SC6/SM9 Graphical Models

Michaelmas Term, 2017

Robin Evans

evans@stats.ox.ac.uk
Department of Statistics
University of Oxford

November 29, 2017

Course Website

The class site is at

`http://www.stats.ox.ac.uk/~evans/gms/`

You'll find

- lecture notes;
- slides;
- problem sheets;
- data sets.

Course Information

There will be four problem sheets and four associated classes.

Part C students, your classes are weeks 3, 5, 7 and HT1. Sign up online for one of the two sessions.

Hand in work by Tuesday, 5pm.

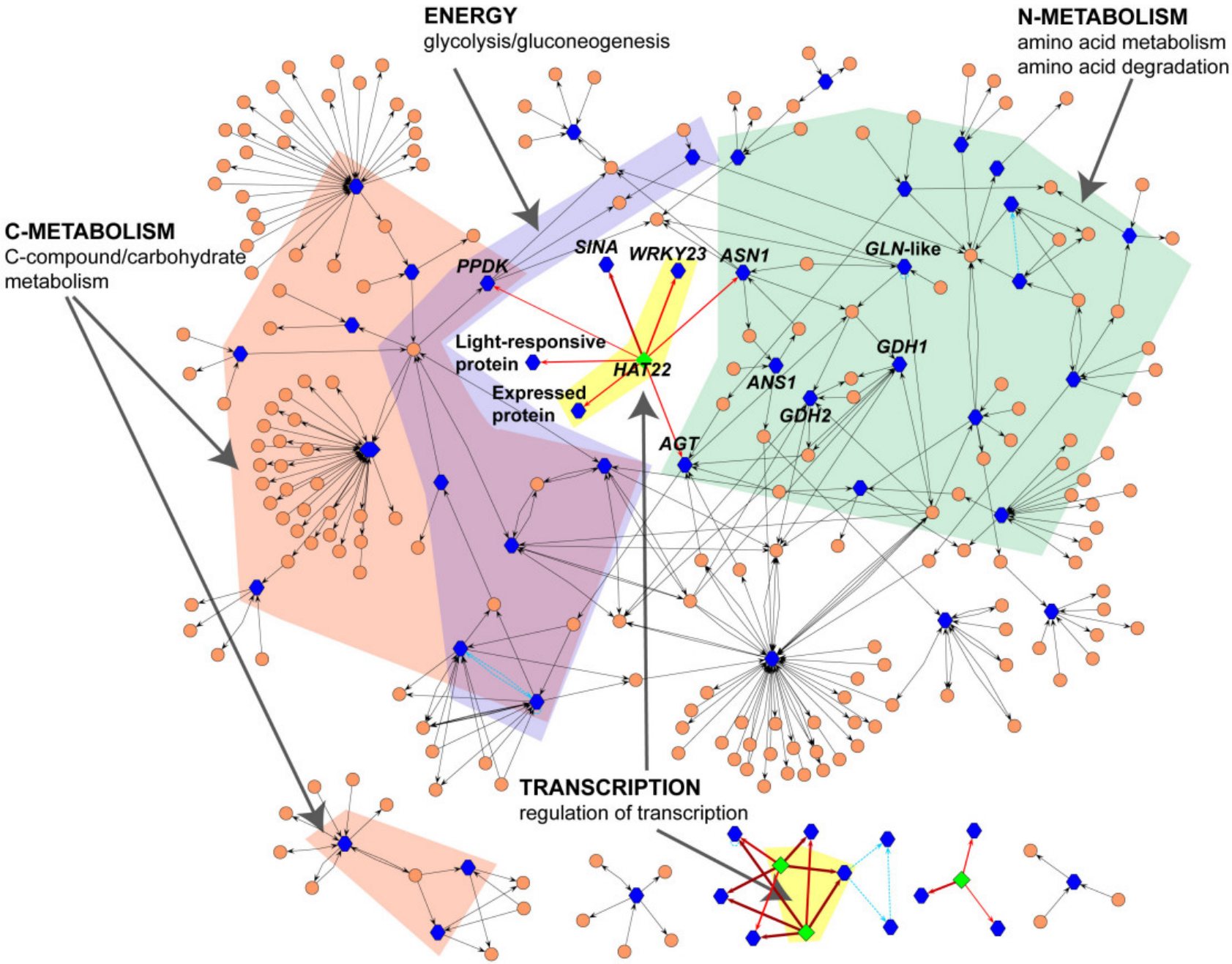
MSc students, classes are at 2pm on Wednesdays, weeks 3, 5, 7, and Thursday week 8 in here (LG.01).

Books

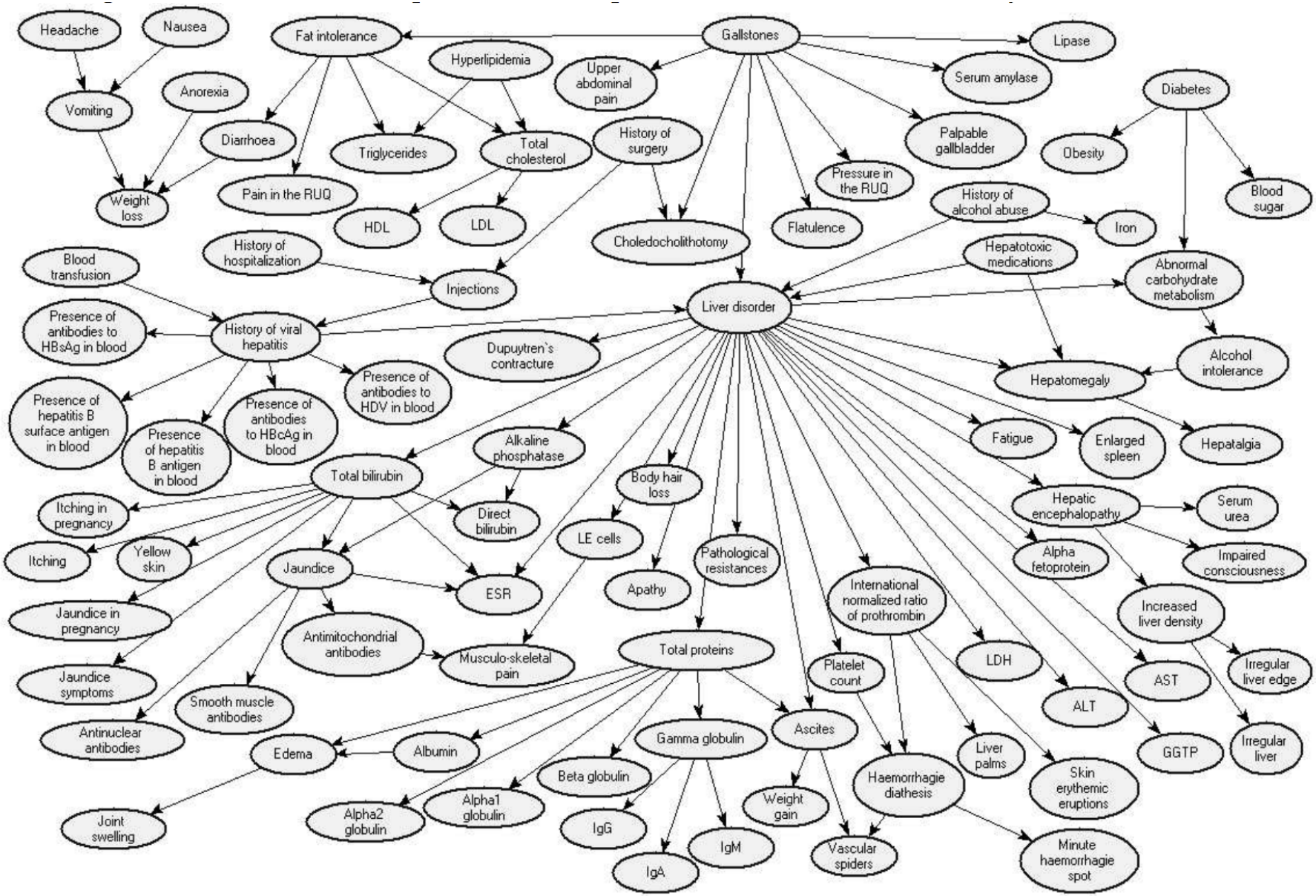
These books might be useful.

- Lauritzen (1996). *Graphical Models*, OUP.
- Wainwright and Jordan (2008). *Graphical Models, Exponential Families, and Variational Inference*. (Available online).
- Pearl (2009). *Causality*, (3rd edition), Cambridge.
- Koller and Friedman (2009), *Probabilistic Graphical Models: Principles and Techniques*, MIT Press.

Gene Regulatory Networks



Medical Diagnosis



Main Issues

There are two main problems with large data sets that we will consider in this course:

- statistical;
  we need to predict outcomes from scenarios that have never been observed (i.e., we need a model).
- computational:
  - we can't store probabilities for all combinations of variables;
  - even if we could, we can't sum/integrate them to find a marginal or conditional probability:

$$P(X = x) = \sum_{\boldsymbol{y}} P(X = x, \boldsymbol{Y} = \boldsymbol{y}).$$

Our solution will be to impose nonparametric structure, in the form of conditional independences.

Conditional Independence

Simpson's Paradox

Death Penalty?	Defendant's Race	
	White	Black
Yes	53	15
No	430	176

Simpson's Paradox

Victim's Race	Death Penalty?	Defendant's Race	
		White	Black
White	Yes	53	11
	No	414	37
Black	Yes	0	4
	No	16	139

Contingency Tables: Some Notation

We will consider multivariate systems of vectors $X_V \equiv (X_v : v \in V)$ for some set $V = \{1, \ldots, p\}$.

Write $X_A \equiv (X_v : v \in A)$ for any $A \subseteq V$.

We assume that each $X_v \in \{1, \ldots, d_v\}$ (usually $d_v = 2$).

If we have n i.i.d. observations write

$$X_V^{(i)} \equiv (X_1^{(i)}, \ldots, X_p^{(i)})^T, \qquad i = 1, \ldots, n.$$

Contingency Tables: Some Notation

We typically summarize categorical data by counts:

aspirin	heart attack
Y	N
Y	Y
N	N
N	N
Y	N
⋮	⋮

	heart attack	
	Y	N
no aspirin	28	656
aspirin	18	658

Write

$$n(x_V) = \sum_{i=1}^{n} \mathbb{1}\{X_1^{(i)} = x_1, \ldots, X_p^{(i)} = x_p\}$$

A **marginal table** only counts some of the variables.

$$n(x_A) = \sum_{x_{V \setminus A}} n(x_A, x_{V \setminus A}).$$

Marginal Table

Victim's Race	Death Penalty?	Defendant's Race	
		White	Black
White	Yes	53	11
	No	414	37
Black	Yes	0	4
	No	16	139

If we sum out the Victim's race...

Death Penalty?	Defendant's Race	
	White	Black
Yes	53	15
No	430	176

Contingency Tables

The death penalty data is on the class website.

```
> deathpen <- read.table("deathpen.txt", header=TRUE)
> deathpen

  DeathPen Defendant Victim freq
1      Yes     White  White   53
2       No     White  White  414
3      Yes     Black  White   11
4       No     Black  White   37
5      Yes     White  Black    0
6       No     White  Black   16
7      Yes     Black  Black    4
8       No     Black  Black  139
```

Contingency Tables

We can fit models on it in R:

```
> summary(glm(freq ~ Victim*Defendant + Victim*DeathPen,
+                 family=poisson, data=deathpen))
```

```
Coefficients:
                            Estimate Std. Error
(Intercept)                  4.93737    0.08459
VictimWhite                 -1.19886    0.16812
DefendantWhite              -2.19026    0.26362
DeathPenYes                 -3.65713    0.50641
VictimWhite:DefendantWhite   4.46538    0.30408
VictimWhite:DeathPenYes      1.70455    0.52373

Residual deviance:    5.394  on 2  degrees of freedom
```

(So $p \approx 0.07$ in hypothesis test of model fit.)

Contingency Tables

If we fit the marignal table over the races of Victim and Defendant, the parameters involving 'Defendant' are the same.

```
> summary(glm(freq ~ Victim*Defendant,
+                 family=poisson, data=deathpen))
```

```
Coefficients:
                          Estimate Std. Error
(Intercept)                4.26970    0.08362
VictimWhite               -1.09164    0.16681
DefendantWhite            -2.19026    0.26360
VictimWhite:DefendantWhite  4.46538    0.30407
```

Undirected Graphical Models

Multivariate Data

```
> library(ggm)
> data(marks)
> dim(marks)

[1] 88  5

> head(marks, 8)

  mechanics vectors algebra analysis statistics
1        77      82      67       67         81
2        63      78      80       70         81
3        75      73      71       66         81
4        55      72      63       70         68
5        63      63      65       70         63
6        53      61      72       64         73
7        51      67      65       65         68
8        59      70      68       62         56
```

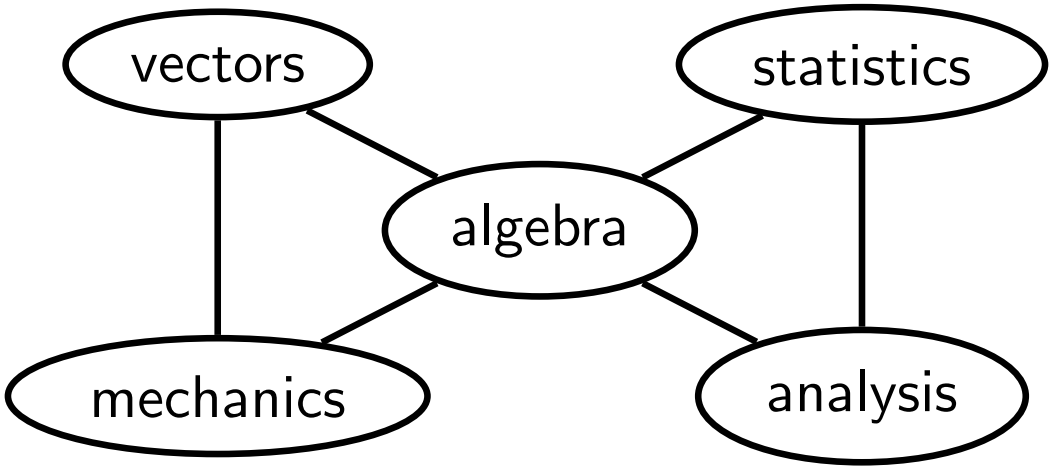
Multivariate Data

```
> sapply(marks, mean)

 mechanics    vectors    algebra   analysis statistics
      39.0       50.6       50.6       46.7       42.3

> cor(marks)

           mechanics vectors algebra analysis statistics
mechanics      1.000   0.553   0.546    0.410      0.389
vectors        0.553   1.000   0.610    0.485      0.436
algebra        0.546   0.610   1.000    0.711      0.665
analysis       0.410   0.485   0.711    1.000      0.607
statistics     0.389   0.436   0.665    0.607      1.000
```

Multivariate Data

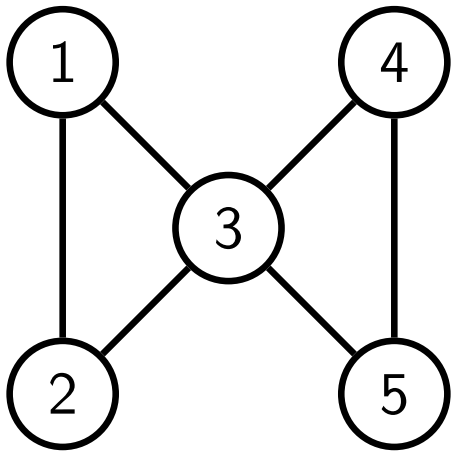
```
> conc <- solve(cov(marks))  # concentration matrix
> round(1000*conc, 2)

           mechanics vectors algebra analysis statistics
mechanics       5.24   -2.43   -2.72     0.01      -0.15
vectors        -2.43   10.42   -4.72    -0.79      -0.16
algebra        -2.72   -4.72   26.94    -7.05      -4.70
analysis        0.01   -0.79   -7.05     9.88      -2.02
statistics     -0.15   -0.16   -4.70    -2.02       6.45
```

Undirected Graphs



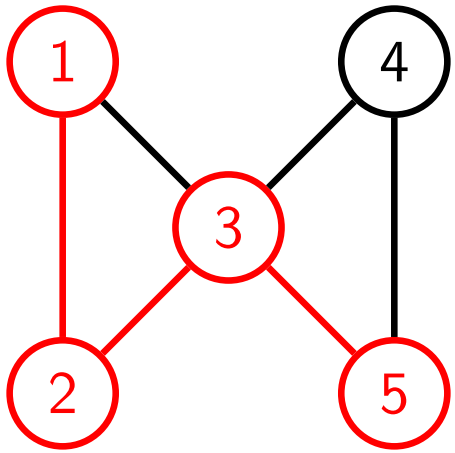
	mech	vecs	alg	anlys	stats
mechanics	5.24	-2.43	-2.72	0.01	-0.15
vectors	-2.43	10.42	-4.72	-0.79	-0.16
algebra	-2.72	-4.72	26.94	-7.05	-4.70
analysis	0.01	-0.79	-7.05	9.88	-2.02
statistics	-0.15	-0.16	-4.70	-2.02	6.45

Undirected Graphs



$$V = \{1, 2, 3, 4, 5\}$$
$$E = \{\{1, 2\}, \{1, 3\}, \{2, 3\}, \{3, 4\}, \{3, 5\}, \{4, 5\}\}.$$

Paths



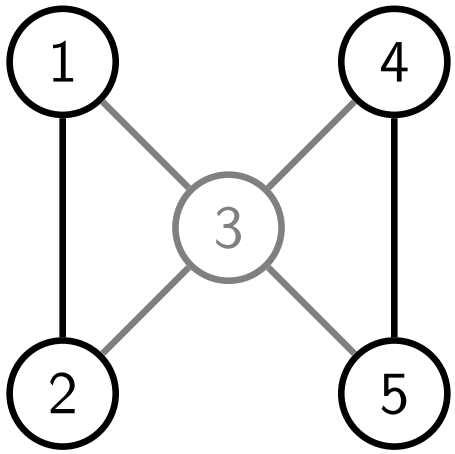
Paths:

$$\pi_1 : 1 - 2 - 3 - 5$$

$$\pi_2 : 3$$

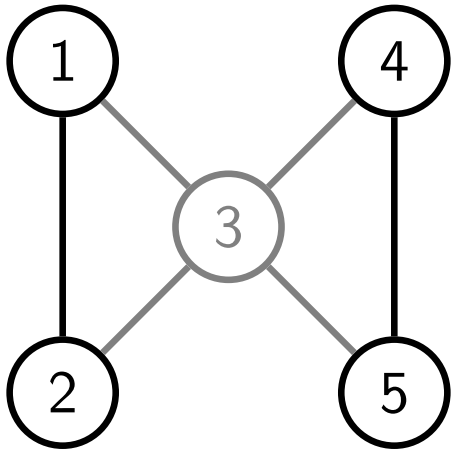
Note that paths may consist of one vertex and no edges.

Induced Subgraph



The **induced subgraph** $\mathcal{G}_{\{1,2,4,5\}}$ drops any edges that involve $\{3\}$.

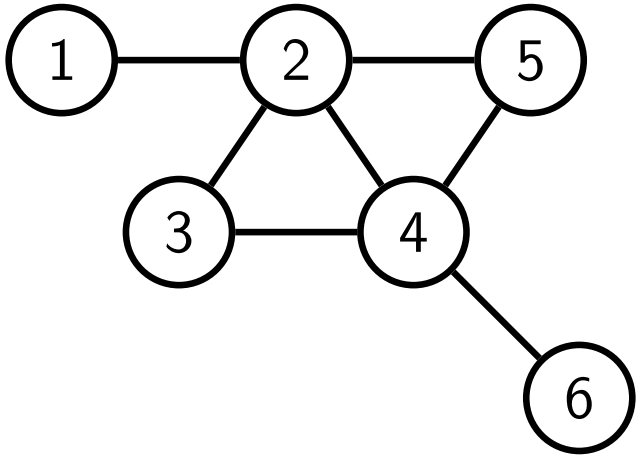
Separation



All paths between $\{1, 2\}$ and $\{5\}$ pass through $\{3\}$.

Hence $\{1, 2\}$ and $\{5\}$ are **separated** by $\{3\}$.

Cliques and Running Intersection



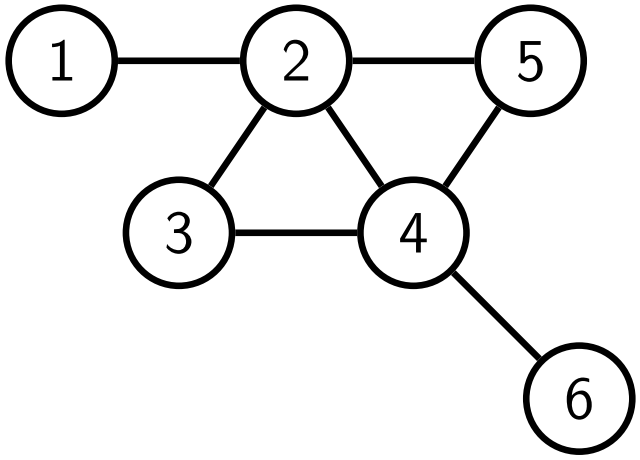
Cliques:

$$\{1,2\} \qquad \{2,3,4\} \qquad \{2,4,5\} \qquad \{4,6\}.$$

Separator sets:

$$\emptyset \qquad \{2\} \qquad \{2,4\} \qquad \{4\}.$$

Cliques and Running Intersection



A different ordering of the cliques:

$$\{2,3,4\} \qquad \{2,4,5\} \qquad \{4,6\} \qquad \{1,2\}.$$

Separator sets:

$$\emptyset \qquad \{2,4\} \qquad \{4\} \qquad \{2\}.$$

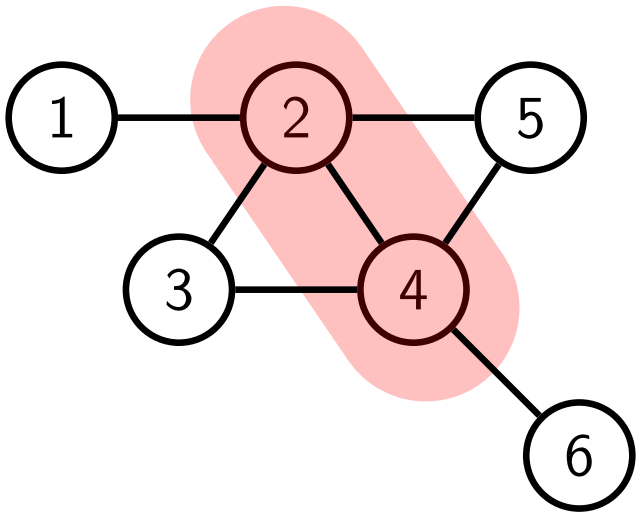
Any ordering works in this case as long $\{1,2\}$ and $\{4,6\}$ aren't the first two entries.

Estimation

Given a decomposition of the graph, we have an associated conditional independence: e.g. $(\{1,3\},\{2,4\},\{5,6\})$ suggests

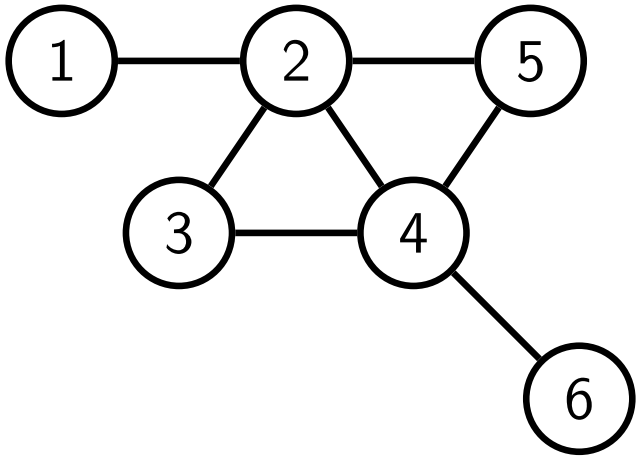
$$X_1, X_3 \perp\!\!\!\perp X_5, X_6 \mid X_2, X_4$$

$$p(x_{123456}) \cdot p(x_{24}) = p(x_{1234}) \cdot p(x_{2456}).$$



And $p(x_{1234})$ and $p(x_{2456})$ are Markov with respect to $\mathcal{G}_{1234}$ and $\mathcal{G}_{2456}$ respectively.

Estimation



Repeating this process on each subgraph we obtain:

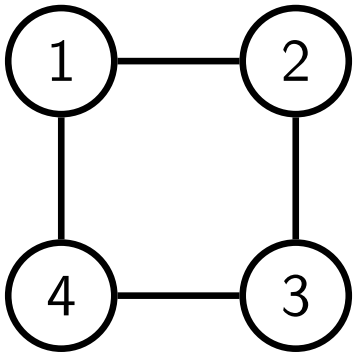
$$p(x_{123456}) \cdot p(x_{24}) \cdot p(x_2) \cdot p(x_4) = p(x_{12}) \cdot p(x_{234}) \cdot p(x_{245}) \cdot p(x_{46}).$$

i.e.

$$p(x_{123456}) = \frac{p(x_{12}) \cdot p(x_{234}) \cdot p(x_{245}) \cdot p(x_{46})}{p(x_{24}) \cdot p(x_2) \cdot p(x_4)}.$$

Non-Decomposable Graphs

But can't we do this for any factorization?



No! Although

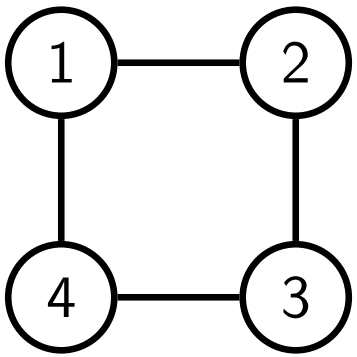
$$p(x_{1234}) = \psi_{12}(x_{12}) \cdot \psi_{23}(x_{23}) \cdot \psi_{34}(x_{34}) \cdot \psi_{14}(x_{14}),$$

the ψs are constrained by the requirement that

$$\sum_{x_{1234}} p(x_{1234}) = 1.$$

These is no nice representation of the ψ_Cs in terms of p.

Non-Decomposable Graphs



If we 'decompose' without a complete separator set then we introduce constraints between the separate terms:

$$p(x_{1234}) = p(x_1 \mid x_2, x_4) \cdot p(x_3 \mid x_2, x_4),$$

but how to ensure that $X_2 \perp\!\!\!\perp X_4 \mid X_1, X_3$?

Iterative Proportional Fitting

The Iterative Proportional Fitting Algorithm

function IPF(collection of margins $q(x_{C_i})$)
  set $p(x_V)$ to uniform distribution;
  while $\max_i \max_{x_{C_i}} |p(x_{C_i}) - q(x_{C_i})| >$ tol **do**
    for i in $1, \ldots, k$ **do**
      update $p(x_V)$ to $p(x_{V \setminus C_i} \mid x_{C_i}) \cdot q(x_{C_i})$;
    end for
  end while
  return distribution p with margins $p(x_{C_i}) = q(x_{C_i})$.
end function

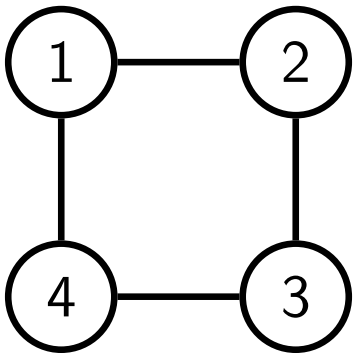
If any distribution satisfying $p(x_{C_i}) = q(x_{C_i})$ for each $i = 1, \ldots, k$ exists, then the algorithm converges to the **unique distribution** with those margins and which is Markov with respect to the graph with cliques $C_1, \ldots, C_k$.

Some Data

		$X_2 = 0$		$X_2 = 1$	
		$X_1 = 0$	1	0	1
$X_4 = 0$	$X_3 = 0$	5	10	18	1
	1	0	3	4	0
$X_4 = 1$	0	24	0	9	3
	1	1	2	2	7

Margins

Suppose we want to fit the 4-cycle model:



The relevant margins are:

$n(x_{12})$	$X_2 = 0$	1
$X_1 = 0$	30	33
1	15	11

$n(x_{23})$	$X_3 = 0$	1
$X_2 = 0$	39	6
1	31	13

$n(x_{34})$	$X_4 = 0$	1
$X_3 = 0$	34	36
1	7	12

$n(x_{14})$	$X_4 = 0$	1
$X_1 = 0$	27	36
1	14	12

Start with a Uniform Table

		$X_2 = 0$		$X_2 = 1$	
		$X_1 = 0$	1	0	1
$X_4 = 0$	$X_3 = 0$	5.56	5.56	5.56	5.56
	1	5.56	5.56	5.56	5.56
$X_4 = 1$	0	5.56	5.56	5.56	5.56
	1	5.56	5.56	5.56	5.56

Set Margin X_1, X_2 to Correct Value

		$X_2 = 0$		$X_2 = 1$	
		$X_1 = 0$	1	0	1
$X_4 = 0$	$X_3 = 0$	7.5	3.75	8.25	2.75
	1	7.5	3.75	8.25	2.75
$X_4 = 1$	0	7.5	3.75	8.25	2.75
	1	7.5	3.75	8.25	2.75

Replace

$$p^{(i+1)}(x_1, x_2, x_3, x_4) = p^{(i)}(x_1, x_2, x_3, x_4) \cdot \frac{n(x_1, x_2)}{p^{(i)}(x_1, x_2)}$$

Set Margin X_2, X_3 to Correct Value

		$X_2 = 0$		$X_2 = 1$	
		$X_1 = 0$	1	0	1
$X_4 = 0$	$X_3 = 0$	13	6.5	11.62	3.88
	1	2	1	4.88	1.62
$X_4 = 1$	0	13	6.5	11.62	3.88
	1	2	1	4.88	1.62

Replace

$$p^{(i+1)}(x_1, x_2, x_3, x_4) = p^{(i)}(x_1, x_2, x_3, x_4) \cdot \frac{n(x_2, x_3)}{p^{(i)}(x_2, x_3)}$$

Set Margin X_3, X_4 to Correct Value

		$X_2 = 0$		$X_2 = 1$	
		$X_1 = 0$	1	0	1
$X_4 = 0$	$X_3 = 0$	12.63	6.31	11.29	3.76
	1	1.47	0.74	3.59	1.2
$X_4 = 1$	0	13.37	6.69	11.96	3.99
	1	2.53	1.26	6.16	2.05

Replace

$$p^{(i+1)}(x_1, x_2, x_3, x_4) = p^{(i)}(x_1, x_2, x_3, x_4) \cdot \frac{n(x_3, x_4)}{p^{(i)}(x_3, x_4)}$$

Set Margin X_1, X_4 to Correct Value

		$X_2 = 0$		$X_2 = 1$	
		$X_1 = 0$	1	0	1
$X_4 = 0$	$X_3 = 0$	11.76	7.36	10.52	4.39
	1	1.37	0.86	3.35	1.4
$X_4 = 1$	0	14.15	5.74	12.66	3.42
	1	2.67	1.08	6.52	1.76

Replace

$$p^{(i+1)}(x_1, x_2, x_3, x_4) = p^{(i)}(x_1, x_2, x_3, x_4) \cdot \frac{n(x_1, x_4)}{p^{(i)}(x_1, x_4)}$$

Notice that sum of first column is now 29.96.

Set Margin X_1, X_2 to Correct Value

		$X_2 = 0$		$X_2 = 1$	
		$X_1 = 0$	1	0	1
$X_4 = 0$	$X_3 = 0$	11.78	7.37	10.53	4.39
	1	1.37	0.86	3.34	1.39
$X_4 = 1$	0	14.14	5.73	12.64	3.42
	1	2.68	1.09	6.54	1.77

Eventually:

Waiting for this process to converge leads to the MLE:

		$X_2 = 0$		$X_2 = 1$	
		$X_1 = 0$	1	0	1
$X_4 = 0$	$X_3 = 0$	11.76	7.33	10.5	4.4
	1	1.38	0.86	3.35	1.4
$X_4 = 1$	0	14.18	5.72	12.66	3.44
	1	2.68	1.08	6.48	1.76

Gaussian Graphical Models

The Multivariate Gaussian Distribution

Let $X_V \sim N_p(0, \Sigma)$, where $\Sigma \in \mathbb{R}^{p \times p}$ is a symmetric positive definite matrix.

$$\log p(x_V; \Sigma) = -\frac{1}{2} \log |\Sigma| - \frac{1}{2} x_V^T \Sigma^{-1} x_V + \text{const.}$$

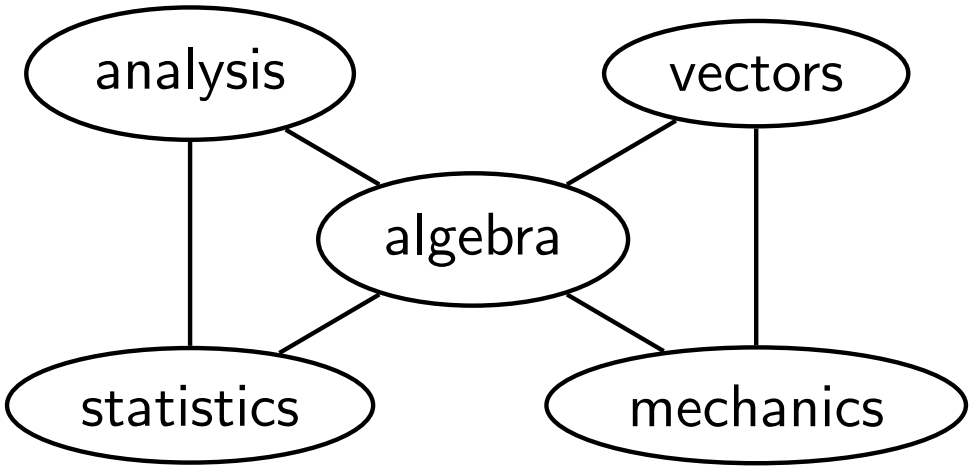
The log-likelihood for Σ is

$$l(\Sigma) = -\frac{n}{2} \log |\Sigma| - \frac{n}{2} \operatorname{tr}(S\Sigma^{-1})$$

where S is the sample covariance matrix, and this is maximized by choosing $\hat{\Sigma} = S$.

Gaussian Graphical Models

We have $X_a \perp\!\!\!\perp X_b \mid X_{V\setminus\{a,b\}}$ if and only if $k_{ab} = 0$.



	mechanics	vectors	algebra	analysis	statistics
mechanics	k_{11}	k_{12}	k_{13}	0	0
vectors		k_{22}	k_{23}	0	0
algebra			k_{33}	k_{34}	k_{35}
analysis				k_{44}	k_{45}
statistics					k_{55}

Likelihood

From Lemma 4.23, we have

$$\log p(x_V) + \log p(x_S) = \log p(x_A, x_S) + \log p(x_B, x_S).$$

This becomes

$$x_V^T \Sigma^{-1} x_V + x_S^T (\Sigma_{SS})^{-1} x_S - x_{AS}^T (\Sigma_{AS,AS})^{-1} x_{AS} - x_{SB}^T (\Sigma_{SB,SB})^{-1} x_{SB} = 0$$

But can rewrite each term in the form $x_V^T M x_V$, e.g.:

$$x_{AS}^T (\Sigma_{AS,AS})^{-1} x_{AS} = x_V^T \begin{pmatrix} (\Sigma_{AS,AS})^{-1} & 0 \\ 0 \quad 0 & 0 \end{pmatrix} x_V$$

Equating terms gives:

$$\Sigma^{-1} = \begin{pmatrix} (\Sigma_{AS,AS})^{-1} & 0 \\ 0 \quad 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & & \\ 0 & & (\Sigma_{SB,SB})^{-1} \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & (\Sigma_{SS})^{-1} & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

Maximum Likelihood Estimation

Iterating this process with a decomposable graph shows that:

$$\Sigma^{-1} = \sum_{i=1}^{k} \left\{ (\Sigma_{C_i,C_i})^{-1} \right\}_{C_i,C_i} - \sum_{i=1}^{k} \left\{ (\Sigma_{S_i,S_i})^{-1} \right\}_{S_i,S_i}.$$

For maximum likelihood estimation, using Lemma 4.23 we have

$$\begin{aligned} \hat{\Sigma}^{-1} &= \sum_{i=1}^{k} \left\{ (\hat{\Sigma}_{C_i,C_i})^{-1} \right\}_{C_i,C_i} - \sum_{i=1}^{k} \left\{ (\hat{\Sigma}_{S_i,S_i})^{-1} \right\}_{S_i,S_i} \\ &= \sum_{i=1}^{k} \left\{ (W_{C_i,C_i})^{-1} \right\}_{C_i,C_i} - \sum_{i=1}^{k} \left\{ (W_{S_i,S_i})^{-1} \right\}_{S_i,S_i} \end{aligned}$$

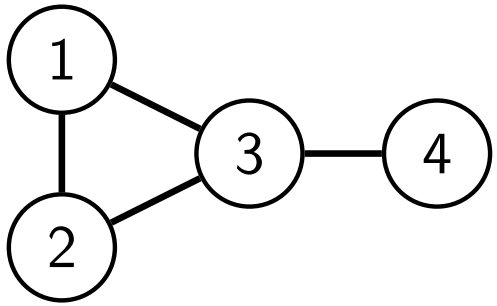
where $W_{CC} = \frac{1}{n} \sum_i X_C^{(i)} X_C^{(i)T}$ is the sample covariance matrix.

Example

```
> true_inv          # true concentration matrix

     [,1] [,2] [,3] [,4]
[1,]  1.0  0.3  0.2  0.0
[2,]  0.3  1.0 -0.1  0.0
[3,]  0.2 -0.1  1.0  0.3
[4,]  0.0  0.0  0.3  1.0

> solve(true_inv)  # Sigma

      [,1]   [,2]  [,3]   [,4]
[1,]  1.17 -0.382 -0.30  0.090
[2,] -0.38  1.136  0.21 -0.063
[3,] -0.30  0.209  1.19 -0.356
[4,]  0.09 -0.063 -0.36  1.107

> # rmvnorm is in the mvtnorm package
> dat <- rmvnorm(1000, mean=rep(0,4), sigma = solve(true_inv))
> W <- cov(dat)     # sample covariance
```

Example

Fit the model with decomposition $(\{1,2\},\{3\},\{4\})$:



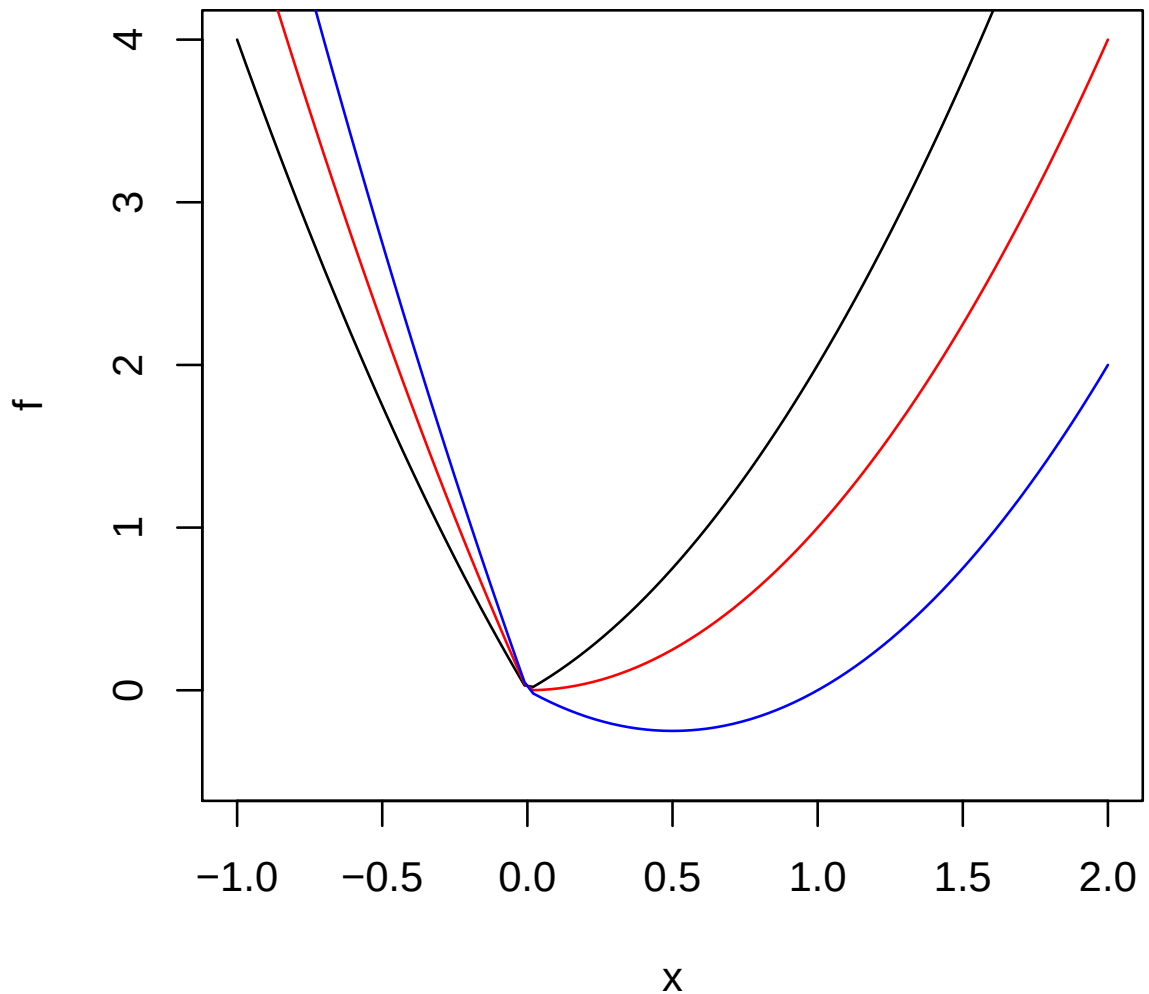

```
> K_hat = matrix(0, 4, 4)
> K_hat[1:3, 1:3] = solve(W[1:3, 1:3])
> K_hat[3:4, 3:4] = K_hat[3:4, 3:4] + solve(W[3:4, 3:4])
> K_hat[3, 3] = K_hat[3, 3] - 1/W[3, 3]
> K_hat

      [,1]    [,2]    [,3]  [,4]
[1,] 1.079  0.2851  0.2298 0.000
[2,] 0.285  0.9930 -0.0687 0.000
[3,] 0.230 -0.0687  1.0017 0.296
[4,] 0.000  0.0000  0.2958 1.082
```

Note this is close to the true concentration matrix.

The Lasso

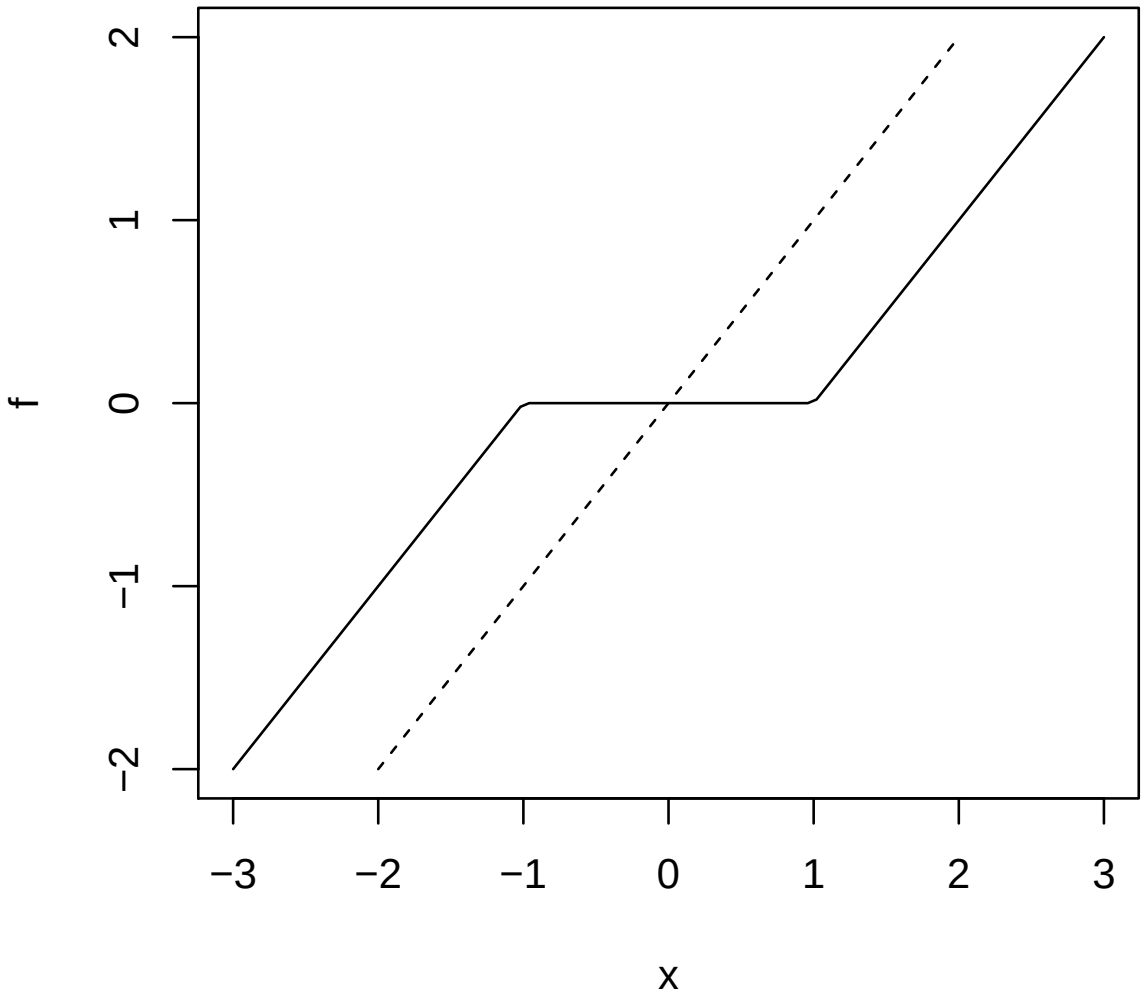
Cusps

$$f(x) = x^2 - ax + 2|x|, \qquad a = 1, a = 2, a = 3.$$

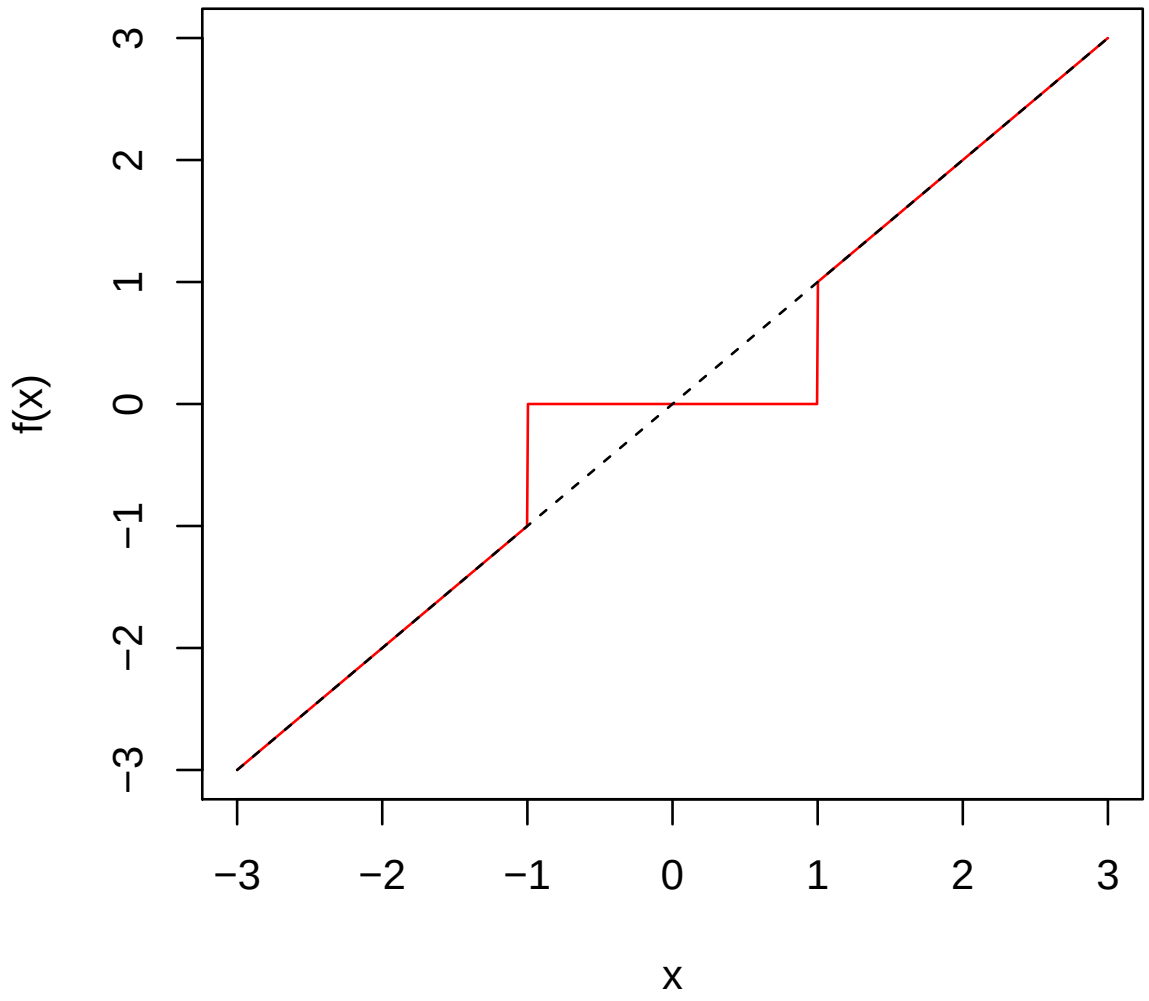


Soft Thresholding

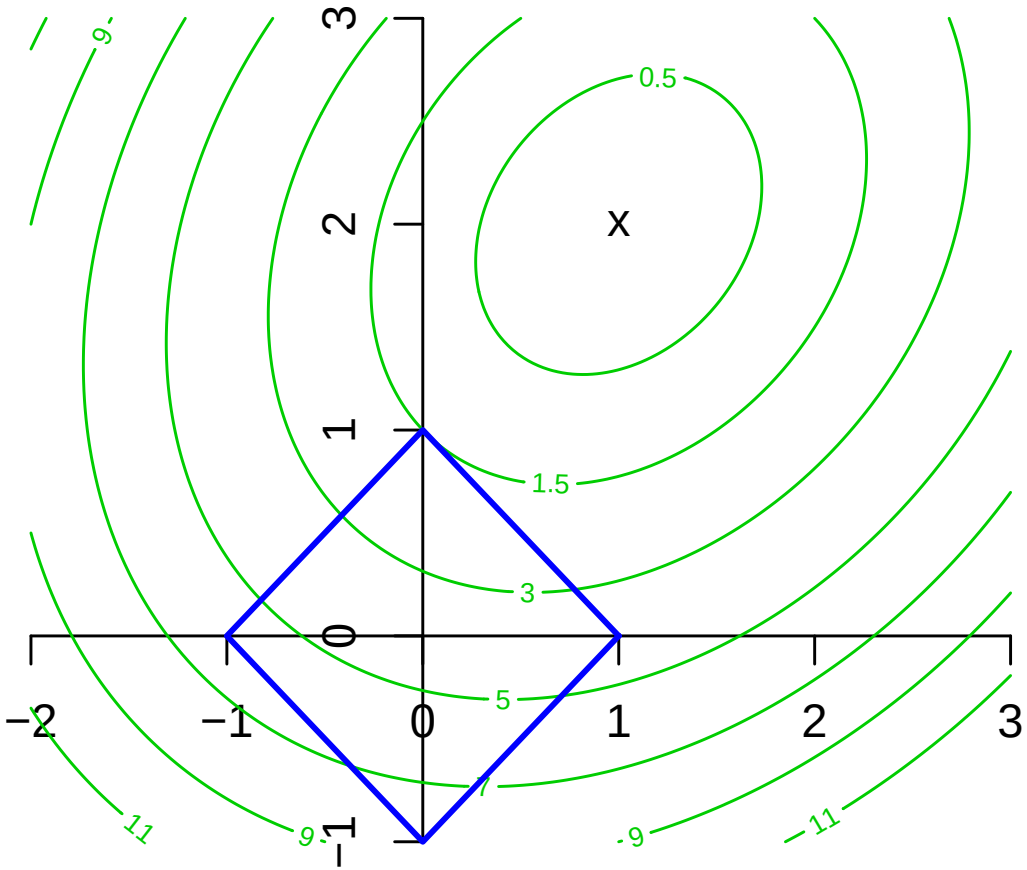
$f(x) = \text{sign}(x)(|x| - \lambda)_+$ for $x \in (-5, 5)$ and $\lambda = 1$.



Hard Thresholding (Significance Tests)



Sparsity



Riboflavin Data

The Riboflavin production dataset is available in R's `hdi` package; it consists of $p = 4088$ gene expression measurements in 71 cells, and also measures Riboflavin production.

Here is some code to load it.

```
> library(hdi)
> data("riboflavin")
> Y <- riboflavin[,1]  # response variable
> X <- as.matrix(riboflavin[,2])  # some preprocessing!
> class(X) <- "numeric"
> X <- as.data.frame(X)
> dim(X)  # n=71, p=4088

[1]   71 4088
```

Riboflavin Data

We would like to find a small subset of genes that explain the Riboflavin production as well as possible, without overfitting.

```
> lm0 <- lm(Y ~ 1, data=X)    # fit a null model
> # make a formula for the maximal model with all variables
> form <- paste("~ ", paste(names(X), collapse=" + "),
+                 sep="")
> substr(form, 1, 50)

[1] "~ AADK_at + AAPA_at + ABFA_at + ABH_at + ABNA_at +"

> # stepAIC(lm0, scope=form)  # doesn't work!
```

The `stepAIC()` function in R seems unable to deal with systems of this size (in principle it ought to work though).

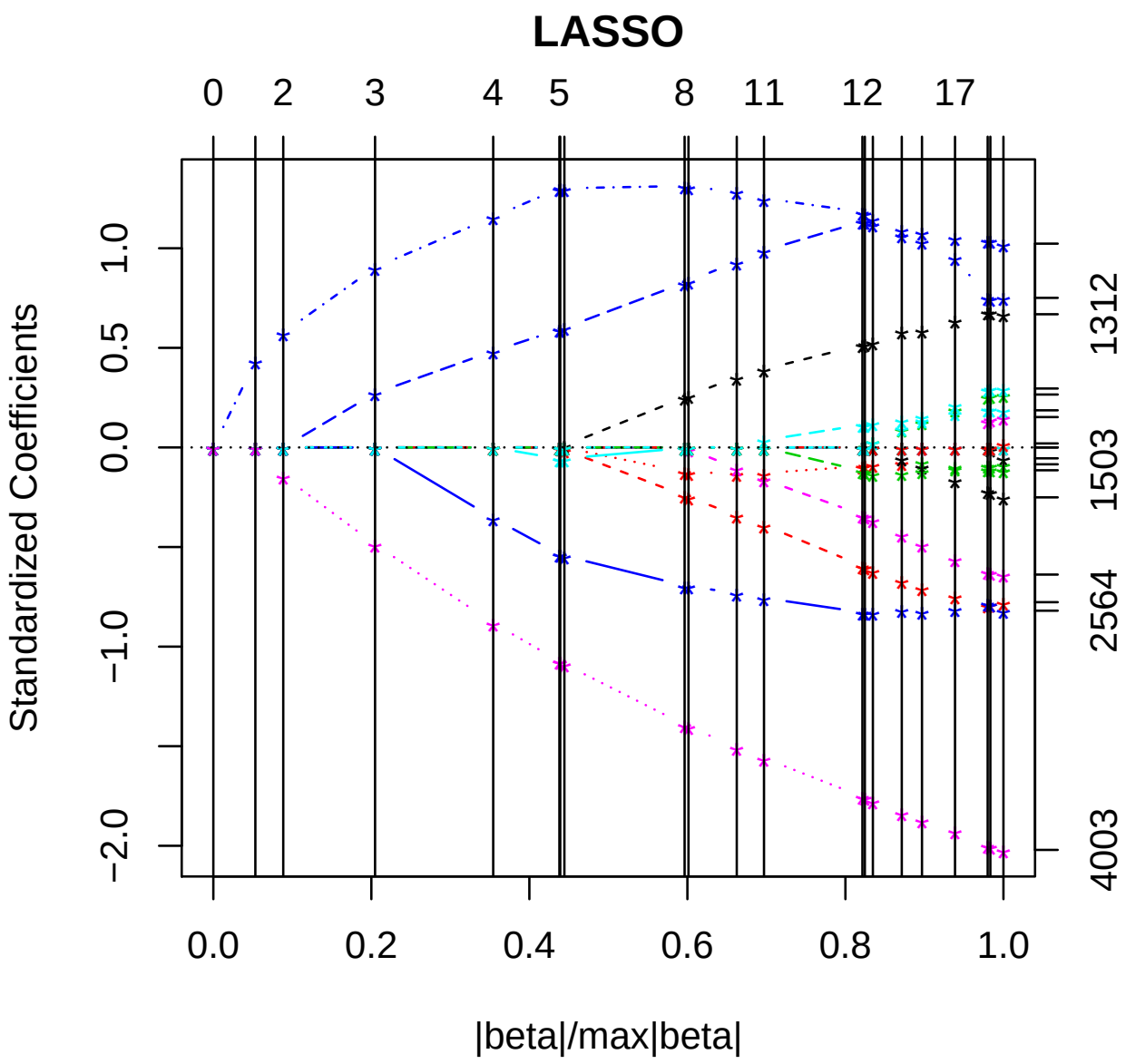
Riboflavin Data

On the other hand, we can use the lasso to select variables and fit the model all at once.

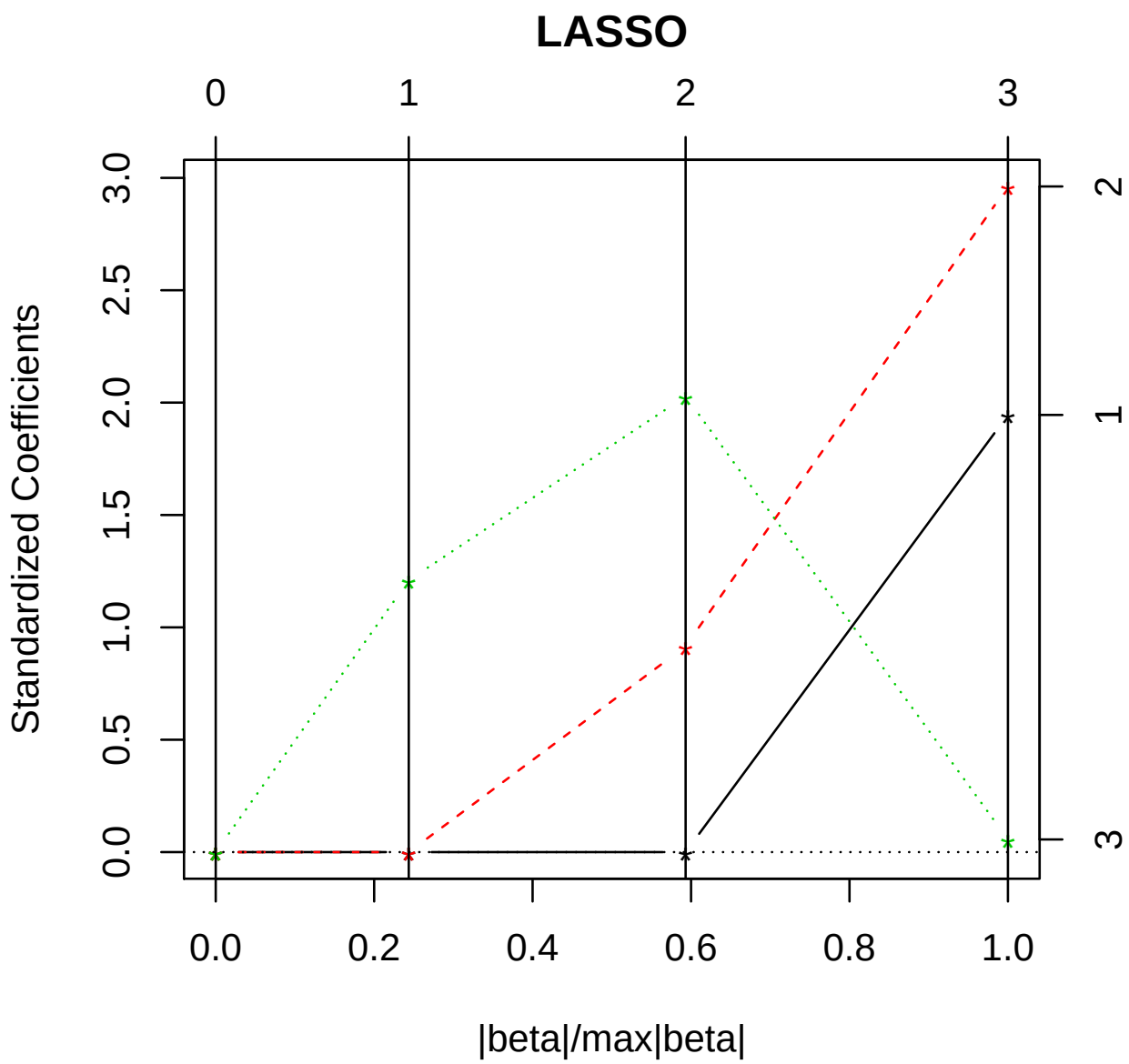
The `lars` package gives an algorithm (called LARS) that can fit the entire lasso solution path (i.e. for all λ).

```
> library(lars)
> out <- lars(x=as.matrix(X), y=Y, max.steps = 20)

There are more than 500 variables and n<m;
You may wish to restart and set use.Gram=FALSE

> ## plot(out)
```

Lasso Solution Path



Irrepresentability



Sachs et al. Data

Sachs et al. measured the quantity of 11 signalling proteins in 7,466 cells.

```
> dat <- read.table("sachs_et_al.txt", header=TRUE)
> head(dat)

  PIP3 Plcg PIP2  PKC PKA Raf  Mek  Erk P38 Jnk Akt
1 58.8  8.8 18.3 17.0 414  26 13.2  6.6  45  40  17
2  8.1 12.3 16.8  3.4 352  36 16.5 18.6  16  62  32
3 13.0 14.6 10.2 11.4 403  59 44.1 14.9  32  20  32
4  1.3 23.1 13.5 13.7 528  73 82.8  5.8  29  23  12
5 24.8  5.2  9.7  4.7 305  34 19.8 21.1  26  81  46
6 10.9 17.6 22.1 13.7 610  19  3.8 11.9  49  58  26

> S <- cov(dat)
```

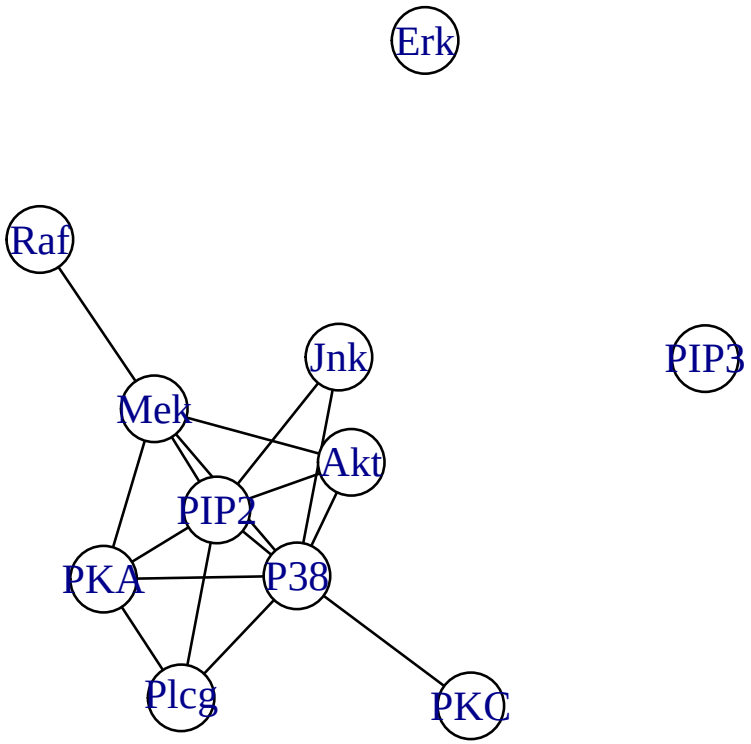
Sachs et al. Data

The `glasso` package runs the coordinate descent algorithm.

```
> library(glasso)
> out <- glassopath(S,
+           rholist = 10^seq(from=3, to=5, length=21),
+           penalize.diagonal = FALSE, trace=0)
```

Sachs et al. Data

Here is the graph for $\lambda = 10^4$.



Directed Graphical Models

Directed Graphs

We have so far used **undirected graphs**.

Directed graphs give each edge an orientation.

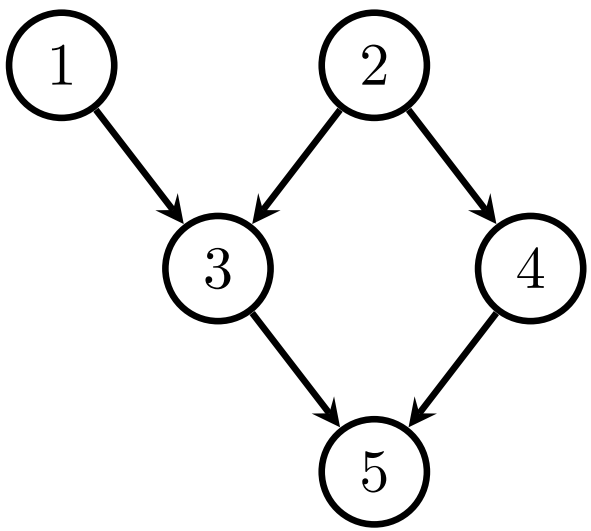
A directed graph $\mathcal{G}$ is a pair (V, D), where

- V is a set of vertices;
- D is a set of ordered pairs of vertices (i, j) such that $i, j \in V$ and $i \neq j$.

If $(i, j) \in D$ we write $i \to j$.

$V = \{1, 2, 3, 4, 5\}$

$D = \{(1, 3), (2, 3), (2, 4), (3, 5), (4, 5)\}$



Acyclicity

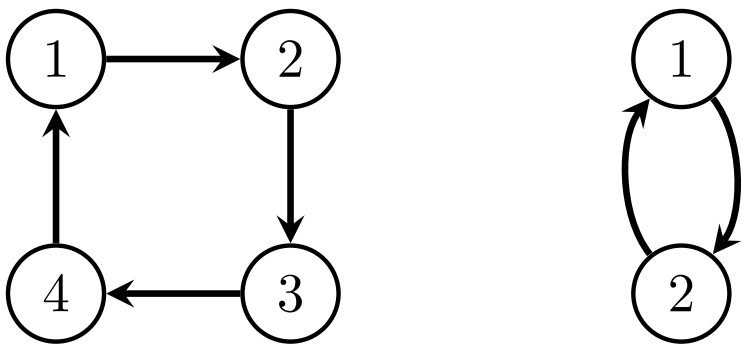
Paths are sequences of adjacent vertices, without repetition:

$$1 \to 3 \leftarrow 2 \to 4 \to 5 \qquad\qquad 1 \to 3 \to 5.$$

The path is **directed** if all the arrows point away from the start.

(A path of length 0 is just a single vertex.)

A **directed cycle** is a directed path from i to $j \neq i$, together with $j \to i$.



Graphs that contain no directed cycles are called **acyclic**. or more specifically, **directed acyclic graphs** (DAGs).

All the directed graphs we consider are acyclic.

Happy Families

$$i \to j \quad \begin{cases} i \in \mathrm{pa}_{\mathcal{G}}(j) & i \text{ is a parent of } j \\ j \in \mathrm{ch}_{\mathcal{G}}(i) & j \text{ is a child of } i \end{cases}$$

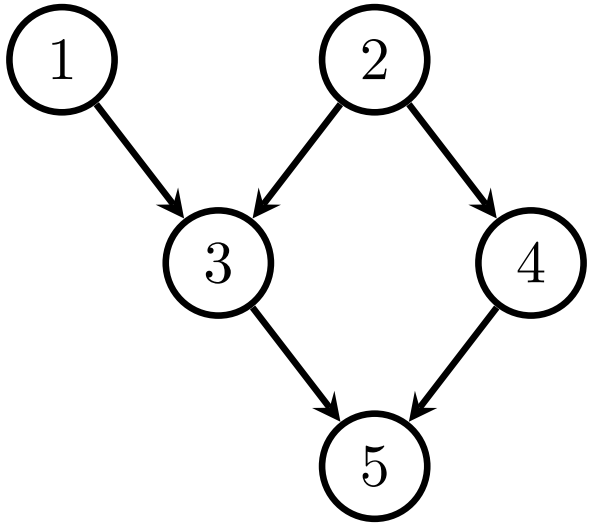
$$\begin{array}{c} a \to \cdots \to b \\ \text{or } a = b \end{array} \quad \begin{cases} a \in \mathrm{an}_{\mathcal{G}}(b) & a \text{ is an ancestor of } b \\ b \in \mathrm{de}_{\mathcal{G}}(a) & b \text{ is a descendant of } a \end{cases}$$

If $w \notin \mathrm{de}_{\mathcal{G}}(v)$ then w is a **non-descendant** of v:

$$\mathrm{nd}_{\mathcal{G}}(v) = V \setminus \mathrm{de}_{\mathcal{G}}(v).$$

(Notice that no v is a non-descendant of itself).

Examples



$$\mathrm{pa}_{\mathcal{G}}(3) = \{1, 2\}$$
$$\mathrm{ch}_{\mathcal{G}}(5) = \emptyset$$

$$\mathrm{an}_{\mathcal{G}}(4) = \{2, 4\}$$
$$\mathrm{de}_{\mathcal{G}}(1) = \{1, 3, 5\}$$
$$\mathrm{nd}_{\mathcal{G}}(1) = \{2, 4\}.$$

Topological Orderings

If the graph is acyclic, we can find a **topological ordering**: i.e. one in which no vertex comes before any of its parents. (Proof: induction)

Topological orderings:

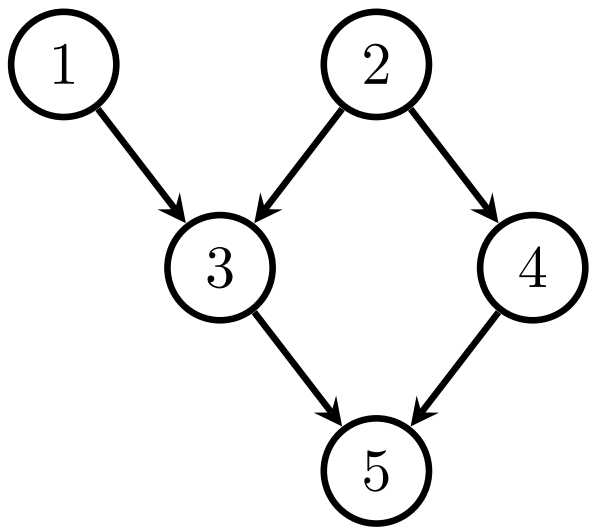
$1, 2, 3, 4, 5$

$1, 2, 4, 3, 5$

$2, 1, 3, 4, 5$

$2, 1, 4, 3, 5$

$2, 4, 1, 3, 5$



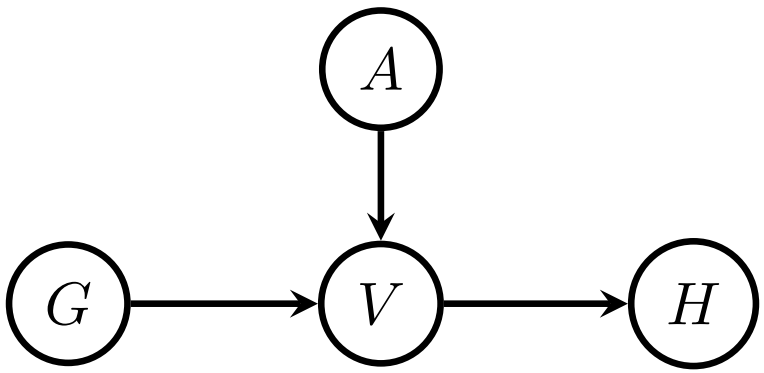
Parameter Estimation

G : group assigned to patient;

A : patient's age in years;

V : whether patient received flu vaccine;

H : patient hospitalized with respiratory problems;

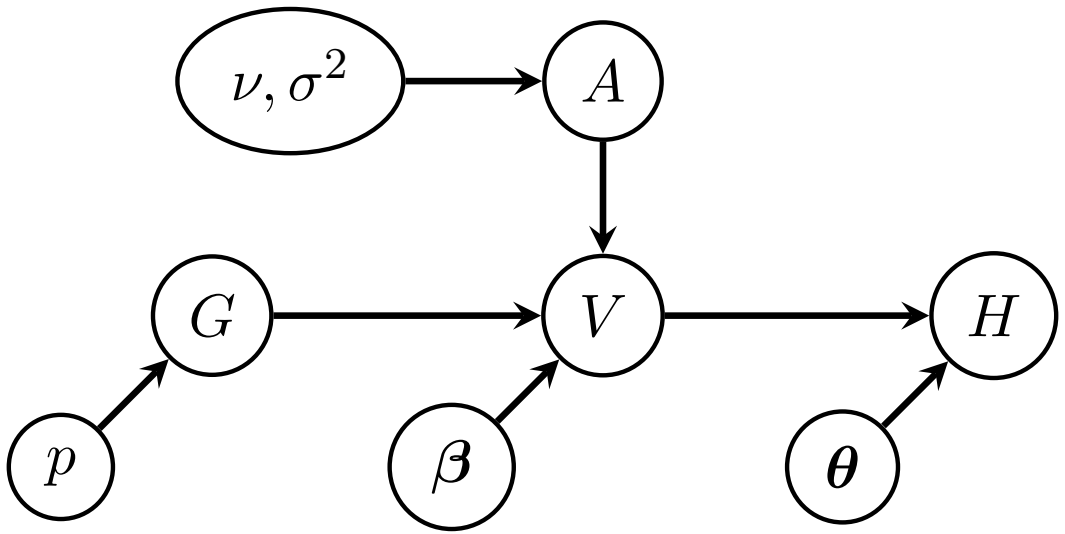


Parameter Estimation

We can model the data (G_i, A_i, V_i, H_i) as

$$\begin{aligned}
\text{group} &: G_i \sim \text{Bernoulli}(p); \\
\text{age} &: A_i \sim N(\nu, \sigma^2); \\
\text{vaccine} &: V_i \mid A_i, G_i \sim \text{Bernoulli}(\mu_i) \text{ where} \\
&\qquad \text{logit}\, \mu_i = \beta_0 + \beta_1 A_i + \beta_2 G_i. \\
\text{hospital} &: H_i \mid V_i \sim \text{Bernoulli}(\text{expit}(\theta_0 + \theta_1 V_i)).
\end{aligned}$$

Assuming independent priors:

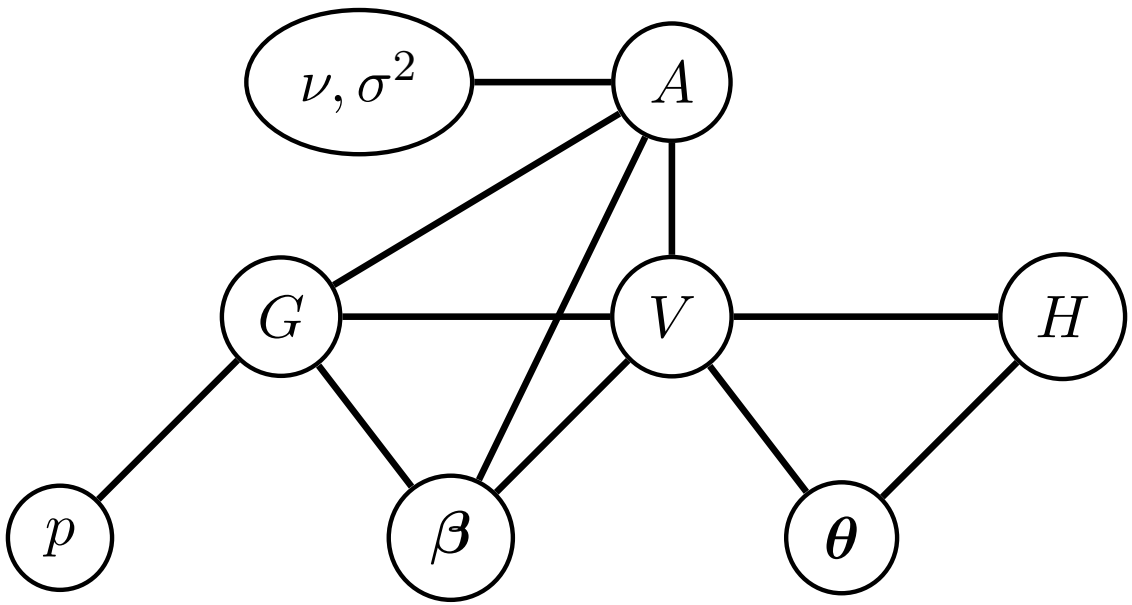


Bayesian Inference

From our argument, we have

$$\begin{aligned}\pi(\boldsymbol{\beta} \mid G, A, V, H) &= \pi(\boldsymbol{\beta} \mid G, A, V) \\ &\propto p(V \mid A, G, \boldsymbol{\beta}) \cdot \pi(\boldsymbol{\beta}).\end{aligned}$$

Looking at the moral graph we see

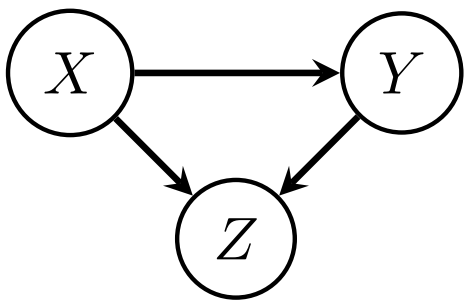


Markov Equivalence

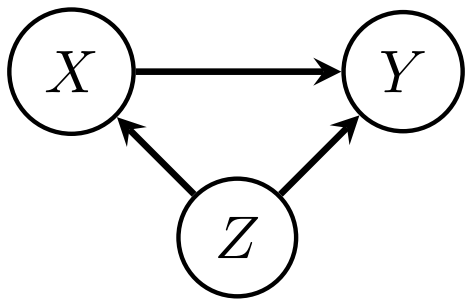
All undirected graphs induce distinct models.

$$v \not\sim w \qquad \iff \qquad X_v \perp\!\!\!\perp X_w \mid X_{V \setminus \{v,w\}} \text{ implied}$$

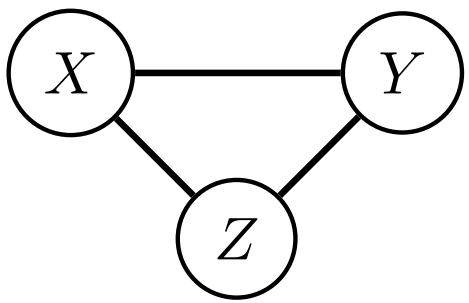
The same is not true for directed graphs:



$$p(x) \cdot p(y \mid x) \cdot p(z \mid x, y)$$

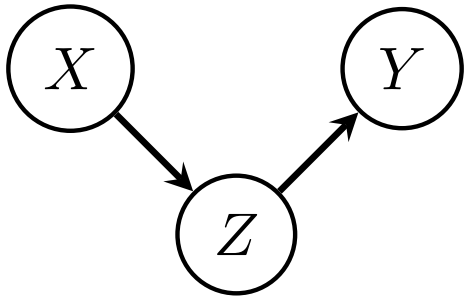


$$p(z) \cdot p(x \mid z) \cdot p(y \mid x, z)$$



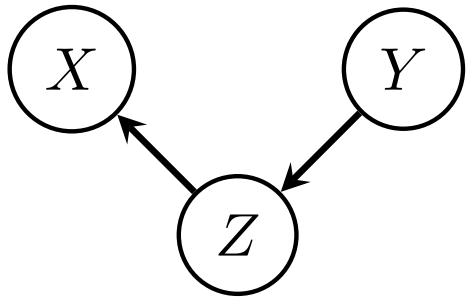
$$\psi_{XYZ}(x, y, z)$$

Markov Equivalence



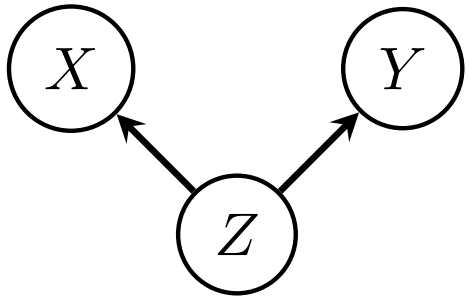
$$p(x) \cdot p(z \mid x) \cdot p(y \mid z)$$

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



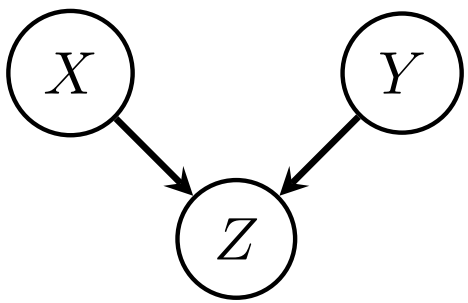
$$p(y) \cdot p(z \mid y) \cdot p(x \mid z)$$

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



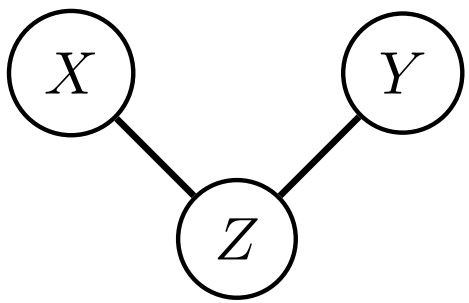
$$p(z) \cdot p(x \mid z) \cdot p(y \mid z)$$

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



$$p(x) \cdot p(y) \cdot p(z \mid x, y)$$

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

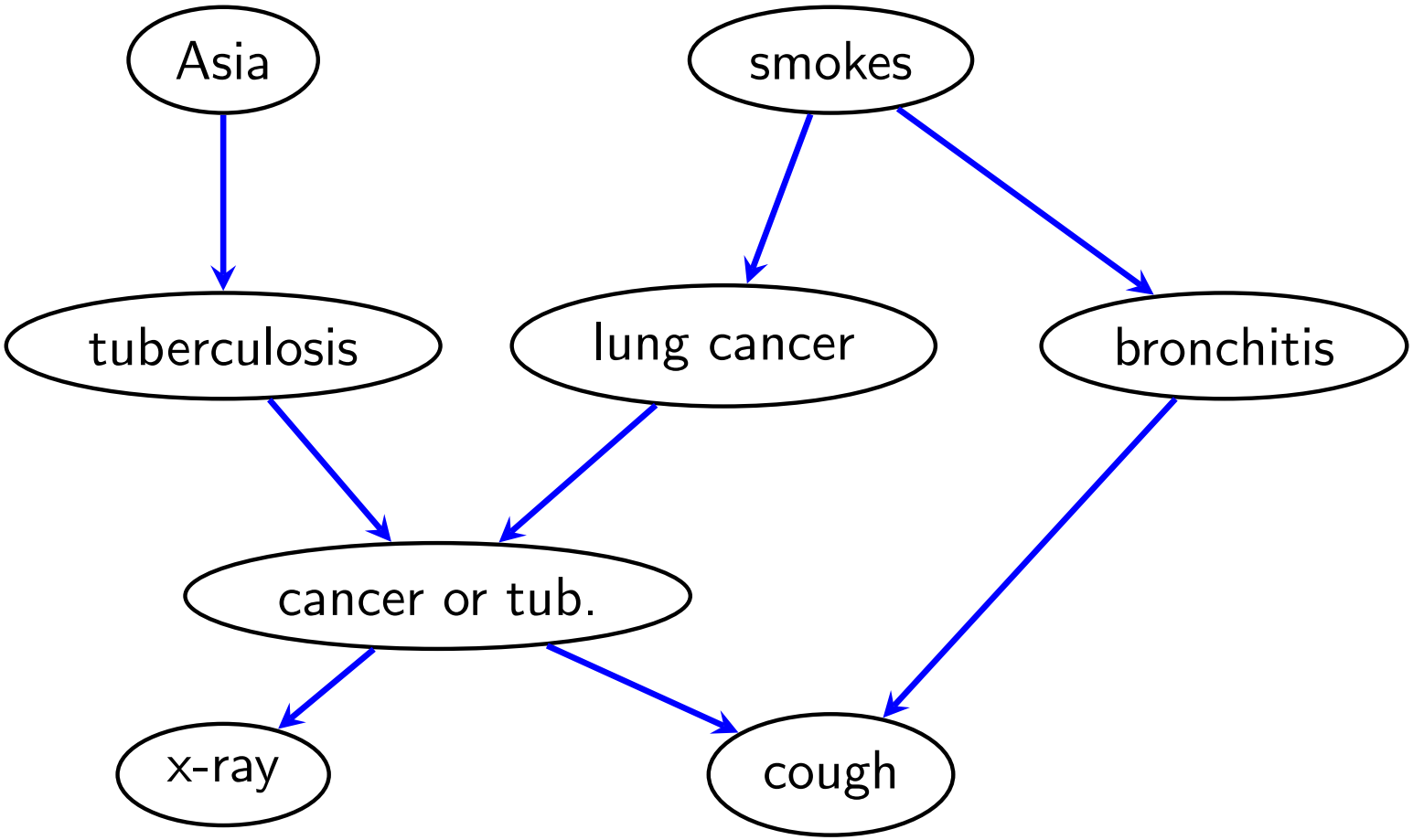


$$\psi_{XZ}(x, z) \cdot \psi_{YZ}(y, z)$$

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

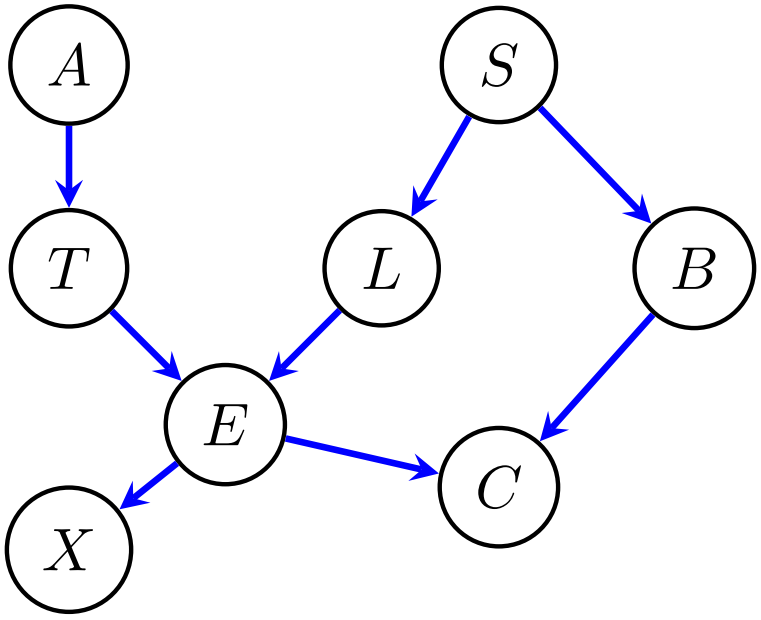
Expert Systems

Expert Systems



The 'Chest Clinic' network, a fictitious diagnostic model.

Variables



A has the patient recently visited southern Asia?

S does the patient smoke?

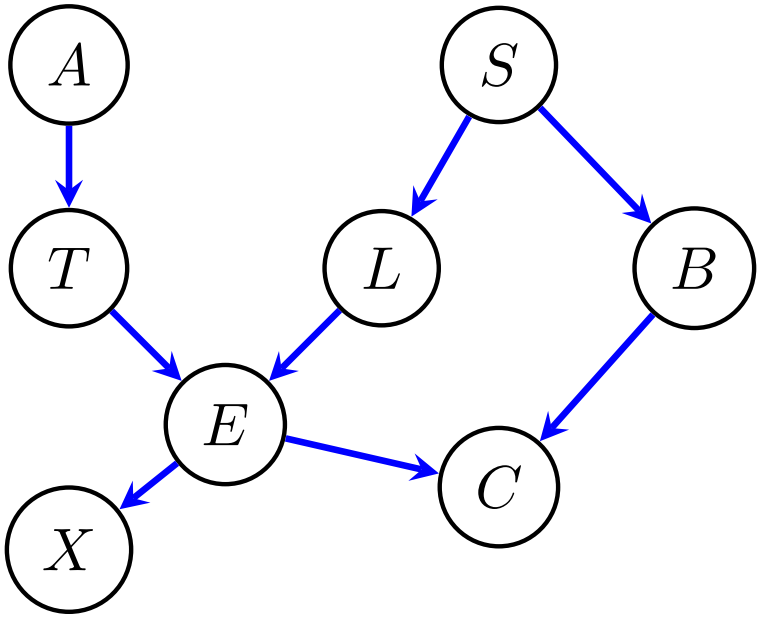
T,C,B Tuberculosis, lung cancer, bronchitis.

E logical: Tuberculosis OR lung cancer.

X shadow on chest X-ray?

C does the patient have a persistent cough?

Conditional Probability Tables



We have our factorization:

$$p(a, s, t, l, b, e, x, c) = p(a) \cdot p(s) \cdot p(t \mid a) \cdot p(l \mid s) \cdot p(b \mid s) \cdot \\ \cdot p(e \mid t, l) \cdot p(x \mid e) \cdot p(c \mid e, b).$$

Assume that we are given each of these factors. How could we calculate $p(l \mid x, c, a, s)$?

Probabilities

$p(a) =$

yes	no
0.01	0.99

$p(s) =$

yes	no
0.5	0.5

$p(t \mid a) =$

A	yes	no
yes	0.05	0.95
no	0.01	0.99

$p(l \mid s) =$

S	yes	no
yes	0.1	0.9
no	0.01	0.99

$p(b \mid s) =$

S	yes	no
yes	0.6	0.4
no	0.3	0.7

$p(x \mid e) =$

E	yes	no
yes	0.98	0.02
no	0.05	0.95

$p(c \mid b, e) =$

B	E	yes	no
yes	yes	0.9	0.1
	no	0.8	0.2
no	yes	0.7	0.3
	no	0.1	0.9

Factorizations

$$p(l \mid x, c, a, s) = \frac{p(l, x, c \mid a, s)}{\sum_l p(l, x, c \mid a, s)}$$

From the graph $p(l, x, c \mid a, s)$ is

$$\sum_{t,e,b} p(t \mid a) \cdot p(l \mid s) \cdot p(b \mid s) \cdot p(e \mid t, l) \cdot p(x \mid e) \cdot p(c \mid e, b).$$

But this is:

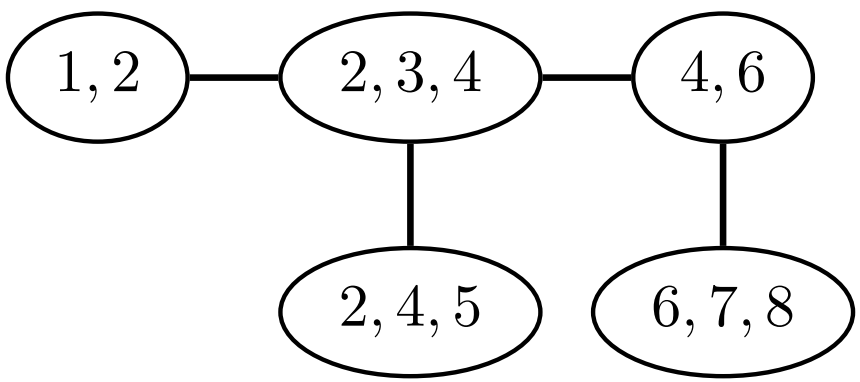
$$p(l \mid s) \sum_e p(x \mid e) \left(\sum_b p(b \mid s) \cdot p(c \mid e, b) \right) \left(\sum_t p(t \mid a) \cdot p(e \mid t, l) \right).$$

Junction Trees

A **junction tree**:

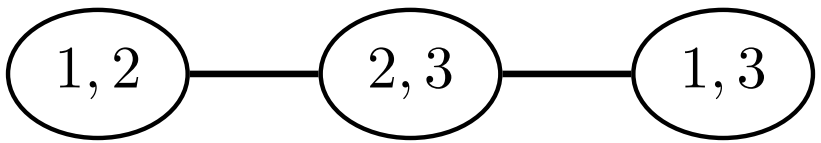
- is a connected undirected graph without cycles (a tree);
- has vertices C_i that consist of **subsets** of a set V;
- satsifies the property that if $C_i \cap C_j = S$ then every vertex on the (unique) path from C_i to C_j contains S.

Example.



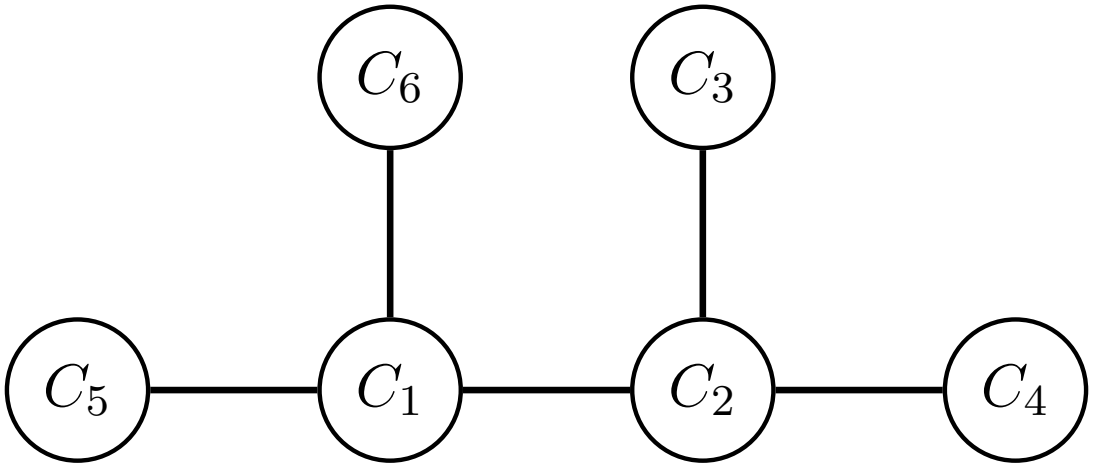
Junction Trees

The following graph is **not** a junction tree:



Junction Trees

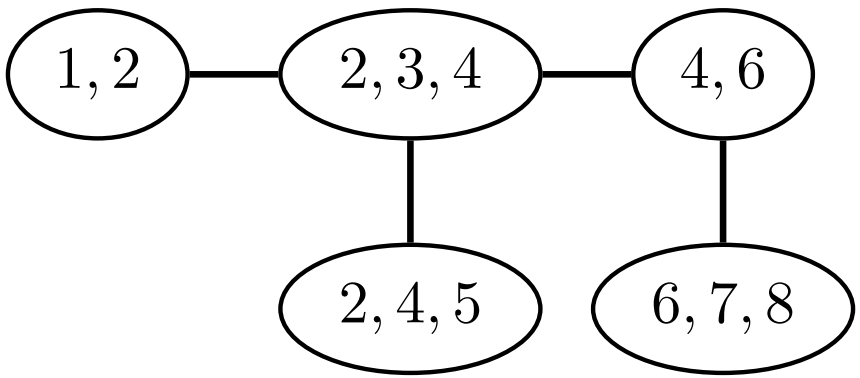
Junction trees can be constructed directly from sets of cliques satisfying running intersection.



$$C_i \cap \bigcup_{j<i} C_j = C_i \cap C_{\sigma(i)}.$$

Example: Junction Trees and RIP

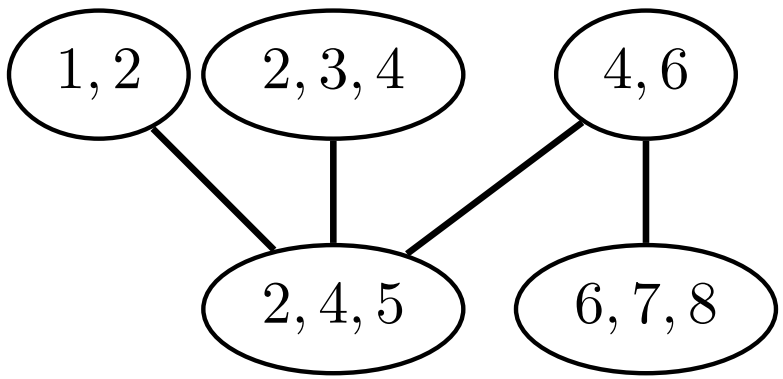
Given sets $\{1, 2\}$, $\{2, 3, 4\}$, $\{2, 4, 5\}$, $\{4, 6\}$, $\{6, 7, 8\}$, we can build this tree:



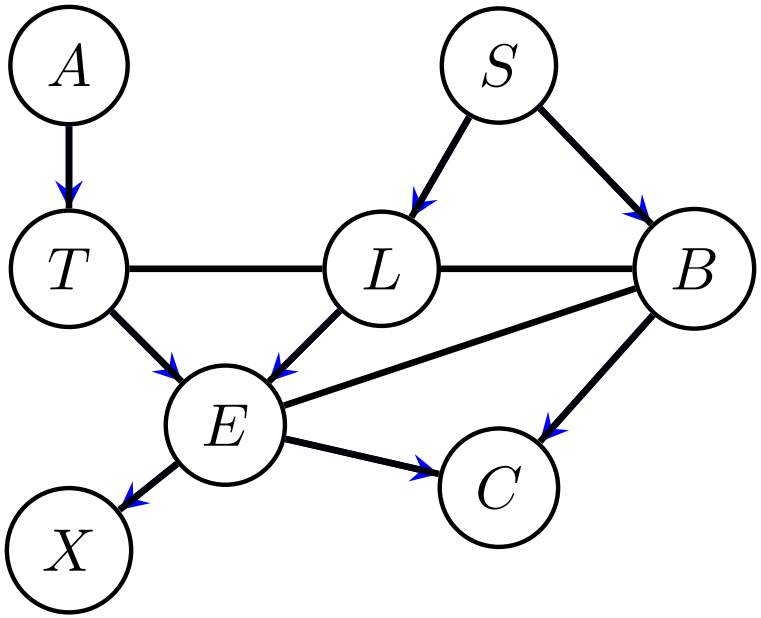
Example: Junction Trees and RIP

Equally, we could use a different ordering:

$$\{6,7,8\},\{4,6\},\{2,4,5\},\{1,2\},\{2,3,4\}.$$



Forming A Junction Tree



Steps to Forming a Junction Tree:

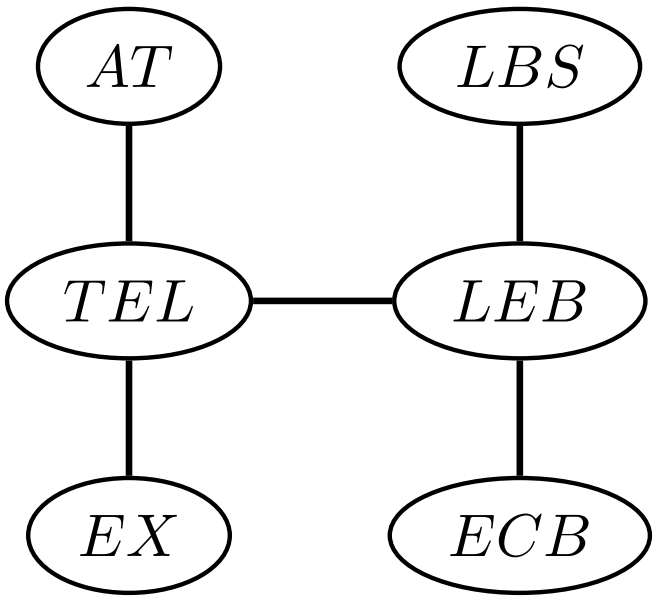
Moralize

Drop directions

Triangulate (add edges to get a decomposable graph)

Forming A Junction Tree

Finally, form the tree of cliques.



Initialization

$p(a) =$

yes	no
0.01	0.99

$p(s) =$

yes	no
0.5	0.5

$p(t \mid a) =$

A	yes	no
yes	0.05	0.95
no	0.01	0.99

$p(l \mid s) =$

S	yes	no
yes	0.1	0.9
no	0.01	0.99

$p(b \mid s) =$

S	yes	no
yes	0.6	0.4
no	0.3	0.7

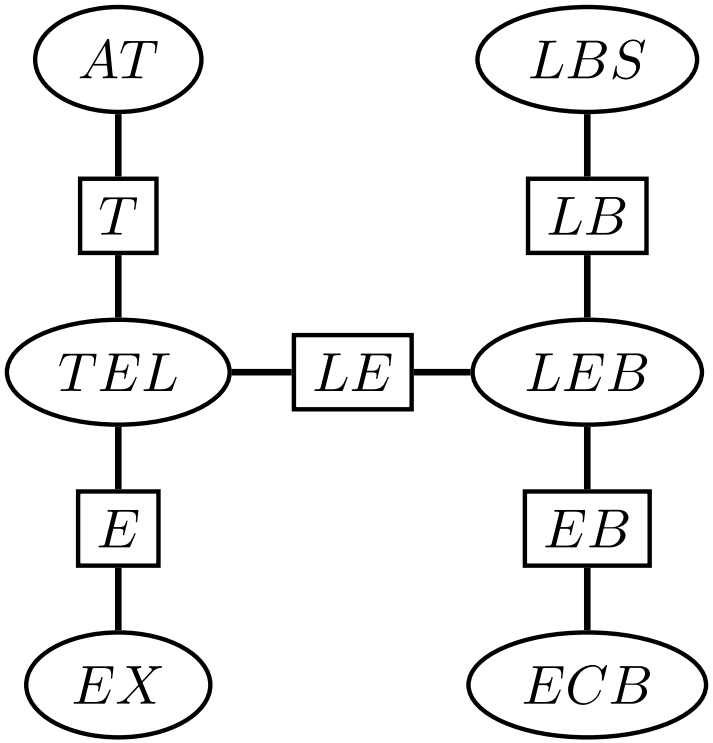
$p(x \mid e) =$

E	yes	no
yes	0.98	0.02
no	0.05	0.95

$p(c \mid b, e) =$

B	E	yes	no
yes	yes	0.9	0.1
	no	0.8	0.2
no	yes	0.7	0.3
	no	0.1	0.9

Initialization

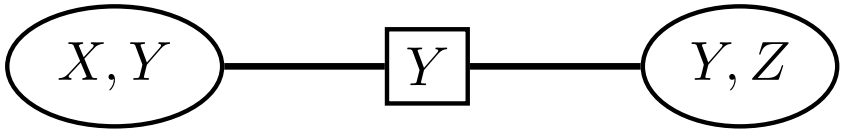


Can set, for example:

$$\psi_{AT}(a,t) = p(a) \cdot p(t \mid a) \qquad \psi_{LBS}(l,b,s) = p(s) \cdot p(l \mid s) \cdot p(b \mid s)$$
$$\psi_{TEL}(t,e,l) = p(e \mid t,l) \qquad \psi_{ELB}(e,l,b) = 1$$
$$\psi_{EX}(e,x) = p(x \mid e) \qquad \psi_{ECB}(e,c,b) = p(c \mid e,b).$$

Updating / Message Passing

Suppose we have two vertices and one separator set.



$\psi_{XY}(x, y)$

		$y = 0$	1
x	0	0.3	0.9
	1	0.7	0.1

$\psi_Y(y)$

$y = 0$	1
1	1

$\psi_{YZ}(y, z)$

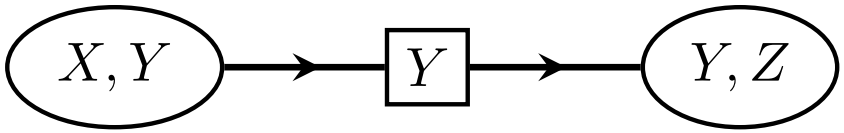
		$z = 0$	1
y	0	0.3	0.1
	1	0.2	0.4

Initialize with

$$\psi_{XY}(x, y) = p(x \mid y) \qquad \psi_{YZ}(y, z) = p(z \mid y) \cdot p(y) \qquad \psi_Y(y) = 1.$$

Updating / Message Passing

Suppose we have two vertices and one separator set.



$\psi_{XY}(x, y)$

		$y = 0$	1
x	0	0.3	0.9
	1	0.7	0.1

$\psi_Y(y)$

$y = 0$	1
1	1

$\psi_{YZ}(y, z)$

		$z = 0$	1
y	0	0.3	0.1
	1	0.2	0.4

Pass message from X, Y to Y, Z. We set

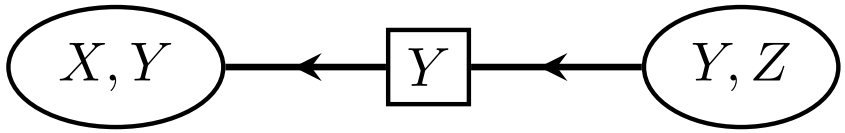
$$\psi'_Y(y) = \sum_x \psi_{XY}(x, y) = (1, 1);$$

$$\psi'_{YZ}(y, z) = \frac{\psi'_Y(y)}{\psi_Y(y)} \psi_{YZ}(y, z) = \psi_{YZ}(y, z).$$

So in this case nothing changes.

Updating / Message Passing

Suppose we have two vertices and one separator set.



$\psi_{XY}(x, y)$

x \ y	$y = 0$	1
0	0.3	0.9
1	0.7	0.1

$\psi'_Y(y)$

$y = 0$	1
1	1

$\psi'_{YZ}(y, z)$

y \ $z = 0$	1
0	0.3	0.1
1	0.2	0.4

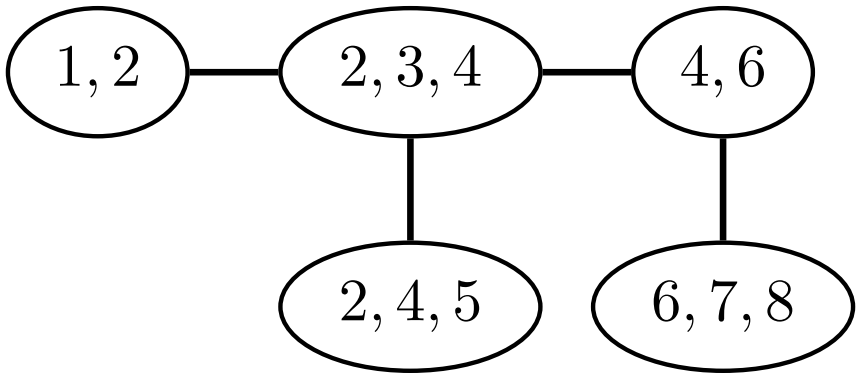
Pass message from Y, Z to X, Y. We set

$$\psi''_Y(y) = \sum_x \psi_{YZ}(y, z) = (0.4, 0.6);$$

$$\psi'_{XY}(x, y) = \frac{\psi''_Y(y)}{\psi'_Y(y)} \psi_{XY}(x, y) = \begin{matrix} 0.12 & 0.54 \\ 0.28 & 0.06 \end{matrix}.$$

And now we note that $\psi'_{XY}(x, y) = p(x, y)$ as intended.

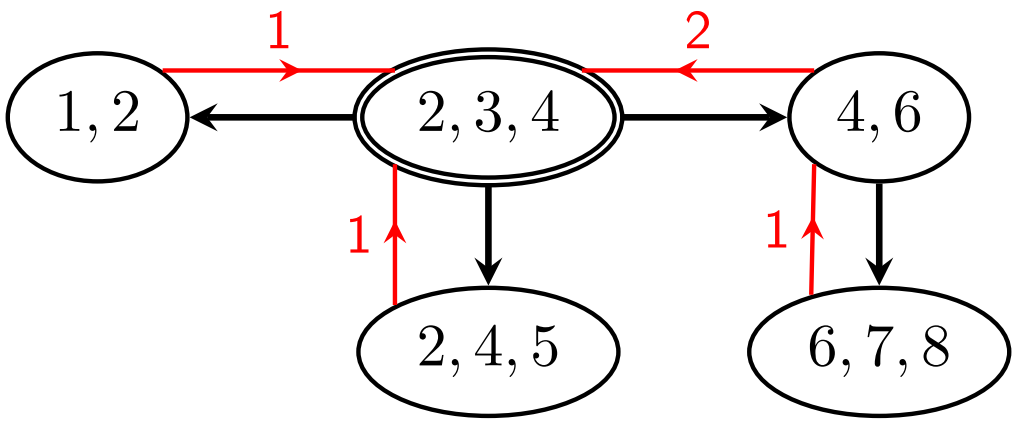
Rooting



Given a tree, we can pick any vertex as a ‘root’, and direct all edges away from it.

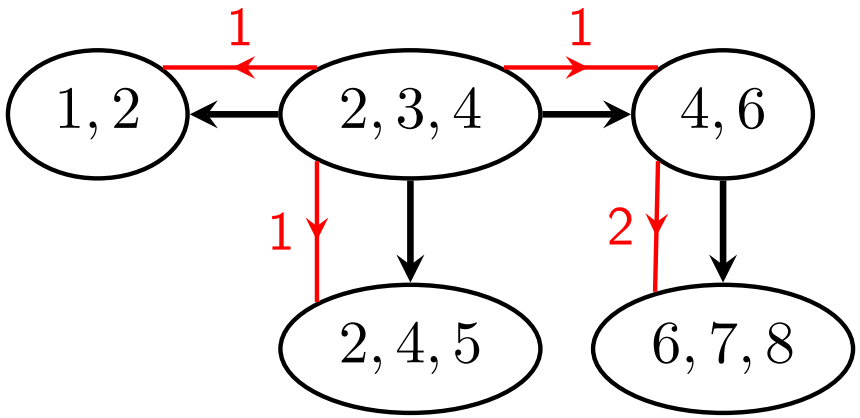
Collection and Distribution

function COLLECT(rooted tree $\mathcal{T}$, potentials ψ_t)
    let $1 < \ldots < k$ be a topological ordering of $\mathcal{T}$
    for t in $k, \ldots, 2$ **do**
        send message from ψ_t to $\psi_{\sigma(t)}$;
    end for
    return updated potentials ψ_t
end function



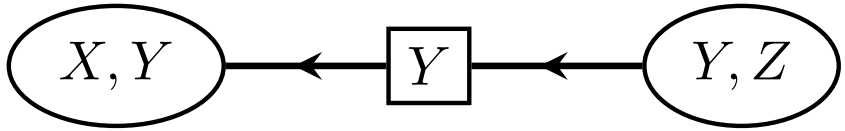
Collection and Distribution

function DISTRIBUTE(rooted tree $\mathcal{T}$, potentials ψ_t)
    let $1 < \ldots < k$ be a topological ordering of $\mathcal{T}$
    for t in $2, \ldots, k$ **do**
        send message from $\psi_{\sigma(t)}$ to ψ_t;
    end for
    return updated potentials ψ_t
end function



Evidence

Now, suppose we want to calculate $p(x \mid z = 0)$.



$\psi_{XY}(x, y)$

		$y = 0$	1
x	0	0.12	0.54
	1	0.28	0.06

$\psi_Y(y)$

$y = 0$	1
0.4	0.6

$\psi_{YZ}(y, z)$

		$z = 0$	1
y	0	0.6	0
	1	0.4	0

Replace $\psi_{YZ}(y, z)$ with $p(y \mid z = 0)$.

Pass message from Y, Z to X, Y. We set

$$\psi_Y(y) = \sum_x \psi_{YZ}(y, z) = (0.60.4);$$

$$\psi'_{XY}(x, y) = \frac{\psi''_Y(y)}{\psi'_Y(y)} \psi_{XY}(x, y) = \begin{matrix} 0.18 & 0.36 \\ 0.42 & 0.04 \end{matrix}.$$

And now calculate $\sum_y \psi_{XY}(x, y) = (0.54, 0.46)$.

From the Chest Clinic Network

Marginal Probability Tables:

ψ_{EX} :

E	yes	no
yes	0.06	0
no	0.05	0.89

ψ_{AT} :

A	yes	no
yes	5×10^{-4}	0.01
no	0.01	0.98

ψ_{LBS} :

L	B	yes	no
yes	yes	0.03	0
	no	0.02	0
no	yes	0.27	0.15
	no	0.18	0.35

ψ_{LEB} :

L	E	yes	no
yes	yes	0.03	0.02
	no	0	0
no	yes	0	0.01
	no	0.41	0.52

ψ_{TEL} :

T	E	yes	no
yes	yes	5.72×10^{-4}	0
	no	0.01	0
no	yes	0.05	0
	no	0	0.94

ψ_{ECB} :

B	E	yes	no
yes	yes	0.03	0
	no	0.02	0.01
no	yes	0.33	0.08
	no	0.05	0.47

From the Chest Clinic Network

Suppose now that we have a shadow on the chest X-ray:

ψ_{EX} :

E	yes	no
yes	0.58	-
no	0.42	-

ψ_{AT} :

A	yes	no
yes	0	0.01
no	0.09	0.9

ψ_{LBS} :

L	B	yes	no
yes	yes	0.27	0.01
yes	no	0.18	0.03
no	yes	0.15	0.08
no	no	0.1	0.19

ψ_{LEB} :

L	E	yes	no
yes	yes	0.28	0.21
yes	no	0	0
no	yes	0.04	0.05
no	no	0.19	0.24

ψ_{TEL} :

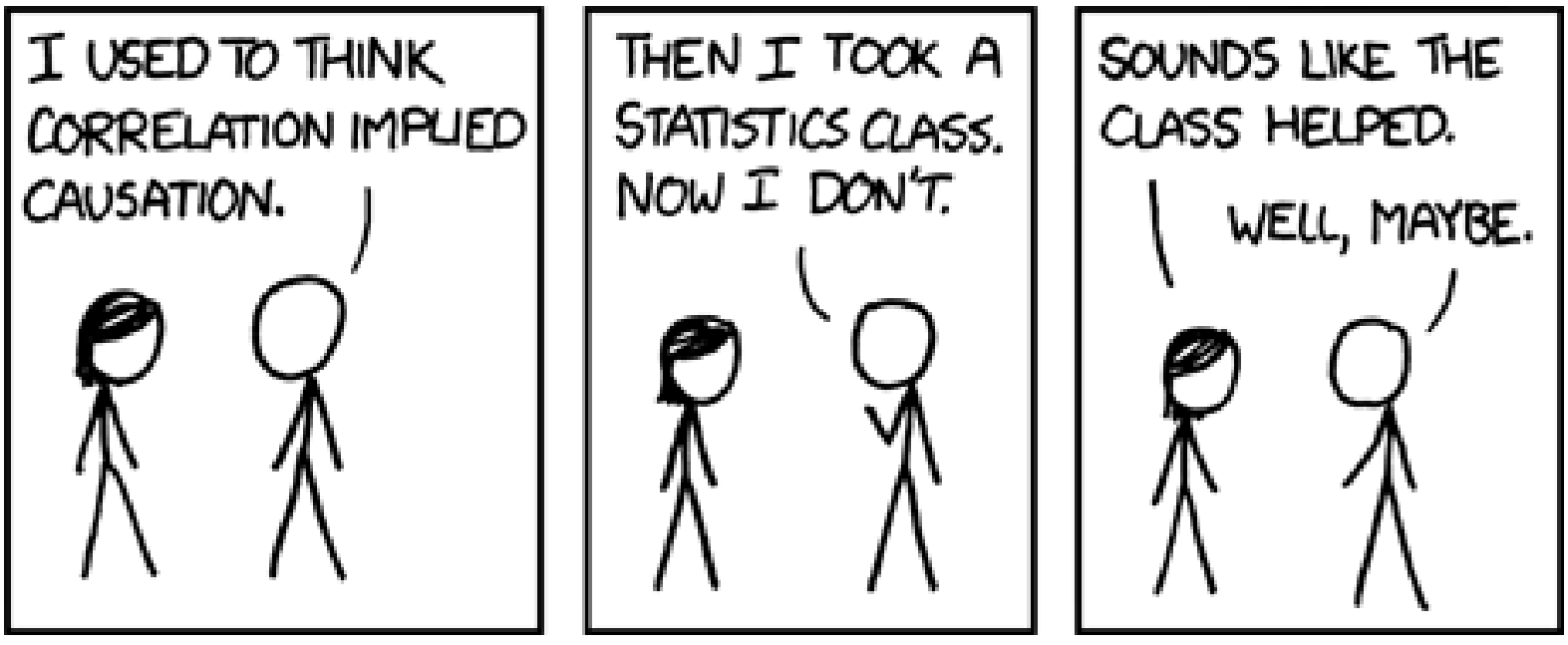
T	E	yes	no
yes	yes	0.01	0
yes	no	0.09	0
no	yes	0.48	0
no	no	0	0.42

ψ_{ECB} :

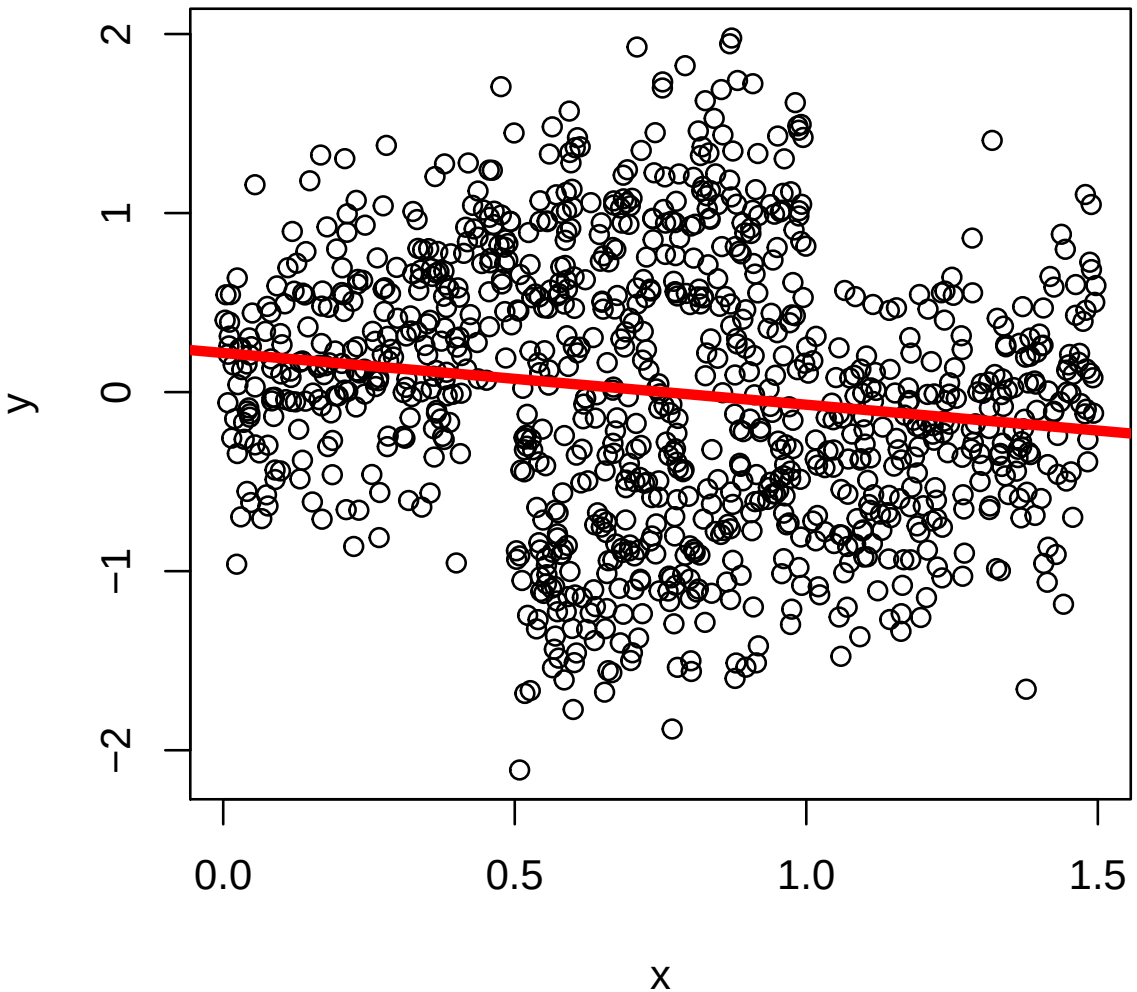
B	E	yes	no
yes	yes	0.29	0.03
yes	no	0.18	0.08
no	yes	0.15	0.04
no	no	0.02	0.21

Causal Inference

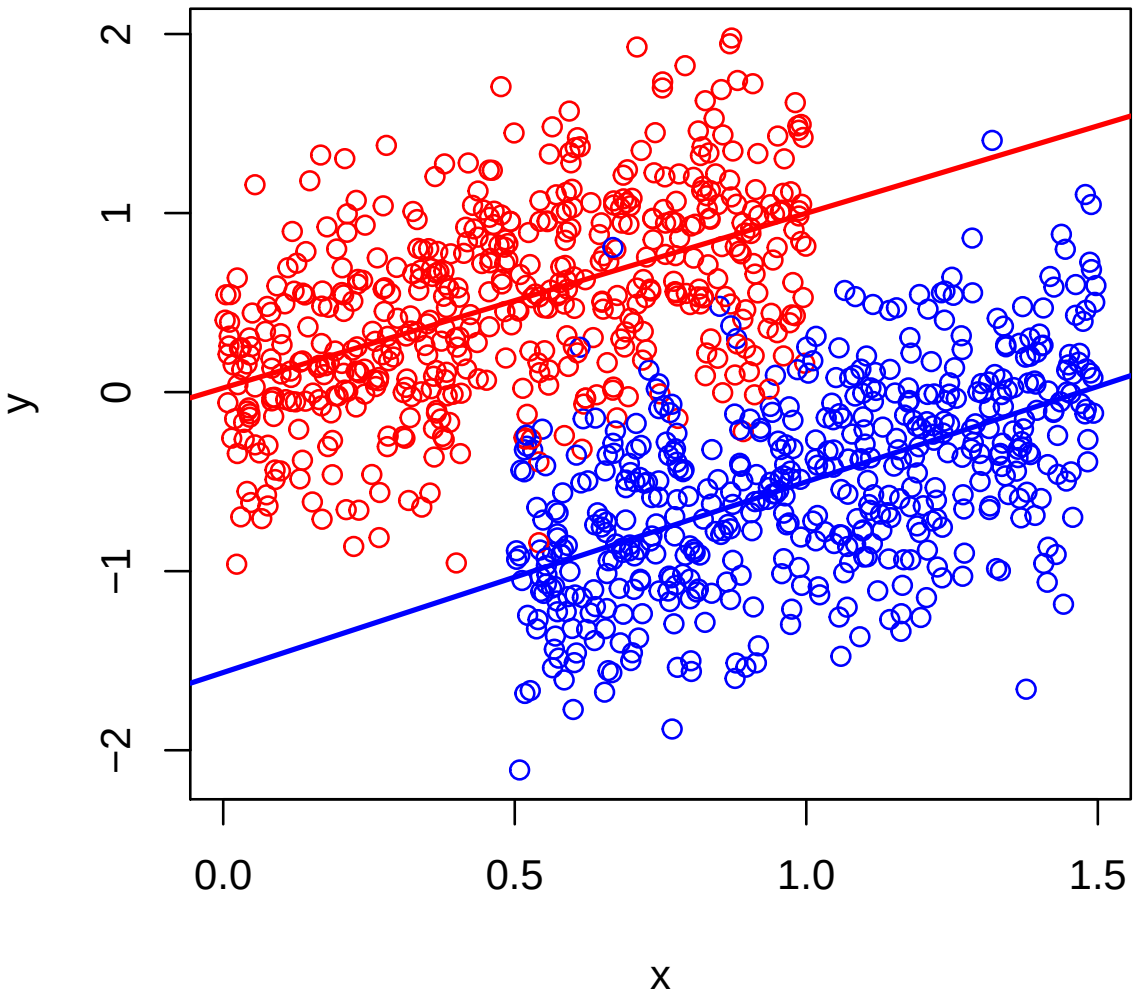
Correlation



Controlling for Covariates

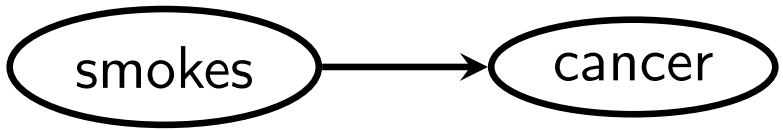


Controlling for Covariates



Causation

Example. Smoking is strongly predictive of lung cancer. So maybe smoking causes lung cancer to develop.

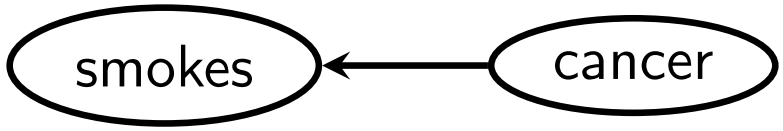


BUT: how do we know that this is a causal relationship? And what do we mean by that?

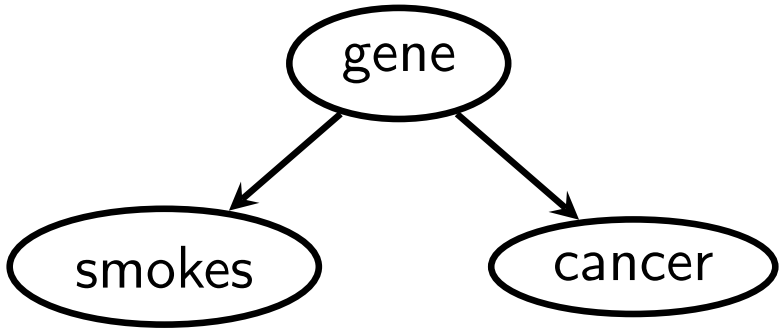
The central question is: "if we stop people from smoking, will they be less likely to get lung cancer?"

That is: does this 'intervention' on one variable change the distribution of another variable?

Alternative Explanations



Reverse Causation. Lung cancer causes smoking: people with (undiagnosed) lung cancer smoke to soothe irritation in the lungs.



Confounding / Common Cause. There is a gene that makes people likely to smoke, and also more likely to get lung cancer.

Example

Suppose we take 32 men and 32 women, ask them whether they smoke and check for lung damage.

	women			men	
	not smoke	smoke		not smoke	smoke
no damage	21	6		6	6
damage	3	2		2	18

Marginally, there is clearly a strong relationship between smoking and damage

	not smoke	smoke
no damage	27	12
damage	5	20

$$P(D = 1 \mid S = 1) = \frac{5}{8} \qquad P(D = 1 \mid S = 0) = \frac{5}{32}.$$

Example

This might suggest that if we had prevented them all from smoking, only $\frac{5}{32} \times 64 = 10$ would have had damage, whereas if we had made them all smoke, $\frac{5}{8} \times 64 = 40$ would have damage.

But: both smoking and damage are also correlated with gender, so this effect may be inaccurate. If we repeat this separately for men and women:

no-one smoking:

$$\frac{3}{21+3} \times 32 + \frac{2}{6+2} \times 32 = 12$$

everyone smoking

$$\frac{2}{6+2} \times 32 + \frac{18}{18+6} \times 32 = 32.$$

Compare these to 10 and 40.

‘do’ notation

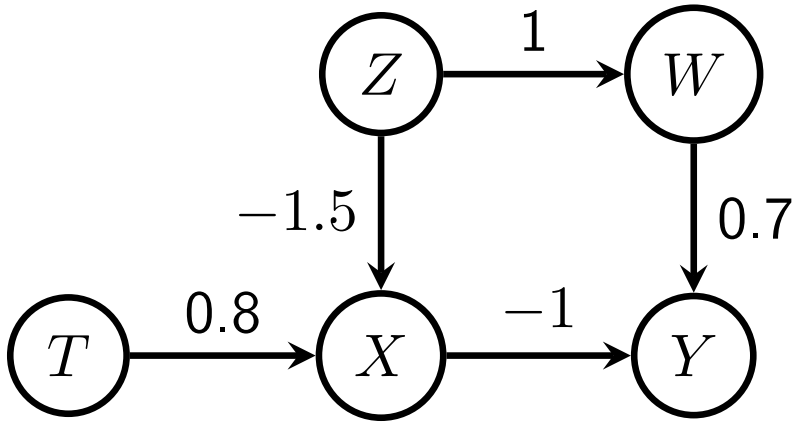
In this example there is a difference between predicting damage when we ‘observe’ that someone smokes . . .

$$P(D = 1 \mid S = 1) = \frac{5}{8},$$

. . . and prediciting damage when we intervene to make someone smoke:

$$P(D = 1 \mid do(S = 1)) = \frac{32}{64} = \frac{1}{2}.$$

Gaussian




```
> set.seed(513)
> n <- 1e3
> Z <- rnorm(n)
> T <- rnorm(n)
> W <- Z + rnorm(n)
> X <- 0.8*T - 1.5*Z + rnorm(n)
> Y <- 0.7*W     - X + rnorm(n)
```

Back-Door Paths

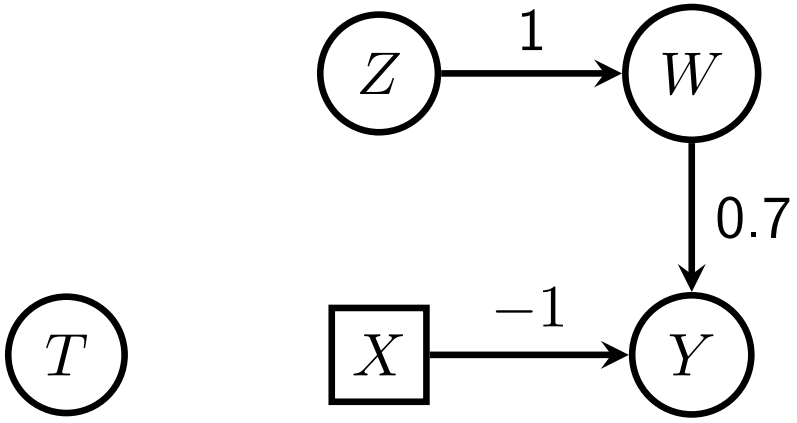
```
> summary(lm(Y ~ X))$coefficients[,1:2]

            Estimate Std. Error
(Intercept)    0.035       0.04
X             -1.285       0.02

> summary(lm(Y ~ X + Z))$coefficients[,1:2]

            Estimate Std. Error
(Intercept)    0.043      0.038
X             -1.024      0.032
Z              0.645      0.062

> summary(lm(Y ~ X + W))$coefficients[,1:2]

            Estimate Std. Error
(Intercept)    0.029      0.031
X             -1.011      0.019
W              0.668      0.027
```

Instruments

Adding in unnecessary variables to the regression generally increases the variance.

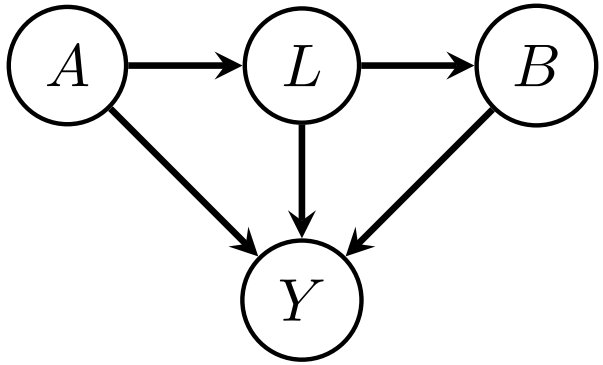
```
> summary(lm(Y ~ X + W + T))$coefficients[,1:2]

            Estimate Std. Error
(Intercept)    0.029      0.031
X             -1.006      0.022
W              0.671      0.027
T             -0.018      0.036

> summary(lm(Y ~ X + W + Z))$coefficients[,1:2]

            Estimate Std. Error
(Intercept)    0.028      0.031
X             -1.026      0.026
W              0.682      0.031
Z             -0.053      0.061
```

Simulating Intervention




```
> Z <- rnorm(n)
> T <- rnorm(n)
> W <- Z + rnorm(n)
> X <- rnorm(n)   # set X independently
> Y <- 0.7*W - X + rnorm(n)
> summary(lm(Y ~ X))$coefficients[,1:2]

             Estimate Std. Error
(Intercept)    -0.04      0.045
X              -1.05      0.044
```

Example: HIV Treatment



A treatment with AZT (an HIV drug);
L opportunisitic infection;
B treatment with antibiotics;
Y survival at 5 years.

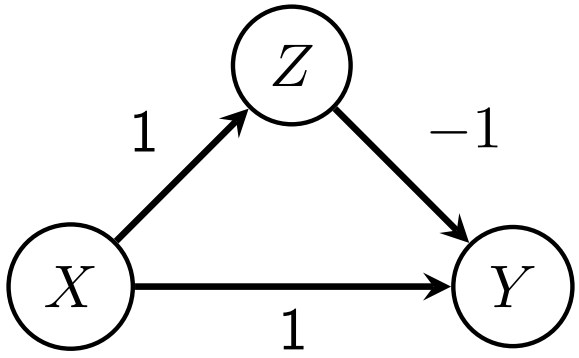
$$p(a, l, b, y) = p(a) \cdot p(l \mid a) \cdot p(b \mid l) \cdot p(y \mid a, l, b)$$
$$p(l, y \mid do(a, b)) = p(l \mid a) \cdot p(y \mid a, l, b)$$
$$p(y \mid do(a, b)) = \sum_l p(l \mid a) \cdot p(y \mid a, l, b).$$

Model Selection and Causal Discovery

Finding Graphs

```
> head(dat)

      X     Y     Z
1  1.15  0.20  0.38
2  0.90 -1.57  1.26
3  0.79  1.52 -0.03
4  1.15 -0.74  2.47
5  0.74  0.78  0.40
6 -0.15  1.14 -1.04

> round(cov(dat),2)

     X     Y     Z
X 0.99  0.01  1.02
Y 0.01  1.98 -0.98
Z 1.02 -0.98  2.06
```

Extra Independences




```
> n <- 1000
> X <- rnorm(n)
> Z <- X + rnorm(n)
> Y <- X - Z + rnorm(n)
> summary(lm(Y ~ X))$coefficients  # no significant effect of X on

             Estimate Std. Error t value Pr(>|t|)
(Intercept)     0.036      0.046    0.78     0.43
X              -0.086      0.045   -1.88     0.06
```

The PC Algorithm

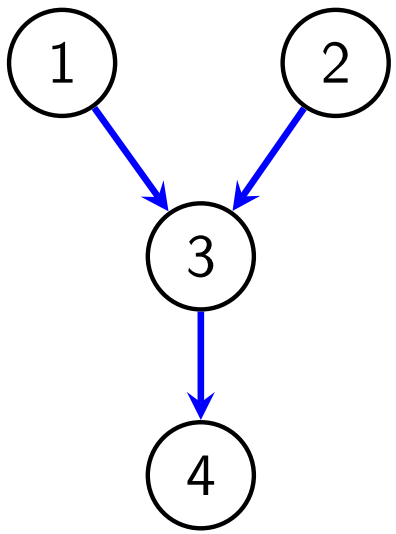
Start with a complete undirected graph, $\mathcal{H}$.

- For every pair of vertices i, j, test the marginal independence $X_i \perp\!\!\!\perp X_j$.
  If it holds, remove $i - j$ from $\mathcal{H}$.
- For every remaining edge i, j and $k \in V \setminus \{i, j\}$, test $X_i \perp\!\!\!\perp X_j \mid X_k$.
  If it holds, remove $i - j$ from $\mathcal{H}$.
- For every remaining edge i, j and $\{k, l\} \subseteq V \setminus \{i, j\}$, test $X_i \perp\!\!\!\perp X_j \mid X_k, X_l$.
  If it holds, remove $i - j$ from $\mathcal{H}$.
- ...

In fact, if suffices to consider subsets of the neighbours of i, or the neighbours of j.

Example

Consider the following true graph and its implied pairwise independences.



$$X_1 \perp\!\!\!\perp X_2$$

$$X_1 \perp\!\!\!\perp X_4 \mid X_3$$

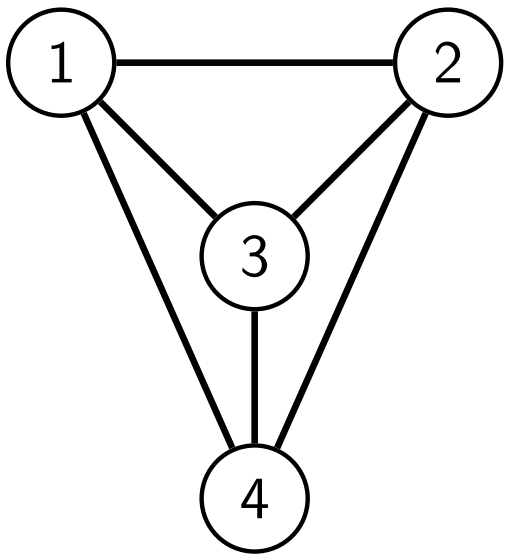
$$X_1 \perp\!\!\!\perp X_4 \mid X_2, X_3$$

$$X_2 \perp\!\!\!\perp X_4 \mid X_3$$

$$X_2 \perp\!\!\!\perp X_4 \mid X_1, X_3$$

Example

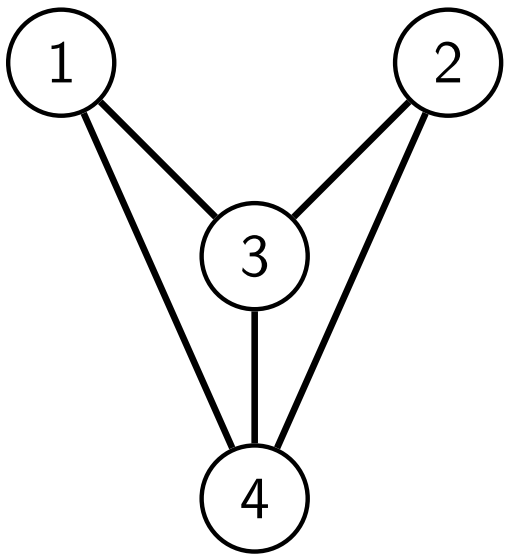
Start with a complete graph:



We have $X_1 \perp\!\!\!\perp X_2$, but no other marginal independences.

Example

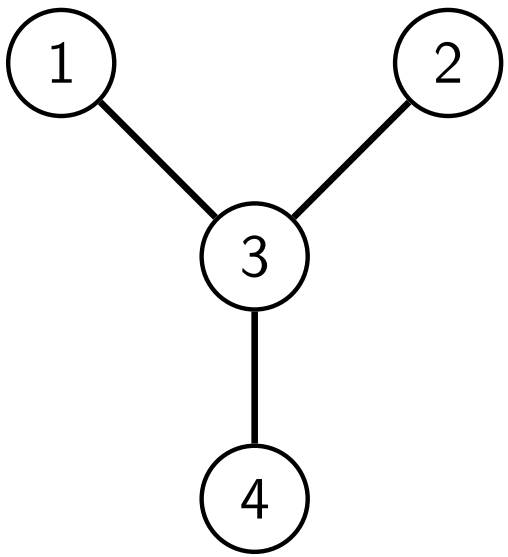
Start with a complete graph:



Now test $X_i \perp\!\!\!\perp X_j \mid X_k$ for each remaining edge $i - j$ and other variable k.
This gives $X_1 \perp\!\!\!\perp X_4 \mid X_3$ and $X_2 \perp\!\!\!\perp X_4 \mid X_3$.

Example

We have recovered the correct skeleton.



We would continue to test, but should find only dependence.

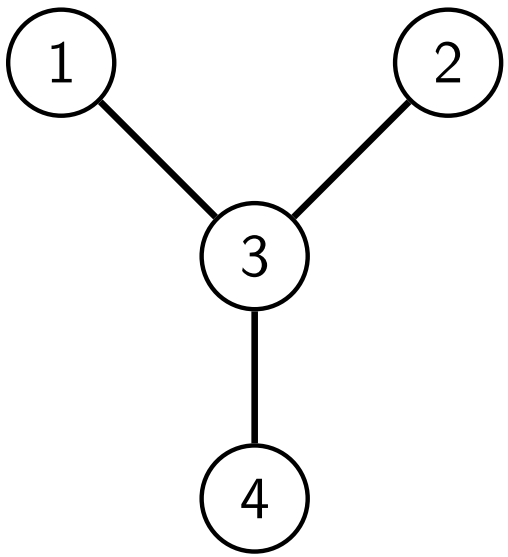
Can we orient the edges?

We found $X_1 \perp\!\!\!\perp X_2$ so we must have $1 \to 3 \leftarrow 2$.

Since we didn't find $X_1 \perp\!\!\!\perp X_4$, we must have $3 \to 4$ to avoid a v-structure.

Example

Start with a complete graph:



We would continue to test, but should find only dependence.

The PC Algorithm

function SKELETON(distribution $p(x_V)$)
    Start with complete undirected graph $\mathcal{H}$;
    for k in $0, 1, \ldots, p-2$ **do**
        for every $i \sim j$ in $\mathcal{H}$ **do**
            for $C \subseteq \mathrm{bd}_{\mathcal{H}}(i) \setminus \{j\}$ or $C \subseteq \mathrm{bd}_{\mathcal{H}}(j) \setminus \{i\}$ with $|C| = k$ **do**
                if $X_i \perp\!\!\!\perp X_j \mid X_C \, [p(x_V)]$ **then**
                    remove $i - j$ edge from $\mathcal{H}$;
                    record $SepSet(i, j) = C$;
                    exit loop over C and move to next edge in $\mathcal{H}$.
                end if
            end for
        end for
    end for
    return $\mathcal{H}$, collection of $Sepset(i, j)$s.
end function

The PC Algorithm

function ORIENT(Skeleton $\mathcal{H}$, collection of $Sepset(i, j)$s)
  for every triple $i - k - j$ in $\mathcal{H}$ with $i \not\sim j$ **do**
    if $k \notin SepSet(i, j)$ **then**
      orient $i \rightarrow k \leftarrow j$.
    end if
  end for
  return $\mathcal{H}$, collection of $Sepset(i, j)$s.
end function

Example

Consider the mathematics test marks again

```
> data(marks, package = "ggm")
> C <- cor(marks)
> n <- 88
> C

           mechanics vectors algebra analysis statistics
mechanics       1.00    0.55    0.55     0.41       0.39
vectors         0.55    1.00    0.61     0.49       0.44
algebra         0.55    0.61    1.00     0.71       0.66
analysis        0.41    0.49    0.71     1.00       0.61
statistics      0.39    0.44    0.66     0.61       1.00
```

Example

Consider the mathematics test marks again

```
> f <- function(x) 0.5*log((1+x)/(1-x))
> sqrt(n-3)*f(C)

           mechanics vectors algebra analysis statistics
mechanics        Inf     5.7     5.7      4.0        3.8
vectors          5.7     Inf     6.5      4.9        4.3
algebra          5.7     6.5     Inf      8.2        7.4
analysis         4.0     4.9     8.2      Inf        6.5
statistics       3.8     4.3     7.4      6.5        Inf
```

Comparing to a $N(0, 1)$, we would reject the possibility of any marginal independences.

Example

Now try conditional independences with sets of size one.

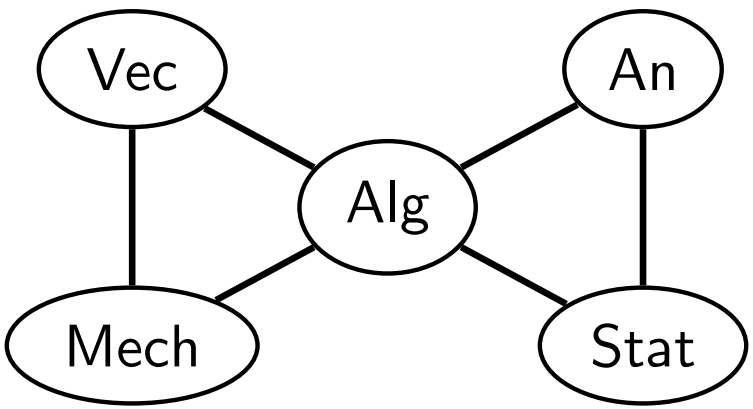
```
> S <- c(2,3,4)  # pick subset of varaibles
> Cp <- solve(C[S,S])  # compute inverse matrix
> Cp <- Cp/sqrt(diag(Cp)*rep(diag(Cp),each=3))  # get partial cors
> sqrt(n-3-1)*f(Cp)

          vectors algebra analysis
vectors       Inf    -4.2    -0.85
algebra    -4.22     Inf    -6.34
analysis   -0.85    -6.3      Inf
```

Comparing to a $N(0,1)$, we would accept that Analysis is independent of Mechanics conditional on Vectors.

Example

Repeating this process we would obtain

$$\begin{aligned} \text{Analysis} &\perp\!\!\!\perp \text{Mechanics} \mid \text{Vectors} \\ \text{Statistics} &\perp\!\!\!\perp \text{Mechanics} \mid \text{Vectors} \\ \text{Analysis} &\perp\!\!\!\perp \text{Vectors} \mid \text{Algebra} \\ \text{Statistics} &\perp\!\!\!\perp \text{Vectors} \mid \text{Algebra} \end{aligned}$$



There are two implied v-structures.

Two more edges can be oriented to avoid more v-structures and cycles.

Gibbs Sampling

Gibbs Sampling

Suppose

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \sim N_2 \left(0, \begin{pmatrix} 1 & \rho \\ \rho & 1 \end{pmatrix} \right)$$

so

$$K = \Sigma^{-1} = \frac{1}{1-\rho^2} \begin{pmatrix} 1 & -\rho \\ -\rho & 1 \end{pmatrix}.$$

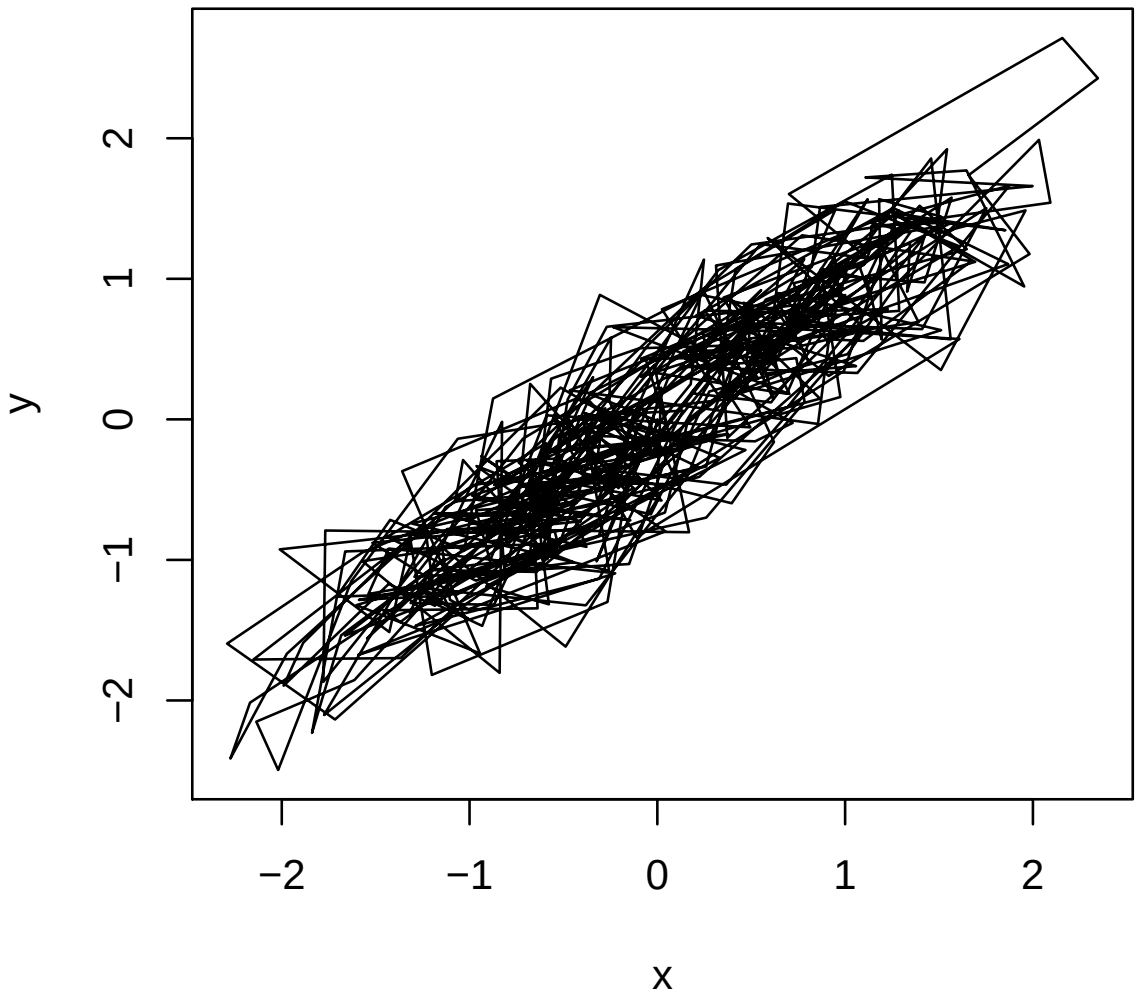
Then

$$\begin{aligned} X_1 \mid X_2 = x_2 &\sim N\left(\rho x_2, (1-\rho)^2\right) \\ X_2 \mid X_1 = x_1 &\sim N\left(\rho x_1, (1-\rho)^2\right) \end{aligned}$$

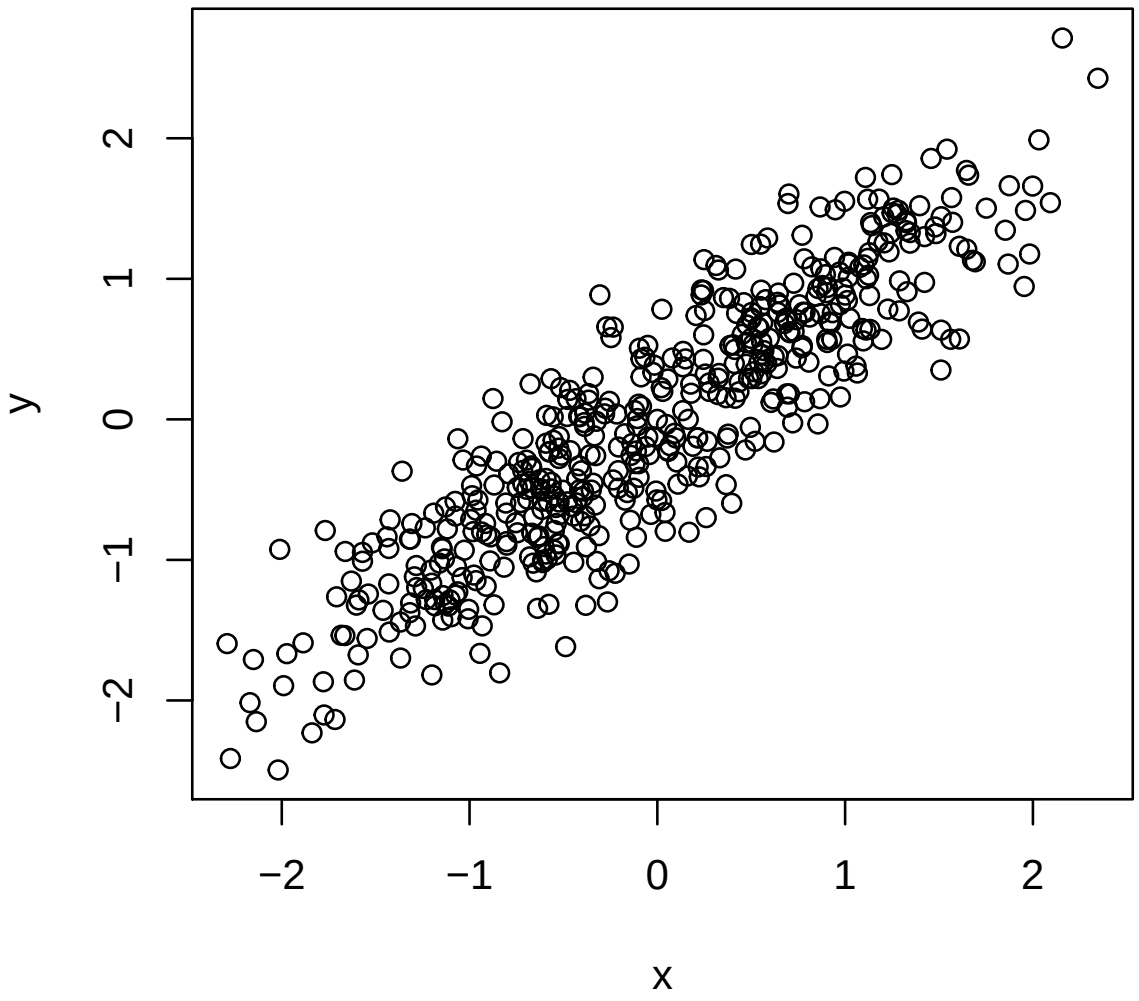
Gibbs Sampler

```
> ## Gaussian Gibbs sampler
> rho <- 0.9  ## correlation
> N <- 500  ## number of samples
> x <- y <- numeric(N)
> x[1] <- y[1] <- 0
>
> for (i in 2:N) {
+   x[i] <- rnorm(1, mean=rho*y[i-1], sd=sqrt(1-rho^2))
+   y[i] <- rnorm(1, mean=rho*x[i], sd=sqrt(1-rho^2))
+ }
>
> plot(x,y, type="l")
```

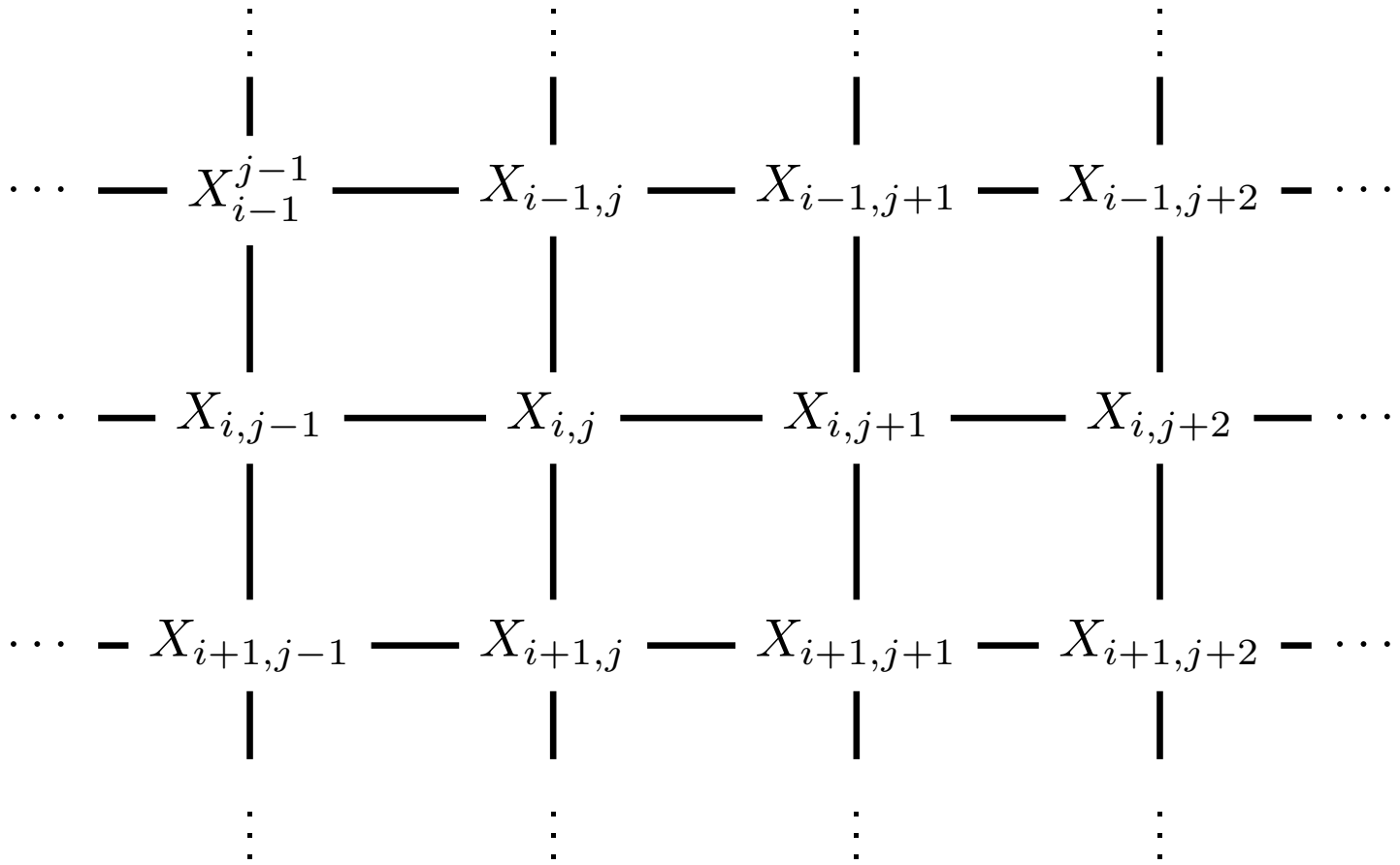
Gibbs Sampler



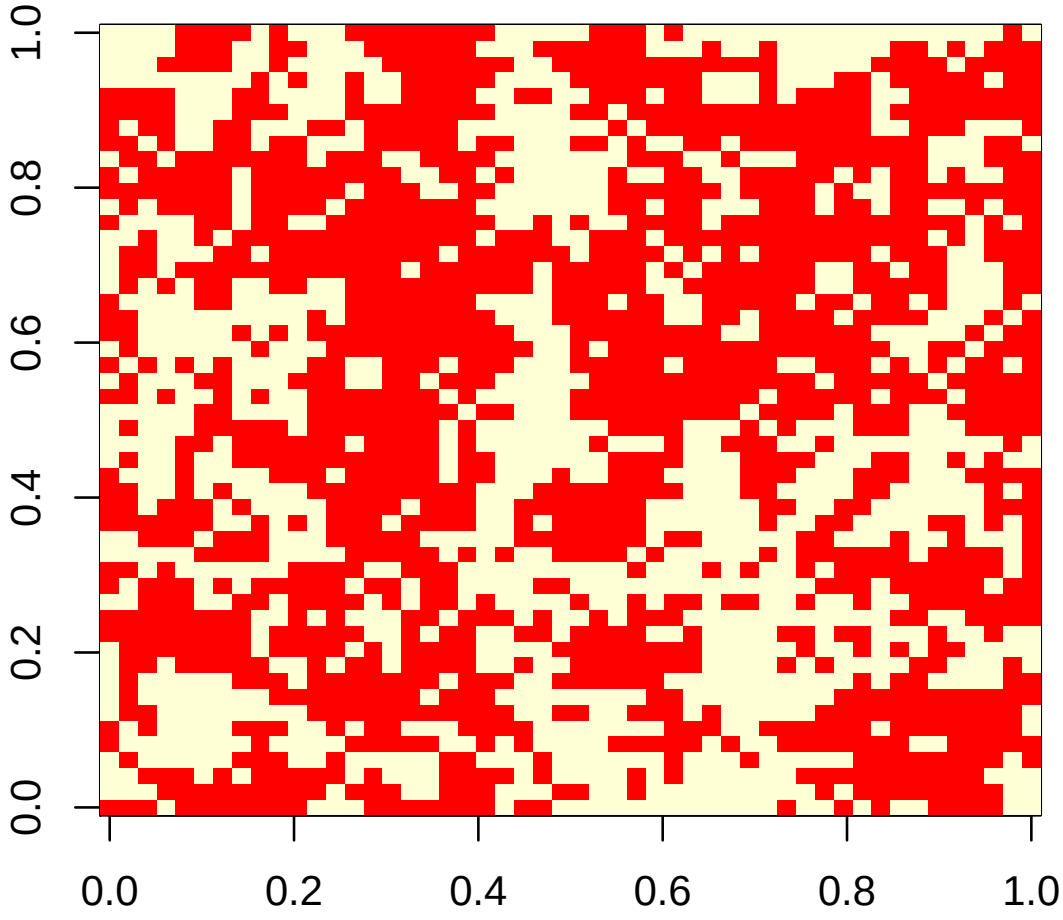
Gibbs Sampler



The Ising Model

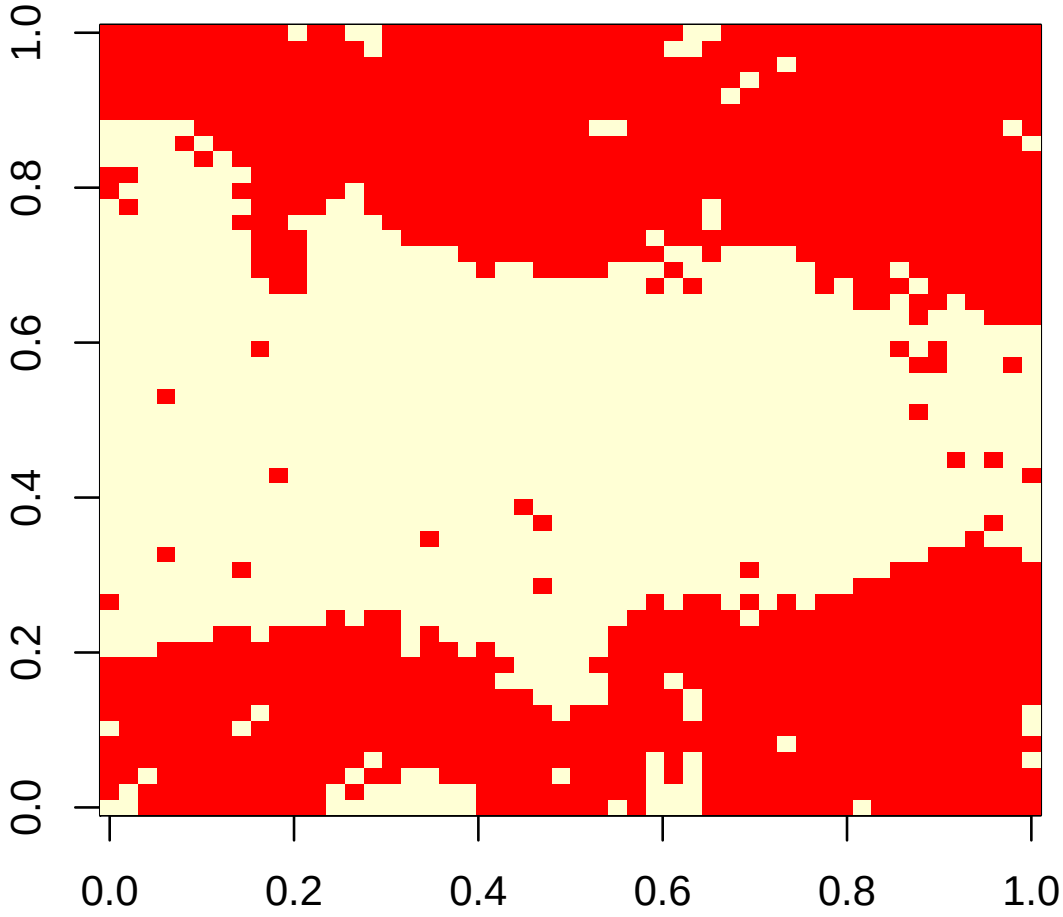


The Ising Model



50×50 grid, sample from $\theta = 0.15$.

The Ising Model



50×50 grid, sample from $\theta = 0.25$.

The Ising Model: Code

```
> ## function to perform Gibbs updates
> iterate = function(x, N, theta=0.5) {
+   n1 <- nrow(x); n2 <- ncol(x)

+   for (it in 1:N) {
+     for (i in 1:n1) for (j in 1:n2) {
+       rw <- (max(1,i-1):min(n1,i+1))
+       cl <- (max(1,j-1):min(n2,j+1))
+       cur <- sum(x[rw,cl]) - x[i,j]
+       prob = exp(cur*theta)/c(exp(cur*theta) + exp(-cur*theta))
+       x[i,j] <- 2*rbinom(1,1,prob)-1
+     }
+   }
+   x
+ }
```

The Ising Model: Code

```
> ## generage data set
> set.seed(123)
> n <- 50; theta = 0.25
> x <- matrix(2*rbinom(n^2,1,.5)-1, n, n)
> x = iterate(x,100, theta=theta)
> image(x)
```