Advanced Machine Learning

Learning Graphical Models

Learning fully observed and partially observed BN

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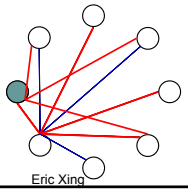


Lecture 14, August 13, 2009

Reading:

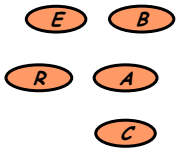
Inference and Learning

- A BN *M* describes a unique probability distribution *P*
- Typical tasks:
  - Task 1: How do we answer **queries** about P?
    - We use **inference** as a name for the process of computing answers to such queries
    - So far we have learned several algorithms for exact and approx. inference
  - Task 2: How do we estimate a **plausible model** M from data D?
    i. We use **learning** as a name for the process of obtaining point estimate of M.
    ii. But for *Bayesian*, they seek $p(M \mid D)$, which is actually an **inference** problem.
    iii. When not all variables are observable, even computing point estimate of M need to do **inference** to impute the *missing data*.

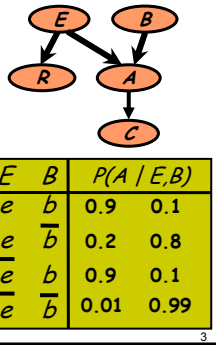
Learning Graphical Models

The goal:

Given set of independent samples (***assignments*** of random variables), find the ***best*** (the most likely?) graphical model (both the graph and the CPDs)



(B,E,A,C,R)=(T,F,F,T,F)
(B,E,A,C,R)=(T,F,T,T,F)
……..
(B,E,A,C,R)=(F,T,T,T,F)

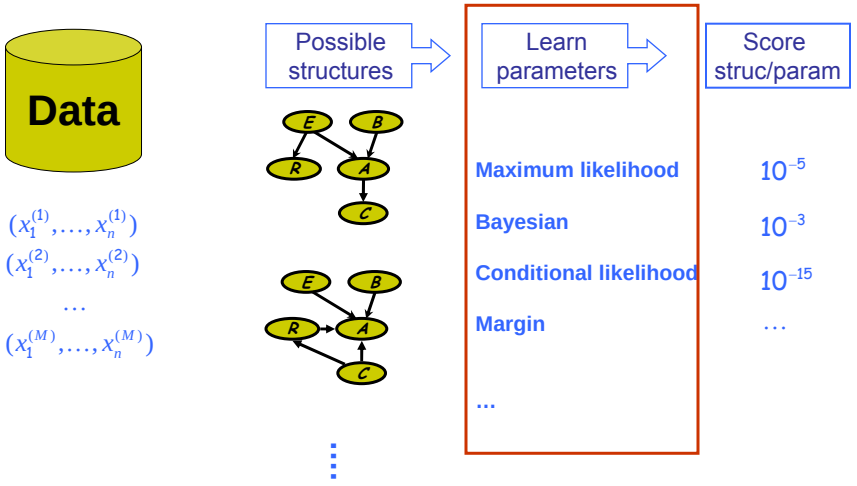


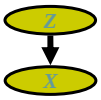
E	B	P(A | E,B)	
e	b	0.9	0.1
e	$\bar{b}$	0.2	0.8
$\bar{e}$	b	0.9	0.1
$\bar{e}$	$\bar{b}$	0.01	0.99

Learning Graphical Models

- Scenarios:
  - completely observed GMs
    - directed √
    - undirected √
  - partially observed GMs
    - directed √
    - undirected (an open research topic)
- Estimation principles:
  - Maximal likelihood estimation (MLE) √
  - Bayesian estimation
  - Maximal conditional likelihood
  - Maximal "Margin"
- We use **learning** as a name for the process of estimating the parameters, and in some cases, the topology of the network, from data.

Score-based approach





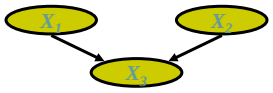
ML Parameter Est. for completely observed GMs of given structure

- The data:

  $\{(z^{(1)},x^{(1)}), (z^{(2)},x^{(2)}), (z^{(3)},x^{(3)}), \ldots (z^{(N)},x^{(N)})\}$

The basic idea underlying MLE

- Likelihood
  (for now let's assume that the structure is given):



$$L(\boldsymbol{\theta} \mid X) = p(X \mid \boldsymbol{\theta}) = p(X_1 \mid \theta_1)\, p(X_2 \mid \theta_2)\, p(X_3 \mid X_3, X_3; \theta_3)$$

- Log-Likelihood:

$$l(\boldsymbol{\theta} \mid X) = \log p(X \mid \boldsymbol{\theta}) = \log p(X_1 \mid \theta_1) + \log p(X_2 \mid \theta_2) + \log p(X_3 \mid X_3, X_3, \theta_3)$$

- Data log-likelihood

$$l(\boldsymbol{\theta} \mid DATA) = \log \prod_n p(X_n \mid \boldsymbol{\theta})$$
$$= \sum_n \log p(X_{n,1} \mid \theta_1) + \sum_n \log p(X_{n,2} \mid \theta_2) + \sum_n \log p(X_{n,3} \mid X_{n,1} X_{n,2}, \theta_3)$$

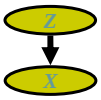
- MLE

$$\{\theta_1, \theta_2, \theta_3\}_{MLE} = \arg\max l(\boldsymbol{\theta} \mid DATA)$$

$$\theta_1^* = \arg\max \sum_n \log p(X_{n,1} \mid \theta_1), \quad \theta_2^* = \arg\max \sum_n \log p(X_{n,2} \mid \theta_2), \quad \theta_3^* = \arg\max \sum_n \log p(X_{n,3} \mid X_{n,1} X_{n,2}, \theta_3)$$

Example 1: conditional Gaussian

- The completely observed model:
  - Z is a class indicator vector



$$Z = \begin{bmatrix} Z^1 \\ Z^2 \\ \vdots \\ Z^M \end{bmatrix}, \quad \text{where } Z^m = [0,1], \text{ and } \sum_m Z^m = 1$$

and a datum is in class i w.p. π_i

$$p(z^i = 1 \mid \pi) = \pi_i = \pi_1^{z^1} \times \pi_2^{z^2} \times \ldots \times \pi_M^{z^M}$$

All except one of these terms will be one

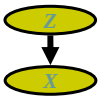
$$p(z) = \prod_m \pi_m^{z^m}$$

  - X is a conditional Gaussian variable with a class-specific mean

$$p(x \mid z^m = 1, \mu, \sigma) = \frac{1}{(2\pi\sigma^2)^{1/2}} \exp\left\{ \frac{1}{2\sigma^2} (x - \mu_m)^2 \right\}$$

$$p(x \mid z, \mu, \sigma) = \prod_m N(x \mid \mu_m, \sigma)^{z^m}$$

Example 1: conditional Gaussian



- Data log-likelihood

$$l(\boldsymbol{\theta} \mid D) = \log \prod_n p(z_n, x_n) = \log \prod_n p(z_n \mid \pi) p(x_n \mid z_n, \mu, \sigma)$$

$$= \sum_n \log p(z_n \mid \pi) + \sum_n \log p(x_n \mid z_n, \mu, \sigma)$$

$$= \sum_n \log \prod_m \pi_m^{z_n^m} + \sum_n \log \prod_m N(x_n \mid \mu_m, \sigma)^{z_n^m}$$

$$= \sum_n \sum_m z_n^m \log \pi_m - \sum_n \sum_m z_n^m \frac{1}{2\sigma^2}(x_n - \mu_m)^2 + C$$

- MLE

$$\pi_m^* = \arg\max l(\boldsymbol{\theta} \mid D), \quad \Rightarrow \frac{\partial}{\partial \pi_m} l(\boldsymbol{\theta} \mid D) = 0, \forall m, \quad \text{s.t.} \sum_m \pi_m = 1$$

$$\Rightarrow \pi_m^* = \sum_n z_n^m / N = n_m / N$$

the fraction of samples of class m

$$\mu_m^* = \arg\max l(\boldsymbol{\theta} \mid D), \quad \Rightarrow \mu_m^* = \frac{\sum_n z_n^m x_n}{\sum_n z_n^m} = \frac{\sum_n z_n^m x_n}{n_m}$$

the average of samples of class m

Example 2: HMM: two scenarios

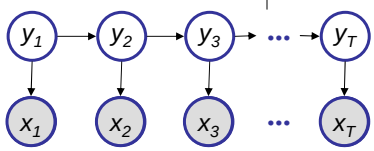
- **Supervised learning**: estimation when the "right answer" is known
  - **Examples:**
    GIVEN: a genomic region $x = x_1 \ldots x_{1,000,000}$ where we have good (experimental) annotations of the CpG islands
    GIVEN: the casino player allows us to observe him one evening, as he changes dice and produces 10,000 rolls
- **Unsupervised learning**: estimation when the "right answer" is unknown
  - **Examples:**
    GIVEN: the porcupine genome; we don't know how frequent are the CpG islands there, neither do we know their composition
    GIVEN: 10,000 rolls of the casino player, but we don't see when he changes dice
- **QUESTION:** Update the parameters θ of the model to maximize $P(x|\theta)$ --- Maximal likelihood (ML) estimation

Recall definition of HMM

- Transition probabilities between any two states

$$p(y_t^j = 1 \mid y_{t-1}^i = 1) = a_{i,j},$$

or $$p(y_t \mid y_{t-1}^i = 1) \sim \text{Multinomial}(a_{i,1}, a_{i,2}, \ldots, a_{i,M}), \forall i \in \mathbb{I}.$$



- Start probabilities

$$p(y_1) \sim \text{Multinomial}(\pi_1, \pi_2, \ldots, \pi_M).$$

- Emission probabilities associated with each state

$$p(x_t \mid y_t^i = 1) \sim \text{Multinomial}(b_{i,1}, b_{i,2}, \ldots, b_{i,K}), \forall i \in \mathbb{I}.$$

or in general: $$p(x_t \mid y_t^i = 1) \sim \text{f}(\cdot \mid \theta_i), \forall i \in \mathbb{I}.$$

Supervised ML estimation

- Given $x = x_1 \ldots x_N$ for which the true state path $y = y_1 \ldots y_N$ is known,
  - **Define:**

    A_{ij} = # times state transition $i \to j$ occurs in $\mathbf{y}$

    B_{ik} = # times state i in $\mathbf{y}$ emits k in $\mathbf{x}$

  - **We can show that the maximum likelihood parameters θ are:**

$$a_{ij}^{ML} = \frac{\#(i \to j)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=2}^T y_{n,t-1}^i y_{n,t}^j}{\sum_n \sum_{t=2}^T y_{n,t-1}^i} = \frac{A_{ij}}{\sum_{j'} A_{ij'}}$$

$$b_{ik}^{ML} = \frac{\#(i \to k)}{\#(i \to \bullet)} = \frac{\sum_n \sum_{t=1}^T y_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^T y_{n,t}^i} = \frac{B_{ik}}{\sum_{k'} B_{ik'}}$$

  - **What if x is continuous? We can treat $\{(x_{n,t}, y_{n,t}) : t = 1:T, n = 1:N\}$ as $N \times T$ observations of, e.g., a Gaussian, and apply learning rules for Gaussian …**

Supervised ML estimation, ctd.

- **Intuition:**
  - When we know the underlying states, the best estimate of θ is the average frequency of transitions & emissions that occur in the training data
- **Drawback:**
  - Given little data, there may be **overfitting**:
    - $P(x|\theta)$ is maximized, but θ is unreasonable
      0 probabilities – VERY BAD
- **Example:**
  - Given 10 casino rolls, we observe
    `x = 2, 1, 5, 6, 1, 2, 3, 6, 2, 3`
    `y = F, F, F, F, F, F, F, F, F, F`
  - Then: $a_{FF} = 1$; $a_{FL} = 0$
    $b_{F1} = b_{F3} = .2$;
    $b_{F2} = .3$; $b_{F4} = 0$; $b_{F5} = b_{F6} = .1$

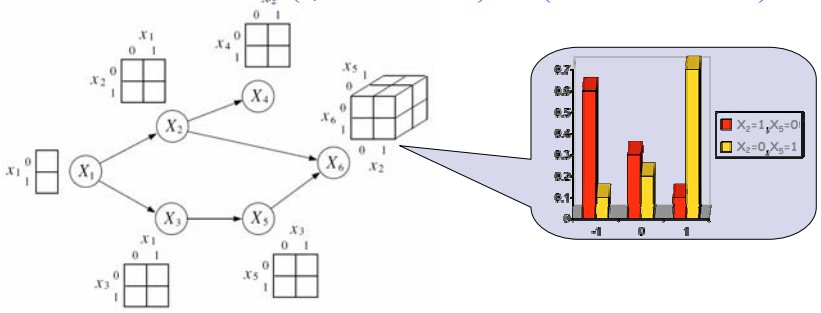
Pseudocounts

- Solution for small training sets:
  - Add pseudocounts
    A_{ij} = # times state transition $i \to j$ occurs in $\mathbf{y}$ + R_{ij}
    B_{ik} = # times state i in $\mathbf{y}$ emits k in $\mathbf{x}$ + S_{ik}
  - R_{ij}, S_{ij} are pseudocounts representing our prior belief
  - Total pseudocounts: $R_i = \Sigma_j R_{ij}$, $S_i = \Sigma_k S_{ik}$,
    - --- "strength" of prior belief,
    - --- total number of imaginary instances in the prior
- Larger total pseudocounts ⇒ strong prior belief
- Small total pseudocounts: just to avoid 0 probabilities --- smoothing
- This is equivalent to Bayesian est. under a uniform prior with "parameter strength" equals to the pseudocounts

MLE for general BN parameters

- If we assume the parameters for each CPD are globally independent, and all nodes are **fully observed**, then the log-likelihood function decomposes into a sum of local terms, one per node:

$$\ell(\theta; D) = \log p(D \mid \theta) = \log \prod_{x_2} \left(\prod_i p(x_{n,i} \mid \mathbf{x}_{n,\pi_i}, \theta_i) \right) = \sum_i \left(\sum_n \log p(x_{n,i} \mid \mathbf{x}_{n,\pi_i}, \theta_i) \right)$$

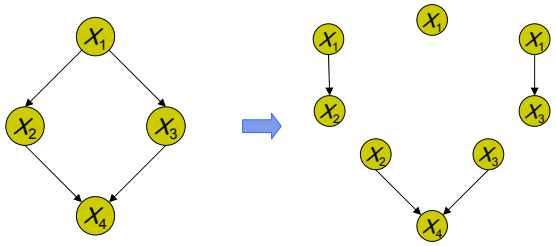


Example: decomposable likelihood of a directed model

- Consider the distribution defined by the directed acyclic GM:

$$p(x \mid \theta) = p(x_1 \mid \theta_1)\, p(x_2 \mid x_1, \theta_1)\, p(x_3 \mid x_1, \theta_3)\, p(x_4 \mid x_2, x_3, \theta_1)$$

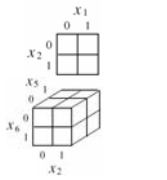
- This is exactly like learning four separate small BNs, each of which consists of a node and its parents.



E.g.: MLE for BNs with tabular CPDs

- Assume each CPD is represented as a table (multinomial) where

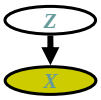
$$\theta_{ijk} \overset{\text{def}}{=} p(X_i = j \mid X_{\pi_i} = k)$$



  - Note that in case of multiple parents, $\mathbf{X}_{\pi_i}$ will have a composite state, and the CPD will be a high-dimensional table
  - The sufficient statistics are counts of family configurations

$$n_{ijk} \overset{\text{def}}{=} \sum_n x_{n,i}^j x_{n,\pi_i}^k$$

- The log-likelihood is $\ell(\theta; \mathcal{D}) = \log \prod_{i,j,k} \theta_{ijk}^{n_{ijk}} = \sum_{i,j,k} n_{ijk} \log \theta_{ijk}$
- Using a Lagrange multiplier to enforce $\sum_j \theta_{ijk} = 1$, we get: $\theta_{ijk}^{ML} = \frac{n_{ijk}}{\sum_{i,j',k} n_{ij'k}}$



Learning partially observed GMs

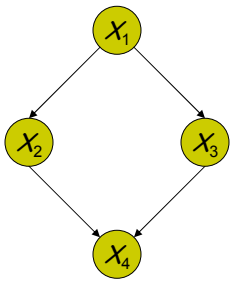
- The data:

$\{(x^{(1)}), (x^{(2)}), (x^{(3)}), \ldots (x^{(N)})\}$

What if some nodes are not observed?

- Consider the distribution defined by the directed acyclic GM:

$$p(x \mid \theta) = p(x_1 \mid \theta_1)\, p(x_2 \mid x_1, \theta_1)\, p(x_3 \mid x_1, \theta_3)\, p(x_4 \mid x_2, x_3, \theta_1)$$



- Need to compute $p(x_H|x_V)$ → inference

Recall: EM Algorithm

- A way of maximizing likelihood function for latent variable models. Finds MLE of parameters when the original (hard) problem can be broken up into two (easy) pieces:
  1. Estimate some "missing" or "unobserved" data from observed data and current parameters.
  2. Using this "complete" data, find the maximum likelihood parameter estimates.
- Alternate between filling in the latent variables using the best guess (posterior) and updating the parameters based on this guess:
  - E-step: $q^{t+1} = \arg\max_q F(q, \theta^t)$
  - M-step: $\theta^{t+1} = \arg\max_\theta F(q^{t+1}, \theta^t)$
- In the M-step we optimize a lower bound on the likelihood. In the E-step we close the gap, making bound=likelihood.

EM for general BNs

while not converged

% E-step

for each node i

$ESS_i = 0$ % reset expected sufficient statistics

for each data sample n

do inference with $X_{n,H}$

for each node i

$$ESS_i += \left\langle SS_i(x_{n,i}, x_{n,\pi_i}) \right\rangle_{p(x_{n,H}|x_{n,-H})}$$

% M-step

for each node i

$\theta_i := \text{MLE}(ESS_i)$

Example: HMM

- **Supervised learning**: estimation when the "right answer" is known
  - **Examples:**

    GIVEN: a genomic region $x = x_1 \ldots x_{1,000,000}$ where we have good (experimental) annotations of the CpG islands

    GIVEN: the casino player allows us to observe him one evening, as he changes dice and produces 10,000 rolls
- **Unsupervised learning**: estimation when the "right answer" is unknown
  - **Examples:**

    GIVEN: the porcupine genome; we don't know how frequent are the CpG islands there, neither do we know their composition

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- **QUESTION:** Update the parameters θ of the model to maximize $P(x|\theta)$ -- Maximal likelihood (ML) estimation

The Baum Welch algorithm

- The complete log likelihood

$$\ell_c(\boldsymbol{\theta};\mathbf{x},\mathbf{y}) = \log p(\mathbf{x},\mathbf{y}) = \log \prod_n \left(p(y_{n,1}) \prod_{t=2}^{T} p(y_{n,t} \mid y_{n,t-1}) \prod_{t=1}^{T} p(x_{n,t} \mid x_{n,t}) \right)$$

- The expected complete log likelihood

$$\langle \ell_c(\boldsymbol{\theta};\mathbf{x},\mathbf{y}) \rangle = \sum_n \left(\langle y_{n,1}^i \rangle_{p(y_{n,1}|\mathbf{x}_n)} \log \pi_i \right) + \sum_n \sum_{t=2}^{T} \left(\langle y_{n,t-1}^i y_{n,t}^j \rangle_{p(y_{n,t-1},y_{n,t}|\mathbf{x}_n)} \log a_{i,j} \right) + \sum_n \sum_{t=1}^{T} \left(x_{n,t}^k \langle y_{n,t}^i \rangle_{p(y_{n,t}|\mathbf{x}_n)} \log b_{i,k} \right)$$

- EM
  - The **E** step

$$\gamma_{n,t}^i = \langle y_{n,t}^i \rangle = p(y_{n,t}^i = 1 \mid \mathbf{x}_n)$$

$$\xi_{n,t}^{i,j} = \langle y_{n,t-1}^i y_{n,t}^j \rangle = p(y_{n,t-1}^i = 1, y_{n,t}^j = 1 \mid \mathbf{x}_n)$$

  - The **M** step ("symbolically" identical to MLE)

$$\pi_i^{ML} = \frac{\sum_n \gamma_{n,1}^i}{N} \qquad a_{ij}^{ML} = \frac{\sum_n \sum_{t=2}^{T} \xi_{n,t}^{i,j}}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i} \qquad b_{ik}^{ML} = \frac{\sum_n \sum_{t=1}^{T} \gamma_{n,t}^i x_{n,t}^k}{\sum_n \sum_{t=1}^{T-1} \gamma_{n,t}^i}$$

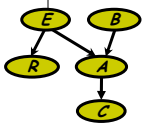
Unsupervised ML estimation

- Given $x = x_1 \ldots x_N$ for which the true state path $y = y_1 \ldots y_N$ is unknown,
  - **EXPECTATION MAXIMIZATION**

0. Starting with our best guess of a model M, parameters θ:
1. Estimate A_{ij}, B_{ik} in the training data
   - How? $A_{ij} = \sum_{n,t} \langle y_{n,t-1}^i y_{n,t}^j \rangle$ $B_{ik} = \sum_{n,t} \langle y_{n,t}^i \rangle x_{n,t}^k$,
2. Update θ according to A_{ij}, B_{ik}
   - Now a "supervised learning" problem
3. Repeat 1 & 2, until convergence

This is called the Baum-Welch Algorithm

We can get to a provably more (or equally) likely parameter set θ each iteration



ML Structural Learning for completely observed GMs

$(x_1^{(1)},\ldots,x_n^{(1)})$
$(x_1^{(2)},\ldots,x_n^{(2)})$
…
$(x_1^{(M)},\ldots,x_n^{(M)})$

Information Theoretic Interpretation of ML

$$
\begin{aligned}
\ell(\theta_G, G; D) &= \log p(D \mid \theta_G, G) \\
&= \log \prod_n \left(\prod_i p(x_{n,i} \mid \mathbf{x}_{n,\pi_i(G)}, \theta_{i\mid\pi_i(G)}) \right) \\
&= \sum_i \left(\sum_n \log p(x_{n,i} \mid \mathbf{x}_{n,\pi_i(G)}, \theta_{i\mid\pi_i(G)}) \right) \\
&= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \frac{count(x_i, \mathbf{x}_{\pi_i(G)})}{M} \log p(x_i \mid \mathbf{x}_{\pi_i(G)}, \theta_{i\mid\pi_i(G)}) \right) \\
&= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \hat{p}(x_i, \mathbf{x}_{\pi_i(G)}) \log p(x_i \mid \mathbf{x}_{\pi_i(G)}, \theta_{i\mid\pi_i(G)}) \right)
\end{aligned}
$$

From sum over data points to sum over count of variable states

Information Theoretic Interpretation of ML (con'd)

$$
\begin{aligned}
\ell(\theta_G, G; D) &= \log \hat{p}(D \mid \theta_G, G) \\
&= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \hat{p}(x_i, \mathbf{x}_{\pi_i(G)}) \log \hat{p}(x_i \mid \mathbf{x}_{\pi_i(G)}, \theta_{i|\pi_i(G)}) \right) \\
&= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \hat{p}(x_i, \mathbf{x}_{\pi_i(G)}) \log \frac{\hat{p}(x_i, \mathbf{x}_{\pi_i(G)}, \theta_{i|\pi_i(G)})}{\hat{p}(\mathbf{x}_{\pi_i(G)})} \frac{\hat{p}(x_i)}{\hat{p}(x_i)} \right) \\
&= M \sum_i \left(\sum_{x_i, \mathbf{x}_{\pi_i(G)}} \hat{p}(x_i, \mathbf{x}_{\pi_i(G)}) \log \frac{\hat{p}(x_i, \mathbf{x}_{\pi_i(G)}, \theta_{i|\pi_i(G)})}{\hat{p}(\mathbf{x}_{\pi_i(G)}) \hat{p}(x_i)} \right) - M \sum_i \left(\sum_{x_i} \hat{p}(x_i) \log p(x_i) \right) \\
&= M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)}) - M \sum_i \hat{H}(x_i)
\end{aligned}
$$

Decomposable score and a function of the graph structure

Structural Search

- How many graphs over *n* nodes? $O(2^{n^2})$
- How many trees over *n* nodes? $O(n!)$
- But it turns out that we can find exact solution of an optimal tree (under MLE)!
  - Trick: in a tree each node has only one parent!
  - Chow-liu algorithm

Chow-Liu tree learning algorithm

- Objection function:

$$\ell(\theta_G, G; D) = \log \hat{p}(D \mid \theta_G, G) = M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)}) - M \sum_i \hat{H}(x_i) \quad \Rightarrow \quad \boxed{C(G) = M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)})}$$

- Chow-Liu:
  - For each pair of variable x_i and x_j
    - Compute empirical distribution: $\hat{p}(X_i, X_j) = \frac{count(x_i, x_j)}{M}$
    - Compute mutual information: $\hat{I}(X_i, X_j) = \sum_{x_i, x_j} \hat{p}(x_i, x_j) \log \frac{\hat{p}(x_i, x_j)}{\hat{p}(x_i)\hat{p}(x_j)}$
  - Define a graph with node $x_1, \ldots, x_n$
    - Edge (I,j) gets weight $\hat{I}(X_i, X_j)$

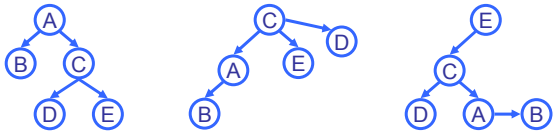
Chow-Liu algorithm (con'd)

- Objection function:

$$\ell(\theta_G, G; D) = \log \hat{p}(D \mid \theta_G, G) = M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)}) - M \sum_i \hat{H}(x_i) \quad \Rightarrow \quad \boxed{C(G) = M \sum_i \hat{I}(x_i, \mathbf{x}_{\pi_i(G)})}$$

- Chow-Liu:

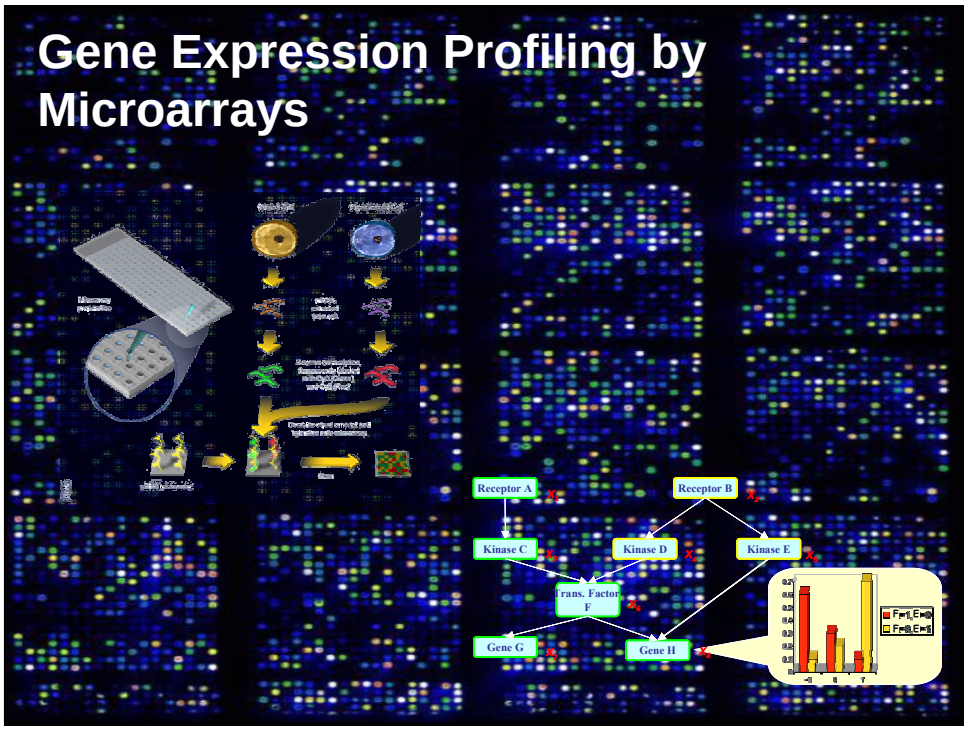
  Optimal tree BN
  - Compute maximum weight spanning tree
  - Direction in BN: pick any node as root, do breadth-first-search to define directions
  - I-equivalence:



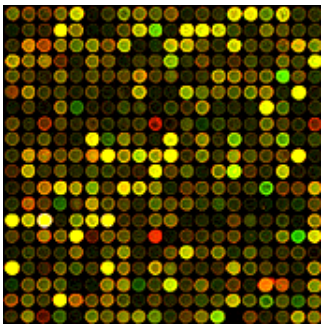
$$C(G) = I(A,B) + I(A,C) + I(C,D) + I(C,E)$$

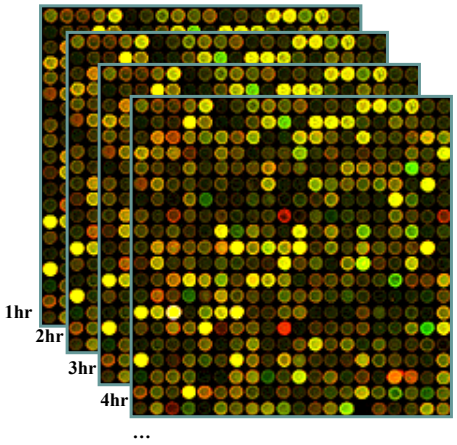
Structure Learning for general graphs

- Theorem:
  - The problem of learning a BN structure with at most *d* parents is NP-hard for any (fixed) $d \geq 2$
- Most structure learning approaches use heuristics
  - Exploit score decomposition
  - Two heuristics that exploit decomposition in different ways
    - Greedy search through space of node-orders
    - Local search of graph structures

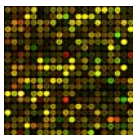


Microarray Data



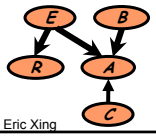


Structure Learning Algorithms



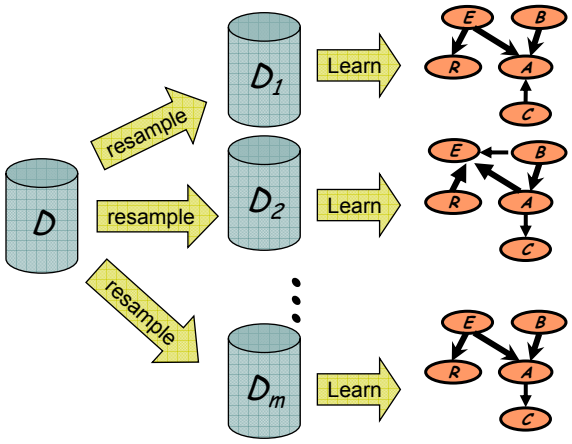
Expression data

Learning Algorithm



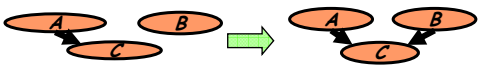
- Structural EM (Friedman 1998)
  - The original algorithm
- Sparse Candidate Algorithm (Friedman et al.)
  - Discretizing array signals
  - Hill-climbing search using local operators: add/delete/swap of a single edge
  - Feature extraction: Markov relations, order relations
  - Re-assemble high-confidence sub-networks from features
- Module network learning (Segal et al.)
  - Heuristic search of structure in a "module graph"
  - Module assignment
  - Parameter sharing
  - Prior knowledge: possible regulators (TF genes)

Scoring Networks



Learning GM structure

- Learning of best CPDs *given DAG* is easy
  - collect statistics of values of each node given specific assignment to its parents
- Learning of the graph topology (structure) is NP-hard
  - heuristic search must be applied, generally leads to a **locally** optimal network
- Overfitting
  - It turns out, that richer structures give higher likelihood P(D|G) to the data (adding an edge is always preferable)



$$P(C \mid A) \leq P(C \mid A, B)$$

  - more parameters to fit => more freedom => always exist more "optimal" CPD(C)
- We prefer *simpler* (more explanatory) networks
  - **Practical** scores **regularize** the likelihood improvement complex networks.

Learning (sparse) GGM

- Multivariate Gaussian over all continuous expressions

$$p([x_1,...,x_n]) = \frac{1}{(2\pi)^{\frac{n}{2}} |\Sigma|^{\frac{1}{2}}} \exp\left\{-\tfrac{1}{2}(\vec{x}-\mu)^T \Sigma^{-1}(\vec{x}-\mu)\right\}$$

- The precision matrix $K=\Sigma^{-1}$ reveals the topology of the (undirected) network

$$E(x_i \mid x_{-i}) = \sum_j (K_{ij}/K_{ii}) x_j$$

  - Edge ~ $|K_{ij}| > 0$

- Learning Algorithm: Covariance selection
  - Want a sparse matrix
    - Regression for each node with degree constraint (Dobra et al.)
    - Regression for each node with hierarchical Bayesian prior (Li, et al)
    - Graphical Lasso (we will describe it shortly)

Learning Ising Model (i.e. pairwise MRF)

- Assuming the nodes are discrete, and edges are weighted, then for a sample x_d, we have

$$P(\mathbf{x}_d|\Theta) = \exp\left(\sum_{i\in V}\theta_{ii}^t x_{d,i} + \sum_{(i,j)\in E}\theta_{ij}x_{d,i}x_{d,j} - A(\Theta)\right)$$

- **Graph lasso** has been used to obtain a sparse estimate of *E* with continuous *X*

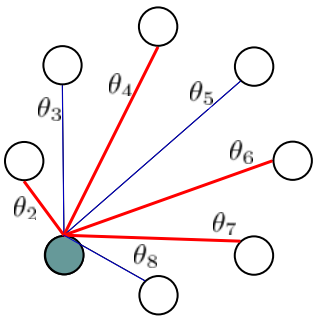
- We can use graphical L_1 regularized logistic regression to obtain a sparse estimate of with discrete *X*

Recall lasso

$$\hat{\theta}_i \;=\; \arg\min_{\theta_i} l(\theta_i) + \lambda_1 \| \theta_i \|_1$$

where $l(\theta_i) = \log P(y_i|\mathbf{x}_i, \theta_i)$.

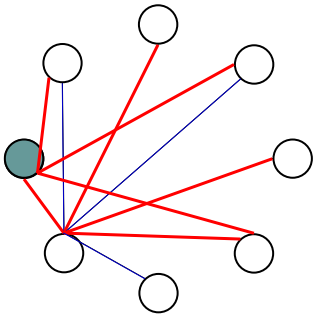
Graph Regression



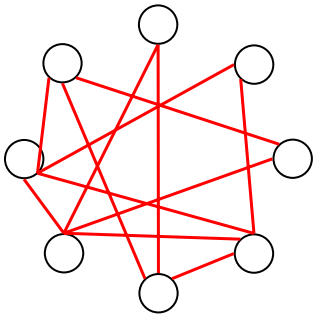
Lasso:

$$\hat{\theta} \;=\; \arg\min_{\theta} \sum_{t=1}^{T} l(\theta) + \lambda_1 \| \theta \|_1$$

Graph Regression



Graph Regression



Consistency

- **Theorem**: for the graphical regression algorithm, under certain verifiable conditions (omitted here for simplicity):

$$\mathbb{P}\left[\hat{G}(\lambda_n) \neq G\right] = \mathcal{O}\left(\exp\left(-Cn^{\epsilon}\right)\right) \to 0$$

Note the from this theorem one should see that the regularizer is not actually used to introduce an "artificial" sparsity bias, but a devise to ensure consistency under finite data and high dimension condition.

Learning GM

- Learning of best CPDs *given DAG* is easy
  - collect statistics of values of each node given specific assignment to its parents
- Learning of the graph topology (structure) is NP-hard
  - heuristic search must be applied, generally leads to a **locally** optimal network
- We prefer *simpler* (more explanatory) networks
  - **Regularized graph regression**