Machine Learning Summer School

Lecture 3: Learning parameters and structure

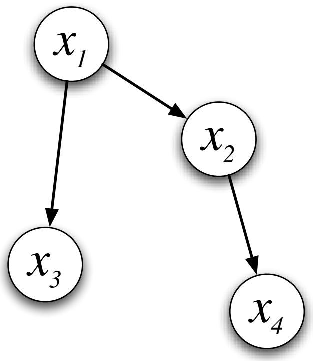
Zoubin Ghahramani
zoubin@eng.cam.ac.uk
http://learning.eng.cam.ac.uk/zoubin/

Department of Engineering
University of Cambridge, UK

Machine Learning Department
Carnegie Mellon University, USA

August 2009

Learning parameters



$$p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_4|x_2)$$

θ_2

x_1 \ x_2			
	0.2	*0.3*	*0.5*
	0.1	*0.6*	*0.3*

Assume each variable x_i is discrete and can take on K_i values.

The parameters of this model can be represented as 4 tables: θ_1 has K_1 entries, θ_2 has $K_1 \times K_2$ entries, etc.

These are called **conditional probability tables** (CPTs) with the following semantics:

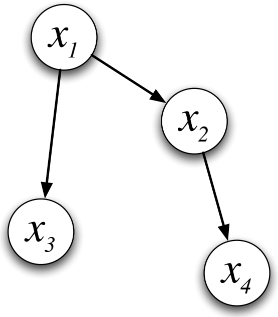
$$p(x_1 = k) = \theta_{1,k} \qquad p(x_2 = k'|x_1 = k) = \theta_{2,k,k'}$$

If node i has M parents, θ_i can be represented either as an $M+1$ dimensional table, or as a 2-dimensional table with $\left(\prod_{j \in \mathrm{pa}(i)} K_j\right) \times K_i$ entries by collapsing all the states of the parents of node i. Note that $\sum_{k'} \theta_{i,k,k'} = 1$.

Assume a data set $\mathcal{D} = \{\mathbf{x}^{(n)}\}_{n=1}^{N}$.

How do we learn θ from $\mathcal{D}$?

Learning parameters



Assume a data set $\mathcal{D} = \{\mathbf{x}^{(n)}\}_{n=1}^{N}$. How do we learn $\boldsymbol{\theta}$ from $\mathcal{D}$?

$$p(\mathbf{x}|\boldsymbol{\theta}) = p(x_1|\theta_1)p(x_2|x_1,\theta_2)p(x_3|x_1,\theta_3)p(x_4|x_2,\theta_4)$$

Likelihood:

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{n=1}^{N} p(\mathbf{x}^{(n)}|\boldsymbol{\theta})$$

Log Likelihood:

$$\log p(\mathcal{D}|\boldsymbol{\theta}) = \sum_{n=1}^{N} \sum_{i} \log p(x_i^{(n)}|x_{\mathrm{pa}(i)}^{(n)}, \theta_i)$$

This decomposes into sum of functions of θ_i. Each θ_i can be optimized separately:

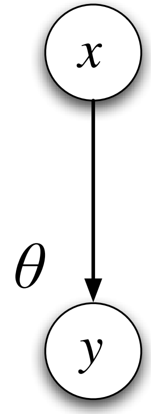
$$\hat{\theta}_{i,k,k'} = \frac{n_{i,k,k'}}{\sum_{k''} n_{i,k,k''}}$$

where $n_{i,k,k'}$ is the number of times in $\mathcal{D}$ where $x_i = k'$ and $x_{\mathrm{pa}(i)} = k$, where k represents a joint configuration of all the parents of i (i.e. takes on one of $\prod_{j \in \mathrm{pa}(i)} K_j$ values)

$$n_2 \quad \begin{array}{c|ccc} & & x_2 & \\ \hline x_1 & 2 & 3 & 0 \\ & 3 & 1 & 6 \end{array} \quad \Rightarrow \quad \theta_2 \quad \begin{array}{c|ccc} & & x_2 & \\ \hline x_1 & 0.4 & 0.6 & 0 \\ & 0.3 & 0.1 & 0.6 \end{array}$$

ML solution: Simply calculate frequencies!

Deriving the Maximum Likelihood Estimate



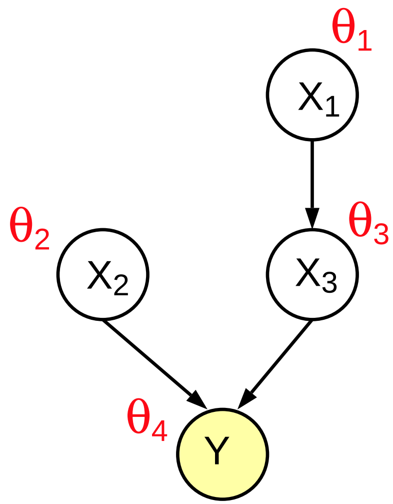
$$p(y|x,\theta) = \prod_{k,\ell} \theta_{k,\ell}^{\delta(x,k)\delta(y,\ell)}$$

Dataset $\mathcal{D} = \{(x^{(n)}, y^{(n)}) : n = 1\ldots, N\}$

$$\begin{aligned}
\mathcal{L}(\theta) &= \log \prod_n p(y^{(n)}|x^{(n)}, \theta) \\
&= \log \prod_n \prod_{k,\ell} \theta_{k,\ell}^{\delta(x^{(n)},k)\delta(y^{(n)},\ell)} \\
&= \sum_{n,k,\ell} \delta(x^{(n)}, k)\delta(y^{(n)}, \ell) \log \theta_{k,\ell} \\
&= \sum_{k,\ell} \left(\sum_n \delta(x^{(n)}, k)\delta(y^{(n)}, \ell) \right) \log \theta_{k,\ell} \;\; = \sum_{k,\ell} n_{k,\ell} \log \theta_{k,\ell}
\end{aligned}$$

Maximize $\mathcal{L}(\theta)$ w.r.t. θ subject to $\sum_\ell \theta_{k,\ell} = 1$ for all k.

Maximum Likelihood Learning with Hidden Variables

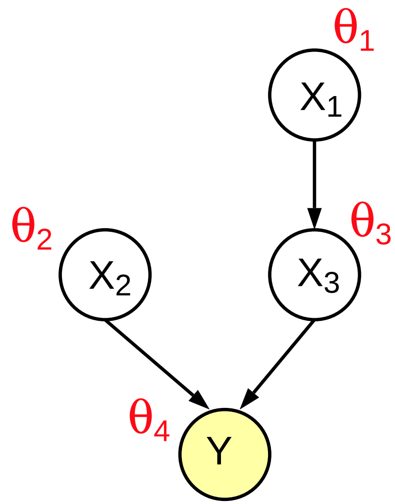


Assume a model parameterised by θ with observable variables Y and hidden variables X

Goal: maximize parameter log likelihood given observed data.

$$\mathcal{L}(\theta) = \log p(Y|\theta) = \log \sum_X p(Y, X|\theta)$$

Maximum Likelihood Learning with Hidden Variables: The EM Algorithm



Goal: maximise parameter log likelihood given observables.

$$\mathcal{L}(\theta) = \log p(Y|\theta) = \log \sum_X p(Y, X|\theta)$$

The Expectation Maximization (EM) algorithm (intuition):

Iterate between applying the following two steps:

- **The E step:** fill-in the hidden/missing variables
- **The M step:** apply complete data learning to filled-in data.

Maximum Likelihood Learning with Hidden Variables: The EM Algorithm

Goal: maximise parameter log likelihood given observables.

$$\mathcal{L}(\theta) = \log p(Y|\theta) = \log \sum_X p(Y, X|\theta)$$

The EM algorithm (derivation):

$$\mathcal{L}(\theta) \quad = \quad \log \sum_X q(X) \frac{p(Y, X|\theta)}{q(X)} \geq \sum_X q(X) \log \frac{p(Y, X|\theta)}{q(X)} = \mathcal{F}(q(X), \theta)$$

- **The E step:** maximize $\mathcal{F}(q(X), \theta^{[t]})$ wrt $q(X)$ holding $\theta^{[t]}$ fixed:

$$q(X) = p(X|Y, \theta^{[t]})$$

- **The M step:** maximize $\mathcal{F}(q(X), \theta)$ wrt θ holding $q(X)$ fixed:

$$\theta^{[t+1]} \leftarrow \mathrm{argmax}_\theta \sum_X q(X) \log p(Y, X|\theta)$$

The E-step requires solving the *inference* problem, finding the distribution over the hidden variables $p(X|Y, \theta^{[t]})$ given the current model parameters. This can be done using **belief propagation** or the **junction tree algorithm**.

Maximum Likelihood Learning without and with Hidden Variables

ML Learning with Complete Data (No Hidden Variables)

Log likelihood decomposes into sum of functions of θ_i. Each θ_i can be optimized separately:

$$\hat{\theta}_{ijk} \leftarrow \frac{n_{ijk}}{\sum_{k'} n_{ijk'}}$$

where n_{ijk} is the number of times in $\mathcal{D}$ where $x_i = k$ and $x_{\mathrm{pa}(i)} = j$.

Maximum likelihood solution: Simply calculate frequencies!

ML Learning with Incomplete Data (i.e. with Hidden Variables)

Iterative EM algorithm

E step: compute expected counts given previous settings of parameters $E[n_{ijk}|\mathcal{D}, \boldsymbol{\theta}^{[t]}]$.

M step: re-estimate parameters using these expected counts

$$\theta_{ijk}^{[t+1]} \leftarrow \frac{E[n_{ijk}|\mathcal{D}, \boldsymbol{\theta}^{[t]}]}{\sum_{k'} E[n_{ijk'}|\mathcal{D}, \boldsymbol{\theta}^{[t]}]}$$

Bayesian Learning

Apply the basic rules of probability to learning from data.

Data set: $\mathcal{D} = \{x_1, \ldots, x_n\}$ Models: m, m' etc. Model parameters: θ

Prior probability of models: $P(m)$, $P(m')$ etc.
Prior probabilities of model parameters: $P(\theta|m)$
Model of data given parameters (likelihood model): $P(x|\theta, m)$

If the data are independently and identically distributed then:

$$P(\mathcal{D}|\theta, m) = \prod_{i=1}^{n} P(x_i|\theta, m)$$

Posterior probability of model parameters:

$$P(\theta|\mathcal{D}, m) = \frac{P(\mathcal{D}|\theta, m)P(\theta|m)}{P(\mathcal{D}|m)}$$

Posterior probability of models:

$$P(m|\mathcal{D}) = \frac{P(m)P(\mathcal{D}|m)}{P(\mathcal{D})}$$

Bayesian parameter learning with no hidden variables

Let n_{ijk} be the number of times ($x_i^{(n)} = k$ and $x_{\mathrm{pa}(i)}^{(n)} = j$) in $\mathcal{D}$.
For each i and j, $\boldsymbol{\theta}_{ij\cdot}$ is a probability vector of length $K_i \times 1$.

Since x_i is a discrete variable with probabilities given by $\boldsymbol{\theta}_{i,j,\cdot}$, the likelihood is:

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_n \prod_i p(x_i^{(n)}|x_{\mathrm{pa}(i)}^{(n)}, \boldsymbol{\theta}) = \prod_i \prod_j \prod_k \theta_{ijk}^{n_{ijk}}$$

If we choose a prior on $\boldsymbol{\theta}$ of the form:

$$p(\boldsymbol{\theta}) = c \prod_i \prod_j \prod_k \theta_{ijk}^{\alpha_{ijk}-1}$$

where c is a normalization constant, and $\sum_k \theta_{ijk} = 1 \; \forall i, j$, then the posterior distribution also has the same form:

$$p(\boldsymbol{\theta}|\mathcal{D}) = c' \prod_i \prod_j \prod_k \theta_{ijk}^{\tilde{\alpha}_{ijk}-1}$$

where $\tilde{\alpha}_{ijk} = \alpha_{ijk} + n_{ijk}$.

This distribution is called the Dirichlet distribution.

Dirichlet Distribution

The Dirichlet distribution is a distribution over the K-dim probability simplex.

Let $\boldsymbol{\theta}$ be a K-dimensional vector s.t. $\forall j : \theta_j \geq 0$ and $\sum_{j=1}^{K} \theta_j = 1$

$$p(\boldsymbol{\theta}|\alpha) = \text{Dir}(\alpha_1, \ldots, \alpha_K) \stackrel{\text{def}}{=} \frac{\Gamma(\sum_j \alpha_j)}{\prod_j \Gamma(\alpha_j)} \prod_{j=1}^{K} \theta_j^{\alpha_j - 1}$$

where the first term is a normalization constant[1] and $E(\theta_j) = \alpha_j / (\sum_k \alpha_k)$

The Dirichlet is conjugate to the multinomial distribution. Let

$$x|\boldsymbol{\theta} \sim \text{Multinomial}(\cdot|\boldsymbol{\theta})$$

That is, $p(x = j|\boldsymbol{\theta}) = \theta_j$. Then the posterior is also Dirichlet:

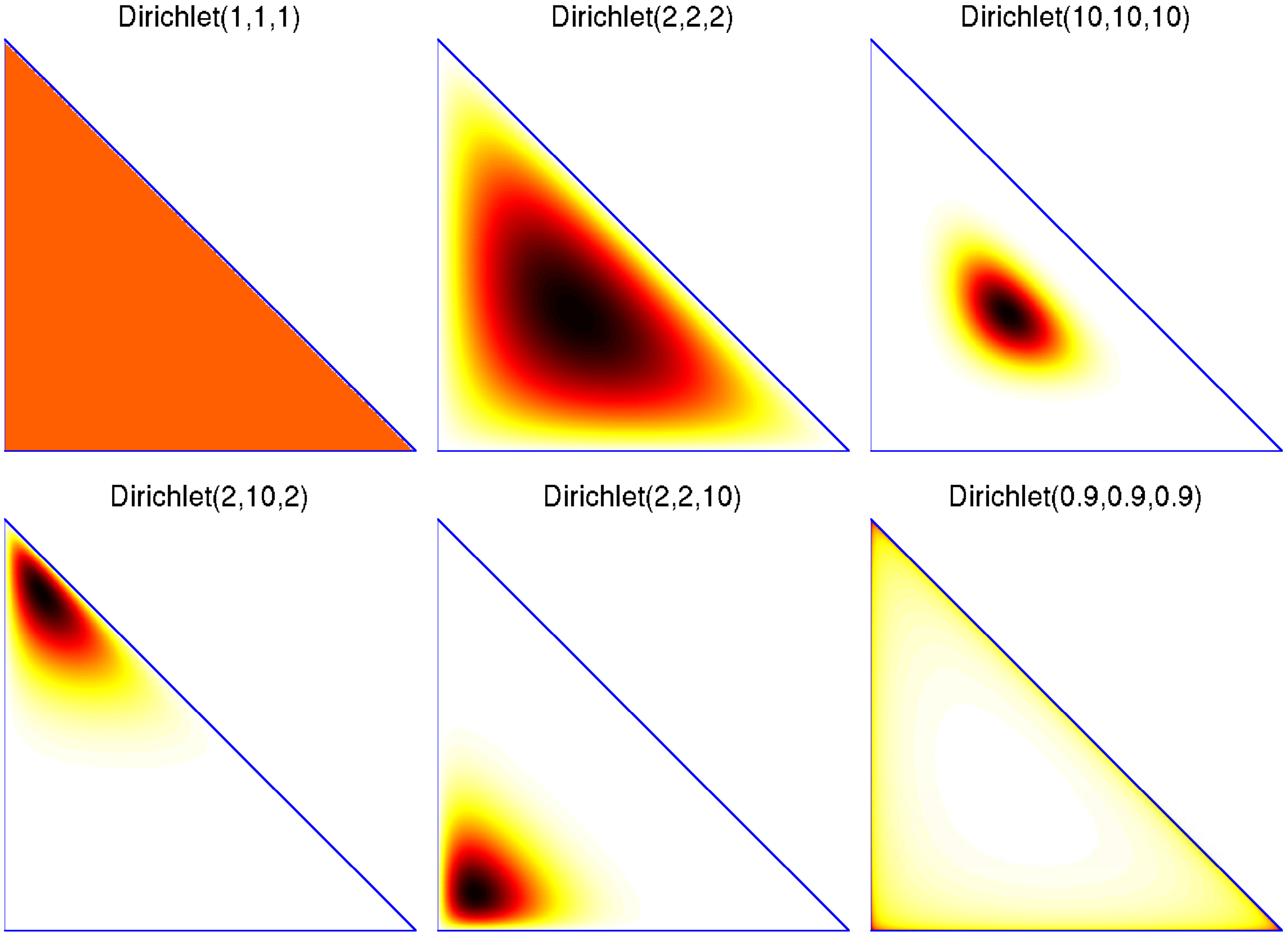
$$\boldsymbol{p(\theta|x = j, \alpha) = \frac{p(x = j|\theta)p(\theta|\alpha)}{p(x = j|\alpha)}} = \text{Dir}(\tilde{\boldsymbol{\alpha}})$$

where $\tilde{\alpha}_j = \alpha_j + 1$, and $\forall \ell \neq j : \tilde{\alpha}_\ell = \alpha_\ell$

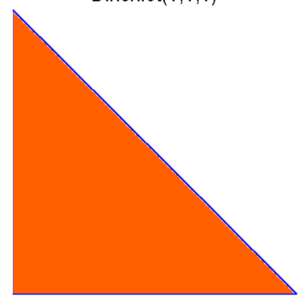
[1] $\Gamma(x) = (x-1)\Gamma(x-1) = \int_0^\infty t^{x-1} e^{-t} dt$. For integer n, $\Gamma(n) = (n-1)!$

Dirichlet Distributions

Examples of Dirichlet distributions over $\boldsymbol{\theta} = (\theta_1, \theta_2, \theta_3)$ which can be plotted in 2D since $\theta_3 = 1 - \theta_1 - \theta_2$:



Example



Assume $\alpha_{ijk} = 1 \ \forall i, j, k$.

This corresponds to a **uniform** prior distribution over parameters θ. This is not a very strong/dogmatic prior, since any parameter setting is assumed a priori possible.

After observed data $\mathcal{D}$, what are the parameter posterior distributions?

$$p(\theta_{ij\cdot}|\mathcal{D}) = \mathrm{Dir}(n_{ij\cdot} + 1)$$

This distribution predicts, for future data:

$$p(x_i = k | x_{\mathrm{pa}(i)} = j, \mathcal{D}) = \frac{n_{ijk} + 1}{\sum_{k'}(n_{ijk'} + 1)}$$

Adding 1 to each of the counts is a form of smoothing called "Laplace's Rule".

Bayesian parameter learning with hidden variables

Notation: let $\mathcal{D}$ be the observed data set, $\mathcal{X}$ be hidden variables, and $\boldsymbol{\theta}$ be model parameters. Assume discrete variables and Dirichlet priors on $\boldsymbol{\theta}$

Goal: to infer $p(\boldsymbol{\theta}|\mathcal{D}) = \sum_{\mathcal{X}} p(\mathcal{X}, \boldsymbol{\theta}|\mathcal{D})$

Problem: since (a)

$$p(\boldsymbol{\theta}|\mathcal{D}) = \sum_{\mathcal{X}} p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{D}) p(\mathcal{X}|\mathcal{D}),$$

and (b) for every way of filling in the missing data, $p(\boldsymbol{\theta}|\mathcal{X}, \mathcal{D})$ is a Dirichlet distribution, and (c) there are exponentially many ways of filling in $\mathcal{X}$, it follows that $p(\boldsymbol{\theta}|\mathcal{D})$ is a mixture of Dirichlets with exponentially many terms!

Solutions:

- Find a single best ("Viterbi") completion of $\mathcal{X}$ (Stolcke and Omohundro, 1993)
- Markov chain Monte Carlo methods
- Variational Bayesian (VB) methods (Beal and Ghahramani, 2003)

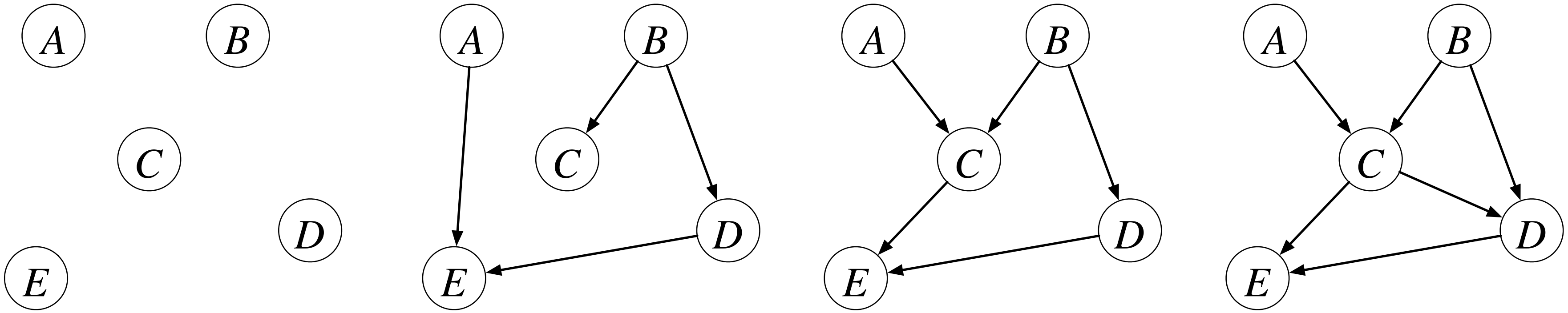
Summary of parameter learning

	Complete (fully observed) data	Incomplete (hidden /missing) data
ML	calculate frequencies	EM
Bayesian	update Dirichlet distributions	MCMC / Viterbi / VB

- For complete data Bayesian learning is not more costly than ML
- For incomplete data VB $\approx$ EM time complexity
- Other parameter priors are possible but Dirichlet is pretty flexible and intuitive.
- For non-discrete data, similar ideas but generally harder inference and learning.

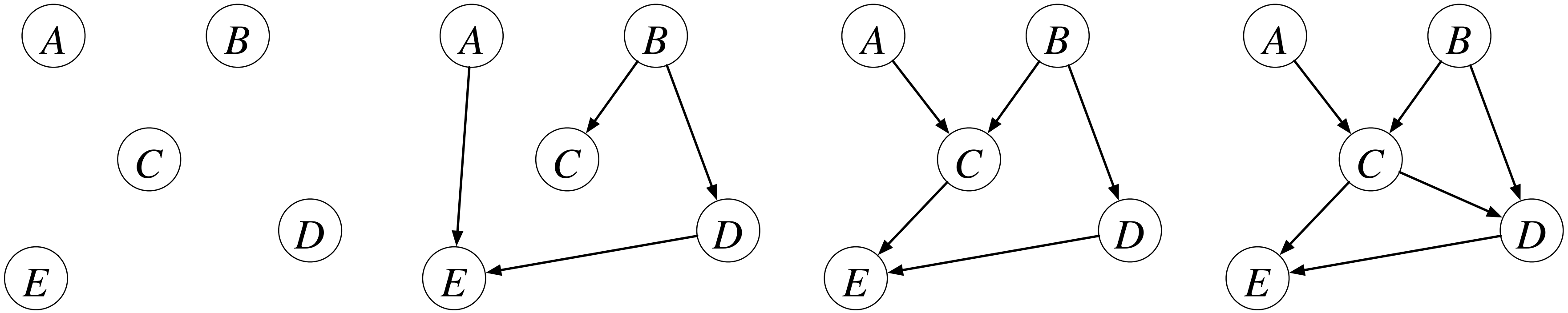
Structure learning

Given a data set of observations of (A, B, C, D, E) can we learn the structure of the graphical model?



Let m denote the graph structure = the set of edges.

Structure learning



Constraint-Based Learning: Use statistical tests of marginal and conditional independence. Find the set of DAGs whose d-separation relations match the results of conditional independence tests.

Score-Based Learning: Use a global score such as the BIC score or Bayesian marginal likelihood. Find the structures that maximize this score.

Score-based structure learning for complete data

Consider a graphical model with structure m, discrete observed data $\mathcal{D}$, and parameters θ. Assume Dirichlet priors.

The Bayesian marginal likelihood score is easy to compute:

$$\text{score}(m) = \log p(\mathcal{D}|m) = \log \int p(\mathcal{D}|\theta, m)p(\theta|m)d\theta$$

$$\text{score}(m) = \sum_i \sum_j \left[\log \Gamma(\sum_k \alpha_{ijk}) - \sum_k \log \Gamma(\alpha_{ijk}) - \log \Gamma(\sum_k \tilde{\alpha}_{ijk}) + \sum_k \log \Gamma(\tilde{\alpha}_{ijk}) \right]$$

where $\tilde{\alpha}_{ijk} = \alpha_{ijk} + n_{ijk}$. **Note that the score decomposes over i.**

One can incorporate structure prior information $p(m)$ as well:

$$\text{score}(m) = \log p(\mathcal{D}|m) + \log p(m)$$

Greedy search algorithm: Start with m. Consider modifications $m \to m'$ (edge deletions, additions, reversals). Accept m' if $\text{score}(m') > \text{score}(m)$. Repeat.

Bayesian inference of model structure: Run MCMC on m.

Bayesian Structural EM for *in*complete data

Consider a graphical model with structure m, observed data $\mathcal{D}$, hidden variables $\mathcal{X}$ and parameters θ

The Bayesian score is generally intractable to compute:

$$\text{score}(m) = p(\mathcal{D}|m) = \int \sum_{\mathcal{X}} p(\mathcal{X}, \theta, \mathcal{D}|m) d\theta$$

Bayesian Structure EM (Friedman, 1998):

1. compute MAP parameters $\hat{\theta}$ for current model m using EM

2. find hidden variable distribution $p(\mathcal{X}|\mathcal{D}, \hat{\theta})$

3. for a small set of candidate structures compute or approximate

$$\text{score}(m') = \sum_{\mathcal{X}} p(\mathcal{X}|\mathcal{D}, \hat{\theta}) \log p(\mathcal{D}, \mathcal{X}|m')$$

4. $m \leftarrow m'$ with highest score

Directed Graphical Models and Causality

Causal relationships are a fundamental component of cognition and scientific discovery.

Even though the independence relations are identical, there is a **causal** difference between

- "smoking" $\rightarrow$ "yellow teeth"
- "yellow teeth" $\rightarrow$ "smoking"

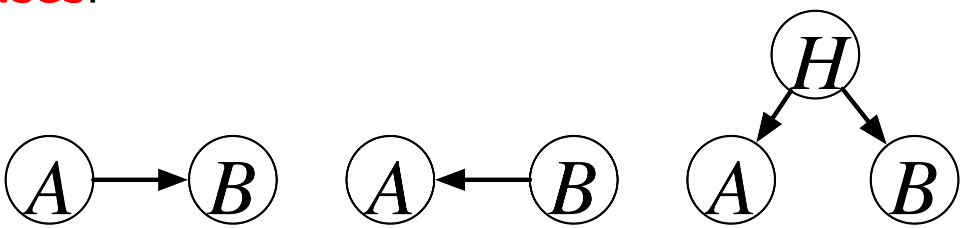
Key idea: interventions and the do-calculus:

$$p(S|Y=y) \neq p(S|\text{do}(Y=y))$$

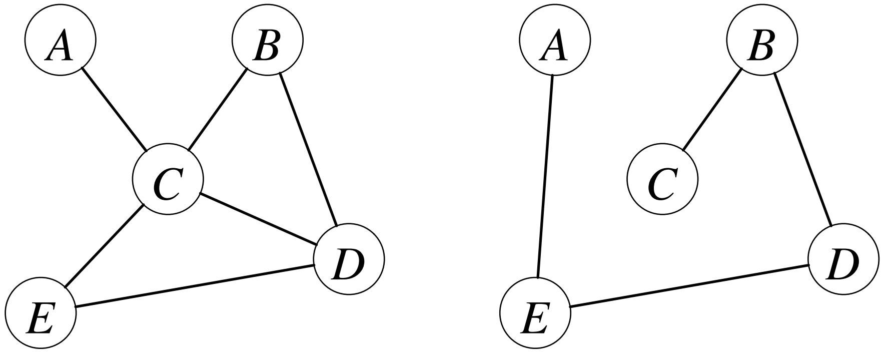
$$p(Y|S=s) = p(Y|\text{do}(S=s))$$

Causal relationships are robust to interventions on the parents.

The **key difficulty** in learning causal relationships from observational data is the presence of **hidden common causes**:



Learning parameters and structure in undirected graphs



$p(\mathbf{x}|\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \prod_j g_j(\mathbf{x}_{C_j}; \boldsymbol{\theta}_j)$ where $Z(\boldsymbol{\theta}) = \sum_{\mathbf{x}} \prod_j g_j(\mathbf{x}_{C_j}; \boldsymbol{\theta}_j)$.

Problem: computing $Z(\boldsymbol{\theta})$ is computationally intractable for general (non-tree-structured) undirected models. Therefore, maximum-likelihood learning of parameters is generally intractable, Bayesian scoring of structures is intractable, etc.

Solutions:

- directly approximate $Z(\boldsymbol{\theta})$ and/or its derivatives (cf. Boltzmann machine learning; contrastive divergence; pseudo-likelihood)
- use approx inference methods (e.g. loopy belief propagation, bounding methods, EP).

See: (Murray and Ghahramani, 2004; Murray et al, 2006) for Bayesian learning in undirected models.

Summary

- Parameter learning in directed models:
  - complete and incomplete data;
  - ML and Bayesian methods
- Structure learning in directed models: complete and incomplete data
- Causality
- Parameter and Structure learning in undirected models

Readings and References

- Beal, M.J. and Ghahramani, Z. (2006) Variational Bayesian learning of directed graphical models with hidden variables. *Bayesian Analysis* 1(4):793–832.
  http://learning.eng.cam.ac.uk/zoubin/papers/BeaGha06.pdf
- Friedman, N. (1998) The Bayesian structural EM algorithm. In *Uncertainty in Artificial Intelligence (UAI-1998)*. http://robotics.stanford.edu/ nir/Papers/Fr2.pdf
- Friedman, N. and Koller, D. (2003) Being Bayesian about network structure. A Bayesian approach to structure discovery in Bayesian networks. *Machine Learning*. 50(1): 95–125.
  http://www.springerlink.com/index/NQ13817217667435.pdf
- Ghahramani, Z. (2004) Unsupervised Learning. In Bousquet, O., von Luxburg, U. and Raetsch, G. *Advanced Lectures in Machine Learning*. 72-112.
  http://learning.eng.cam.ac.uk/zoubin/papers/ul.pdf
- Heckerman, D. (1995) A tutorial on learning with Bayesian networks. In *Learning in Graphical Models*.
  http://research.microsoft.com/pubs/69588/tr-95-06.pdf
- Murray, I.A., Ghahramani, Z., and MacKay, D.J.C. (2006) MCMC for doubly-intractable distributions. In *Uncertainty in Artificial Intelligence (UAI-2006)*.
  http://learning.eng.cam.ac.uk/zoubin/papers/doubly_intractable.pdf
- Murray, I.A. and Ghahramani, Z. (2004) Bayesian Learning in Undirected Graphical Models: Approximate MCMC algorithms. In *Uncertainty in Artificial Intelligence (UAI-2004)*.
  http://learning.eng.cam.ac.uk/zoubin/papers/uai04murray.pdf
- Stolcke, A. and Omohundro, S. (1993) Hidden Markov model induction by Bayesian model merging. In *Advances in Neural Information Processing Systems (NIPS)*.
  http://omohundro.files.wordpress.com/2009/03/stolcke_omohundro93_hmm_induction_bayesian_model_merging.pdf