditional Independence: Stat test: $G$ -statistic

- **Binary or Discrete variables:  $G^2$  test**

$$G = 2 * \sum_i O_i \log \left( \frac{O_i}{E_i} \right)$$

- where  $O_i$ =observed frequencies and  $E_i$ =expected frequencies of the discrete variables.
- The  **$G$ -statistic** follows a **Chi-square distribution** with  $I*(J-1)*(K-1)$  degrees of freedom where  $I$ ,  $J$  and  $K$  are the number of levels of  $X$ ,  $Y$  and  $Z$ , respectively.

$$p - value = pchisq(G, df, lower.tail = FALSE)$$

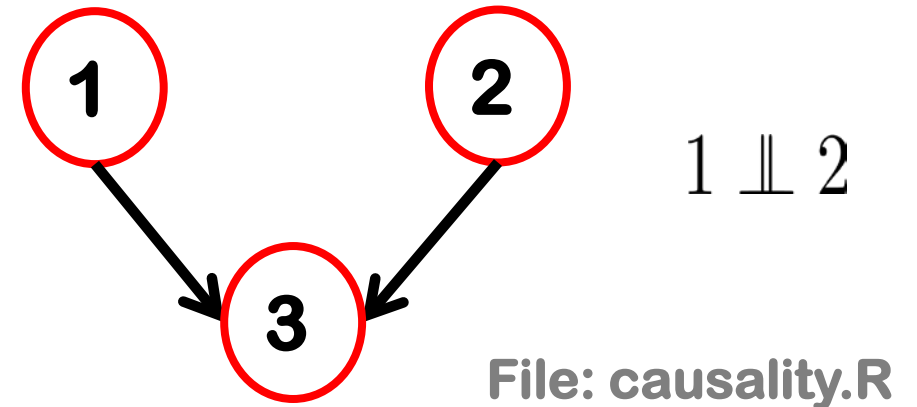
- The null hypothesis of independence is rejected if  $p - value < \alpha$ ; otherwise, we fail to reject the null hypothesis.



# Conditional Independence: Statistical tests

- **Null hypothesis**  $H_0$ : Variables are independent  $\rightarrow$  delete the edge
- **Alternative hypothesis**  $H_1$ : Variables are not independent  $\rightarrow$  keep the edge

Variable type	Test	R function
Continuous	Fisher's Z test	gaussCltest
Discrete	$G^2$ test	disCltest
Binary	$G^2$ test	binCltest



```
> gaussCltest(1,2,s=NULL,suffstat=list(C=cor(dat), n=nrow(dat)))  
[1] 0.7581304
```

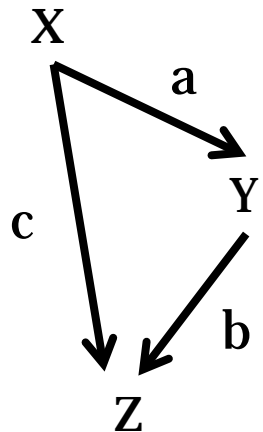
- If  $p\text{-value} < \alpha$  we reject the null hypothesis,  $H_0$  and if  $p\text{-value} > \alpha$  we fail to reject the null hypothesis.

# Constraint-based method: PC Algorithm

- Goal: Test **every pair of adjacent variables** by performing **(un)conditional independence tests** to remove as many spurious associations as possible.
- **Assumptions**:
  1. There are no cyclic causal relations
    - for example,  $X \rightarrow Y$  and  $Y \rightarrow X$
  2. **Causal faithfulness**: Dependencies found by PC algorithm are characteristic of the underlying data distribution.

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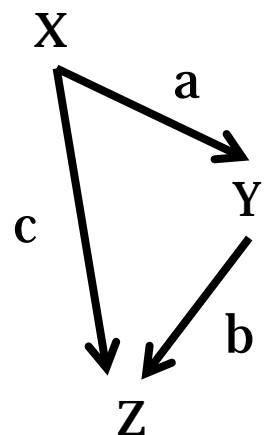


$$\begin{aligned} X &= \epsilon_X \\ Y &= aX + \epsilon_Y \\ Z &= cX + bY + \epsilon_Z \end{aligned}$$

Applying  $d$ -separation does not give us any independence relations between  $X$ ,  $Y$  and  $Z$ .

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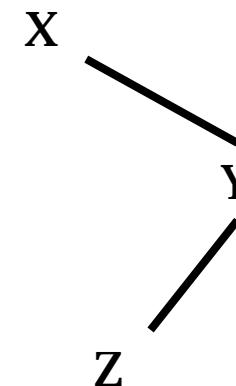


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If

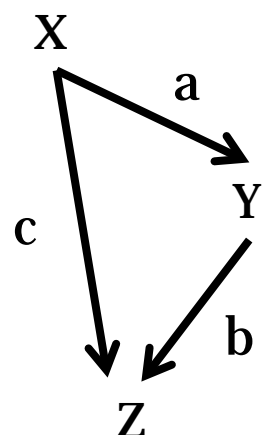
$$a \cdot b + c = 0$$

then  $X$  is independent of  $Z$ !



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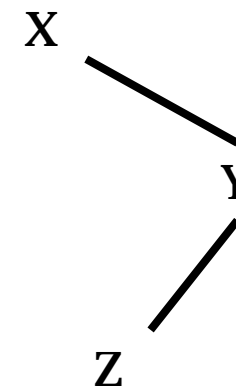


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“Spirtes et al. [2000, Theorem 3.2] show for linear models that this happens with probability zero if we assume that the coefficients are drawn randomly from positive densities.”

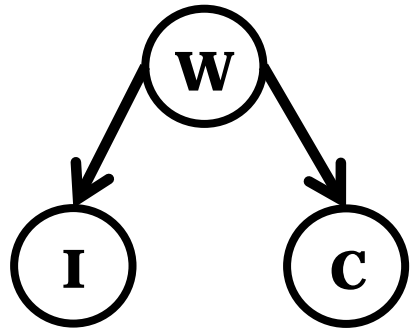
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  3. **Causal sufficiency**: Absence of hidden confounders in the data.

# Constraint-based method: PC Algorithm

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  2. **Causal faithfulness**: Dependencies found by PC algorithm are characteristic of the underlying data distribution.
  3. **Causal sufficiency**: Absence of hidden confounders in the data.
- Steps:
  1. Start with a complete undirected graph.
  2. Perform a **statistical test** for every pair of adjacent variables to test whether an edge between them is spurious or not.
  3. Orient the remaining undirected edges.
- The output of PC algorithm is a **partially directed graph** which represents a Markov equivalent class of graphs.

# PC Algorithm: An example

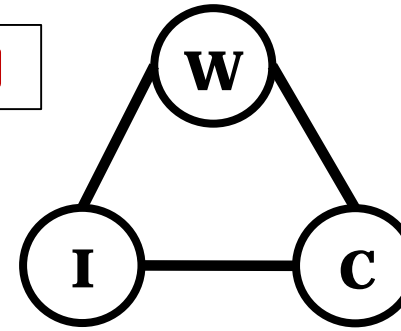


W: Weather  
I: Ice-cream sales  
C: Crime rate

True causal graph

$$I \perp\!\!\!\perp C | W$$

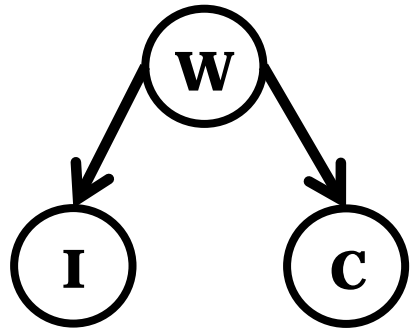
Step 1



A complete undirected graph over variable set  $X = \{W, I, C\}$ .



# PC Algorithm: An example

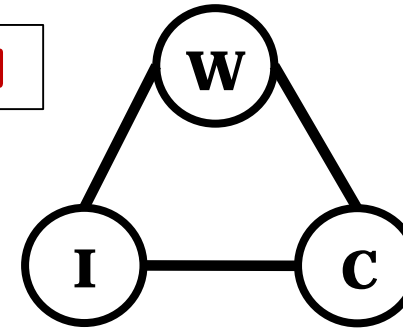


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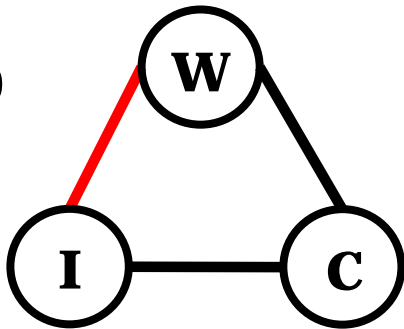
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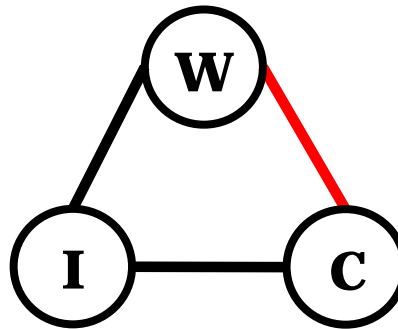
**Step 2:** Perform pairwise CI test with increasing conditioning set size,  $Z$ .

$|Z| = 0$



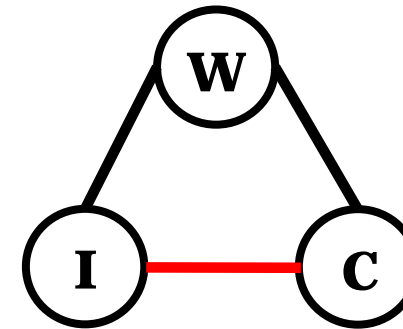
$$I \perp\!\!\!\perp W$$

No



$$C \perp\!\!\!\perp W$$

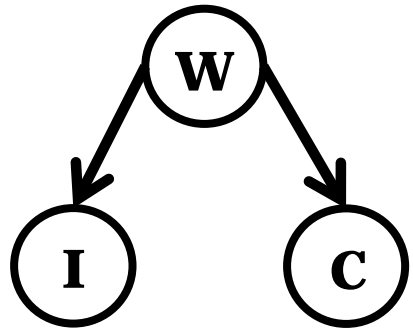
No



$$I \perp\!\!\!\perp C$$

No

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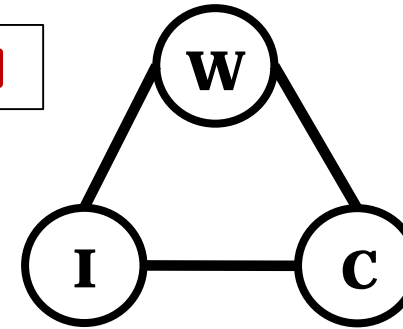


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$$I \perp\!\!\!\perp C | W$$

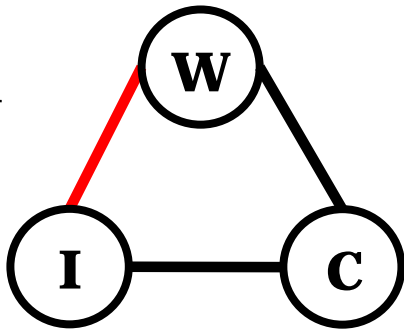
Step 1



A complete undirected graph over variable set  $X = \{W, I, C\}$ .

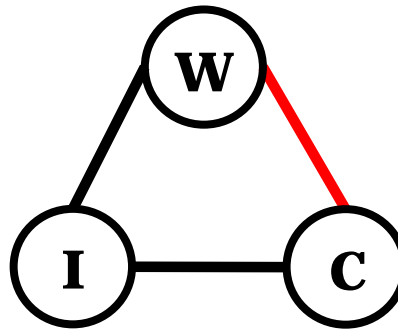
Step 2: Perform pairwise CI test with increasing conditioning set size,  $Z$ .

$|Z| = 1$



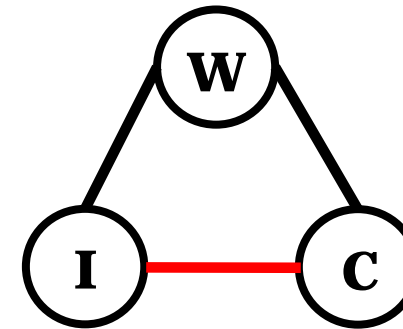
$$I \perp\!\!\!\perp W | C$$

No



$$C \perp\!\!\!\perp W | I$$

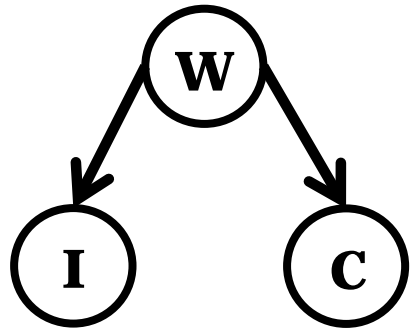
No



$$I \perp\!\!\!\perp C | W$$

Yes

# PC Algorithm: An example

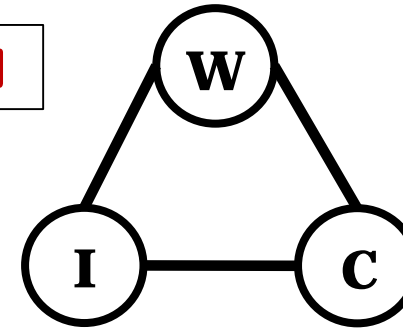


W: Weather  
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True causal graph

$$I \perp\!\!\!\perp C | W$$

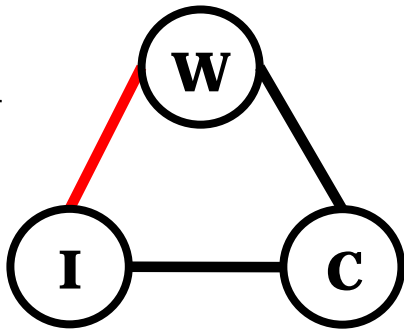
Step 1



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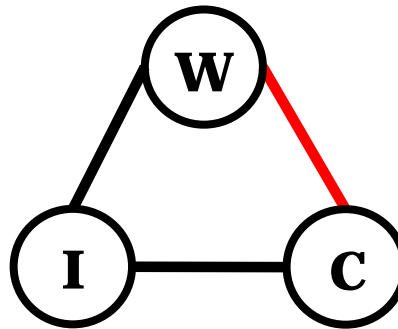
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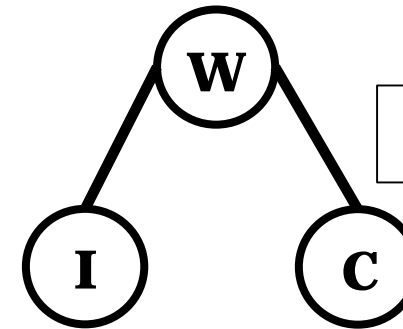
$$I \perp\!\!\!\perp W | C$$

No



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No

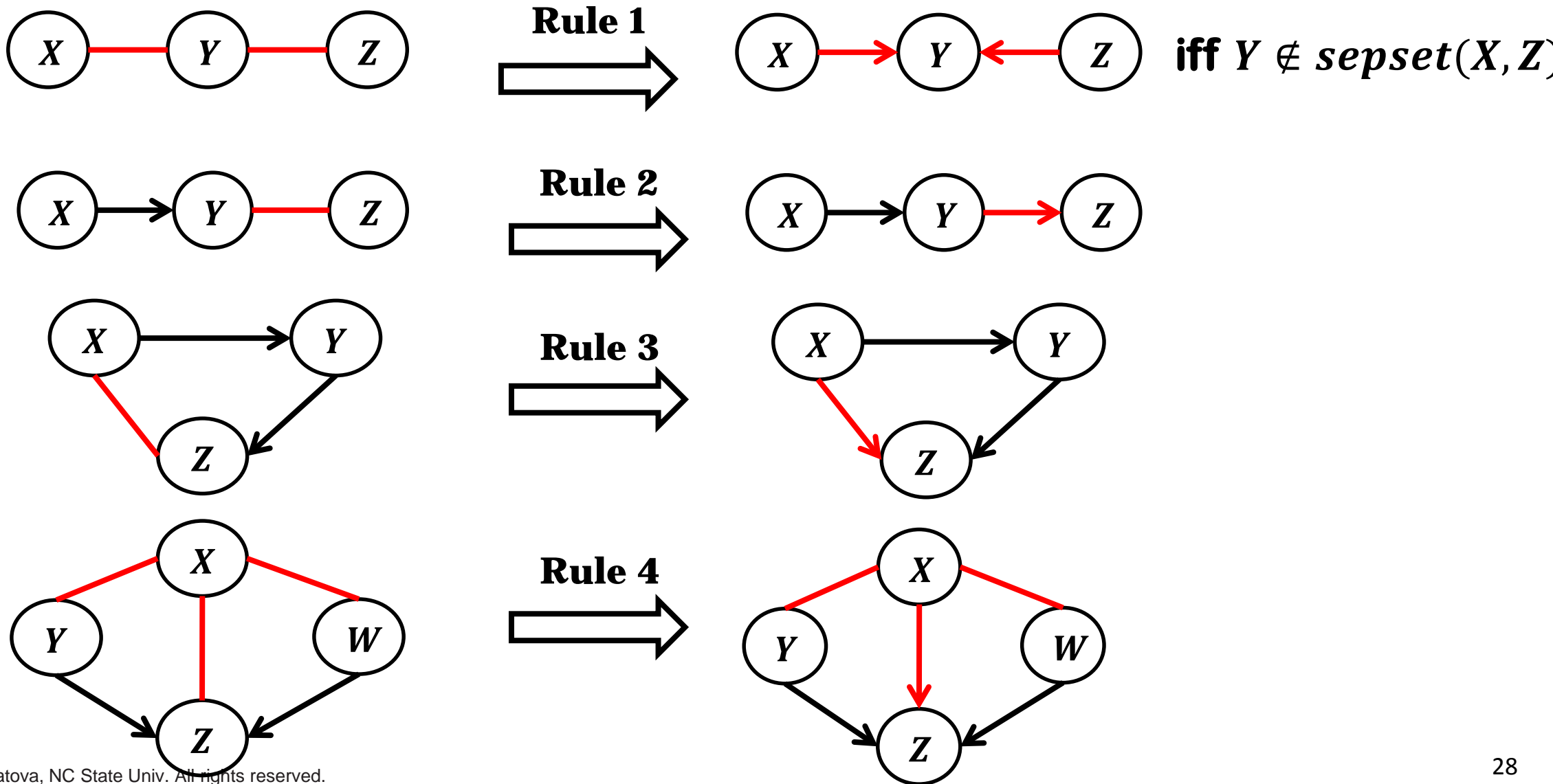


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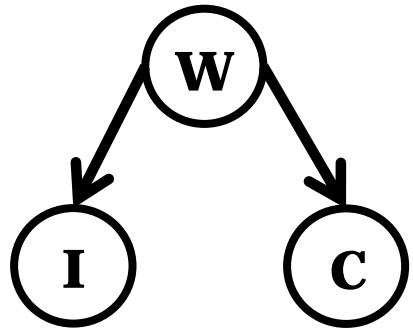
Yes

$$\text{sepset}(I, C) = W$$

# PC algorithm: Orientation Rules



# PC Algorithm: An example



W: Weather  
I: Ice-cream sales  
C: Crime rate

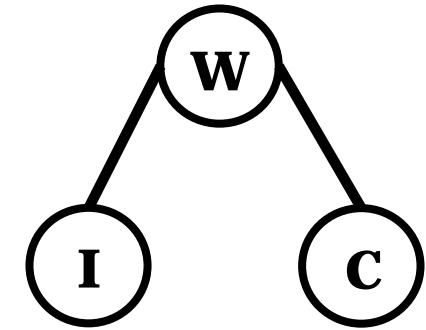
True causal graph

$$I \perp\!\!\!\perp C | W$$

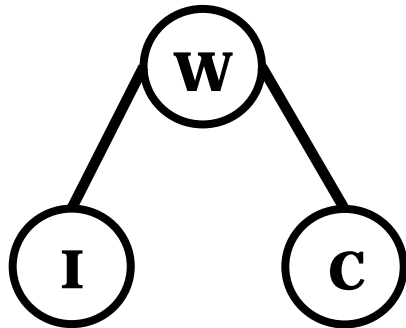
**Step 2: Output**

$$\text{sepset}(I, C) = W$$

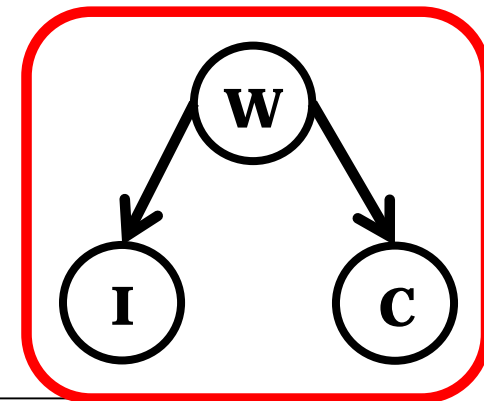
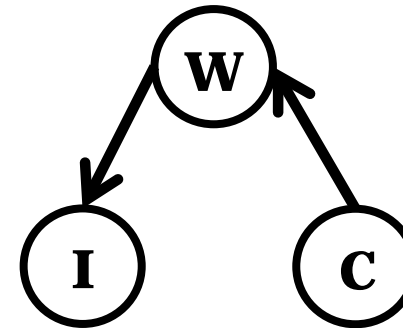
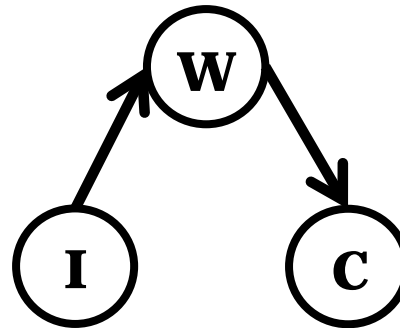
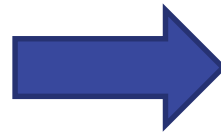
None of the orientation rules apply to this structure.



**Step 3: Output**



A partially directed graph.



A set of Markov equivalent graphs which encode the same conditional independence relationship.

# PC Algorithm: Simulation

File: causality.R

# PC algorithm example

# Causal structure:  $I \leftarrow W \rightarrow C$

$W \leftarrow \text{rnorm}(1000)$

$I \leftarrow 4*W + \text{rnorm}(1000)$

$C \leftarrow 2*W + \text{rnorm}(1000)$

$\text{dat\_3} \leftarrow \text{cbind}(W, I, C)$

$\text{pc\_fit} \leftarrow \text{pc}(\text{suffStat}=\text{list}(C=\text{cor}(\text{dat\_3}), n=\text{nrow}(\text{dat\_3})), \text{indepTest}=\text{gaussCIttest}, \text{alpha}=0.05, \text{labels}=\text{colnames}(\text{dat\_3}), \text{verbose}=\text{TRUE})$

$\text{plot}(\text{pc\_fit}, \text{main}=\text{"Estimated PDAG"})$

# Additive Noise Model (ANM): Linear Non-Gaussian Acyclic Model (LiNGAM)

- Assuming causal sufficiency, exact causal graph can be identified if the data is generated from an additive noise model such that at most  $X$  or  $\epsilon$  is Gaussian.

$$Y = f(X) + \epsilon$$

- Consider a variable set  $X = \{X_1, X_2, \dots, X_n\}$  generated from a structural equation model where  $X$  is a **linear function** of the disturbance variables  $E = \{E_1, E_2, \dots, E_n\}$ , which are **mutually independent and non-Gaussian**.

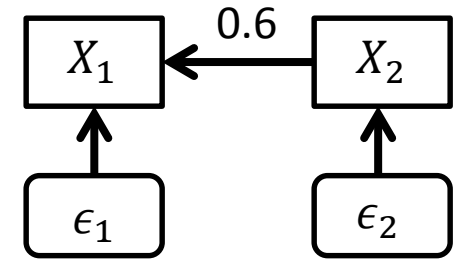
$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 & 0.6 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} + \begin{bmatrix} E_1 \\ E_2 \end{bmatrix}$$

$$X = BX + E$$

$$E = WX$$

- where  $W = I - B$

- How do we estimate  $W$ ? **Independent Component Analysis (ICA)!**



$$\begin{aligned} X_1 &= 0.6 * X_2 + \epsilon_1 \\ X_2 &= \epsilon_2 \end{aligned}$$

# Independent Component Analysis (ICA)

- ICA estimates the mixing matrix,  $W$ , however, the rows in the matrix can be in random order.

$$\begin{bmatrix} E_2 \\ E_1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & -0.6 \end{bmatrix} \begin{bmatrix} X_2 \\ X_1 \end{bmatrix} \quad \xrightarrow{\text{Permute rows}} \quad \begin{bmatrix} E_1 \\ E_2 \end{bmatrix} = \begin{bmatrix} 1 & -0.6 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}$$

The order of rows is incorrect, as  $E_2$  corresponds to  $X_1$  and  $E_1$  to  $X_2$

- An estimate of the coefficient matrix,  $\bar{B}$ , can now be computed using  $\bar{B} = I - \bar{W}$

$$\bar{B} = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 & -0.6 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0.6 \\ 0 & 0 \end{bmatrix}$$



# Estimation Errors in Coefficient Matrix

- However, it is possible to get an estimated coefficient matrix as follows,

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & 0.65 \\ -0.05 & 0 \end{bmatrix}}_{\bar{B}} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} + \begin{bmatrix} E_1 \\ E_2 \end{bmatrix}$$

- In such cases, we need to identify which path coefficients are zero by first permuting the rows and columns of  $\bar{B}$  using a **permutation matrix**  $Q$ , such that it **minimizes the sum of elements in the upper triangular part**.

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 0 & 0.65 \\ -0.05 & 0 \end{bmatrix} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} + \begin{bmatrix} E_1 \\ E_2 \end{bmatrix}$$



$$\begin{bmatrix} X_2 \\ X_1 \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & -0.05 \\ 0.65 & 0 \end{bmatrix}}_{Q\bar{B}Q^T} \begin{bmatrix} X_2 \\ X_1 \end{bmatrix} + \begin{bmatrix} E_2 \\ E_1 \end{bmatrix}$$

- Finally, set the values in the upper triangular matrix to zero.

$$\begin{bmatrix} X_2 \\ X_1 \end{bmatrix} = \underbrace{\begin{bmatrix} 0 & -0.05 \\ 0.65 & 0 \end{bmatrix}}_{Q\bar{B}Q^T} \begin{bmatrix} X_2 \\ X_1 \end{bmatrix} + \begin{bmatrix} E_2 \\ E_1 \end{bmatrix}$$



$$\begin{bmatrix} X_2 \\ X_1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0.65 & 0 \end{bmatrix} \begin{bmatrix} X_2 \\ X_1 \end{bmatrix} + \begin{bmatrix} E_2 \\ E_1 \end{bmatrix}$$

$\tilde{B}$  is strictly lower triangular

# Permutation Algorithm for Large Dimensions

- Computing coefficient matrix using exhaustive search becomes **computationally expensive in large dimensions**.
- An alternative approach,
  1. Set the  $m(m + 1)/2$  smallest (absolute) values in  $\tilde{B}$  to zero where  $m = \#$  of variables in the data.
  2. Test whether the resulting matrix can be permuted to a strict lower triangular matrix.
    - If yes, return the matrix as it contains the causal order of the variables.
    - If not, then set the next smallest (absolute value) element in the matrix to zero and repeat Step 2.

# Prune the coefficient matrix

- The LiNGAM algorithm has additional statistical tests to further prune the edges in the causal structure.
- The steps are as follows,
  1. Find **non-significant edges by applying Wald test** at a significance level of 0.05.
  2. For all the non-significant edges identified by the Wald test.
    - a. Set the least significant edge in the lower triangular matrix  $\tilde{B}$  to zero.
    - b. Test if the **reduced model with one reduced edge fits as good as the full model**.
    - c. Further, perform a **Chi-squared test** on the current model with reduced edge.
    - d. If both the hypotheses are accepted, prune the edge.
  3. Return the updated coefficient matrix  $\tilde{B}$ .

# State-of-the-Art: Causal Discovery

## Improvements to PC algorithm – PC-stable, Conservative PC, PC-Max [3,6]

Improvements to the PC algorithm were proposed to overcome: (i) variable order-dependent output and (ii) errors in orienting edges.

## Causal effect estimation from CPDAGs – IDA [5]

An approach to estimate lower bound of causal effect of a gene on a phenotype was developed to prioritize randomized control experiments. Assuming linearity causal effects can be estimated using linear regression.

## Divide-and-conquer based approaches– Rec, SADA, SAR, CDCD [10,1,4,2]

Divide-and-conquer based approaches perform conditional independence test only on edges that connect different graph partitions thereby reducing errors in statistical tests and improving the quality of output causal graphs.

# State-of-the-Art: Causal Discovery (cont.)

## Additive Noise Models (ANM) – LiNGAM, DirectLiNGAM, PNL [8,9,11,12]

Data generated from the following additive noise model could lead to exact identification of the causal graph if at most one of  $X$  or  $\epsilon$  is Gaussian.

$$Y = g(f(X) + \epsilon)$$

## Robust Conditional Independence tests – CCI, KCIT, RCIT [7,13,14]

Conditional independence tests that utilize kernel matrices and nonlinear regression to better detect independencies between variables.

# Publicly Available Tools for Causal Discovery

Software/Package	Language	Link
<b>pcalg</b>	<b>R</b>	<a href="https://cran.r-project.org/package=pcalg">https://cran.r-project.org/package=pcalg</a>
<b>bnlearn</b>	<b>R</b>	<a href="http://www.bnlearn.com/">http://www.bnlearn.com/</a>
<b>Bayes Net Toolbox</b>	<b>MATLAB</b>	<a href="https://github.com/bayesnet/bnt">https://github.com/bayesnet/bnt</a>
<b>Causal Explorer</b>	<b>MATLAB</b>	<a href="http://proceedings.mlr.press/v3/supplemental/Software_WCCI08_challenge.pdf">http://proceedings.mlr.press/v3/supplemental/Software_WCCI08_challenge.pdf</a>
<b>Tetrad</b>	<b>Java</b>	<a href="http://www.phil.cmu.edu/tetrad/">http://www.phil.cmu.edu/tetrad/</a>

# PC Algorithm: R Example

```
library(pcalg)
```

```
# Initialize the number of variables
```

```
rDAG <- randomDAG(10, prob=0.3, lB=0.1, uB=1)
```

```
# Visualize the generated DAG
```

```
plot(rDAG, main="A sample random DAG")
```

```
# Generate a multivariate data according to rDAG
```

```
data <- rmvDAG(1000, rDAG, errDist="normal")
```

```
# Now let's run the PC algorithm using the data
```

```
suffStat=list(C=cor(data), n=nrow(data))
```

```
pc_fit <- pc(suffStat, indepTest=gaussCIttest, alpha=0.05, labels=colnames(data), verbose=TRUE)
```

```
plot(pc_fit, main="PC Output")
```

```
# Evaluate the estimated graph with the true graph
```

```
shd(rDAG , pc_fit)
```

```
compareGraphs(pc_fit@graph, rDAG)
```

# LiNGAM algorithm: R Example

```
library(pcalg)
```

```
# Initialize the number of variables
```

```
x1 <- runif(1000)
```

```
x2 <- 0.8*x1 + runif(1000)
```

```
data <- cbind(x1, x2)
```

```
# Visualize the distribution
```

```
plot(data[, 1], data[, 2])
```

```
# Now let's run the LiNGAM algorithm using the data
```

```
lingam_fit <- lingam(data, verbose=TRUE)
```

```
show(lingam_fit)
```

```
pc_fit <- pc(suffStat=list(C=cor(data), n=nrow(data)), indepTest=gaussCIttest, alpha=0.05, p=ncol(data))
```

```
plot(pc_fit)
```



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# Constraint-based method: PC Algorithm

- Goal: Test **every pair of adjacent variables** by performing (un)conditional independence tests to remove as many spurious associations as possible.
- Assumptions:
  1. **Causal faithfulness**: Dependencies found by PC algorithm are characteristic of the underlying data distribution.
  2. **Causal sufficiency**: Absence of hidden confounders in the data.
- Steps:
  1. Start with a complete undirected graph.
  2. Perform a **statistical test** for every pair of adjacent variables to test whether an edge between them is spurious or not.
  3. Orient the remaining undirected edges.
- The output of PC algorithm is a **partially directed graph** which represents a Markov equivalent class of graphs.