GRAPHICAL MODEL STRUCTURE LEAERNING

Presented by Zi Wang

A review of MLPP chapter 26

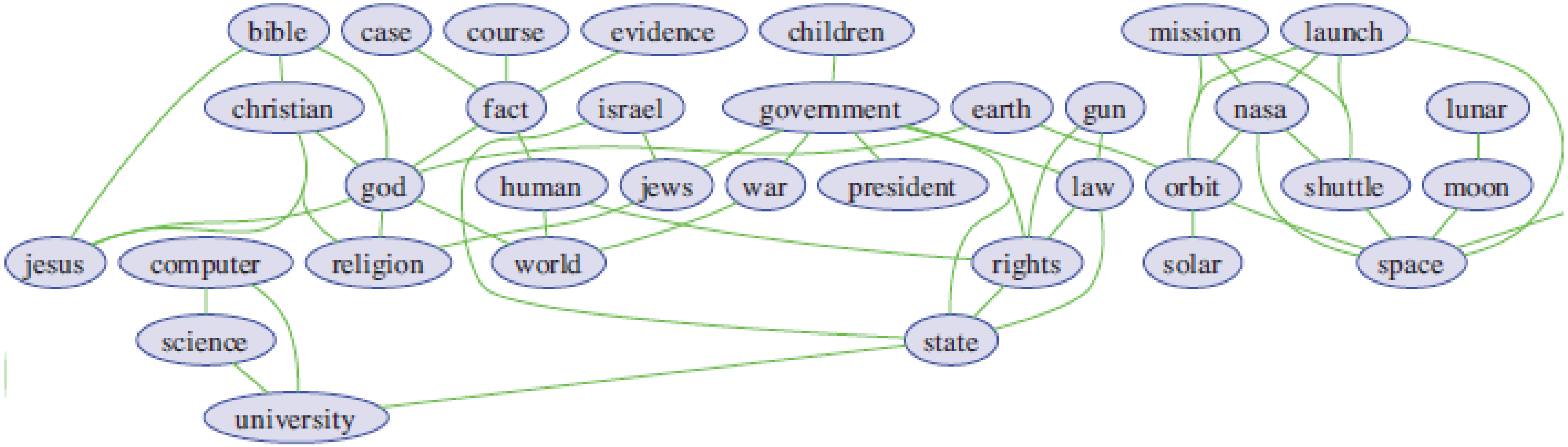
CONTENTS

CONTENTS

- **Structure learning for knowledge discovery**
- Learning tree structures
- Learning DAG structures
- Learning DAG structure with latent variables
- Learning causal DAGs
- Learning undirected Gaussian graphical models
- Learning undirected discrete graphical models

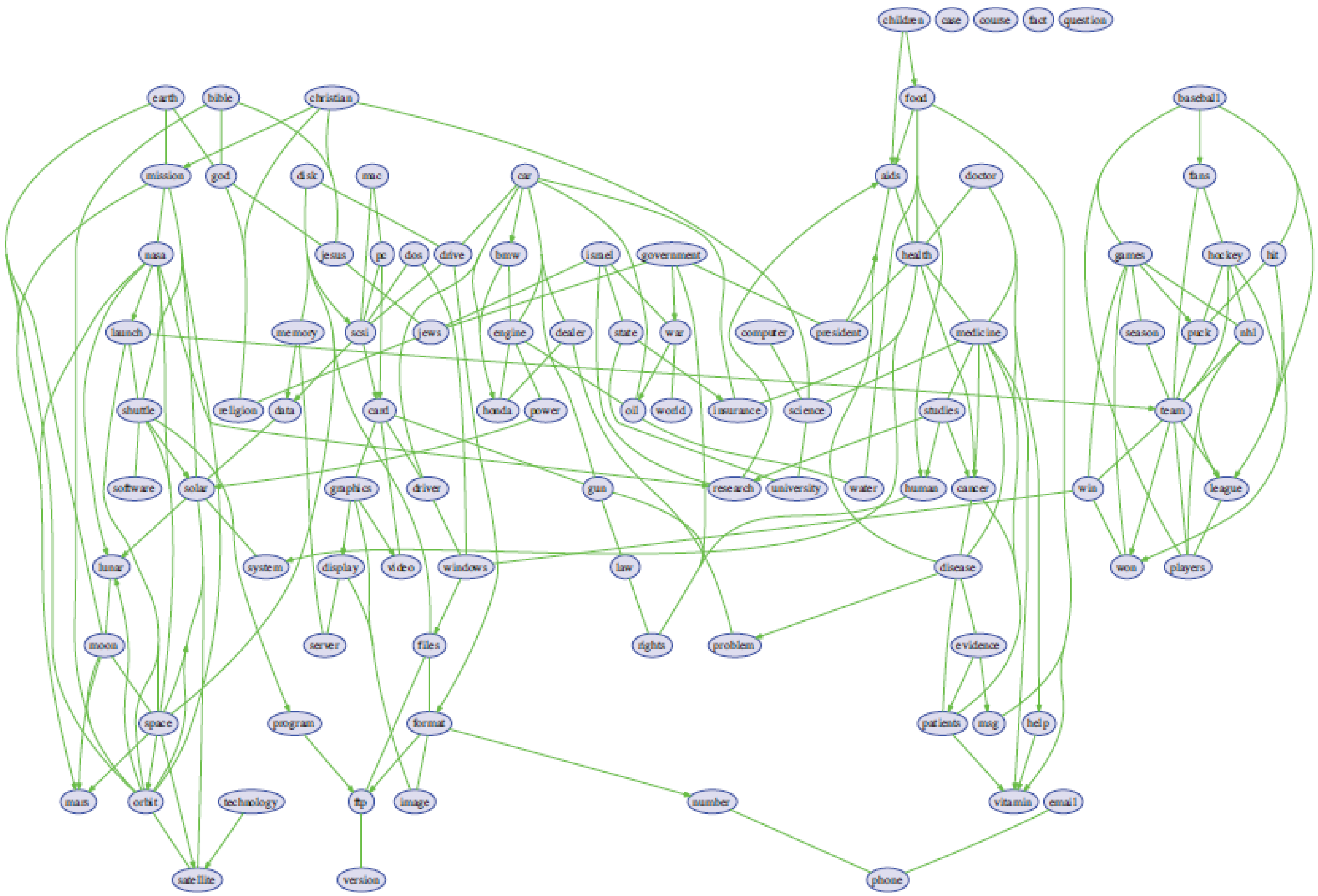
STRUCTURE LEARNING FOR KNOWLEDGE DISCOVERY

- Relevance networks
  - Visualizing mutual information(MI)
  - Dense graph because of disability to capture conditional independence
  - Solution: graphical model



STRUCTURE LEARNING FOR KNOWLEDGE DISCOVERY

- Dependency networks
  - $p(x_t | x_{\neg t})$
  - only its Markov blanket will be chosen as input
  - Sparse graph
- Application
  - Visualization
  - Inference with gibbs sampling



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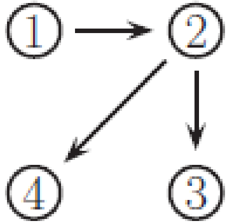
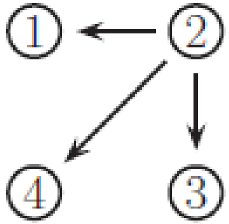
LEARNING TREE STRUCTURES

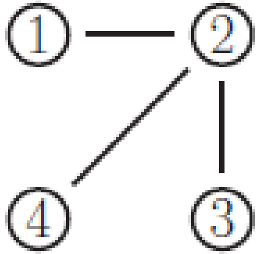
- Equivalence between directed and undirected representation (for trees)

- $p(x_1, x_2, x_3, x_4|T) = p(x_1)p(x_2|x_1)p(x_3|x_2)p(x_4|x_2)$
- $p(x_1, x_2, x_3, x_4|T) = p(x_2)p(x_1|x_2)p(x_3|x_2)p(x_4|x_2)$





- $p(x_1, x_2, x_3, x_4|T) = p(x_1)p(x_2)p(x_3)p(x_4)\frac{p(x_1,x_2)}{p(x_1)p(x_2)}\frac{p(x_2,x_3)}{p(x_2)p(x_3)}\frac{p(x_2,x_4)}{p(x_2)p(x_4)}$
- $p(\vec{x}|T) = \prod_{t \in V} p(x_t) \prod_{(s,t) \in E} \frac{p(x_s,x_t)}{p(x_s)p(x_t)}$



CHOW-LIU ALGORITHM FOR FINDING THE ML TREE STRUCTURE

- Log-likelihood function

$$\begin{aligned}\log p(\mathcal{D}|\boldsymbol{\theta}, T) &= \sum_t \sum_k N_{tk} \log p(x_t = k|\boldsymbol{\theta}) \\ &+ \sum_{s,t} \sum_{j,k} N_{stjk} \log \frac{p(x_s = j, x_t = k|\boldsymbol{\theta})}{p(x_s = j|\boldsymbol{\theta}) p(x_t = k|\boldsymbol{\theta})}\end{aligned}$$

CHOW-LIU ALGORITHM FOR FINDING THE ML TREE STRUCTURE

- Log-likelihood function

$$
\begin{aligned}
\frac{\log p(\mathcal{D}|\boldsymbol{\theta}, T)}{N} \quad = \quad & \sum_{t \in \mathcal{V}} \sum_{k} p_{\text{emp}}(x_t = k) \log p_{\text{emp}}(x_t = k) \\
+ & \sum_{(s,t) \in \mathcal{E}(T)} \mathbb{I}(x_s, x_t | \hat{\boldsymbol{\theta}}_{st})
\end{aligned}
$$

$$
\mathbb{I}(x_s, x_t | \hat{\boldsymbol{\theta}}_{st}) = \sum_{j} \sum_{k} p_{\text{emp}}(x_s = j, x_t = k) \log \frac{p_{\text{emp}}(x_s = j, x_t = k)}{p_{\text{emp}}(x_s = j) p_{\text{emp}}(x_t = k)}
$$

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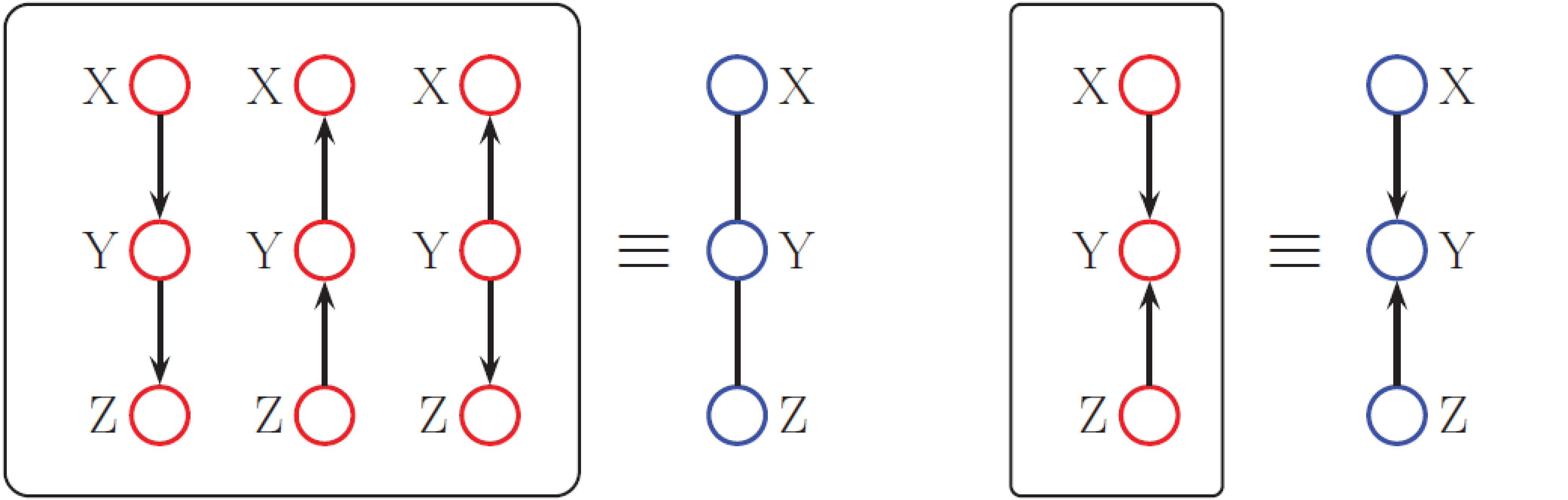
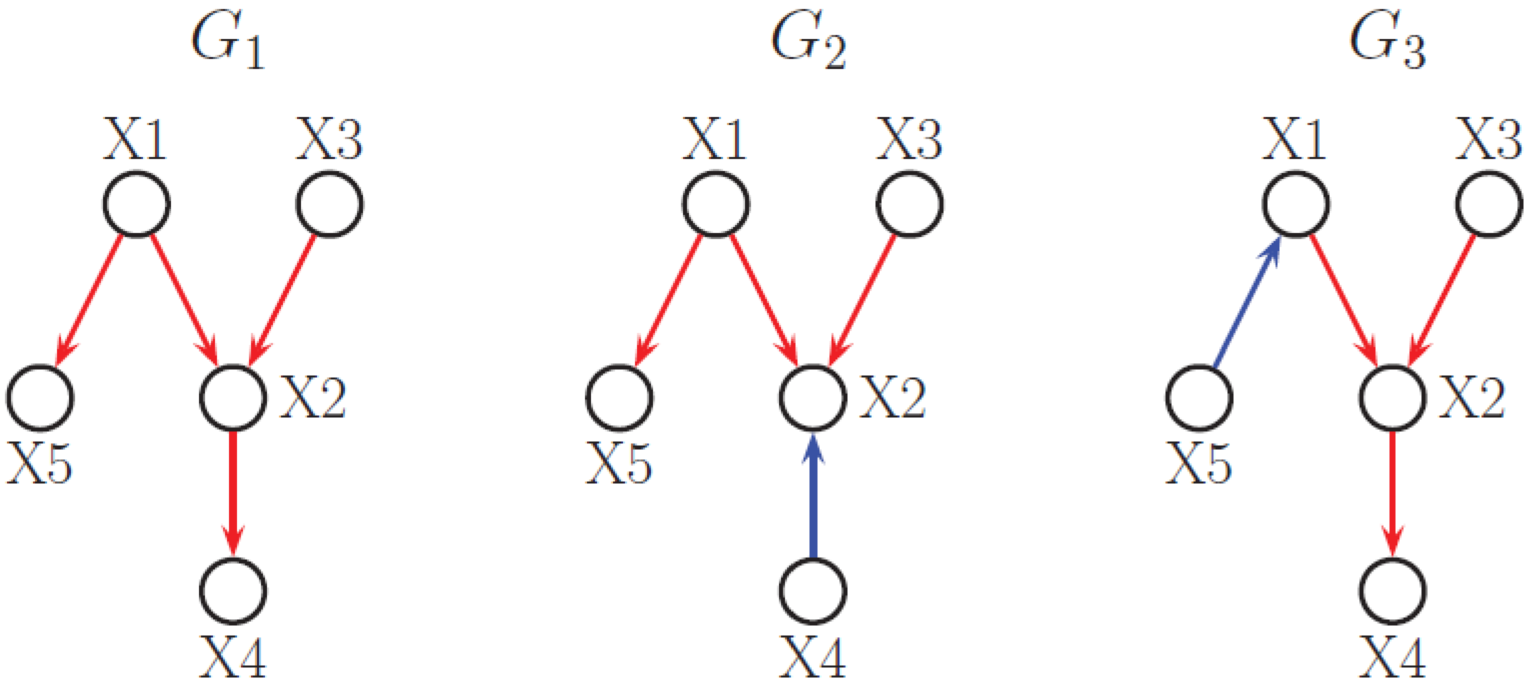
LEARNING DAG STRUCTURES

- Markov Equivalence



MARKOV EQUIVALENCE - EXAMPLE



LEARNING DAG STRUCTURES

- $\theta_{tck} = p(x_t = k | x_{pa(t)} = c)$ where $c = 1 : C_t,\ C_t = K^{d_t},\ d_t = \dim(pa(t))$
- N_{tck} is the number of times node t is in state k and its parents are in state c
- Assumption: no missing data

$$
\begin{aligned}
p(\mathcal{D}|G, \boldsymbol{\theta}) &= \prod_{i=1}^{N} \prod_{t=1}^{V} \mathrm{Cat}(x_{it}|\mathbf{x}_{i,\mathrm{pa}(t)}, \boldsymbol{\theta}_t) \\
&= \prod_{i=1}^{N} \prod_{t=1}^{V} \prod_{c=1}^{C_t} \mathrm{Cat}(x_{it}|\boldsymbol{\theta}_{tc})^{\mathbb{I}(\mathbf{x}_{i,\mathrm{pa}(t)}=c)} \\
&= \prod_{i=1}^{N} \prod_{t=1}^{V} \prod_{c=1}^{C_t} \prod_{k=1}^{K_t} \theta_{tck}^{\mathbb{I}(x_{i,t}=k, \mathbf{x}_{i,\mathrm{pa}(t)}=c)} \\
&= \prod_{t=1}^{V} \prod_{c=1}^{C_t} \prod_{k=1}^{K_t} \theta_{tck}^{N_{tck}}
\end{aligned}
$$

LEARNING DAG STRUCTURES

- Constraints on priors:
  - $p(\theta) = \prod_t p(\theta_t)$ - global prior parameter independence
  - $p(\theta_t) = \prod_c p(\theta_{tc})$ - local prior parameter independence
  - => $p(\theta_{tc}) = Dir(\theta_{tc}|\alpha_{tc})$

- Marginal likelihood
  - $p(D|G) = \prod_{t=1}^{V} \prod_{c=1}^{C_t} \frac{B(N_{tc}+\alpha_{tc})}{B(\alpha_{tc})}$
  - $score\left(N_t, pa(t)\right) = \prod_{c=1}^{C_t} \frac{B(N_{tc}+\alpha_{tc})}{B(\alpha_{tc})}$
  - Recap Chapter 5:
  - $p(\theta|D) = \frac{p(\theta)p(D|\theta)}{p(D)}$ => $\frac{1}{B(\alpha+N)} \prod_t \theta_t^{\alpha_t+N_t-1} = \frac{\frac{1}{B(\alpha)} \prod_t \theta_t^{\alpha_t-1} \prod_t \theta_t^{N_t}}{p(D)}$ => $p(D) = \frac{B(N+\alpha)}{B(\alpha)}$
  - Here just compute the marginal likelihood directly

LEARNING DAG STRUCTURES

- Setting the prior
- $\alpha_{tck} = \alpha p_0\left(x_t = k, x_{pa(t)} = c\ \right) = \alpha / K_t C_t$
- Example:
- $N_1 = (5,3)\ \ N_{21} = (4,1)\ N_{22} = (1,2)$
- $G_1 = \ X_1 \rightarrow X_2 :\ \alpha_1 = (\frac{\alpha}{2}, \frac{\alpha}{2})\ \alpha_{21} = (\frac{\alpha}{4}, \frac{\alpha}{4})\ \alpha_{22} = (\frac{\alpha}{4}, \frac{\alpha}{4})$
- $G_2 = \ X_1 \quad\ X_2 :\ \alpha_1 = (\frac{\alpha}{2}, \frac{\alpha}{2})\ \alpha_{21} = (\frac{\alpha}{2}, \frac{\alpha}{2})\ \alpha_{22} = (\frac{\alpha}{2}, \frac{\alpha}{2})$

X_1	X_2
1	1
1	2
1	1
2	2
1	1
2	1
1	1
2	2

LEARNING DAG STRUCTURES

- Scaling problem: too many possible graphs

$$f(D) = \sum_{i=1}^{D} (-1)^{i+1} \binom{D}{i} 2^{i(D-i)} f(D-i)$$

- Nodes number: 1 2 3 4 5 6
- Graphs number: 1 3 25 543 29281 3781503
- Solutions
  - Greedy hill climbing
  - Sample DAGs from the posterior, e.g. Metropolis Hasting with proposals in greedy search

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LEARNING DAG STRUCTURES WITH LATENT VARIABLES

- Learning DAG structure without complete data

$$p(\mathcal{D}|G) = \int \sum_{\mathbf{h}} p(\mathcal{D}, \mathbf{h}|\boldsymbol{\theta}, G)p(\boldsymbol{\theta}|G)d\boldsymbol{\theta} = \sum_{\mathbf{h}} \int p(\mathcal{D}, \mathbf{h}|\boldsymbol{\theta}, G)p(\boldsymbol{\theta}|G)d\boldsymbol{\theta}$$

- Intractable to compute

APPROXIMATING THE MARGINAL LIKELIHOOD WITH MISSING DATA

- BIC approximation

$$\mathrm{BIC}(G) \triangleq \log p(\mathcal{D}|\hat{\boldsymbol{\theta}}, G) - \frac{\log N}{2} \dim(G)$$

- Cheeseman-Stutz approximation

$$p(\mathcal{D}|G) \approx p(\overline{\mathcal{D}}|G) = \int p(\overline{\mathcal{D}}|\boldsymbol{\theta}, G) p(\boldsymbol{\theta}|G) d\boldsymbol{\theta}$$

$$\log p(\mathcal{D}|G) \approx \log p(\overline{\mathcal{D}}|G) + \log p(\mathcal{D}|\hat{\boldsymbol{\theta}}, G) - \log p(\overline{\mathcal{D}}|\hat{\boldsymbol{\theta}}, G)$$

- Variational Bayes EM

$$p(\boldsymbol{\theta}, \mathbf{z}_{1:N}|\mathcal{D}) \approx q(\boldsymbol{\theta}) q(\mathbf{z}) = q(\boldsymbol{\theta}) \prod_i q(\mathbf{z}_i)$$

STRUCTURAL EM

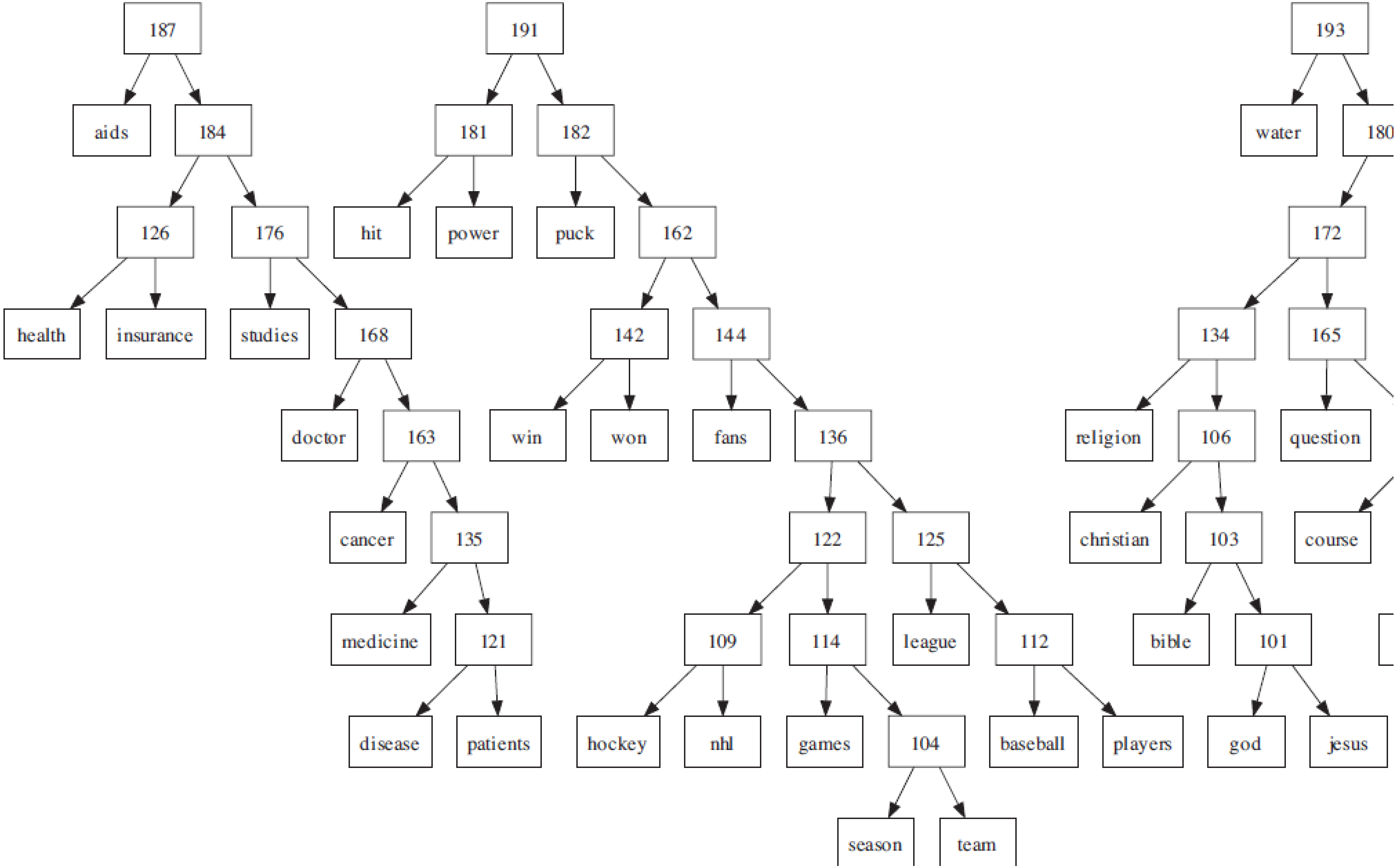
- 0) Initialize a model
- 1) Fill in the data with the current model
- 2) Use the filled-in data to evaluate the score of all the neighbors
- 3) Pick the best neighbor
- 4) Repeat 1),2),3)

$$\text{score}_{\text{BIC}}(G, \mathcal{D}) \triangleq \log p(\mathcal{D}|\hat{\boldsymbol{\theta}}, G) - \frac{\log N}{2}\dim(G) + \log p(G) + \log p(\hat{\boldsymbol{\theta}}|G)$$

- Pro: efficient
- App: learn the phylogenetic tree structure, learn sparse mixture models

DISCOVERING HIDDEN VARIABLES

- Introduce hidden variables to structural signatures, e.g. sets of densely connected nodes
- Latent class model
  - introduce hidden variables with high mutual information with their children
  - Hierarchical latent class model
    - greedy local search algorithm
    - A faster greedy algorithm based on agglomerative hierarchical clustering (Harmeling and Williams 2011)
    - Another approach: Chow-Liu Tree on observed data + add hidden variable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league
112
hockey
nhl
games
104
baseball
players
season
team
193
water
180
172
134
165
religion
106
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christian
103
course
bible
101
god
jesus

STRUCTURAL EQUATION MODELS

SEM: a statistical technique for testing and estimating causal relations using a combination of statistical data and qualitative causal assumptions.

$$x_i = \mu_i + \sum_{j \neq i} w_{ij} x_j + \epsilon_i \qquad \epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{\Psi})$$

$$\mathbf{x} = \mathbf{W}\mathbf{x} + \boldsymbol{\mu} + \boldsymbol{\epsilon} \Rightarrow \mathbf{x} = (\mathbf{I} - \mathbf{W})^{-1}(\boldsymbol{\epsilon} + \boldsymbol{\mu})$$

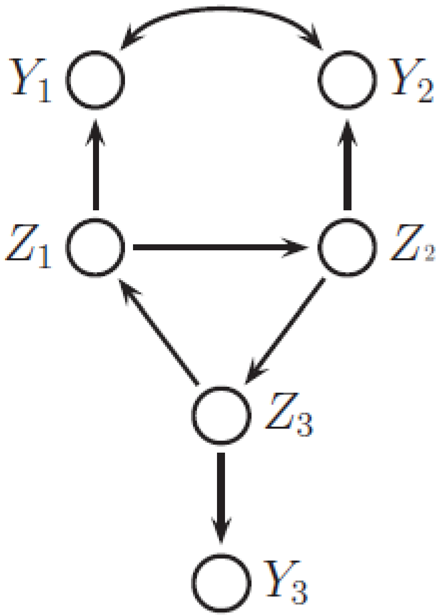
$$p(\mathbf{x}) = \mathcal{N}(\boldsymbol{\mu}, \mathbf{\Sigma})$$

$$\mathbf{\Sigma} = (\mathbf{I} - \mathbf{W})^{-1}\mathbf{\Psi}(\mathbf{I} - \mathbf{W})^{-T}$$

http://en.wikipedia.org/wiki/Structural_equation_modeling

SEM EXAMPLE

$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \\ X_6 \end{pmatrix} = \begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \\ Y_1 \\ Y_2 \\ Y_3 \end{pmatrix} = \begin{pmatrix} 0 & 0 & w_{13} & 0 & 0 & 0 \\ w_{21} & 0 & 0 & 0 & 0 & 0 \\ 0 & w_{32} & 0 & 0 & 0 & 0 \\ w_{41} & 0 & 0 & 0 & 0 & 0 \\ 0 & w_{52} & 0 & 0 & 0 & 0 \\ 0 & 0 & w_{63} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} Z_1 \\ Z_2 \\ Z_3 \\ Y_1 \\ Y_2 \\ Y_3 \end{pmatrix} + \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{pmatrix}$$



$$\boldsymbol{\Psi} = \begin{pmatrix} \Psi_{11} & 0 & 0 & 0 & 0 & 0 \\ 0 & \Psi_{22} & 0 & 0 & 0 & 0 \\ 0 & 0 & \Psi_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & \Psi_{44} & \Psi_{45} & 0 \\ 0 & 0 & 0 & \Psi_{54} & \Psi_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & \Psi_{66} \end{pmatrix}$$

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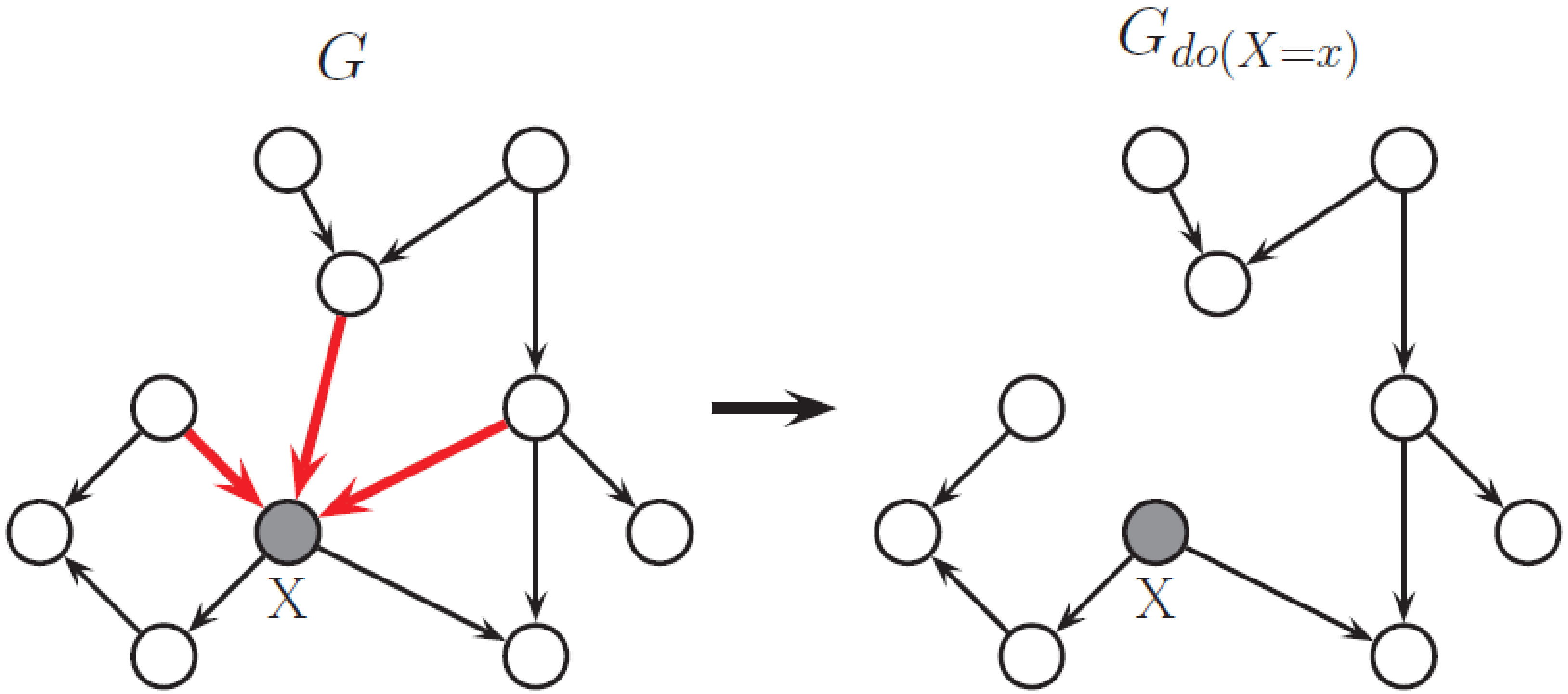
LEARNING CAUSAL DAGS

- Causal models: models which can predict the effects of interventions to, or manipulations of, a system
- Assumptions:
  - Causal Markov assumption
  - Causal sufficiency assumption
- Notations:
  - $do(X_i = x_i)$ – set X_i to be x_i
  - Difference between conditioning on observation and manipulation:
    - P(S=1 | Y=1)>P(S=1)
    - P(S=1 | do(Y=1))=P(S=1)

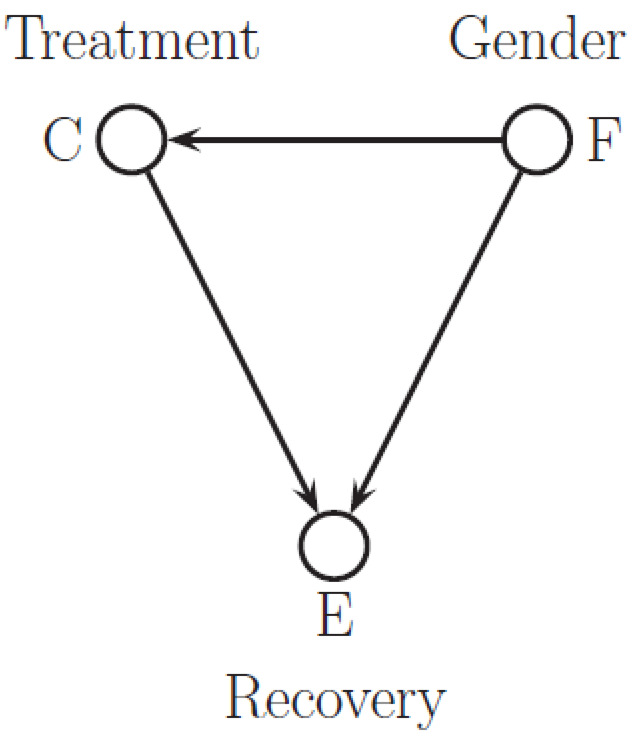
GRAPH SURGERY



SIMPSON'S PARADOX

- Any statistical relationship between two variables can be reversed by including additional factors the analysis
- $P(E|C) > P(E|\neg C)$
- Include additional factor F:
- $P(E|C, F) < P(E|\neg C, F)$
- $P(E|C, \neg F) < P(E|\neg C, \neg F)$
- The statement is not interpreted properly!
- Should be $P(E|do(C)) > P(E|do(\neg C))$

SIMPSON'S PARADOX



Suppose

$$p(E|do(C), F) < p(E|do(\neg C), F)$$

$$p(E|do(C), \neg F) < p(E|do(\neg C), \neg F)$$

We show

$$p(E|do(C)) < p(E|do(\neg C))$$

SIMPSON'S PARADOX

- Proof:
  - $p(F|do(C)) = p(F|do(\neg C)) = p(F)$
  - $p(E|do(C)) = p(E|do(C), F)p(F|do(C)) + p(E|do(C), \neg F)p(\neg F|do(C))$
    $= p(E|do(C), F)p(F) + p(E|do(C), \neg F)p(\neg F)$
  - $p(E|do(\neg C)) = p(E|do(\neg C), F)p(F) + p(E|do(\neg C), \neg F)p(\neg F)$
  - Given $p(E \mid do(C), F) < p(E \mid do(\neg C), F)$ and $p(E \mid do(C), \neg F) < p(E \mid do(\neg C), \neg F)$
  - Conclusion: $p(E|do(C)) < p(E|do(\neg C))$

LEARNING CAUSAL DAG STRUCTURES

- Learning from observational data
  - Learn an PDAG from data
  - Enumerate all the DAGs from the PDAG equivalence class
  - Apply Pearl's do-calculus to compute the magnitude of each causal effect pair
  - Take the minimum of these effects as the lower bound

- Learning from interventional data
  - Control some variables and measure the consequences
  - First skipping over intervention cases
  - Then adding the intervention nodes with constraints

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LEARNING UNDIRECTED GAUSSIAN GRAPHICAL MODELS

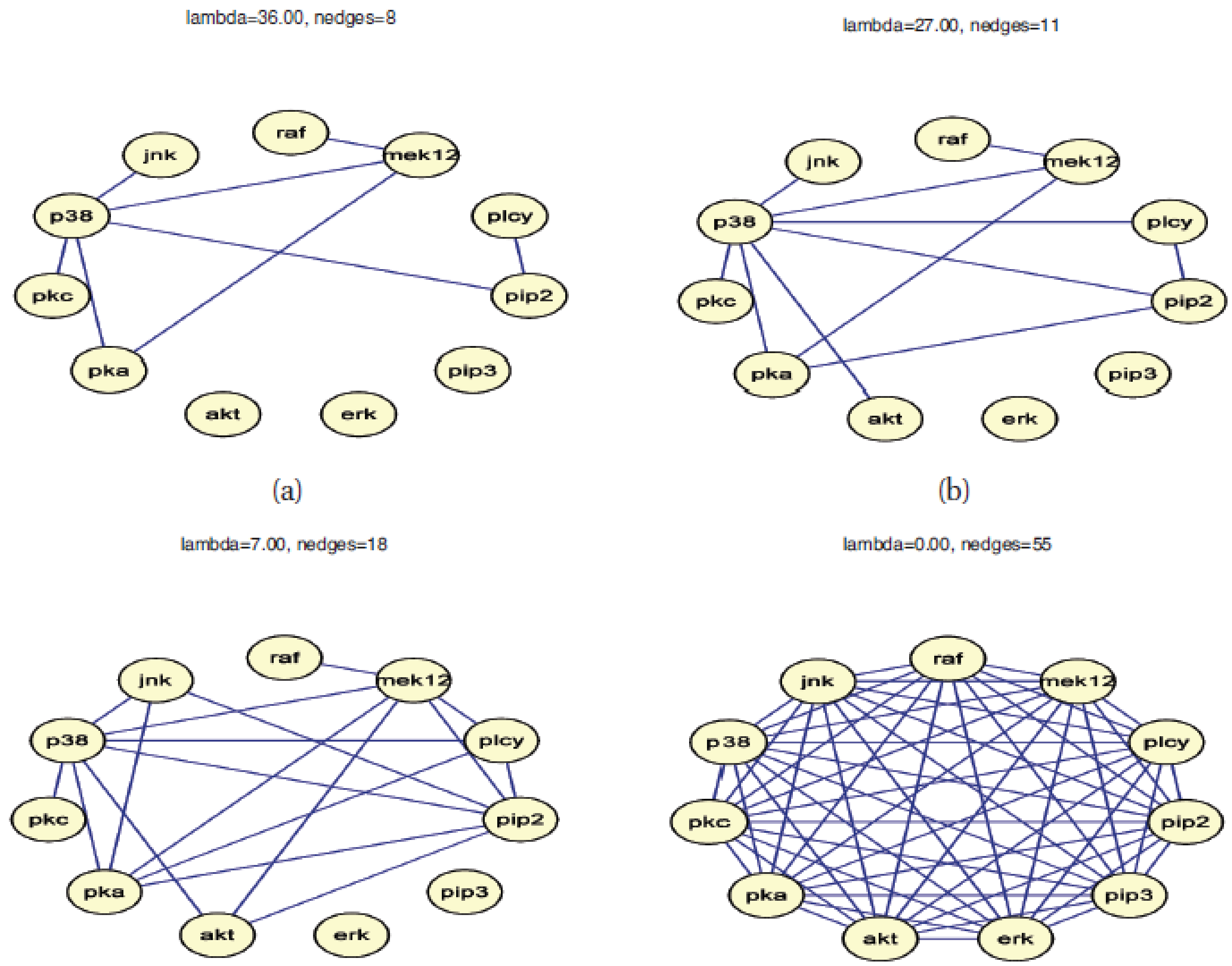
- *MLE for a GGM - covariance estimation*
- $l(\Omega) = \log|\Omega| - tr(S\Omega)$
- $\nabla l(\Omega) = \Omega^{-1} - S$
- Constraints:
  - $\Omega_{st} = 0 \; if \; G_{st} = 0$
  - Ω is positive definite
- Property: $\Sigma_{st} = S_{st}$ if $\mathrm{G_{st}} = 1$ or $\mathrm{s} = \mathrm{t}$

GRAPHICAL LASSO

- $J(\Omega) = -\log|\Omega| + tr(S\Omega) + \lambda||\Omega||_1$
- Convex but non-smooth
- Coordinate descent algorithm

- Shooting algorithm for lasso $\quad \arg\min_x \|Ax - y\|_2^2 + \lambda\|x\|_1$

$$\begin{aligned} S_j &= A_{(:,j)}^T(Ax) - 2(y^TA)_j + (A^TA)_{j,j}x_j^{t-1} \\ x_j^t &\leftarrow \operatorname{sign}(S_j)(|S_j| - \lambda)_+ \end{aligned}$$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lambda=7.00, nedges=18
lambda=0.00, nedges=55
raf
mek12
jnk
p38
plcy
pkc
pip2
pka
pip3
akt
erk

(a)

(b)

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LEARNING UNDIRECTED DISCRETE GRAPHICAL MODELS

- Grapical lasso for CRF

$$\psi_t(y_t, \mathbf{x}) = \begin{pmatrix} \mathbf{v}_{t1}^T\mathbf{x} \\ \mathbf{v}_{t2}^T\mathbf{x} \\ \mathbf{v}_{t3}^T\mathbf{x} \end{pmatrix}, \quad \psi_{st}(y_s, y_t, \mathbf{x}) = \begin{pmatrix} \mathbf{w}_{t11}^T\mathbf{x} & \mathbf{w}_{st12}^T\mathbf{x} & \mathbf{w}_{st13}^T\mathbf{x} \\ \mathbf{w}_{st21}^T\mathbf{x} & \mathbf{w}_{st22}^T\mathbf{x} & \mathbf{w}_{st23}^T\mathbf{x} \\ \mathbf{w}_{st31}^T\mathbf{x} & \mathbf{w}_{st32}^T\mathbf{x} & \mathbf{w}_{st33}^T\mathbf{x} \end{pmatrix}$$

$$\begin{aligned} J &= -\sum_{i=1}^{N}\left[\sum_{t}\log\psi_t(y_{it}, \mathbf{x}_i, \mathbf{v}_t) + \sum_{s=1}^{V}\sum_{t=s+1}^{V}\log\psi_{st}(y_{is}, y_{it}, \mathbf{x}_i, \mathbf{w}_{st})\right] \\ &\quad +\lambda_1\sum_{s=1}^{V}\sum_{t=s+1}^{V}||\mathbf{w}_{st}||_p + \lambda_2\sum_{t=1}^{V}||\mathbf{v}_t||_2^2 \end{aligned}$$

- Thin junction tree – bound the treewidth

SUMMARY

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- Thanks!