Bayesian Model Selection

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Overview

- Bayesian Learning of CPTs
- Dealing with Multiple Models
- Other Scores for Model Comparison
- Searching over Belief Network structures
- Readings: Bishop §3.4, Heckerman tutorial sections 1, 2, 3, 4, 5, 7, 8.1, 11

Learning in Belief Networks

	Known Structure	Unknown Structure
Complete Data	Statistical parameter estimation	Discrete search over structures
Incomplete Data	EM, stochastic sampling methods	Combined search over structures and parameters

(Friedman and Goldszmidt, 1998)

- Data + prior/expert beliefs $\Rightarrow$ Belief networks

Bayesian Learning with Complete Data

- Belief network with m nodes, $x_1, \ldots, x_m$, parameters $\boldsymbol{\theta}$
- Log likelihood

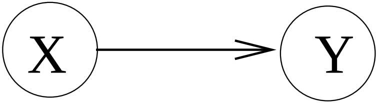
$$
\begin{aligned}
L(\boldsymbol{\theta}; D) &= \sum_{i=1}^{n} \log p(x_1^i, \ldots, x_m^i | \boldsymbol{\theta}) \\
&= \sum_{i=1}^{n} \sum_{j=1}^{m} \log p(x_j^i | pa_j^i, \theta_j)
\end{aligned}
$$

- The likelihood decomposes according to the structure of the network
- $\Rightarrow$ independent estimation problems for MLE

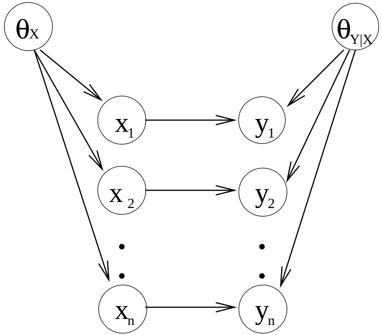
- If priors for each CPT are independent, so are posteriors
- Posterior for each multinomial CPT $P(X_j|Pa_j)$ is Dirichlet with parameters

$$\alpha(X_j = 1|pa_j) + n(X_j = 1|pa_j), \ldots, \\ , \alpha(X_j = r|pa_j) + n(X_j = r|pa_j)$$

Example: $X \rightarrow Y$



- Parameters θ_X, $\theta_{Y|X}$



- Read off from network: complete data $\implies$ posteriors for θ_X and $\theta_{Y|X}$ are independent
- Reduces to 3 separate thumbtack-learning problems

Dealing with Multiple Models

- Let M index possible model structures, with associated parameters $\boldsymbol{\theta}_M$
$$p(M|D) \propto p(D|M)p(M)$$
- For complete data (plus some other assumptions) the marginal likelihood $p(D|M)$ can be computed in closed form
- Making predictions
$$\begin{aligned} p(\mathbf{x}_{n+1}|D) &= \sum_M p(M|D)p(\mathbf{x}_{n+1}|M, D) \\ &= \sum_M p(M|D) \int p(\mathbf{x}_{n+1}|\boldsymbol{\theta}_M, M)p(\boldsymbol{\theta}_M|D, M)\ d\boldsymbol{\theta}_M \end{aligned}$$
- Can approximate $\sum_M$ by keeping the best or the top few models

Comparing models

$$\text{Bayes factor} = \frac{P(D|M_1)}{P(D|M_2)}$$

$$\frac{P(M_1|D)}{P(M_2|D)} = \frac{P(M_1)}{P(M_2)} \cdot \frac{P(D|M_1)}{P(D|M_2)}$$

$$\text{Posterior ratio} = \text{Prior ratio} \times \text{Bayes factor}$$

Strength of evidence from Bayes factor (Kass, 1995; after Jeffreys, 1961)

1 to 3	Not worth more than a bare mention
3 to 20	Positive
20 to 150	Strong
> 150	Very strong

Computing $P(D|M)$

- For the thumbtack example

$$p(D|M) = \frac{\Gamma(\alpha)}{\Gamma(\alpha + n)} \prod_{i=1}^{r} \frac{\Gamma(\alpha_i + n_i)}{\Gamma(\alpha_i)}$$

- The graph $X \longrightarrow Y$ corresponds to 3 separate thumbtack problems for X, $Y|X = \textit{heads}$ and $Y|X = \textit{tails}$

General form of $P(D|M)$ for a discrete belief network

$$p(D|M) = \prod_{i=1}^{m} \prod_{j=1}^{q_i} \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + n_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(\alpha_{ijk} + n_{ijk})}{\Gamma(\alpha_{ijk})}$$

where

- n_{ijk} is the number of cases where $X_i = x_i^k$ and $Pa_i = pa_i^j$
- r_i is the number of states of X_i
- q_i is the number of configurations of the parents of X_i

$$\alpha_{ij} = \sum_{k=1}^{r_i} \alpha_{ijk} \qquad n_{ij} = \sum_{k=1}^{r_i} n_{ijk}$$

- Formula due to Cooper and Herskovits (1992)
- Simply the product of the thumbtack result over all nodes and states of the parents

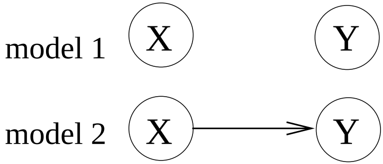
Computation of Marginal Likelihood

Efficient closed form if

- No missing data or hidden variables
- Parameters are independent in prior
- Local distributions are in the exponential family (e.g. multinomial, Gaussian, Poisson, ...)
- Conjugate priors are used

Example

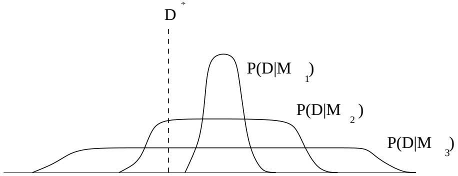
Given data D, compare the two models



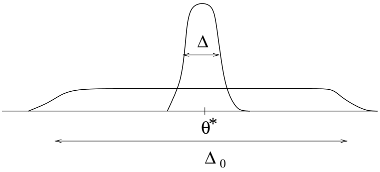
Counts: $hh = 6$, $ht = 2$, $th = 8$, $tt = 4$, from marginal probabilities
$P(X = h) = 0.4$ and $P(Y = h) = 0.7$
Bayes factor $= \frac{P(D|M_1)}{P(D|M_2)} = 1.97$ in favour of model 1
Log Likelihood criterion favours model 2
$\log L(M1) - \log L(M2) = -0.08$

How Bayesian model comparison works

- Consider three models M_1, M_2 and M_3 which are under complex, just right and over complex for a particular dataset D^*
- Note that $P(D|M_i)$ must be *normalized*



- Warning: it can make sense to use a model with an infinite number of parameters (but in a way that the prior is "nice")



- Another view (for a single parameter θ)

$$
\begin{aligned}
P(D|M_i) &= \int p(D|\theta, M_i)p(\theta|M_i)d\theta \\
&\simeq p(D|\theta^*, M_i)p(\theta^*|M_i)\Delta \\
&\simeq p(D|\theta^*, M_i)\frac{\Delta}{\Delta_0}
\end{aligned}
$$

- This last term is known as an *Occam factor*
- The analysis can be extended to multidimensional $\boldsymbol{\theta}$. Pay an Occam factor on each dimension if parameters are well-determined by data; thus models with more parameters can be penalized more

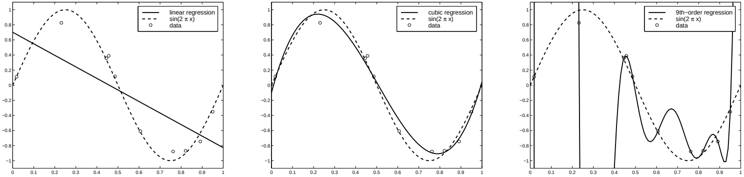
Other scores for comparing models

Above we have used $P(D|M)$ to score models. Other ideas include

- **Maximum likelihood**

$$L(M; D) = \max_{\theta_M} L(\boldsymbol{\theta}_M, M; D)$$

- Bad choice: adding arcs always helps
- Example from supervised learning

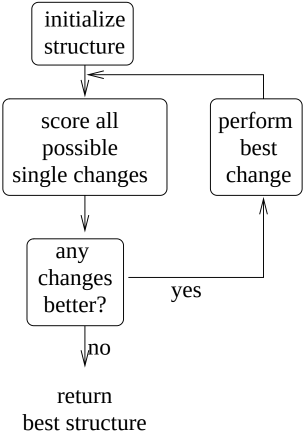


- **Penalize More Complex Models**: e.g. AIC (Akaike Information Criterion), BIC (Bayesian Information Criterion), Structural Risk Minimization (penalize hypothesis classes based on their VC dimension). BIC can be seen as large *n* approximation ot full Bayesian method.
- **Minimum description length**: (Rissanen, Wallace) closely related to Bayesian method
- **Restrict the hypothesis space** to limit the capability for overfitting: but how much?
- **Holdout/Cross-validation**: validate generalization on data withheld during training—but this “wastes” data . . .

Searching over structures

- Number of possible structures over m variables is super-exponential in m
- Finding the BN with the highest marginal likelihood among those structures with at most k parents is NP-hard if $k > 1$ (Chickering, 1995)
- Note: efficient search over trees
- Otherwise, use heuristic methods such as greedy search

Greedy search



Example

College plans of high-school seniors (Heckerman, 1995/6).

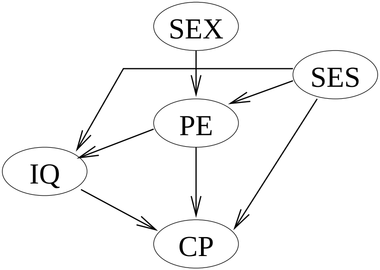
Variables are

- Sex: male, female
- Socioeconomic status: low, low mid, high mid, high
- IQ: low, low mid, high mid, high
- Parental encouragement: low, high
- College plans: yes, no

Priors

- **Structural prior**: SEX has no parents, CP has no children, otherwise uniform
- **Parameter prior**: Uniform distributions

Best network found



- Odd that SES has a direct link to IQ: suggests that a hidden variable is needed
- Searching over structures for visible variables is hard; inferring hidden structure is even harder...

Acknowledgements: this presentation has been greatly aided by the tutorials by Nir Friedman and Moises Goldszmidt
http://www.erg.sri.com/people/moises/tutorial/index.htm
ans David Heckerman
http://research.microsoft.com/~heckerman/