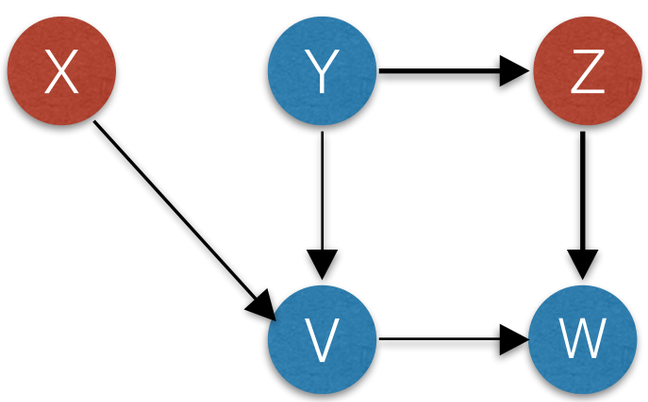
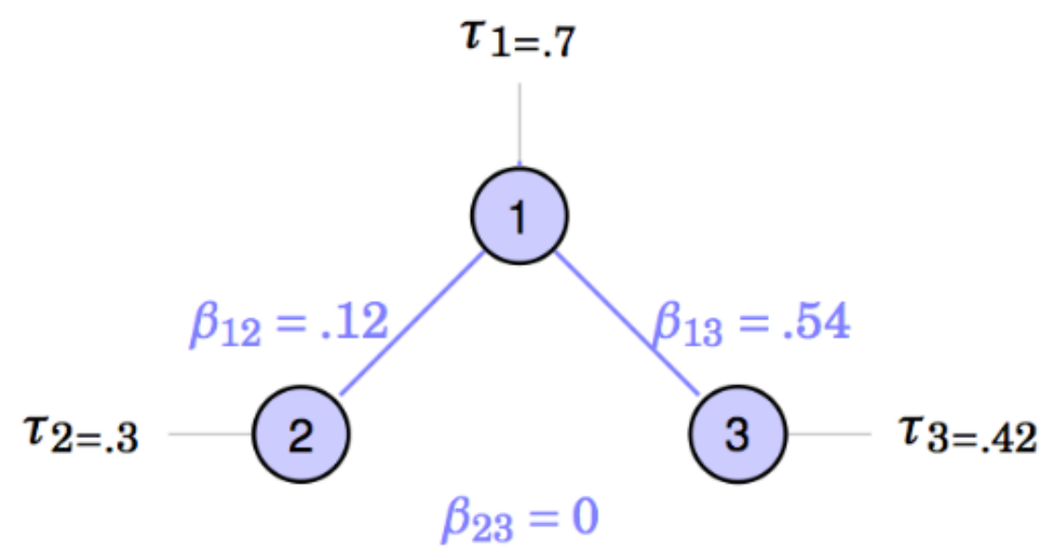
Discovering graphs

from Gaussian and Binary data

week 5



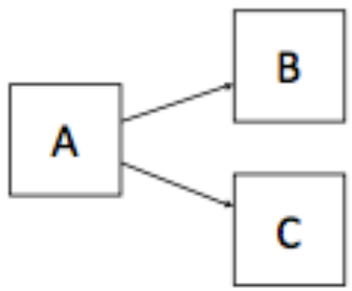


Claudia van Borkulo
University of Groningen/University of Amsterdam

Overview - last week

- About non-temporal causality and conditional independence
- Correlation ≠ causation, but you don't need an experiment to test whether variable A precedes B and not vice versa
- Even from observational data you can infer causal relations!
- What you need are ***conditional independencies (CI)***!
- Focus was on determining implications for CI from a given graph structure (***graph → CI***)

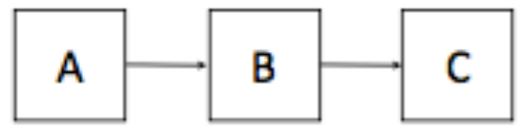
Common Cause



Example:
Village size (A)
causes babies (B)
and storks (C)

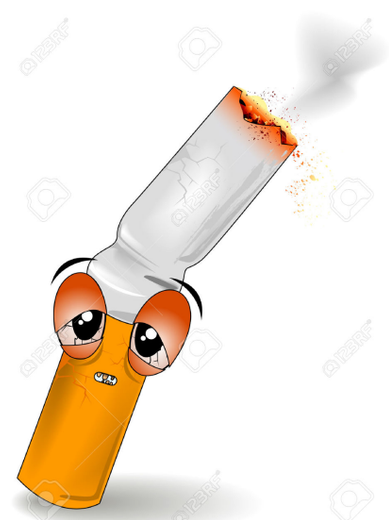
CI:
B and C
conditionally
independent
given A

Chain

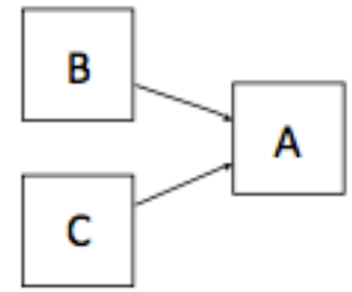


Example:
Smoking (A)
causes tar (B)
causes cancer (C)

CI:
A and C
conditionally
independent
given B



Collider



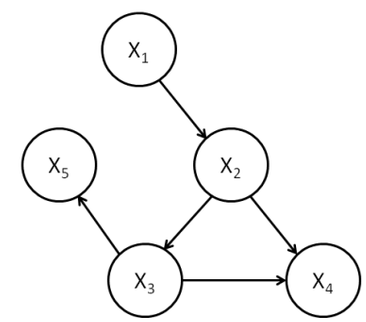
Example:
Firing squad
(B & C)
shoot prisoner (A)

CI:
B and C
conditionally
dependent
given A

Overview

This week:

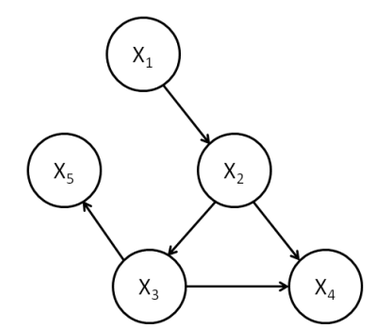
- Alternative for d-separation (ancestral graph)
- Confounds and the back-door criterion



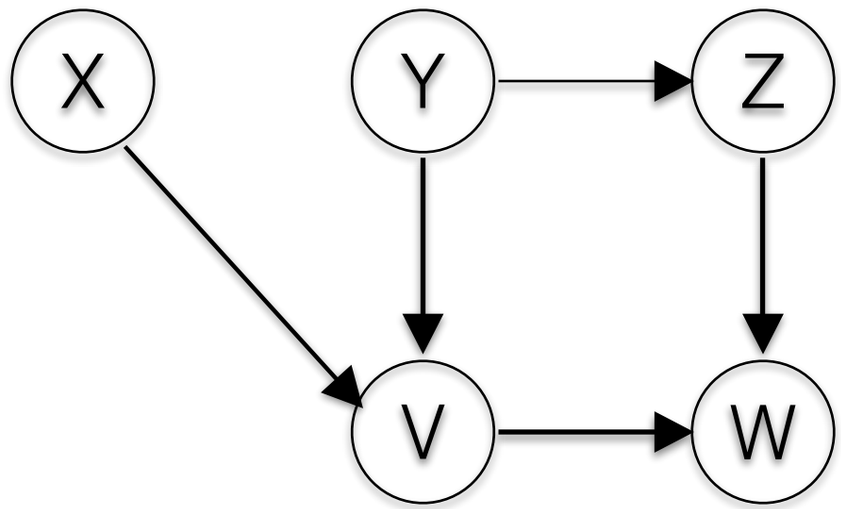
$(X \perp\!\!\!\perp Z \mid Y)$
$(X \perp\!\!\!\perp Z \mid YW)$

- CI (data) → graph structure for gaussian data
- CI (data) → graph structure for binary data (regularization)

$(X \perp\!\!\!\perp Z \mid Y)$
$(X \perp\!\!\!\perp Z \mid YW)$



d-separation (recap)



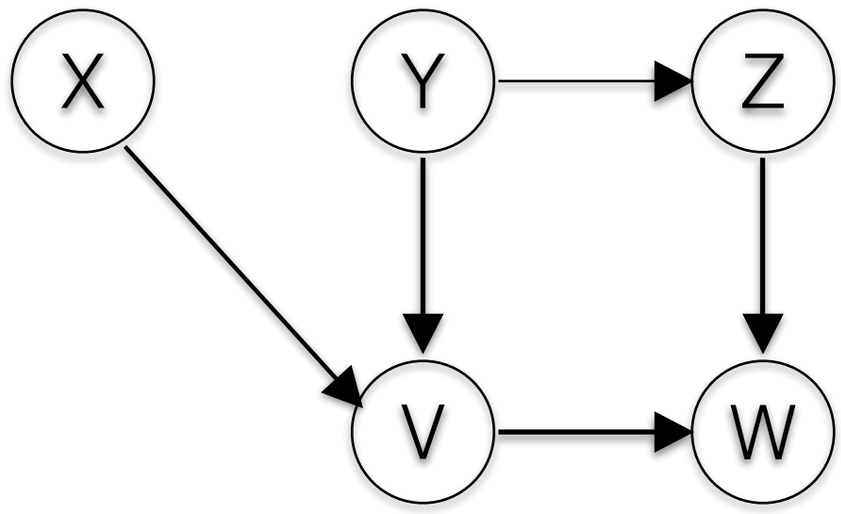
$(X \perp\!\!\!\perp Z \mid Y)$

- $X \rightarrow V \leftarrow Y \rightarrow Z$ blocked
- $X \rightarrow V \rightarrow W \leftarrow Z$ blocked $(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$

- $X \rightarrow V \rightarrow Y \rightarrow Z$ blocked
- $X \rightarrow V \rightarrow W \leftarrow Z$ active ~~$(X \perp\!\!\!\perp Z \mid YW)$~~

alternative: Lauritzen



Lauritzen ($X \perp\!\!\!\perp Z \mid YW$)

1. Make the ***ancestral graph*** (G_{an}); i.e., the variables of interest and all variables that have a directed path *to* those variables $\{W,X,Y,Z\}$

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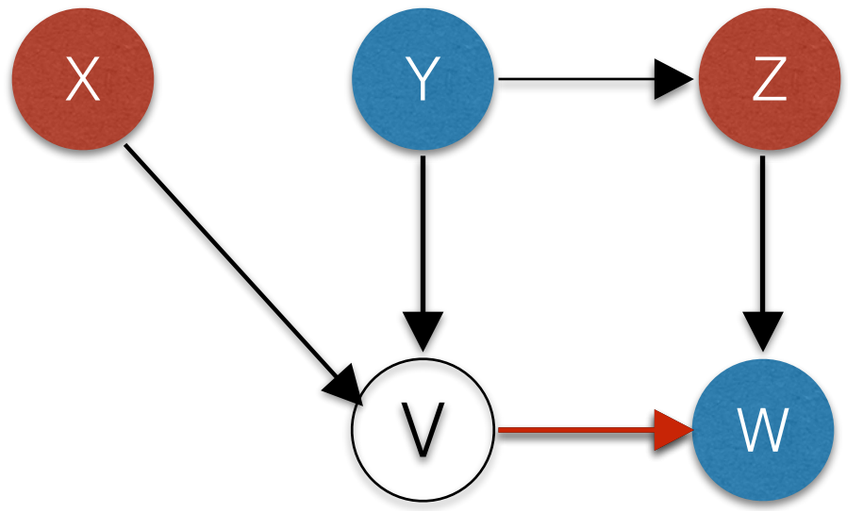

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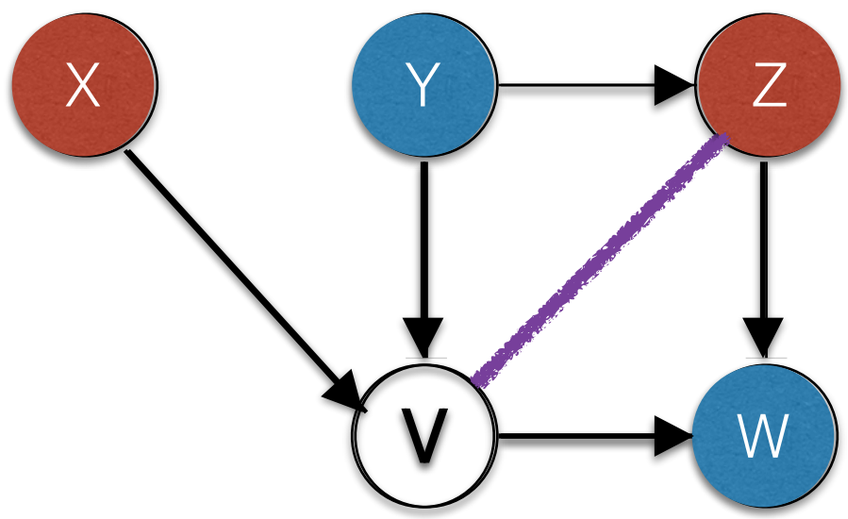
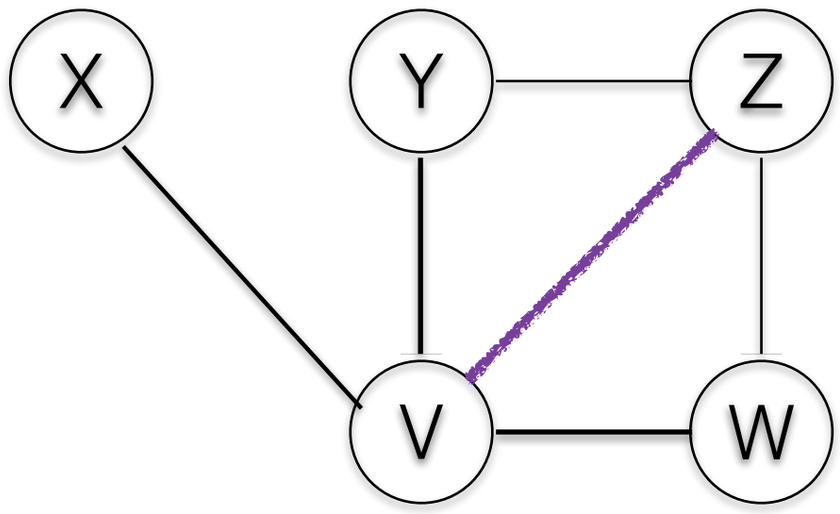


Lauritzen ($X \perp\!\!\!\perp Z \mid YW$)

1. Make the ***ancestral graph*** (G_{an}); i.e., the variables of interest and all variables that have a directed path *to* those variables $\{W,X,Y,Z\}$
2. Make G_{an} ***moral*** (G_{an}^{m}): "***marry the parents***" that have a child in common and convert all arrows into undirected edges

alternative: Lauritzen



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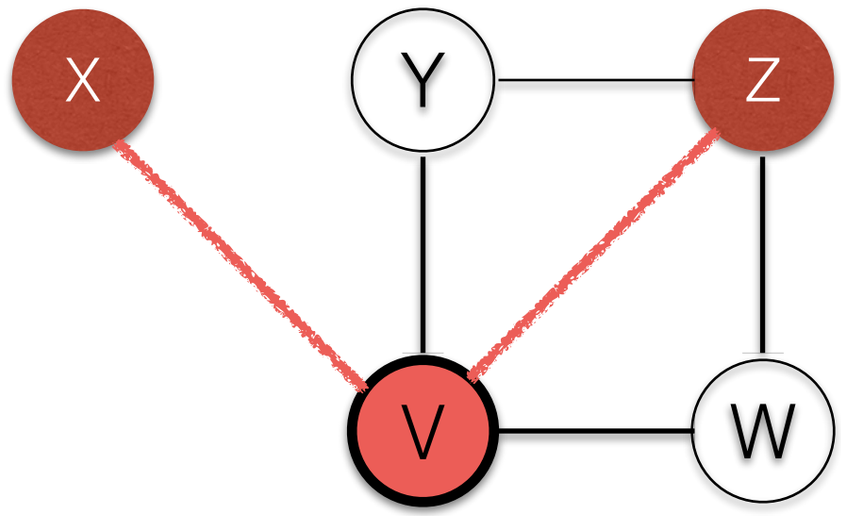

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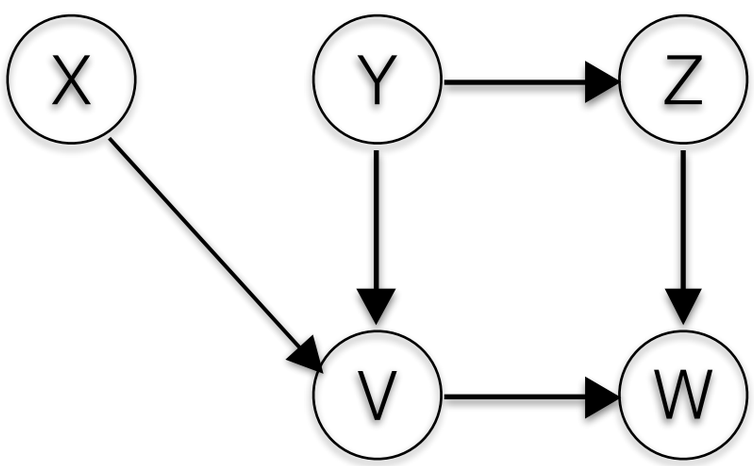
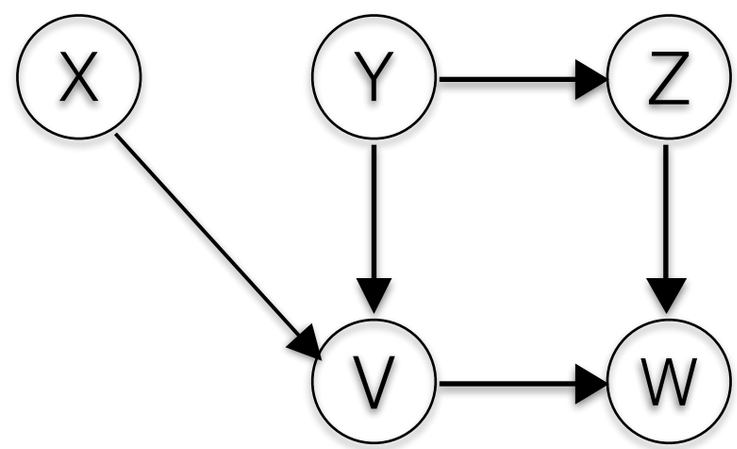
$(X \perp\!\!\!\perp Z \mid YW)$

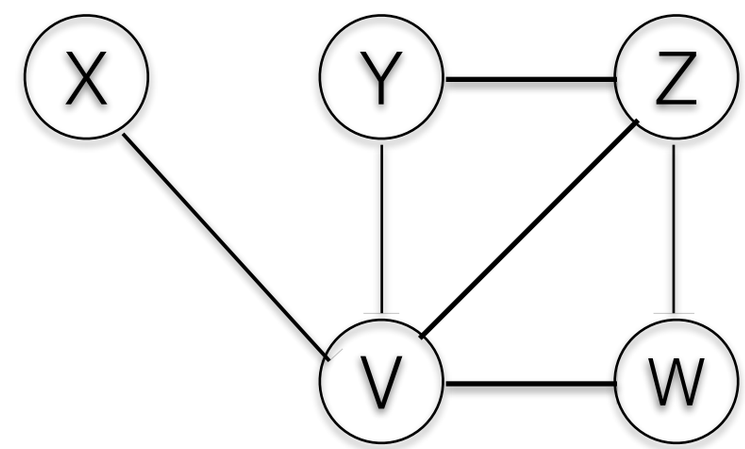
G



G_{an}



$G_{an}{}^{m}$

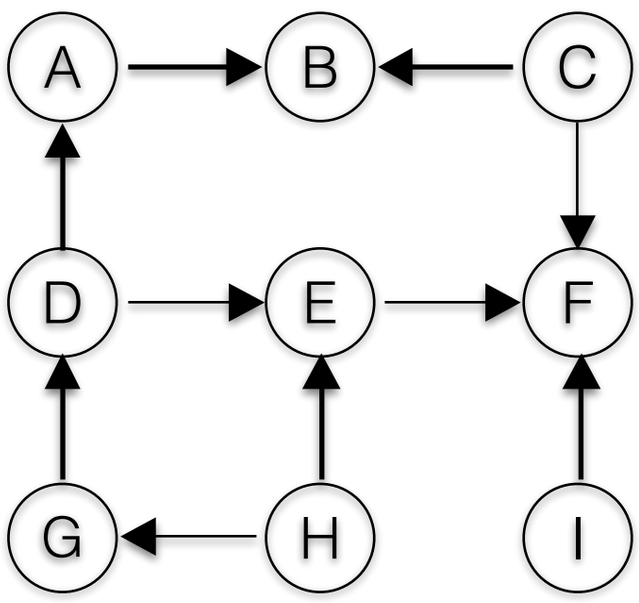


$\cancel{(X \perp\!\!\!\perp Z \mid YW)}$

alternative: Lauritzen

$(D \perp\!\!\!\perp B \mid A, G)$

G

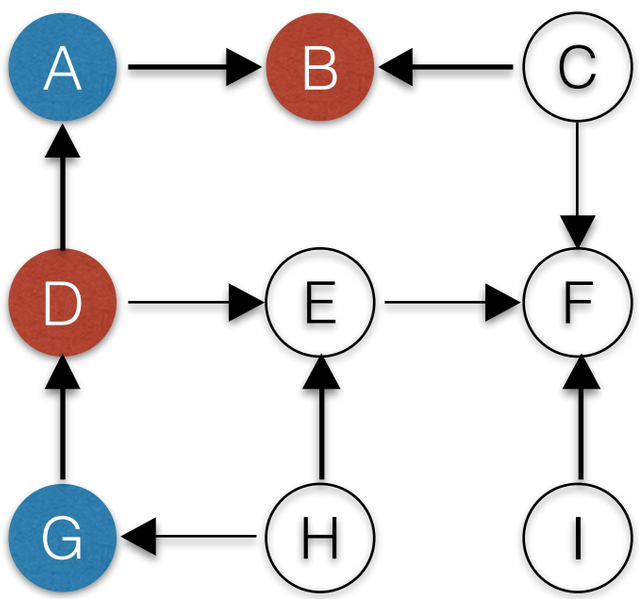


1. variables of interest and all variables that have a directed path *to* those variables

alternative: Lauritzen

$(D \perp\!\!\!\perp B \mid A,G)$

G



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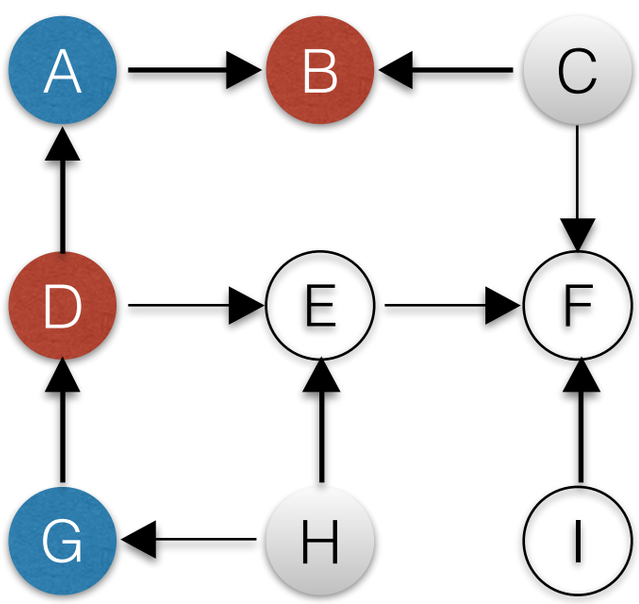

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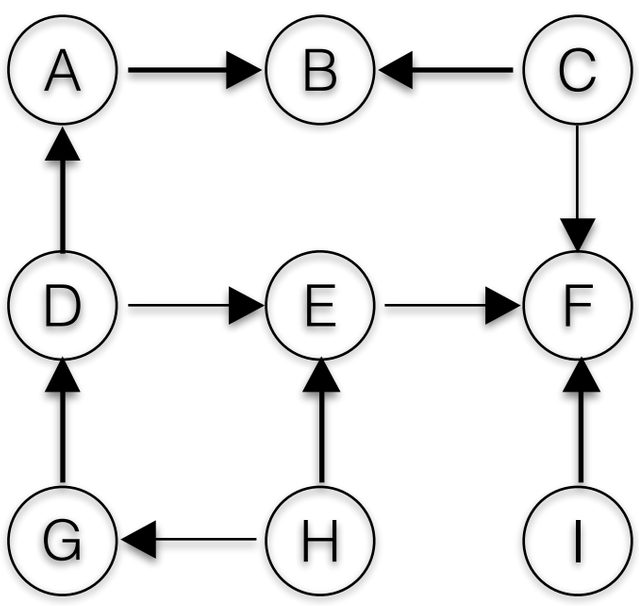
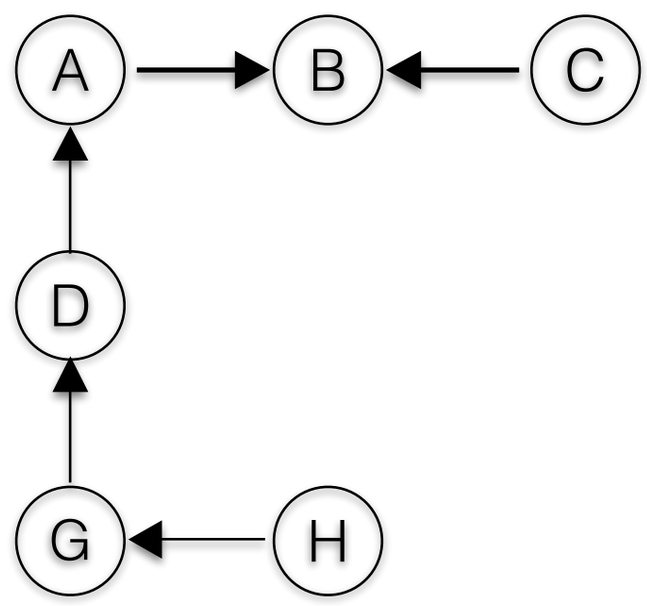


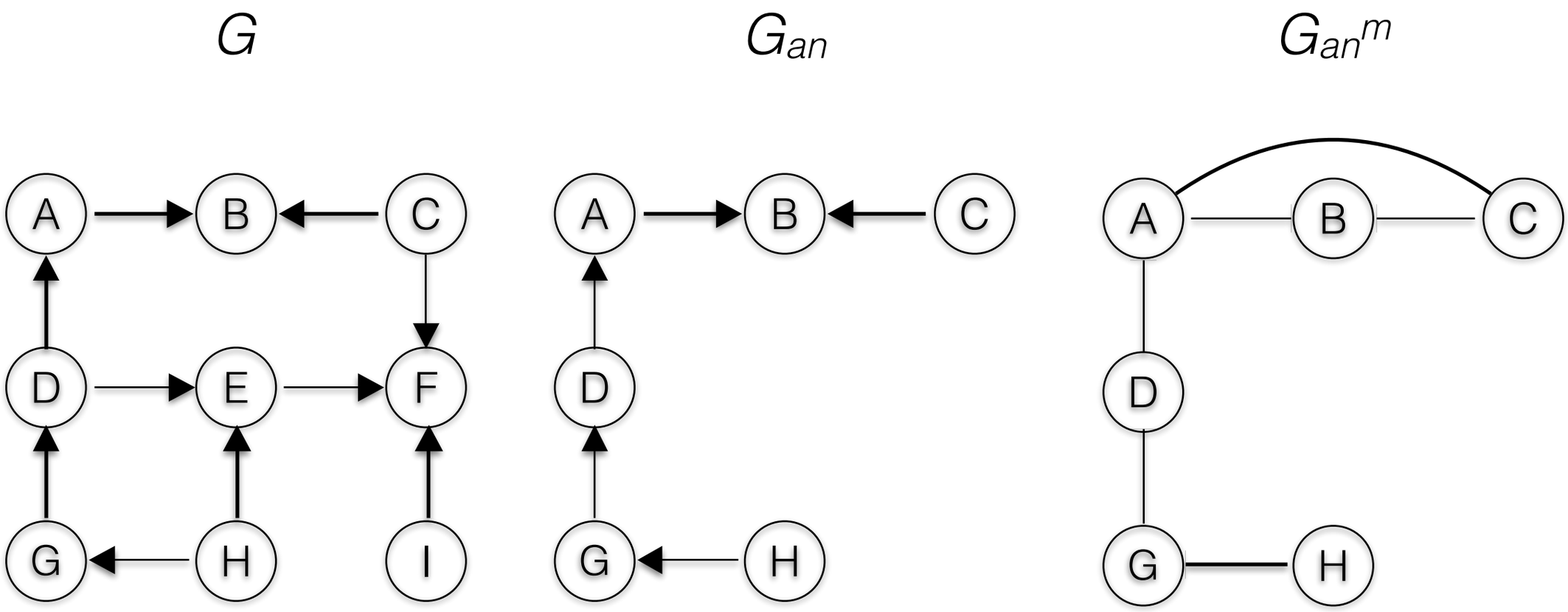
G_{an}



marry the parents

alternative: Lauritzen

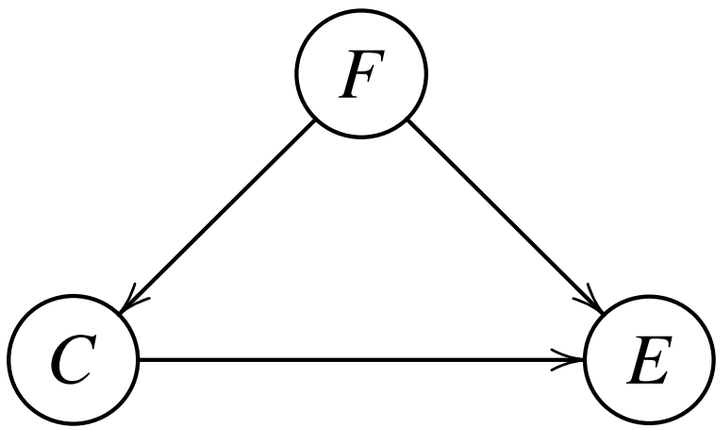
$(D \perp\!\!\!\perp B \mid A,G)$

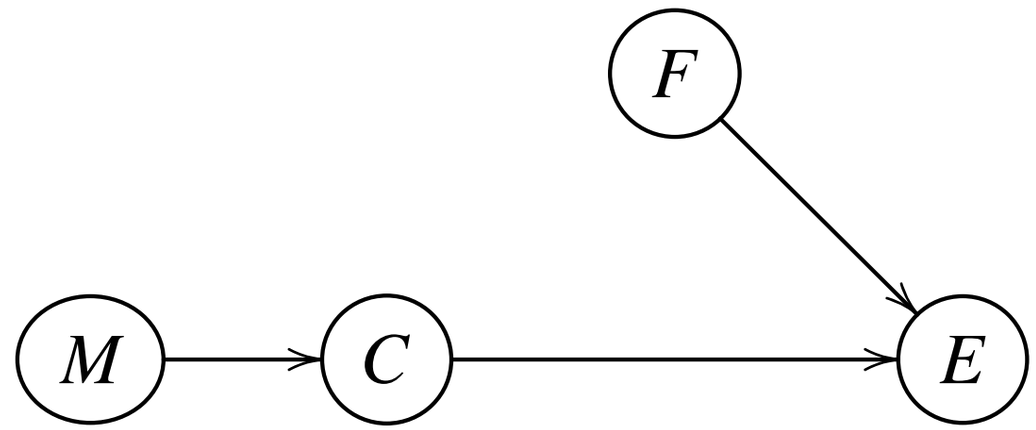


$(D \perp\!\!\!\perp B \mid A,G)$

Confounds and back-doors

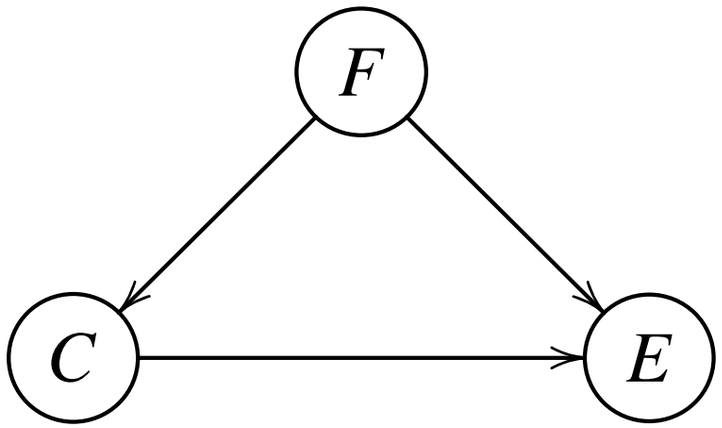
Confounds and back-doors





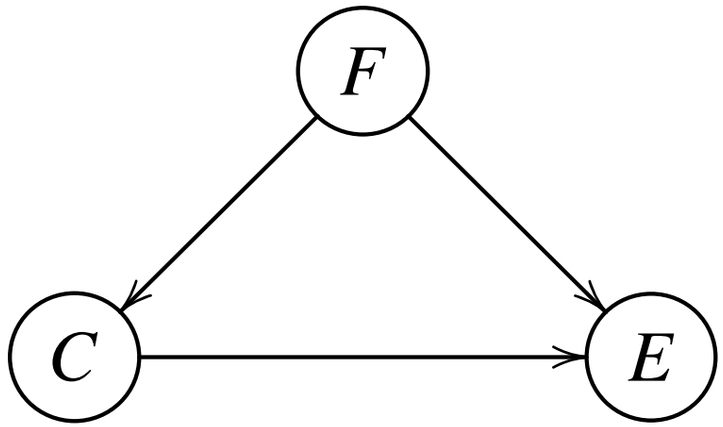
- For the causal interpretation of a graph there is one more thing: *back-doors* and *confounding*
- How can you be sure to infer a causal effect from *C* to *E* when it is possible that there is another variable that causes the relation between *C* and *E*?
- Based on a graph, you can detect confounding variables
- Again, without an experimental design (all influences of other variables are non-systematic)

Confounds and back-doors



Solution***: look for back-doors!***

Confounds and back-doors



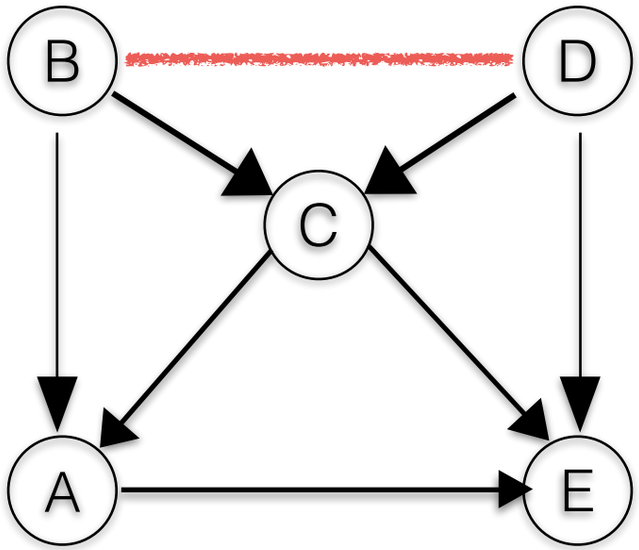
Test: **Back-door criterion**
Tests if a set S of variables is sufficient for identifying $P(E \mid C)$

F satisfies the **back-door criterion** if:

1. F is not a descendant of C, and
2. F blocks all paths from C to E that have an arrow into C.

F is a confound!

Confounds and back-doors

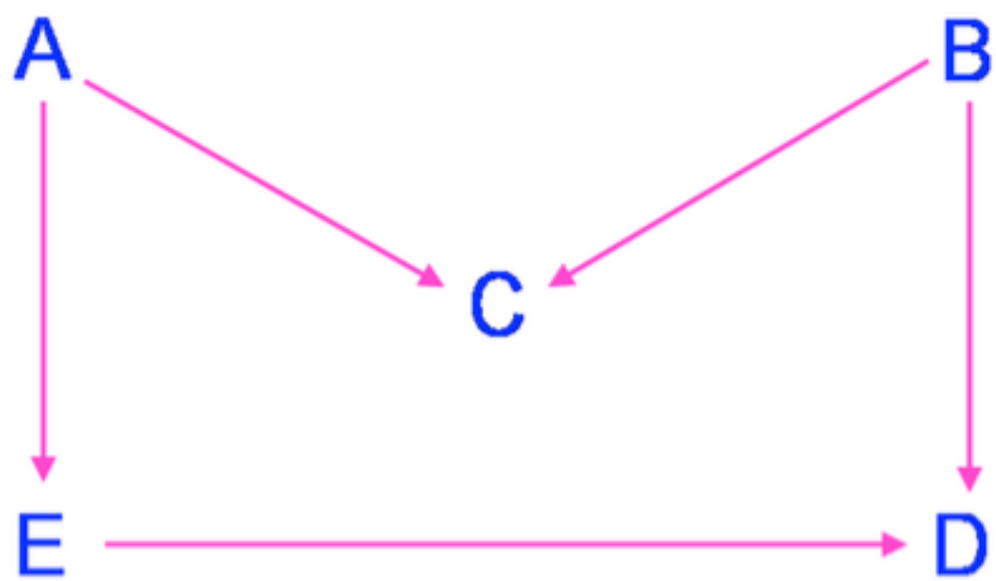


Which back-doors exist from A to E?

1. $A \leftarrow C \rightarrow E$ controling for C blocks path
2. $A \leftarrow B \rightarrow C \rightarrow E$ controling for C blocks path
3. $A \leftarrow B \rightarrow C \leftarrow D \rightarrow E$ controling for C unblocks path
4. $A \leftarrow C \leftarrow D \rightarrow E$ controling for C blocks path

S = {BC} is sufficient to control confouding: $(A \perp\!\!\!\perp E \mid B,C)$

Confounds and back-doors

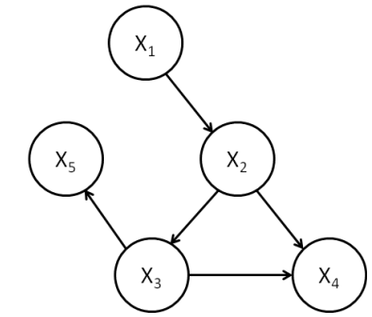


For the effect of E on D, should we control for C?
There are no unblocked back-door paths
S = {} is sufficient to control for confounding

From data (CI) to graph

$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$



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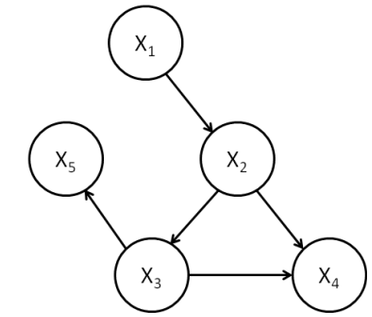
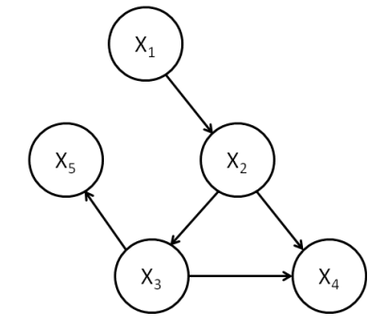


- In daily practice, the graph structure is unknown
- The aim is to infer this from data
- Non-temporal causation
- correlation ≠ causation: but you don't need to perform an experiment
- You need conditional independencies!
- Data:
    1. Find all possible conditional independencies
    2. Draw the undirected graph (multiple directed graphs are possible!)
    3. Infer directions by ruling out certain possibilities (colliders might give clues for directionality)

From data (CI) to graph

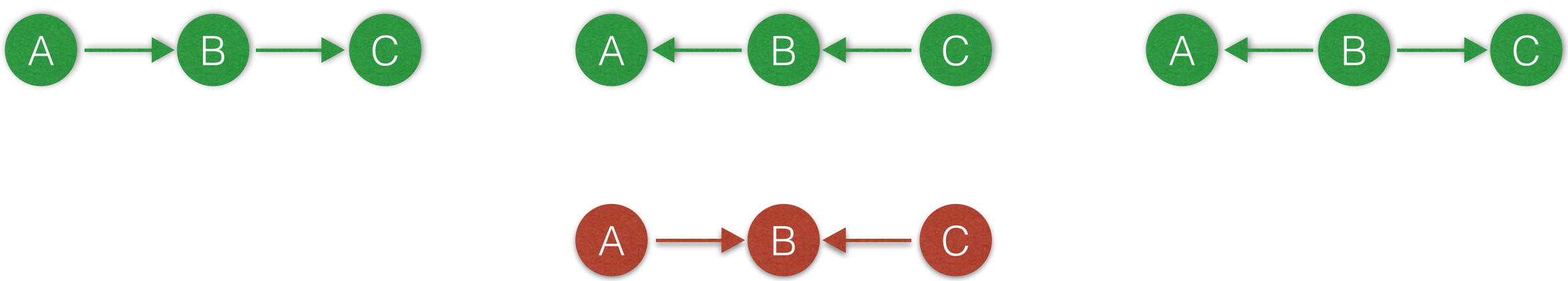
$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$



Example:

- You measured 3 variables {A,B,C}
- Suppose you find: $(A \not\perp\!\!\!\perp C)$ but $(A \perp\!\!\!\perp C \mid B)$

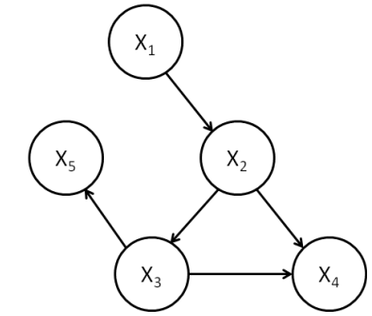


If this were the case, you would have found: $(A \perp\!\!\!\perp C)$ and $(A \not\perp\!\!\!\perp C \mid B)$

From data (CI) to graph

$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$



IC-Algorithm Pearl (1988) (in `R` with package `pcalg`)

Input: a probability distribution *P* of set *V* of variables generated by some underlying DAG

Output: a DAG compatible with *P*

From data (CI) to graph

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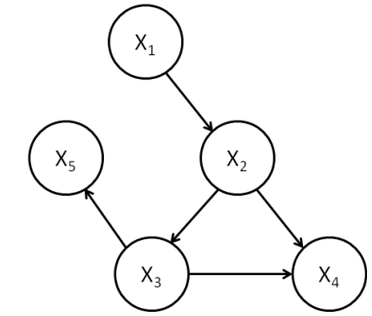

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Input: a probability distribution *P* of set *V* of variables generated by some underlying DAG

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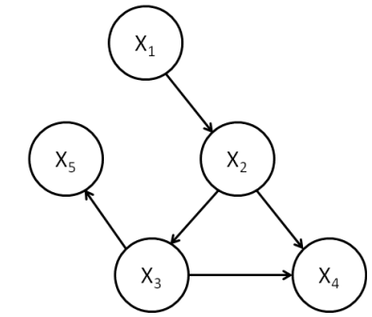
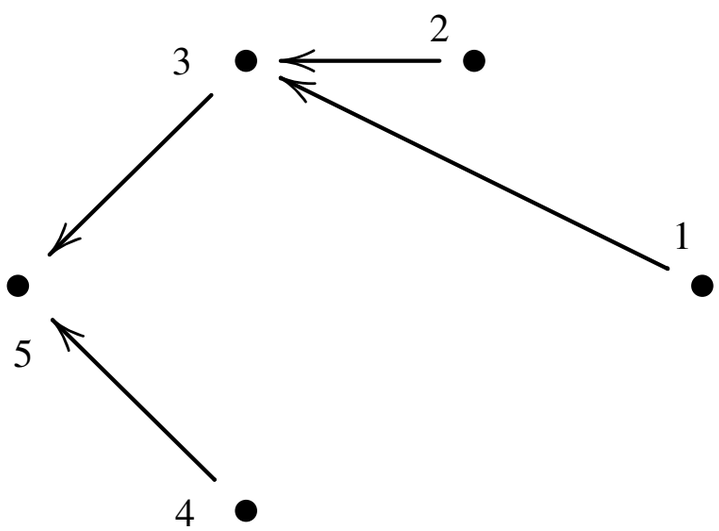
1. For each pair *a* and *b* in V, look for $(a \perp\!\!\!\perp b \mid S_{ab})$. If no such S_{ab} exists, then *a* and *b* are dependent. Draw undirected edges to create the *'skeleton'*.
2. For each trio (*a,b,c*), such that *a* - *c* - *b*, check if $c \in S_{ab}$. If it is, go to step 3. If it is *not*, draw a collider at *c* ($a \rightarrow c \leftarrow b$)
3. Orient as many undirected edges as possible, subject to:
   (i) no new colliders and (ii) no cycles

From data (CI) to graph

$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$





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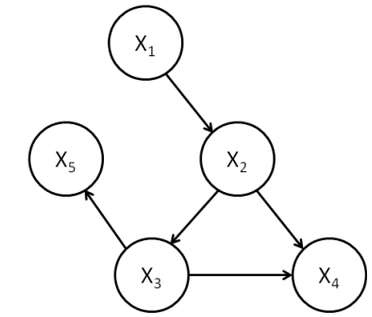
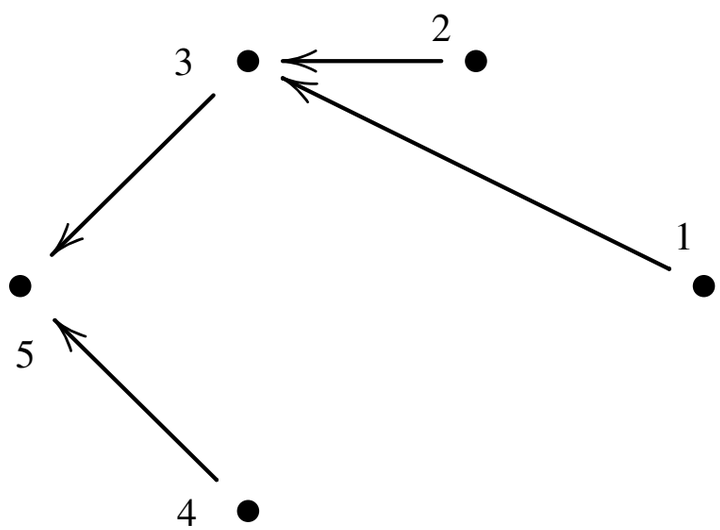
$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$





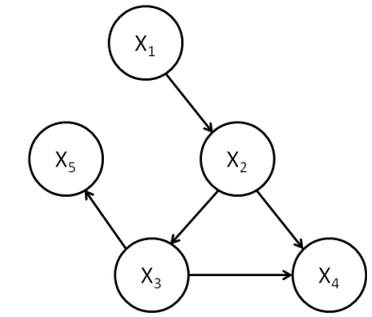
	$r(3,5)$	$r(3,5\|1)$	$r(3,5\|2)$	$r(3,5\|4)$	$\cdots$
$3-5$					

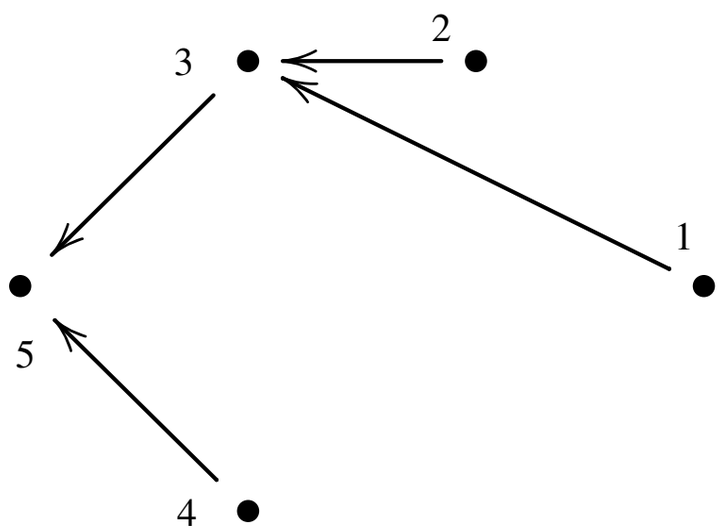
1. For each pair *a* and *b* in V, look for ($a \perp\!\!\!\perp b \mid S_{ab}$). If no such S_{ab} exists, then *a* and *b* are dependent. Draw undirected edges to create the *'skeleton'*.

From data (CI) to graph

$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$





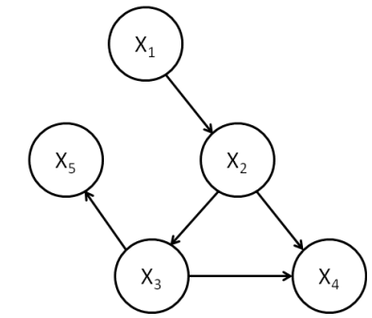
	$r(3,5)$	$r(3,5\|1)$	$r(3,5\|2)$	$r(3,5\|4)$	$\cdots$
$3-5$	TRUE	TRUE	TRUE	TRUE	TRUE

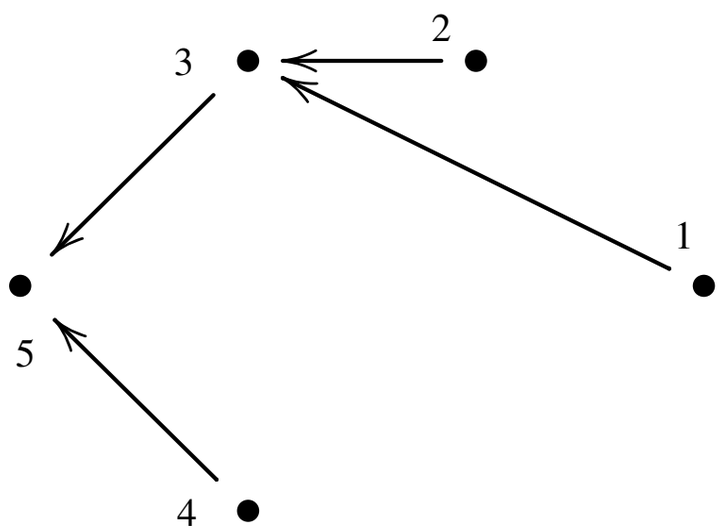
There is no node x in S_{35} such that $(3 \perp\!\!\!\perp 5 \mid x)$ holds; and so connection $3-5$

From data (CI) to graph

$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$



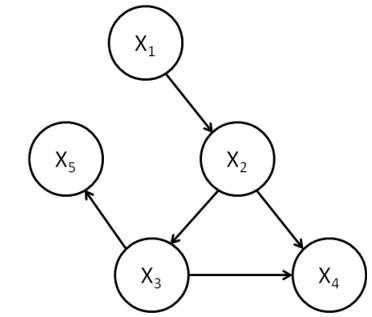


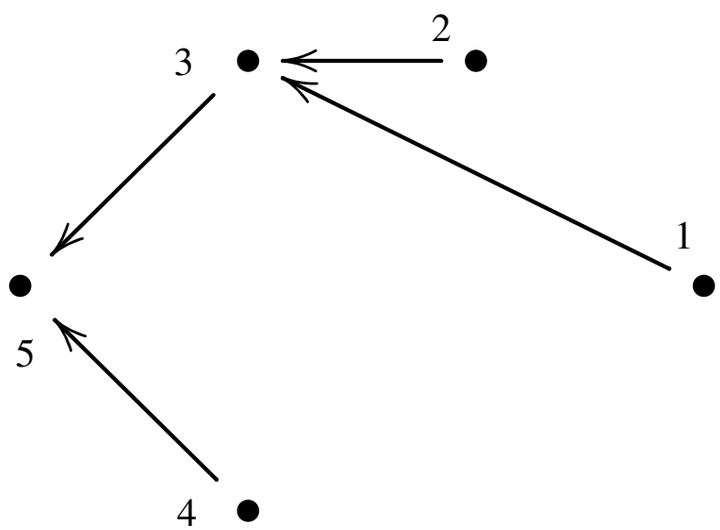
	$r(1,4)$	$r(1,4\|2)$	$r(1,4\|3)$	$r(1,4\|5)$	$\cdots$
$1-4$					

From data (CI) to graph

$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$





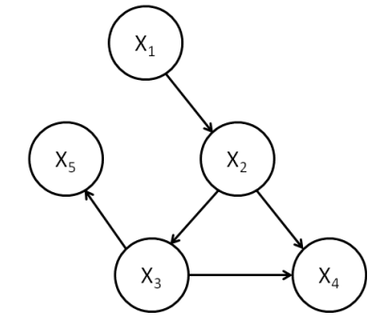
	$r(1,4)$	$r(1,4\|2)$	$r(1,4\|3)$	$r(1,4\|5)$	$\cdots$
$1-4$	FALSE	FALSE	FALSE	TRUE	

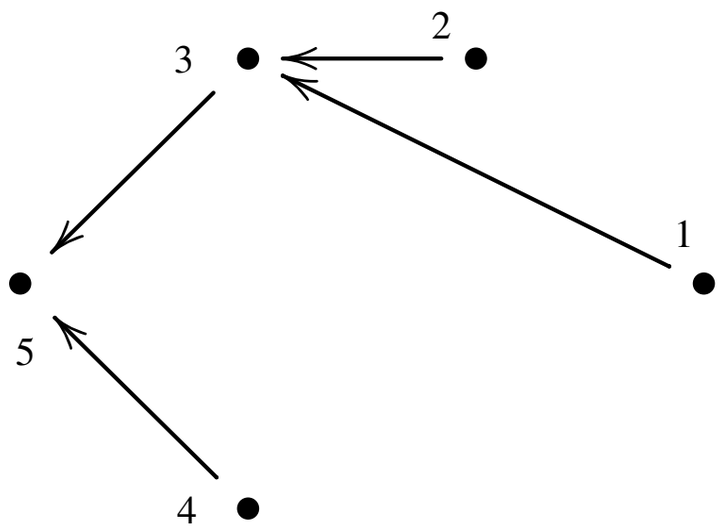
There is no correlation between 1 and 4, and so no (direct) connection $1-4$

From data (CI) to graph

$(X \perp\!\!\!\perp Z \mid Y)$

$(X \perp\!\!\!\perp Z \mid YW)$





	$r(3,4)$	$r(3,4\|1)$	$r(3,4\|2)$	$r(3,4\|5)$	$\cdots$
$3-4$	FALSE	FALSE	FALSE	TRUE	

No correlation between 3 and 4 and so no (direct) connection $3-4$, but 5 is in S_{34} and so a collider $3 \rightarrow 5 \leftarrow 4$ (rule 2 from Pearl, 2993).

2. For each trio (*a,b,c*), such that *a* - *c* - *b*, check if $c \in S_{ab}$. If it is, go to step 3. If it is *not*, draw a collider at *c* ($a \rightarrow c \leftarrow b$)

Example

Data set: 5 variables, 2000 observations

Correlation matrix:

	y	x	z1	z2	z3
y	1.0000000	0.9980315	0.9996026	0.49352081	0.80525205
x	0.9980315	1.0000000	0.9963772	0.53863392	0.77039444
z1	0.9996026	0.9963772	1.0000000	0.47084348	0.81992741
z2	0.4935208	0.5386339	0.4708435	1.00000000	-0.09801633
z3	0.8052520	0.7703944	0.8199274	-0.09801633	1.00000000

Could there be a connection between x and y?

Example

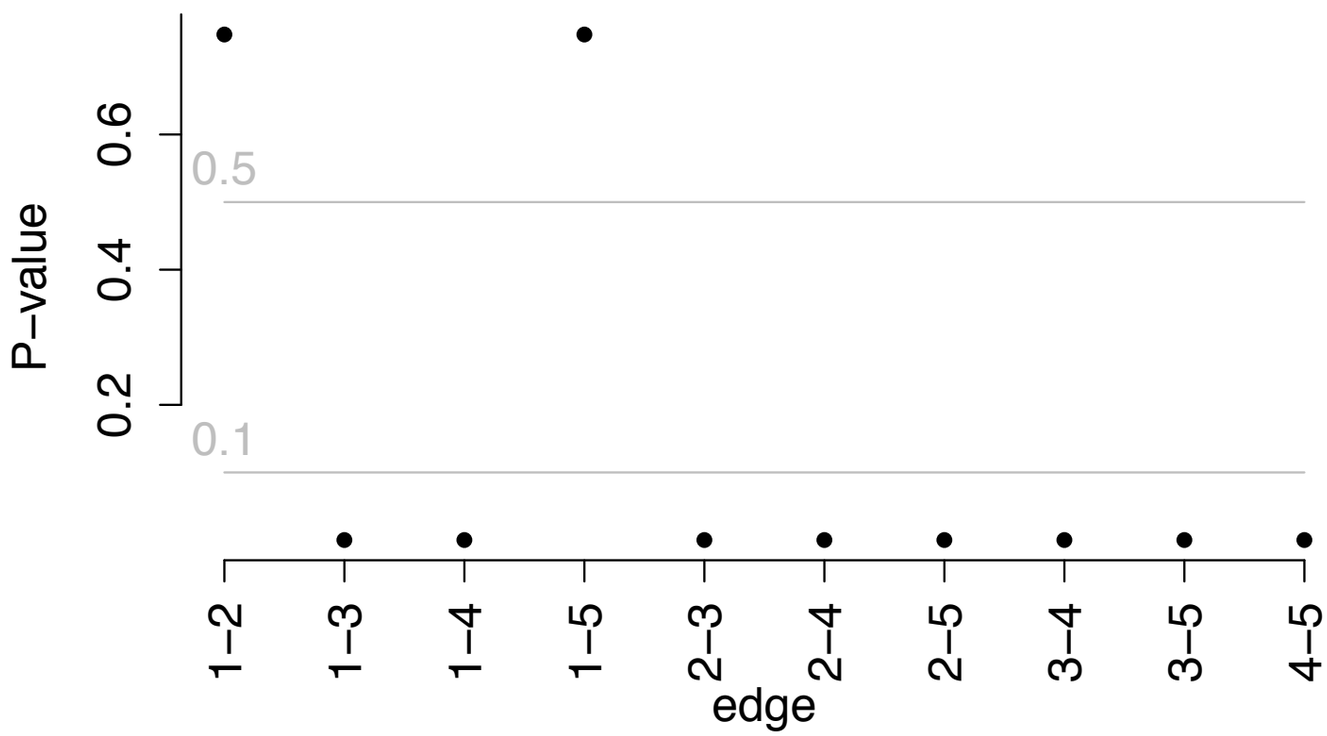
Partial correlations

```
            [,1]       [,2]      [,3]      [,4]       [,5]
[1,]  1.00000000 -0.0275024  0.8965923  0.5139097 -0.07228632
[2,] -0.02750240  1.0000000  0.4620665  0.1127723 -0.63835357
[3,]  0.89659232  0.4620665  1.0000000 -0.4477139  0.39502979
[4,]  0.51390970  0.1127723 -0.4477139  1.0000000 -0.52714707
[5,] -0.07228632 -0.6383536  0.3950298 -0.5271471  1.00000000
```

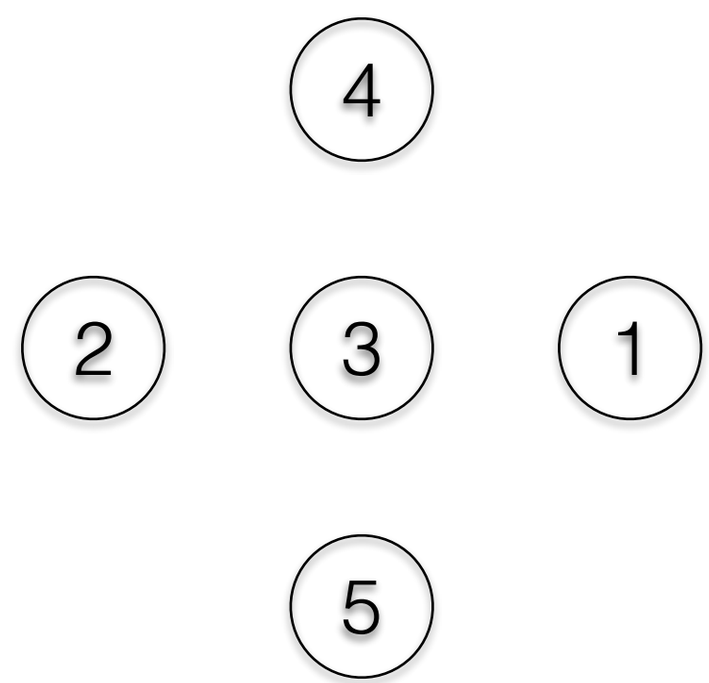
What can you conclude about the relationship between x and y?

Example

Significance partial correlations

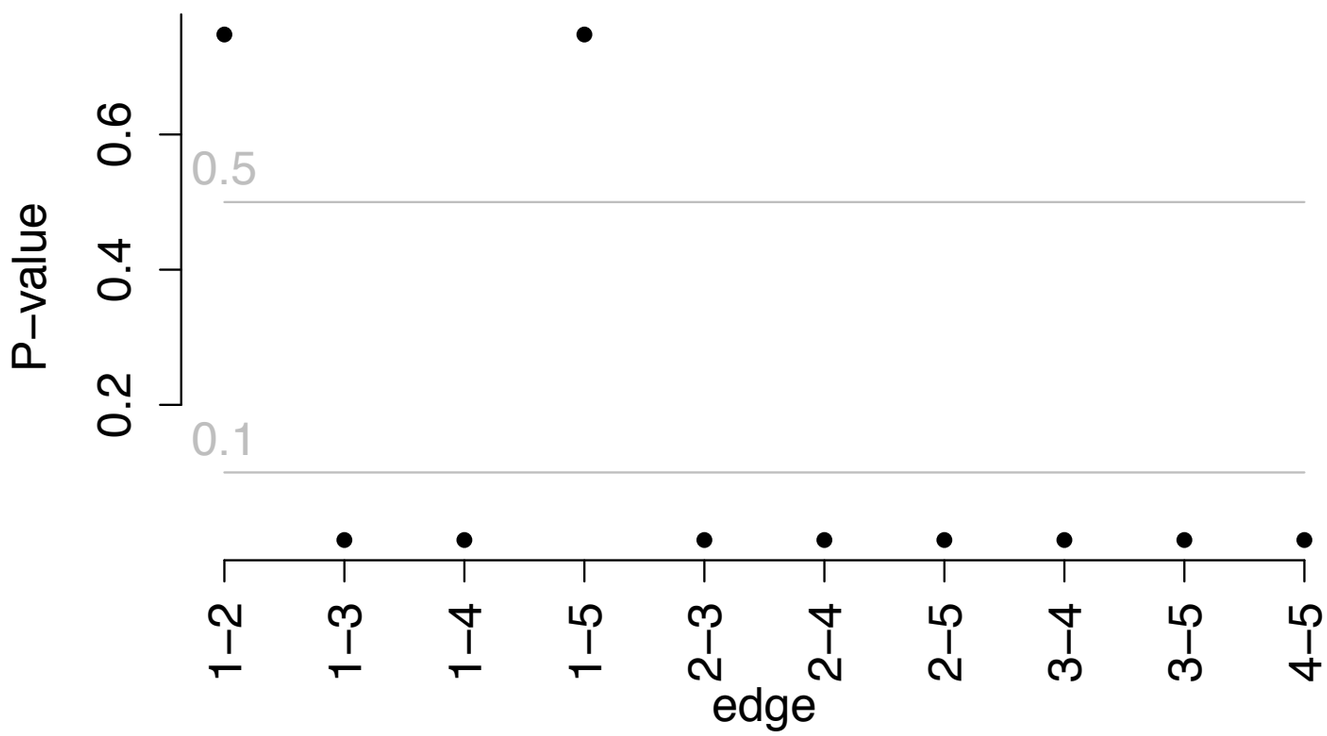


Which connections are likely for these data?

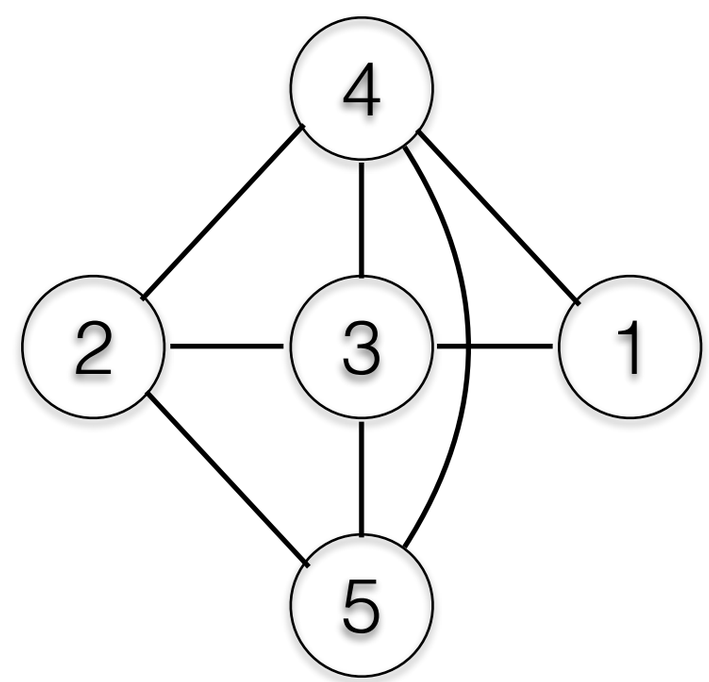


Example

Significance partial correlations



Which connections are likely for these data?



Example

Now, test partial correlations for every possible pair of nodes

```
$ 1-2: Named num [1:8] 0 0 0 0 0.735 ...
 ..- attr(*, "names")= chr [1:8] "" "3" "4" "5" ...
$ 1-3: Named num [1:8] 0 0 0 0 0 0 0 0
 ..- attr(*, "names")= chr [1:8] "" "2" "4" "5" ...
$ 1-4: Named num [1:8] 3.22e-14 0.00 0.00 0.00 0.00 ...
 ..- attr(*, "names")= chr [1:8] "" "2" "3" "5" ...
$ 1-5: Named num [1:8] 0 0 0 0 0 ...
 ..- attr(*, "names")= chr [1:8] "" "2" "3" "4" ...
$ 2-3: Named num [1:8] 0.00 0.00 0.00 0.00 3.85e-05 0.00 0.00 0.00
 ..- attr(*, "names")= chr [1:8] "" "1" "4" "5" ...
$ 2-4: Named num [1:8] 0 0 0 0 0 ...
 ..- attr(*, "names")= chr [1:8] "" "1" "3" "5" ...
$ 2-5: Named num [1:8] 0 0 0 0 0 0 0 0
 ..- attr(*, "names")= chr [1:8] "" "1" "3" "4" ...
$ 3-4: Named num [1:8] 7.26e-13 0.00 0.00 0.00 0.00 ...
 ..- attr(*, "names")= chr [1:8] "" "1" "2" "5" ...
$ 3-5: Named num [1:8] 0 0 0 0 0 ...
 ..- attr(*, "names")= chr [1:8] "" "1" "2" "4" ...
$ 4-5: Named num [1:8] 0.168 0 0 0 0 ...
 ..- attr(*, "names")= chr [1:8] "" "1" "2" "3" ...
```

```
$ 1-2: logi FALSE
$ 1-3: logi TRUE
$ 1-4: logi TRUE
$ 1-5: logi FALSE
$ 2-3: logi TRUE
$ 2-4: logi TRUE
$ 2-5: logi TRUE
$ 3-4: logi FALSE
$ 3-5: logi TRUE
$ 4-5: logi FALSE
```

Example

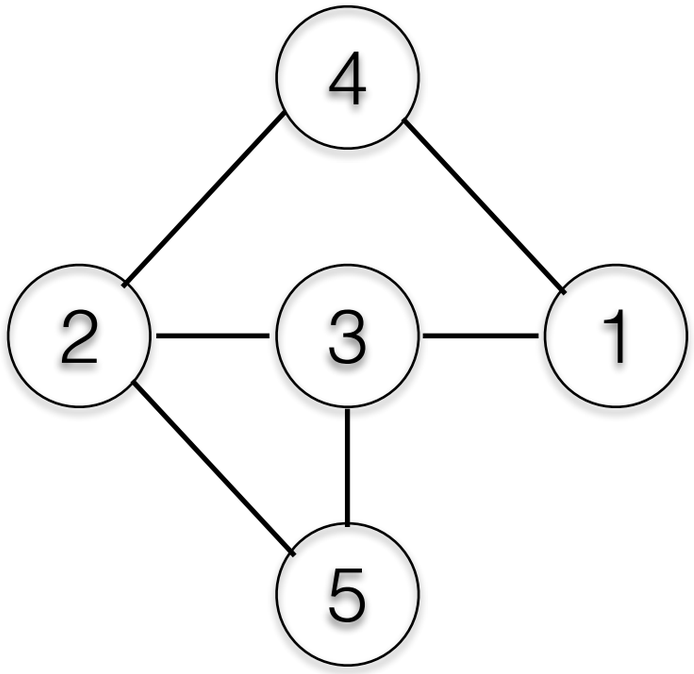
```
$ 1-2: logi FALSE
$ 1-3: logi TRUE
$ 1-4: logi TRUE
$ 1-5: logi FALSE
$ 2-3: logi TRUE
$ 2-4: logi TRUE
$ 2-5: logi TRUE
$ 3-4: logi FALSE
$ 3-5: logi TRUE
$ 4-5: logi FALSE
```

When will a set of P-values lead to TRUE?

Example

```
$ 1-2: logi FALSE
$ 1-3: logi TRUE
$ 1-4: logi TRUE
$ 1-5: logi FALSE
$ 2-3: logi TRUE
$ 2-4: logi TRUE
$ 2-5: logi TRUE
$ 3-4: logi FALSE
$ 3-5: logi TRUE
$ 4-5: logi FALSE
```

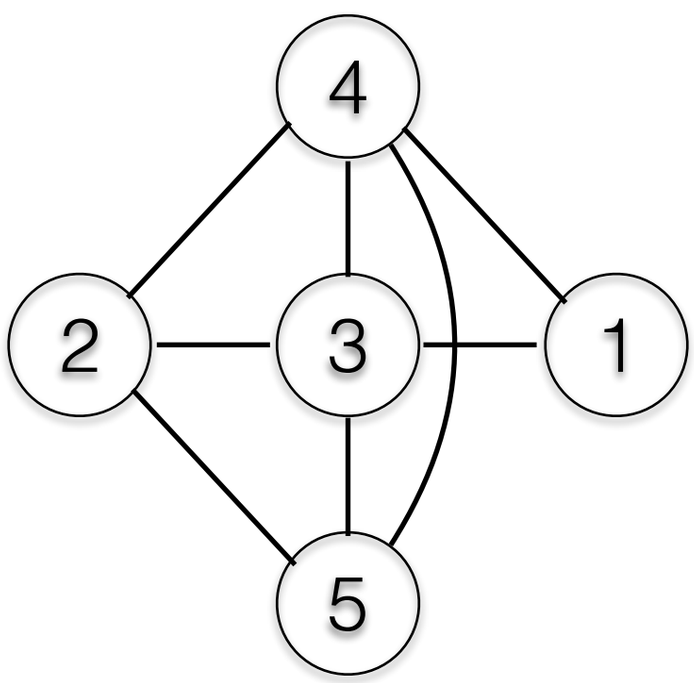
When will a set of P-values lead to TRUE?



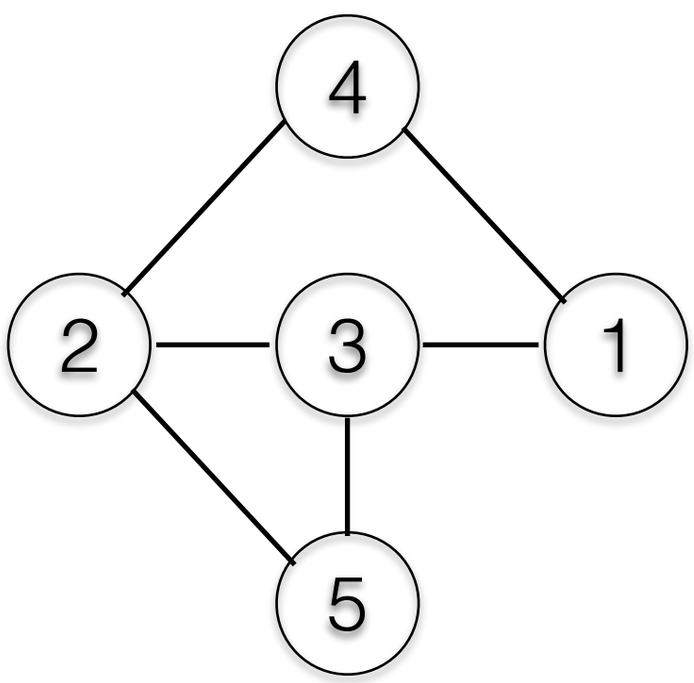
Example

```
$ 1-2: logi FALSE
$ 1-3: logi TRUE
$ 1-4: logi TRUE
$ 1-5: logi FALSE
$ 2-3: logi TRUE
$ 2-4: logi TRUE
$ 2-5: logi TRUE
$ 3-4: logi FALSE
$ 3-5: logi TRUE
$ 4-5: logi FALSE
```

Partial correlations



Controlling for all possible combinations

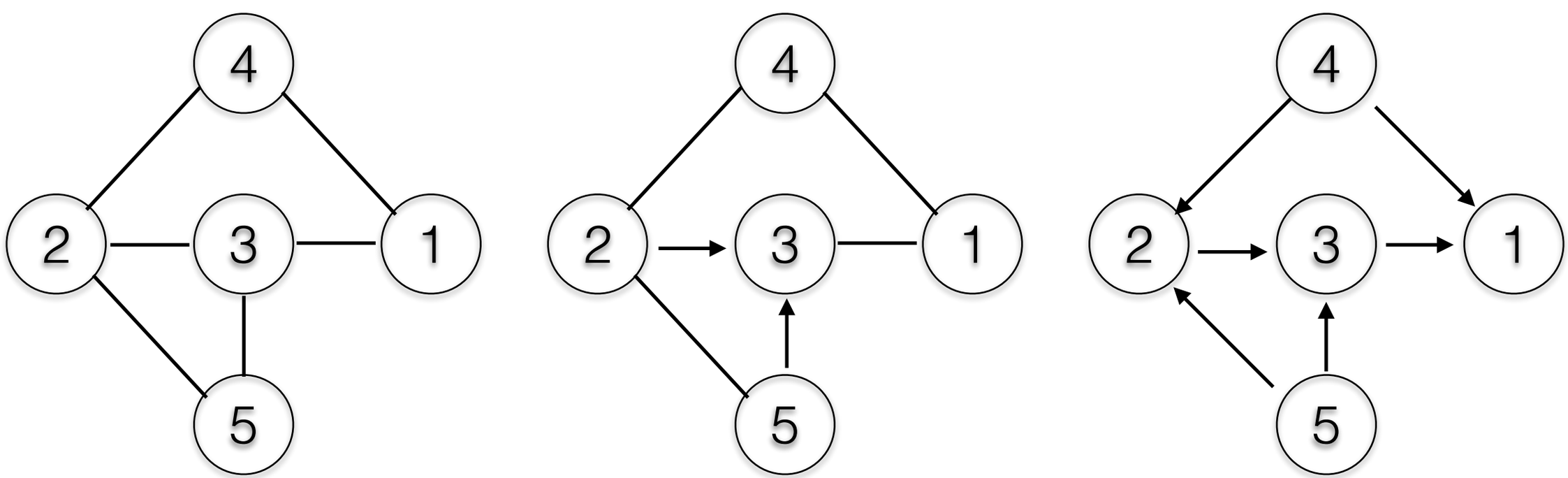


Can you explain the difference?

Example

Finding directions of edges (Pearl's algorithm):

1. For each pair *a* and *b* in V, look for ($a \perp\!\!\!\perp b \mid S_{ab}$). If no such S_{ab} exists, then *a* and *b* are dependent. Draw undirected edges to create the *'skeleton'*.
2. For each trio (*a,b,c*), such that *a* - *c* - *b*, check if $c \in S_{ab}$. If it is, go to step 3. If it is not, draw a collider at *c* ($a \rightarrow c \leftarrow b$)
3. Orient as many undirected edges as possible, subject to:
   (i) no new colliders and (ii) no cycles



Recap

- About causal graphs and how to infer them from data
- To my opinion one really big downside with causal graphs: ***acyclicity***
- While in psychopathology, feedback loops are thought to play an important role in developing and maintaining disorders
- Therefore, let's look at… ***Markov Random Fields***

Markov Random Fields

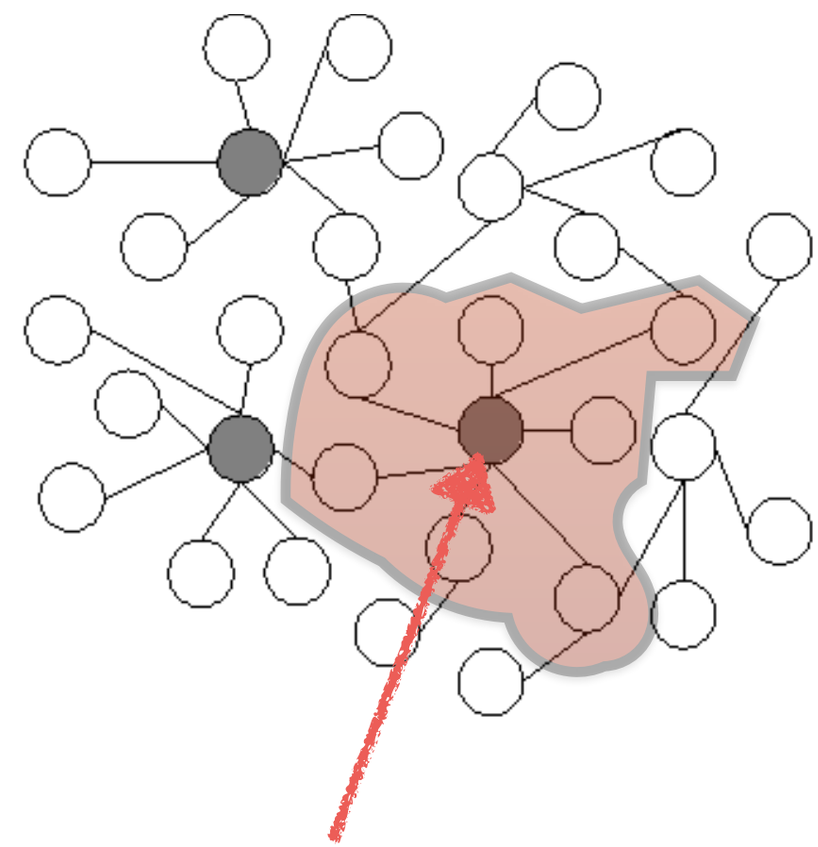
A.k.a. Markov network, undirected graphical model

- Let $G = (V, E)$ be a graph
- Let $\mathbf{X} = (X_1, \ldots, X_{N_v})$ be a set of random variables on V
- $\mathbf{X}$ is a MRF on G if

$$\mathbb{P}_\theta(x_j \mid x_{\setminus j}) = \mathbb{P}_\theta(x_j \mid x_{\mathcal{N}_j})$$

- The probability has the Markov property:

Every set of nodes is conditionally independent of X_A when conditioned on the neighbors of X_A



Markov Random Fields

Ising model

Ising model:

- to explain ferromagnetism
- small dipoles (spins) can be ’spin up’ (+ 1) or ’spin down’ (- 1)
- can be generalized to other *objects* in a network (voter, neuron, tree)
- objects/variables can interact, but only with direct neighbors

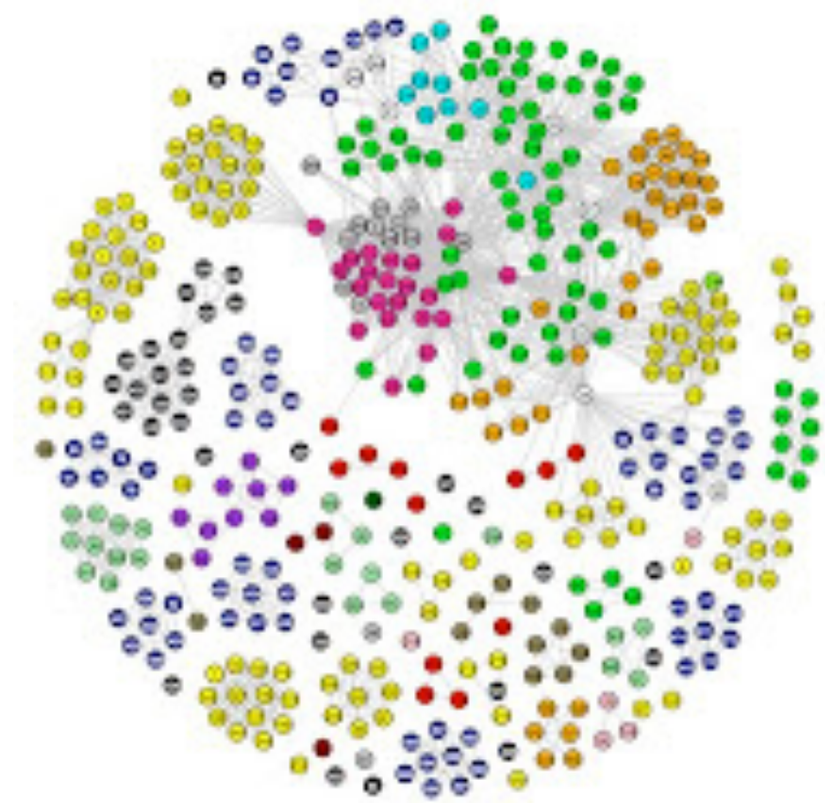
−	−	−	+	−
+	+	−	−	−
−	−	+	−	−
+	+	+	−	−
−	+	−	+	+

Markov Random Fields

Ising model

Psychopathology

- variables are symptoms
- states: present/absent
- N variables: 2^N possible configurations

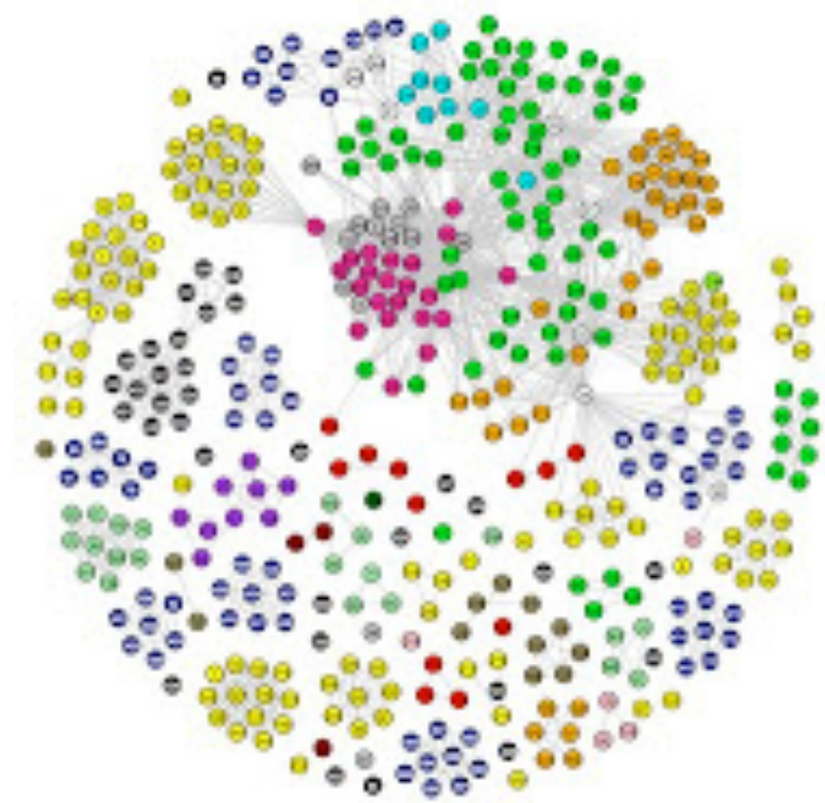


Markov Random Fields

Ising model

Psychopathology

- variables are symptoms
- states: present/absent
- N variables: 2^N possible configurations
- N=28: 268435456 possible configurations



Markov Random Fields

Ising model

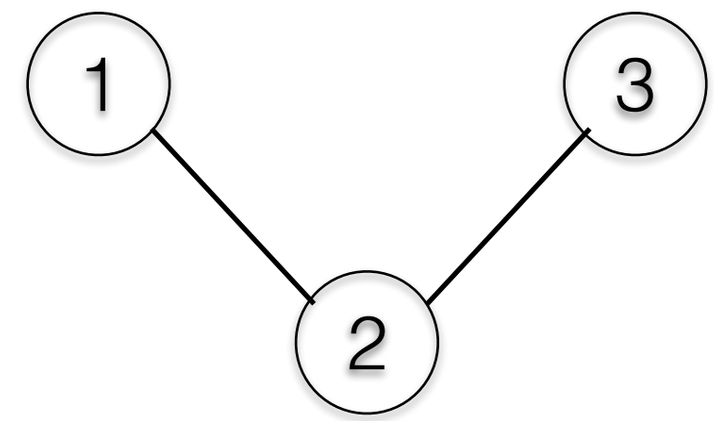
Possible states in network with 3 symptoms:

0 0 0 1 0 1

0 0 1 1 1 0

0 1 0 0 1 1

1 0 0 1 1 1

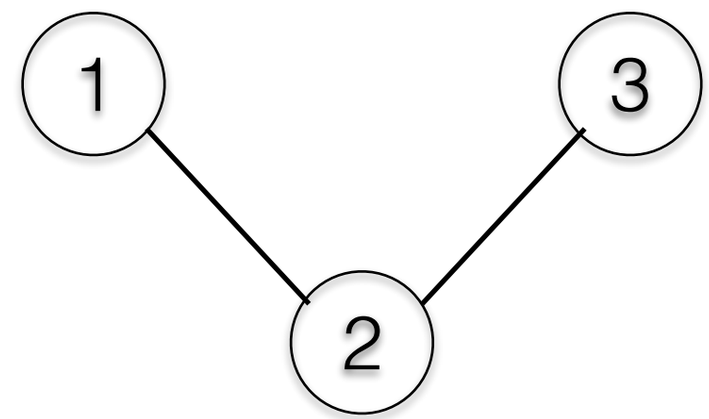


- What is the probability of a particular state?
- Most favourable: configuration that minimizes the ‘energy’
- What is the ‘energy’ of x2=1, given that x1=0 and x3=1?
- $H(x2=1|x1=0,x3=1)$

Markov Random Fields

Ising model

- $H(x2=1|x1=0,x3=1)$: (0,1,1)
- Conceptual level (think about magnets):
  - take state x2 into account
  - and take state x2 *combined* with neighbors' state into account



$$1 + (1*0 + 1*1)$$

x2 x2*x1 x2*x3

- $H(x2=1|x1=0,x3=1)=-(1 + (1*0 + 1*1)) = -2$
- $H(x2=1|x1=0,x3=0)$: (0,1,0)

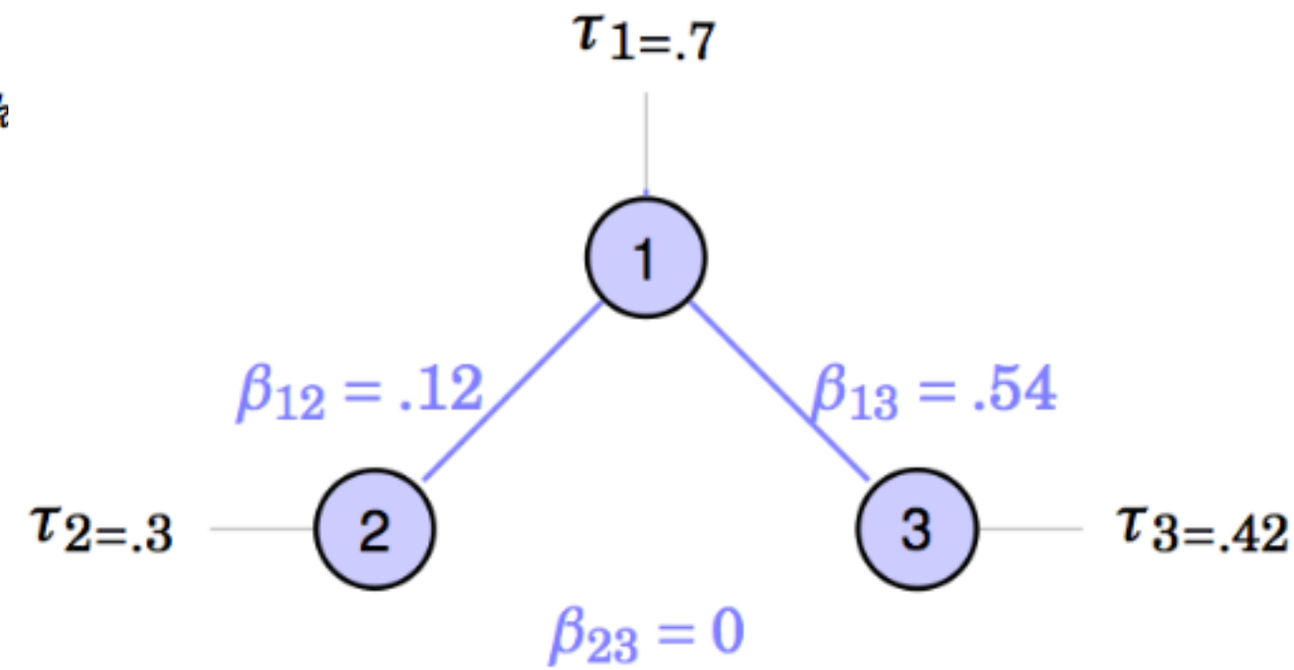
  $-(1 + (1*0 + 1*0)) = -1$
- (0,1,1) is more likely than (0,1,0)

Markov Random Fields

Ising model

- … actually, we just looked at the Hamiltonian:

$$H(x) = -\sum_{j \in V} \tau_j x_j - \sum_{(j,k) \in E} \beta_{jk} x_j x_k$$



τ_j:

- threshold symptom j
- indicative of preferred state of symptom j

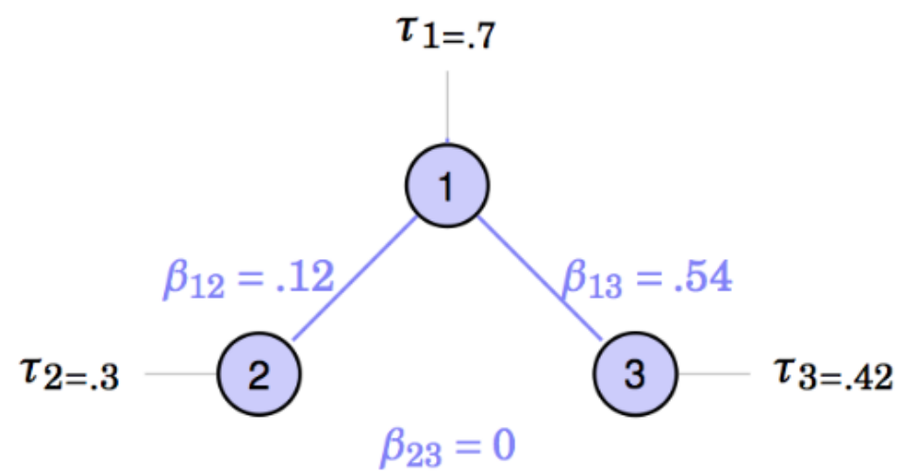
β_{jk}:

- interaction strength between symptoms j and k
- indicative of how symptoms influence each other

Markov Random Fields

Ising model

$$H(x) = -\sum_{j \in V} \tau_j x_j - \sum_{(j,k) \in E} \beta_{jk} x_j x_k$$



configuration	probability	Hamiltonian
1 1 1	P(1 1 1)	$-(\tau_1 + \tau_2 + \tau_3) - (\beta_{12} + \beta_{23} + 0)$
1 1 0	P(1 1 0)	$-(\tau_1 + \tau_2 + 0) - (\beta_{12} + 0 + 0)$
1 0 1	P(1 0 1)	$-(\tau_1 + 0 + \tau_3) - (0 + 0 + 0)$
1 0 0	P(1 0 0)	$-(\tau_1 + 0 + 0) - (0 + 0 + 0)$
0 1 1	P(0 1 1)	$-(0 + \tau_2 + \tau_3) - (0 + \beta_{23} + 0)$
0 1 0	P(0 1 0)	$-(0 + \tau_2 + 0) - (0 + 0 + 0)$
1 0 1	P(1 0 1)	$-(\tau_1 + 0 + \tau_3) - (0 + 0 + 0)$
0 0 0	P(0 0 0)	$-(0 + 0 + 0) - (0 + 0 + 0)$

Markov Random Fields

Ising model

One more step:

From Hamiltonian → Probability

- Divide by all possible energies (of all possible states)

$$\mathbb{P}_{\tau,\beta}(x) = \frac{1}{Z(\tau,\beta)} \exp[-H(x)]$$

- becomes intractable with increasing number of variables

Markov Random Fields

Ising model

but...

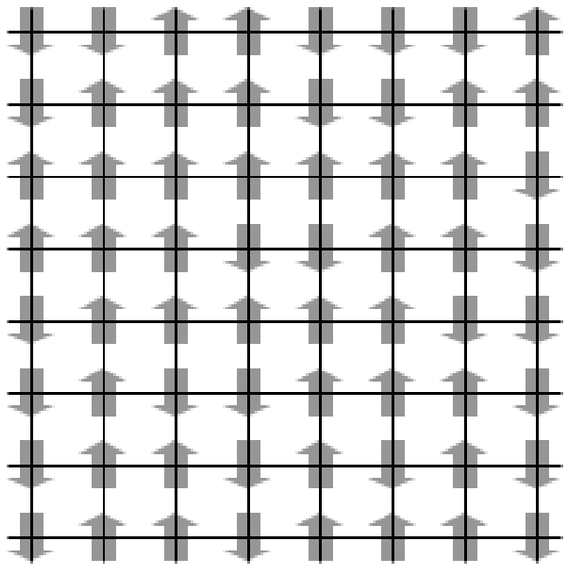
conditional probability of X_j given all other nodes reduces the normalizing constant

$$Z(\tau_j) = 1 + \exp\left[\tau_j + \sum_{k \in V_{\setminus j}} \beta_{jk} x_k\right] \quad \text{(tractable!)}$$

Conditional probability:

$$\mathbb{P}_{\tau,\beta}(x_j \mid x_{\setminus j}) = \frac{\exp\left[\tau_j x_j + x_j \sum_{k \in V_{\setminus j}} \beta_{jk} x_k\right]}{1 + \exp\left[\tau_j + \sum_{k \in V_{\setminus j}} \beta_{jk} x_k\right]}$$

Estimating networks



- Arrangement of spins in ferromagnet is know
- In practice, network structure is unknown
- $\mathscr{L}(\theta \mid x) = P(x \mid \theta)$
- Use Ising model to estimate parameters:
  - interaction parameter β_{jk}
  - threshold parameter τ_j

Estimating networks

Interaction strength between x_j and x_k

Autonomous disposition of x_j

Conditional probability

$$\mathbb{P}_\Theta\left(x_j \middle| x_{\setminus j}\right) = \frac{\exp\left[\tau_j x_j + x_j \sum_{k \in V_{\setminus j}} \beta_{jk} x_k\right]}{1 + \exp\left[\tau_j + \sum_{k \in V_{\setminus j}} \beta_{jk} x_k\right]}$$

x = (x1, x2, …,xn)
xi = 0 or 1
τj: node parameter (threshold)
βjk: pairwise interaction parameter

Estimating networks

Interaction strength between x_j and x_k

Autonomous disposition of x_j

Conditional probability

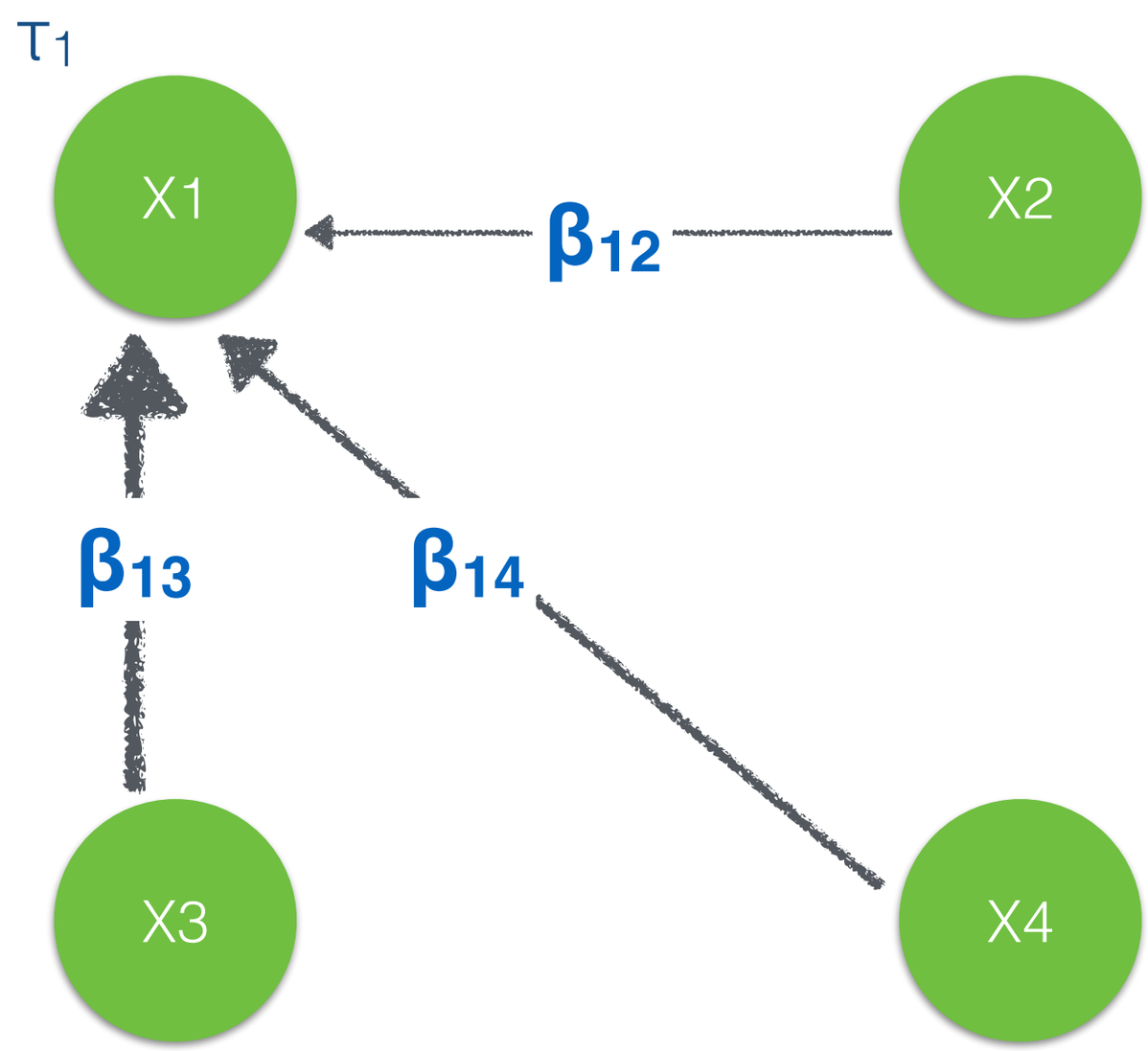
$$\mathbb{P}_\Theta\left(x_j \middle| x_{\setminus j}\right) = \frac{\exp\left[\tau_j x_j + x_j \sum_{k \in V_{\setminus j}} \beta_{jk} x_k\right]}{1 + \exp\left[\underbrace{\tau_j + \sum_{k \in V_{\setminus j}} \beta_{jk} x_k}\right]}$$

$\tau_1 + \beta_{12}X_2 + \beta_{13}X_3 + \ldots$

logistic regression!

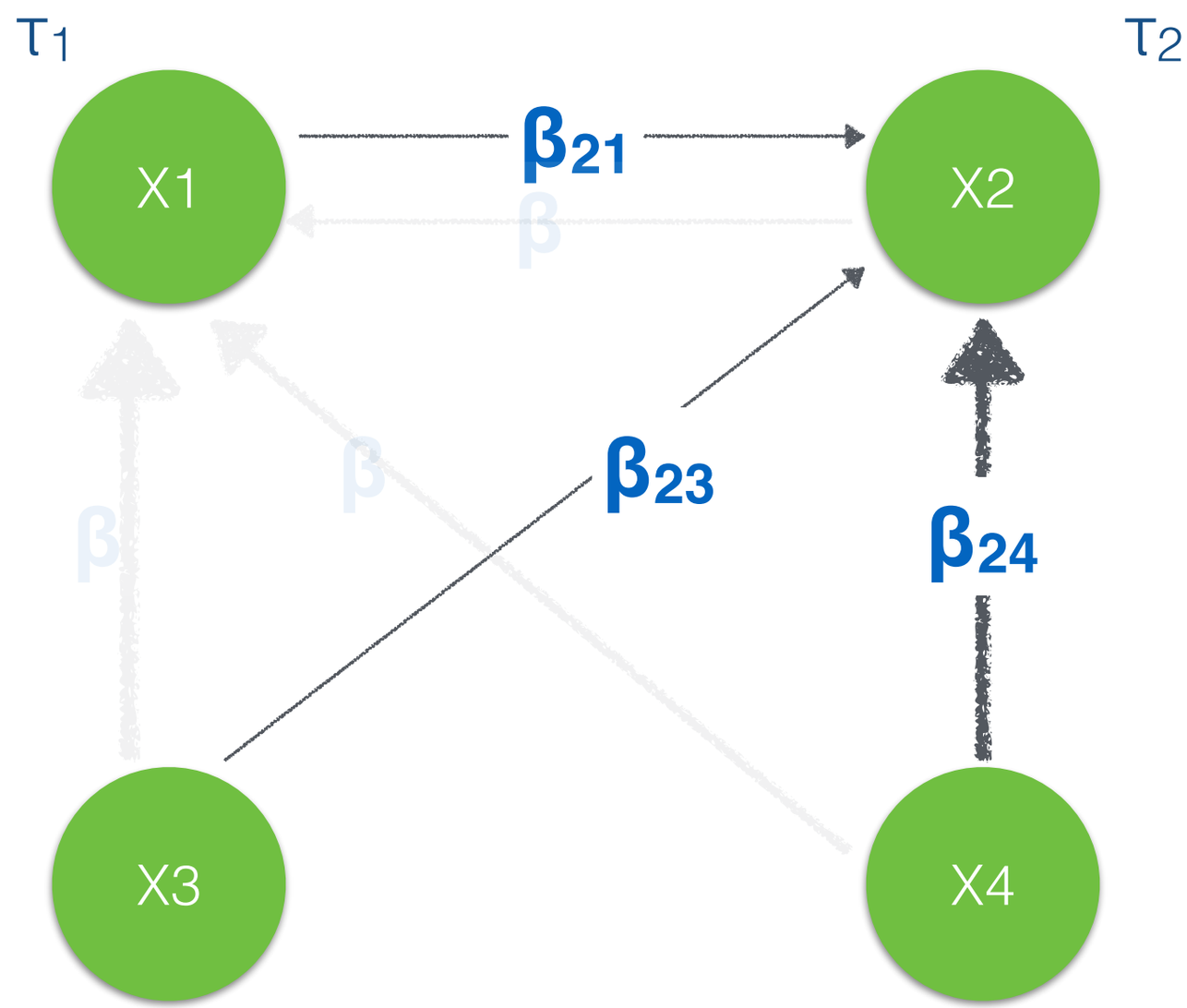
x = (x1, x2, …,xn)
xi = 0 or 1
τj: node parameter (threshold)
βjk: pairwise interaction parameter

Basic idea



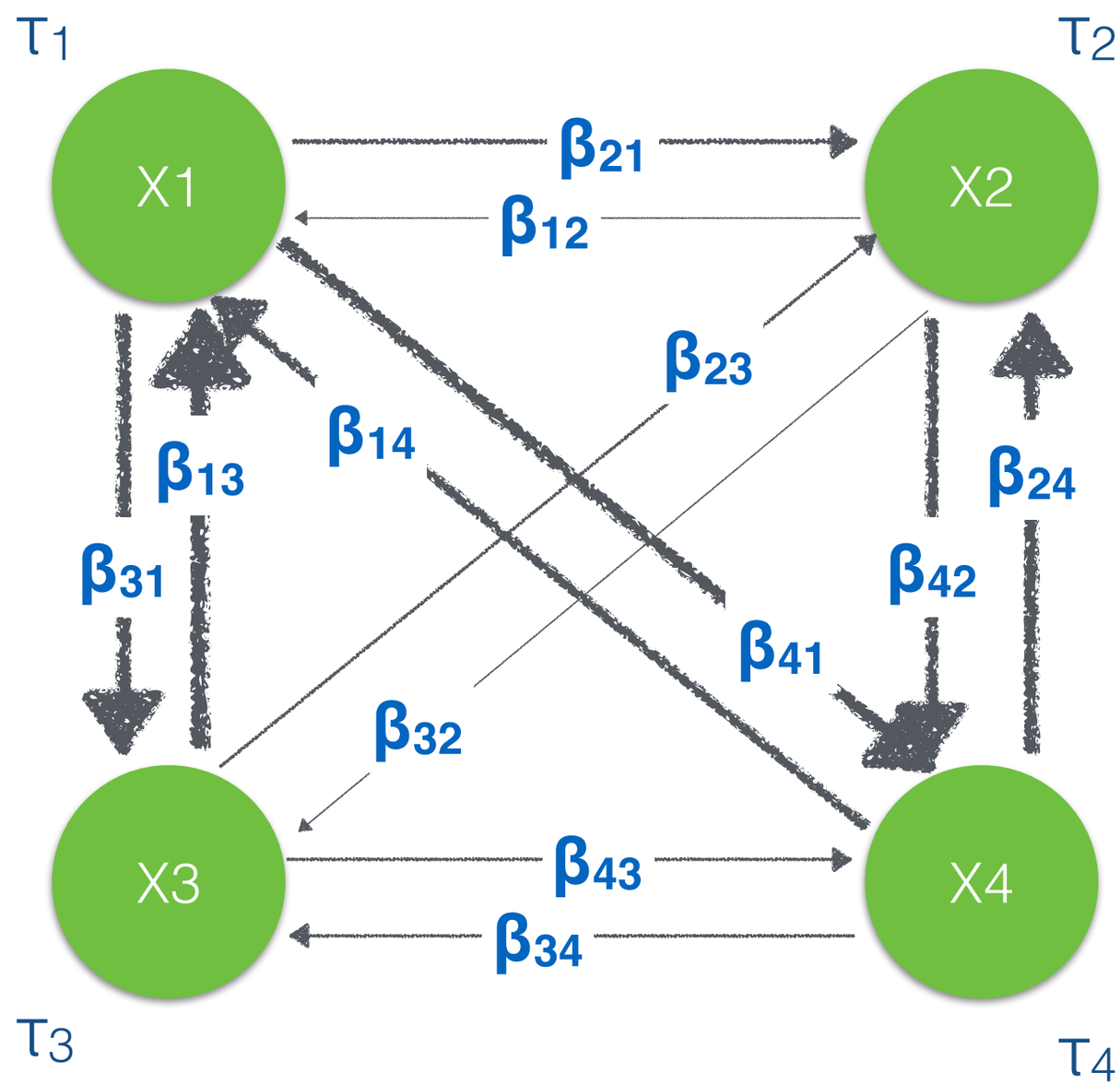
Perform regression of X_1 on all other variables

Basic idea



Repeat this for every variable

Basic idea

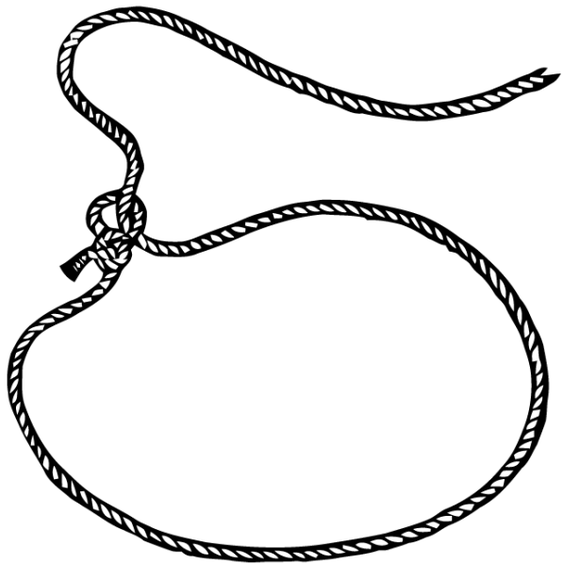


Control model complexity and prevent overfitting:
$\mathcal{L}_1$**-regularized** logistic regression

ℓ_1–regularized logistic regression

What is it and why use it?

- *lasso*: least absolute shrinkage and selection operator (Tibshirani, 1996)
- ensures shrinkage of some regression coefficients
- puts other coefficients to zero (as opposed to ridge regression)
- results in an interpretable network structure



ℓ_1–regularized logistic regression

$$\mathbb{P}_{\tau,\beta}(x_j \mid x_{\setminus j}) = \frac{\exp\left[\tau_j x_j + x_j \sum_{k \in V_{\setminus j}} \beta_{jk} x_k\right]}{1 + \exp\left[\tau_j + \sum_{k \in V_{\setminus j}} \beta_{jk} x_k\right]}$$

- 'as usual': optimizing negative log likelihood
- but with additional constraint

$$\hat{\Theta}_j^{\rho} = \arg\min_{\Theta_j} \left\{ -x_{ij} \cdot \left(\tau_j + \sum_{k \in V_{\setminus j}} \beta_{jk} x_{ik} \right) + \log\left(1 + \exp\left\{ \tau_j + \sum_{k \in V_{\setminus j}} x_{ik} \beta_{jk} \right\} \right) + \rho \sum_{k \in V_{\setminus j}} \left| \beta_{jk} \right| \right\}$$

regularization

- i: independent observations {1, 2, …, n}
- $\hat{\Theta}_j^{\rho}$: matrix with βjk and τj
- ρ: tuning parameter
- `R` package `glmnet`: 100 values of ρ

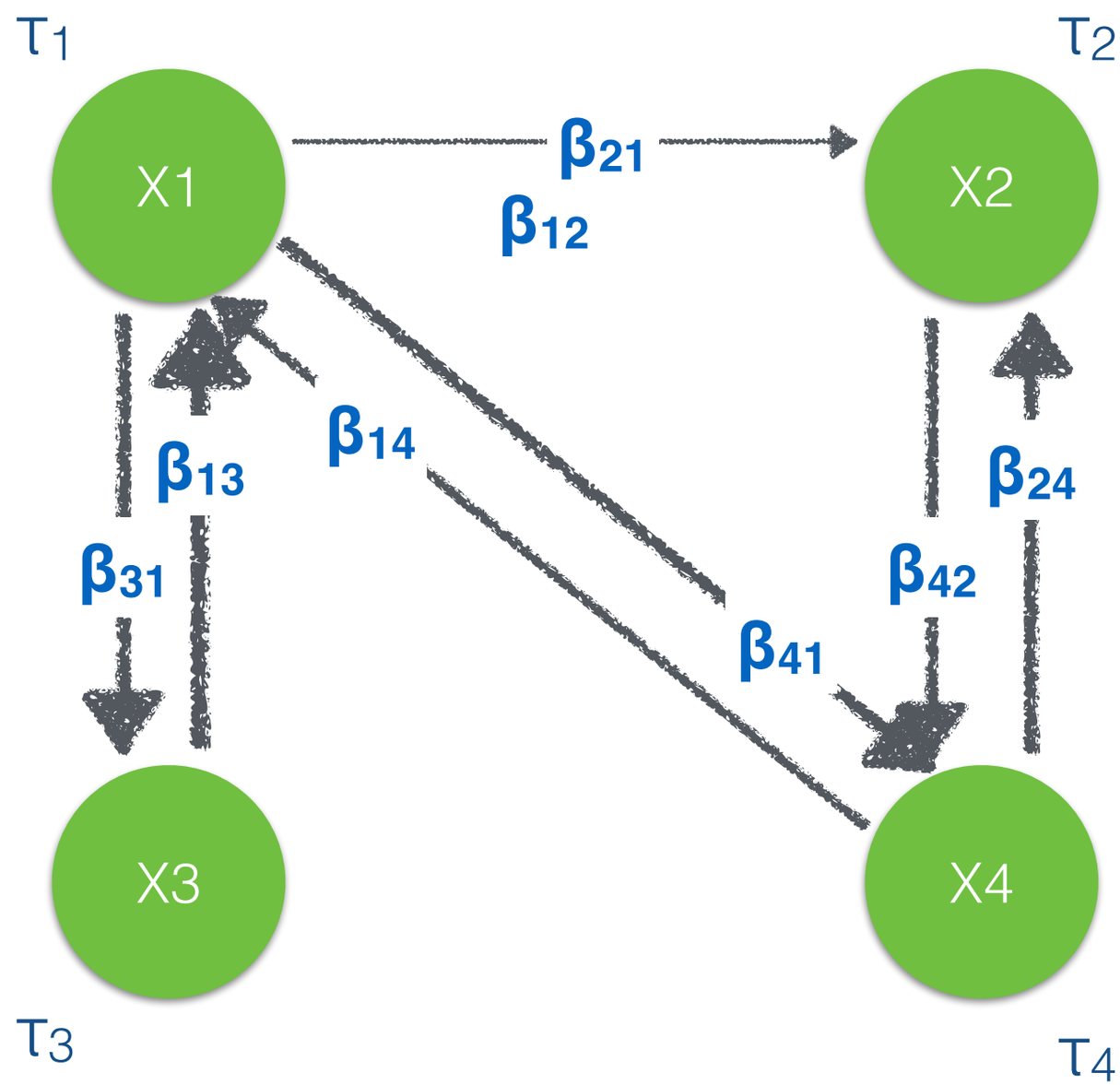
ℓ_1–regularized logistic regression

- Choose tuning parameter with *extended* Bayesian Information Criterion (EBIC)

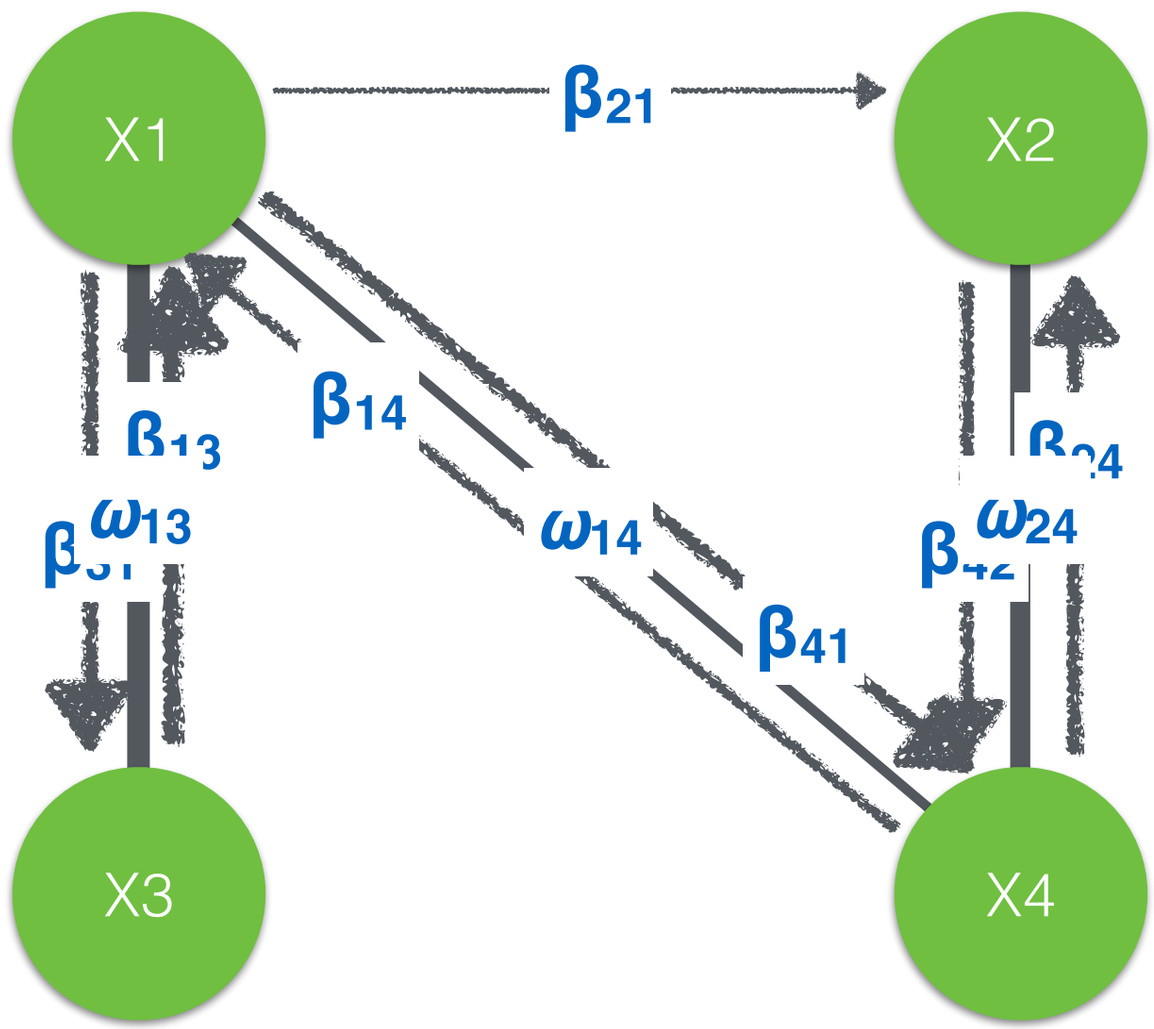
$$\mathrm{BIC}_\gamma(j) = -2\ell(\hat{\Theta}_J) + |J| \cdot \log(n) + 2\gamma|J| \cdot \log(p-1)$$

$$\ell(\hat{\Theta}_j) = \sum_{i=1}^{n} \left(\tau_j x_{ij} + \sum_{k \in V_{\setminus j}} \beta_{jk} x_{ij} x_{ik} - \log(1 + \exp\{\tau_j + \sum_{k \in V_{\setminus j}} x_{ik}\beta_{jk}\}) \right)$$

- |J|: number of neighbours
- n: number of observations
- p-1: number of covariates



- collect regularized parameters
- apply AND/OR rule



AND-rule:

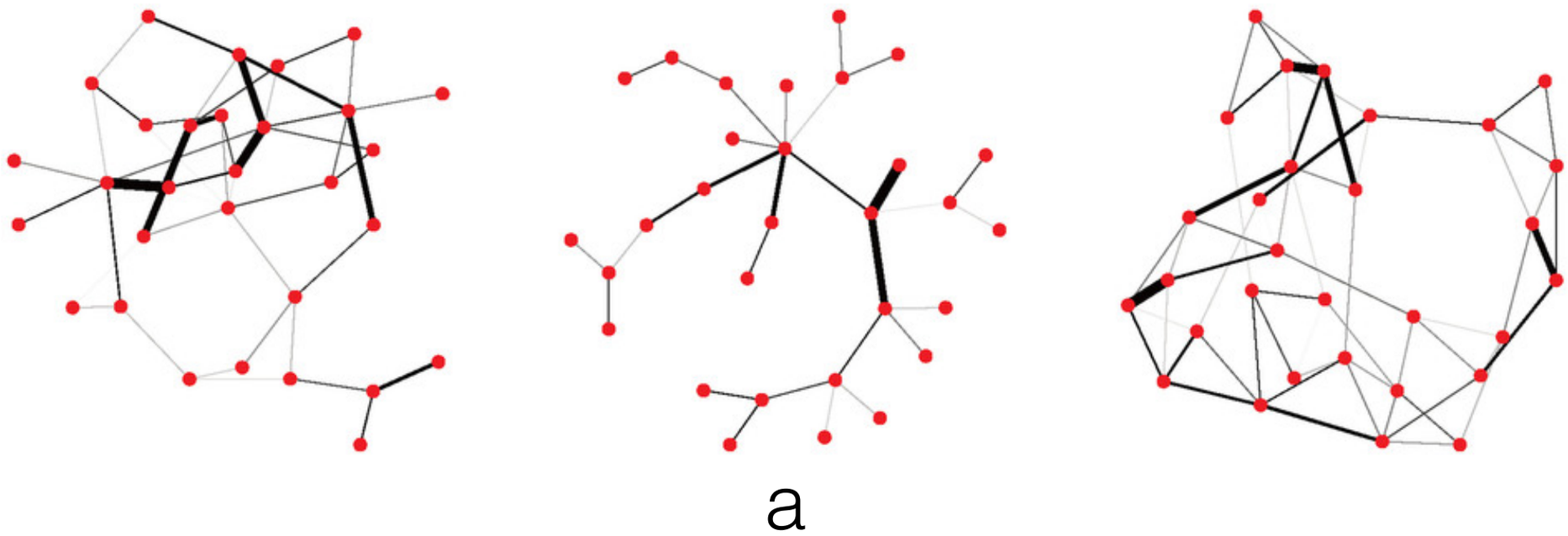
if $\beta_{ij} \neq 0$ AND $\beta_{ji} \neq 0$

then $\omega_{ij} = (\beta_{ij} + \beta_{ji})/2$

else $\omega_{ij} = 0$

eLasso (`R` package `IsingFit`)

True



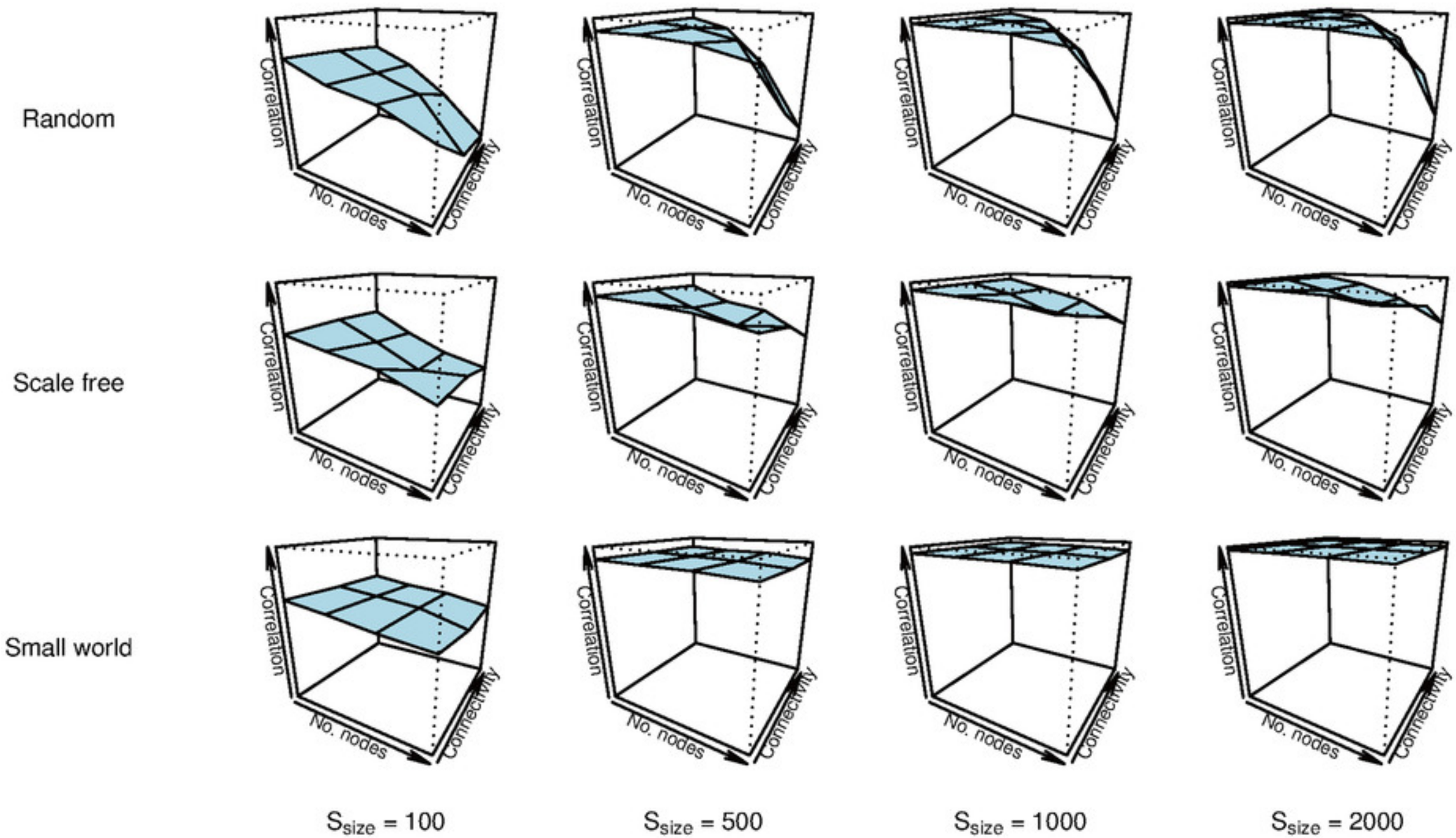
a

Estimated

b

Borkulo, C. D. van, Borsboom, D., Epskamp, S., Blanken, T. F., Boschloo, L., Schoevers, R. A., & Waldorp, L. J. (2014). A new method for constructing networks from binary data. Scientific Reports, 4(5918), 1–10. doi:10.1038/srep05918

Validation study



R package IsingFit

R code:

```
install.packages(‘IsingFit')
library(IsingFit)
res <- IsingFit(x=data, family=“binomial”,
AND=TRUE, gamma=0, plot=TRUE, progressbar=TRUE)
```

Next week

- More information about the final assignment!
- But you can think already about whether you want to analyze continuous or binary data…

See you at the practical!

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