Lecture 15
Model selection/ structure learning

Koller & Friedman chapter 14
Mackay chapter 28

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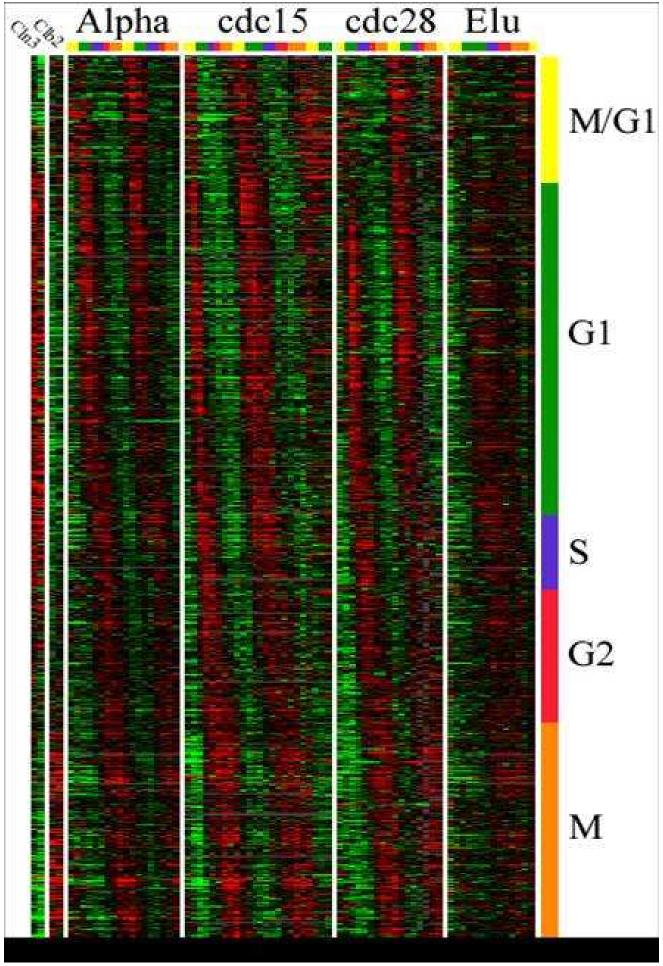
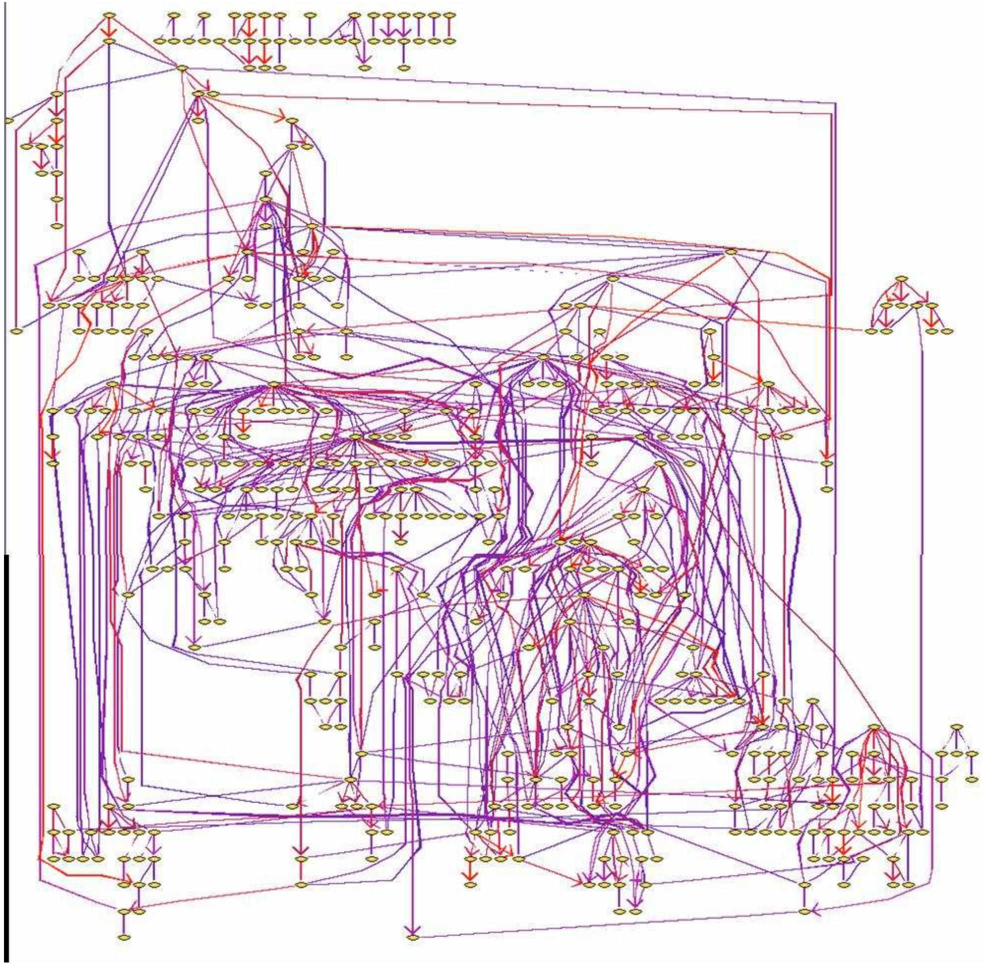
Structure learning: why?

- We often want to learn the structure of the graphical model:
  - Scientific discovery (data mining)
  - Use a good model for prediction, compression, classification etc.
- Often there may be more than one good model
  - Look for features that they all share
  - Average predictions over models

Learning gene regulatory pathways





Structure learning: how?

- Constraint-based approach:
  - Assume some way of testing conditional independencies $X_1 \perp X_2 | X_3$
  - Then construct model consistent with these results
- Search-and-score approach:
  - Define a scoring function for measuring model quality (e.g., marginal likelihood or penalized likelihood)
  - Use a search algorithm to find a (local) maximum of the score

IDENTIFIABILITY

- DAGs are I-equivalent if they encode the same set of conditional independencies, e.g., $X \rightarrow Y \rightarrow Z$ and $X \leftarrow Y \leftarrow Z$ are indistinguishable given just observational data.
- However, $X \rightarrow Y \leftarrow Z$ has a v-structure, which has a unique statistical signature. Hence some arc directions can be inferred from passive observation.
- The set of I-equivalent DAGs can be represented by a PDAG (partially directed acyclic graph).
- Distinguishing between members of an equivalence class requires interventions/ experiments.

Constraint-based approach

- The build-PDAG algorithm from K&F chapter 3 can recover the true DAG up to I-equivalence in $O(N^3 2^d)$ time if we make the following assumptions:
  - The maximum fan-in (number of parents) of any node is d
  - The independence test oracle can handle up to $2d + 2$ variables
  - The underlying distribution P^* is *faithful* to G^* i.e., there are no spurious independencies that are not sanctioned by G^* (G^* is a P-map of P^*).
- This is often called the IC or PC algorithm.

CONSTRAINT-BASED APPROACH

- Bad
  - Faithfulness assumption rules out certain CPDs like noisy-OR.
  - Hard to make a reliable independence test (especially given small data sets) which does not make too many errors (either false positives or false negatives).
  - One misleading independence test result can result in multiple errors in the resulting PDAG, so overall the approach is not very robust to noise.
- Good
  - PC algorithm is less dumb than local search

Independence tests

- An independence test $X \perp Y$ seeks to accept or reject the null hypothesis H_0 that $P^*(X,Y) = P^*(X)P^*(Y)$.
- We need a decision rule that maps data to accept/reject.
- We define a scalar measure of deviance $d(D)$ from the null hypothesis.
- The p-value of a threshold t is the probability of falsely rejecting the null hypothesis:

$$p(t) = P(\{D : d(D) > t\} | H_0, N)$$

- Note that we need to know the size of the data set N (stopping rule) ahead of time!
- We usually choose a threshold t so that the probability of a false rejection is below some significance level $\alpha = 0.05$.

Independence tests

- For discrete data, a common deviance is the χ^2 statistic, which measures how far the counts are from what we would expect given independence:

$$d_{\chi^2}(D) = \sum_{x,y} \frac{(O_{x,y} - E_{x,y})^2}{E_{x,y}} = \sum_{x,y} \frac{(N(x,y) - NP(x)P(y))^2}{NP(x)P(y)}$$

- The p-value requires summing over all datasets of size N:

$$p(t) = P(\{D : d(D) > t\} | H_0, N)$$

- Since this is expensive in general, a standard approximation is to consider the expected distribution of $d(D)$ (under the null hypothesis) as $N \rightarrow \infty$, and use this to define thresholds to achieve a given significance.

Example of classical hypothesis testing

- When spun on edge $N = 250$ times, a Belgian one-euro coin came up heads $Y = 140$ times and tails 110.
- We would like to distinguish two models, or hypotheses: H_0 means the coin is unbiased (so $p = 0.5$); H_1 means the coin is biased (has probability of heads $p \neq 0.5$).
- p-value is “less than 7%”: $p = P(Y \geq 140) + P(Y \leq 110) = 0.066$:

  ```
  n=250; p = 0.5; y = 140;
  p = (1-binocdf(y-1,n,p)) + binocdf(n-y,n,p)
  ```

- If $Y = 141$, we get $p = 0.0497$, so we can reject the null hypothesis at significance level 0.05.
- But is the coin really biased?

Bayesian approach

- We want to compute the posterior ratio of the 2 hypotheses:

$$\frac{P(H_1|D)}{P(H_0|D)} = \frac{P(D|H_1)P(H_1)}{P(D|H_0)P(H_0)}$$

- Let us assume a uniform prior $P(H_0) = P(H_1) = 0.5$.
- Then we just focus on the ratio of the marginal likelihoods:

$$P(D|H_1) = \int_0^1 d\theta \;\; P(D|\theta, H_1)P(\theta|H_1)$$

- For H_0, there is no free parameter, so

$$P(D|H_0) = 0.5^N$$

where N is the number of coin tosses in D.

Parameter prior

- How to compute $P(D|H_1)$?
- Let us assume a beta prior on the coin bias θ

$$P(\theta|\alpha, H_1) = \beta(\theta; \alpha_h, \alpha_t) = \frac{1}{Z(\alpha_h, \alpha_t)} \theta^{\alpha_h - 1}(1-\theta)^{\alpha_t - 1}$$

where

$$Z(\alpha_h, \alpha_t) = \int_0^1 d\theta \quad \theta^{\alpha_h - 1}(1-\theta)^{\alpha_t - 1} = \frac{\Gamma(\alpha_h)\Gamma(\alpha_t)}{\Gamma(\alpha_h + \alpha_t)}$$

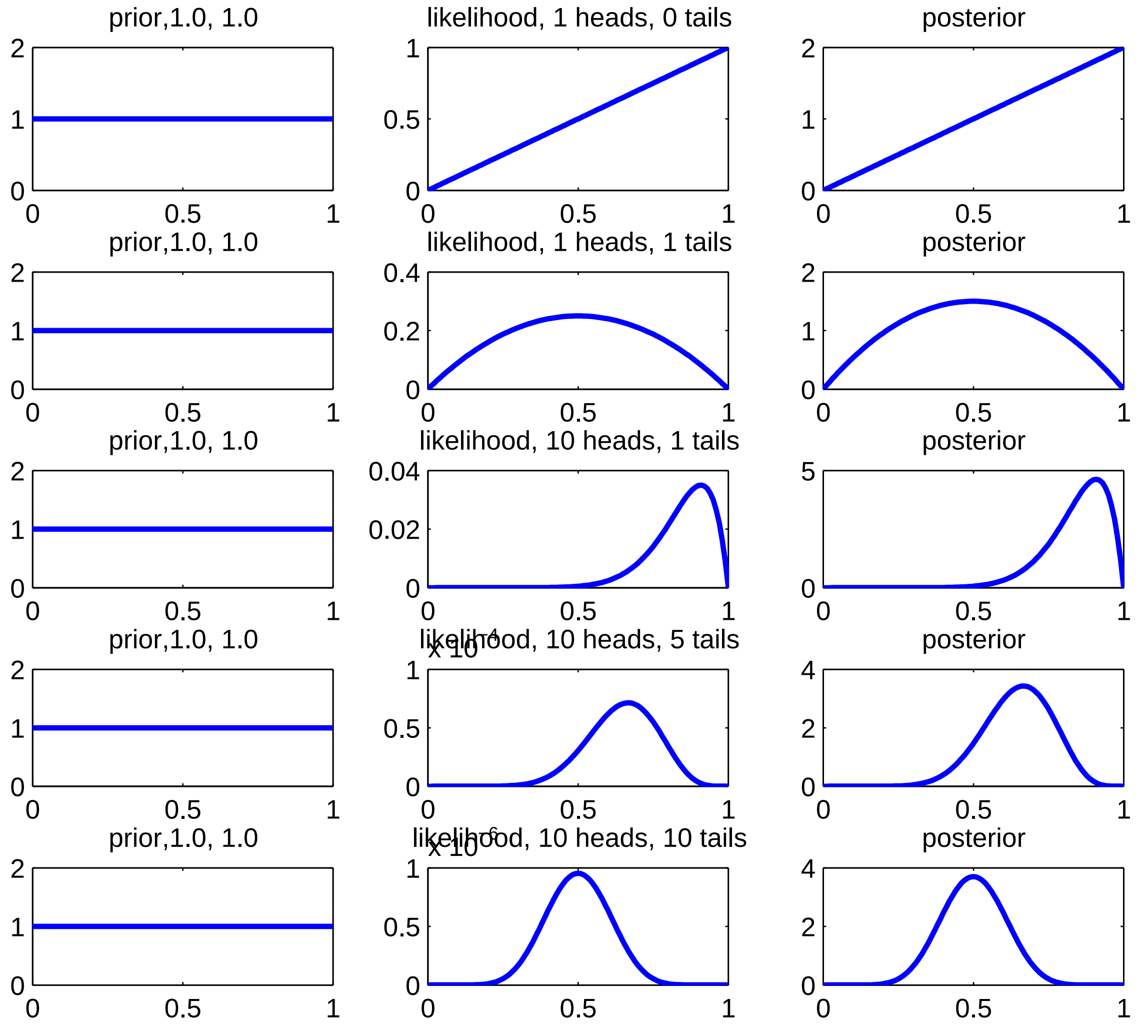
- $\Gamma(n) = (n-1)!$ for positive integers.
- Mean $E\theta = \frac{\alpha_h}{\alpha_h + \alpha_t}$.
- If we set $\alpha_h = \alpha_t = 1$, we get a uniform prior (and $Z = 1$).

Parameter posterior

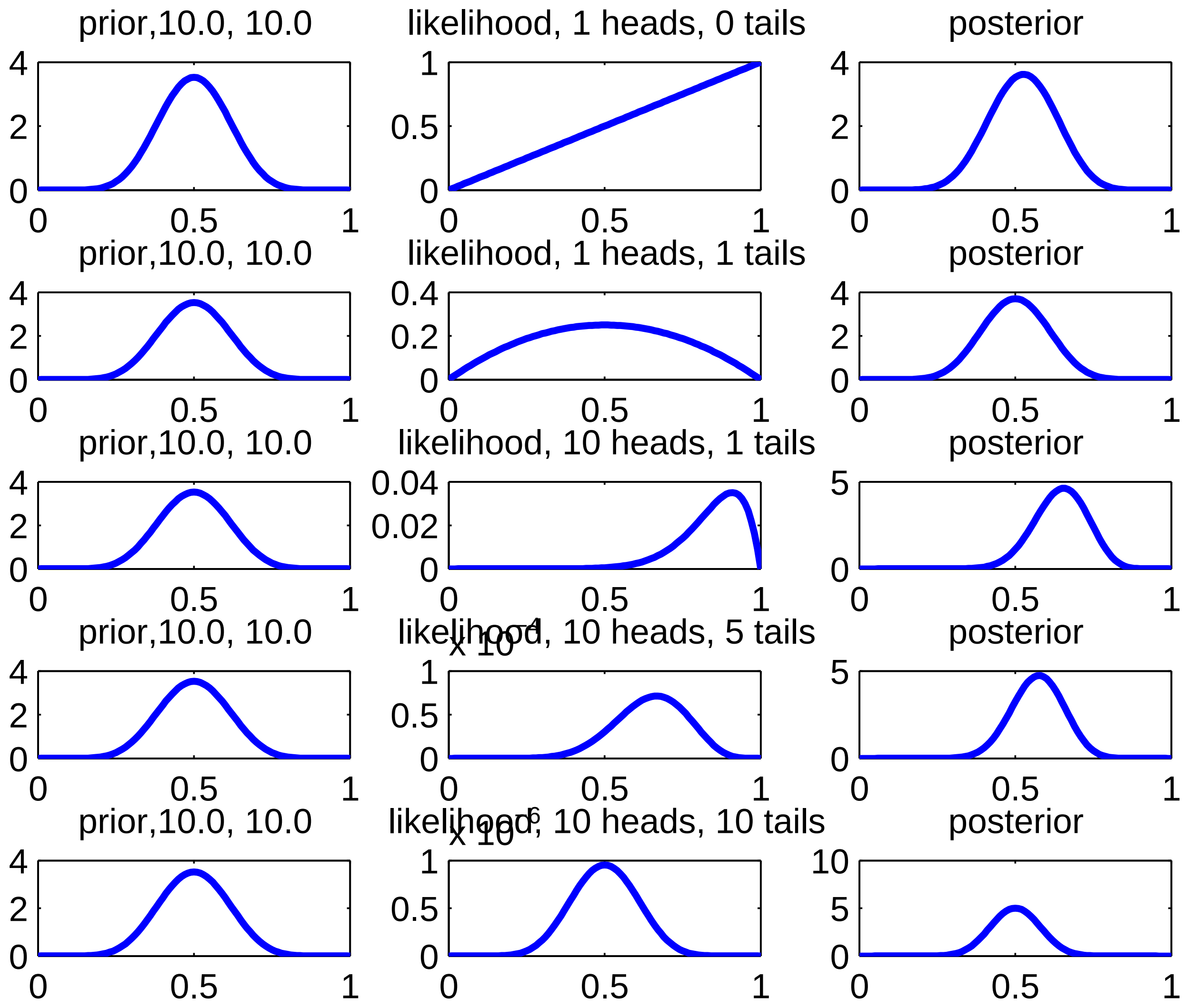
- Suppose we see D_h heads and D_t tails. The parameter posterior is

$$\begin{aligned} P(\theta|D,\alpha) &= \frac{p(\theta|\alpha)P(D|\theta,\alpha)}{P(D|\alpha)} \\ &= \frac{1}{P(D|\alpha)}\frac{1}{Z(\alpha_h,\alpha_t)}\theta^{\alpha_h-1}(1-\theta)^{\alpha_t-1}\theta^{D_h}(1-\theta)^{D_t} \\ &= \beta(\theta;\alpha_h+D_h,\alpha_t+D_t) \end{aligned}$$

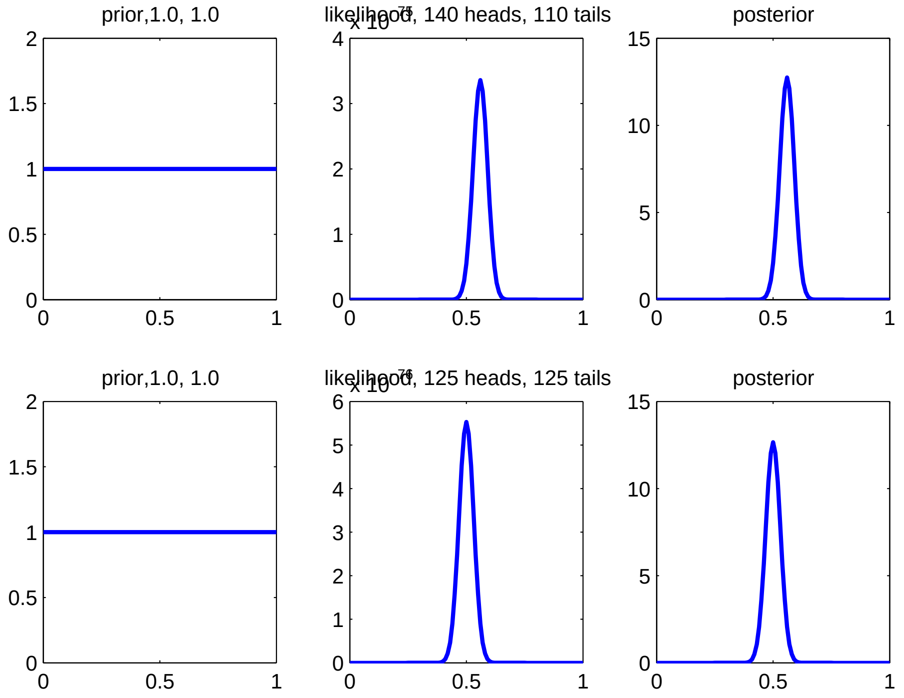
Parameter posterior - small sample, uniform prior



Parameter posterior - small sample, strong prior



Parameter posterior - coin data, uniform prior



```
thetas = 0:0.01:1;
alphaH = 1; alphaT = 1;
prior = betapdf(thetas, alphaH, alphaT);
lik = thetas.^Nh .* (1-thetas).^Nt;
post = betapdf(thetas, alphaH+Nh, alphaT+Nt);
```

Model evidence

- Suppose we see D_h heads and D_t tails. The parameter posterior is

$$
\begin{aligned}
P(\theta|D,\alpha) &= \frac{p(\theta|\alpha)P(D|\theta,\alpha)}{P(D|\alpha)} \\
&= \frac{1}{P(D|\alpha)}\frac{1}{Z(\alpha_h,\alpha_t)}\theta^{\alpha_h-1}(1-\theta)^{\alpha_t-1}\theta^{D_h}(1-\theta)^{D_t} \\
&= \beta(\theta;\alpha_h+D_h,\alpha_t+D_t)
\end{aligned}
$$

where the marginal likelihood (evidence) is

$$
\begin{aligned}
P(D|\alpha) &= \frac{Z(\alpha_h+N_h,\alpha_t+N_t)}{Z(\alpha_h,\alpha_t)} \\
&= \frac{\Gamma(\alpha)}{\Gamma(\alpha+N)}\cdot\frac{\Gamma(\alpha_h+N_h)}{\Gamma(\alpha+N)}\cdot\frac{\Gamma(\alpha_t+N_t)}{\Gamma(\alpha+N)}
\end{aligned}
$$

Sequentially evaluating the evidence

- By the chain rule of probability,

$$P(x_{1:N}) = P(x_1)P(x_2|x_1)P(x_3|x_{1:2})\ldots$$

- Also, after N data cases, $P(X|D_{1:N}) = Dir(\vec{\alpha} + \vec{N})$, so

$$P(X = k|D_{1:N}, \vec{\alpha}) = \frac{N_k + \alpha_k}{\sum_i N_i + \alpha_i} \overset{\text{def}}{=} \frac{N_k + \alpha_k}{N + \alpha}$$

- Suppose $D = H, T, T, H, H, H$. Then

$$\begin{aligned} P(D) &= \frac{\alpha_h}{\alpha} \cdot \frac{\alpha_t}{\alpha + 1} \cdot \frac{\alpha_t + 1}{\alpha + 2} \cdot \frac{\alpha_h + 1}{\alpha + 3} \cdot \frac{\alpha_h + 2}{\alpha + 4} \\ &= \frac{[\alpha_h(\alpha_h + 1)(\alpha_h + 2)]\,[\alpha_t(\alpha_t + 1)]}{\alpha(\alpha + 1)\cdots(\alpha + 4)} \\ &= \frac{[(\alpha_h)\cdots(\alpha_h + N_h - 1)]\,[(\alpha_t)\cdots(\alpha_t + N_t - 1)]}{(\alpha)\cdots(\alpha + N)} \end{aligned}$$

Model evidence

- For integers,

$$
\begin{aligned}
&(\alpha)(\alpha+1)\cdots(\alpha+M-1)\\
&\quad = \frac{(a+M-1)!}{(\alpha-1)!}\\
&\quad = \frac{(a+M-1)(a+M-2)\cdots(a+M-M)(a+M-M-1)\cdots 2\cdot 1}{(a-1)(a-2)\cdots 2\cdot 1}\\
&\quad = \frac{(a+M-1)(a+M-2)\cdots(a)(a-1)\cdots 2\cdot 1}{(a-1)(a-2)\cdots 2\cdot 1}
\end{aligned}
$$

- For reals, we replace $(a-1)!$ with $\Gamma(a)$.

- Hence

$$
\begin{aligned}
P(D) &= \frac{[(\alpha_h)\cdots(\alpha_h+N_h-1)]\,[(\alpha_t)\cdots(\alpha_t+N_t-1)]}{(\alpha)\cdots(\alpha+N)}\\
&= \frac{\Gamma(\alpha)}{\Gamma(\alpha+N)}\cdot\frac{\Gamma(\alpha_h+N_h)}{\Gamma(\alpha+N)}\cdot\frac{\Gamma(\alpha_t+N_t)}{\Gamma(\alpha+N)}
\end{aligned}
$$

Ratio of evidences (Bayes factor)

- We compute the ratio of marginal likelihoods (evidence):

$$\frac{P(H_1|D)}{P(H_0|D)} = \frac{P(D|H_1)}{P(D|H_0)} = \frac{Z(\alpha_h + N_h, \alpha_t + N_t)}{Z(\alpha_h, \alpha_t)} \frac{1}{0.5^N}$$

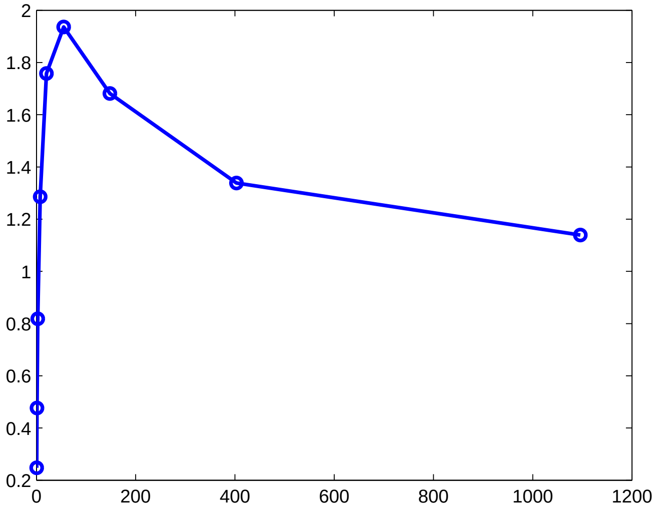
$$= \frac{\Gamma(140+\alpha)\Gamma(110+\alpha)}{\Gamma(250+2\alpha)} \times \frac{\Gamma(2\alpha)}{\Gamma(\alpha)\Gamma(\alpha)} \times 2^{250}$$

- Must work in log domain!

```
alphas = [0.37 1 2.7 7.4 20 55 148 403 1096];
Nh = 140; Nt = 110; N = Nh+Nt;
numer = gammaln(Nh+alphas) + gammaln(Nt+alphas) + gammaln
denom = gammaln(N+2*alphas) + 2*gammaln(alphas);
r = exp(numer ./ denom);
```

So, is the coin biased or not?

- We plot the likelihood ratio vs hyperparameter α:



- For a uniform prior, $\frac{P(H_1|D)}{P(H_0|D)} = 0.48$, (weakly) favoring the fair coin hypothesis H_0!
- At best, for $\alpha = 50$, we can make the biased hypothesis twice as likely.
- Not as dramatic as saying "we reject the null hypothesis (fair coin) with significance 6.6%".

From coins to dice

- Likelihood: binomial → multinomial

$$P(D|\vec{\theta}) = \prod_i \theta_i^{N_i}$$

- Prior: beta → Dirichlet

$$P(\vec{\theta}|\vec{\alpha}) = \frac{1}{Z(\vec{\alpha})} \prod_i \theta_i^{\alpha_i - 1}$$

where

$$Z(\vec{\alpha}) = \frac{\prod_i \Gamma(\alpha_i)}{\Gamma(\sum_i \alpha_i)}$$

- Posterior: beta → Dirichlet

$$P(\vec{\theta}|D) = Dir(\vec{\alpha} + \vec{N})$$

- Evidence (marginal likelihood)

$$P(D|\vec{\alpha}) = \frac{Z(\vec{\alpha} + \vec{N})}{Z(\vec{\alpha})} = \frac{\prod_i \Gamma(\alpha_i + N_i)}{\prod_i \Gamma(\alpha_i)} \frac{\Gamma(\sum_i \alpha_i)}{\Gamma(\sum_i \alpha_i + N_i)}$$

From dice to tabular Bayes nets

- If we assume global parameter independence, the evidence decomposes into one term per node:

$$P(D|G) = \prod_i P(D(X_i, X_{\pi_i})|\vec{\alpha}_i)$$

- If we also assume local parameter independence, each node term decomposes into a product over rows (conditioning cases):

$$\begin{aligned} P(D|G) &= \prod_i \prod_{k \in Val(\pi_i)} P(D(X_i, X_{\pi_i} = k)|\vec{\alpha}_{i,\cdot,k}) \\ &= \prod_i \prod_{k \in Val(\pi_i)} \frac{Z(\vec{\alpha}_{i,\cdot,k} + N_{i,\cdot,k})}{Z(\vec{\alpha}_{i,\cdot,k})} \\ &= \prod_i \prod_{k \in Val(\pi_i)} \left[\prod_j \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})} \right] \left[\frac{\Gamma(\sum_j \alpha_{ijk})}{\Gamma(\sum_j \alpha_{ijk} + N_{ijk})} \right] \end{aligned}$$

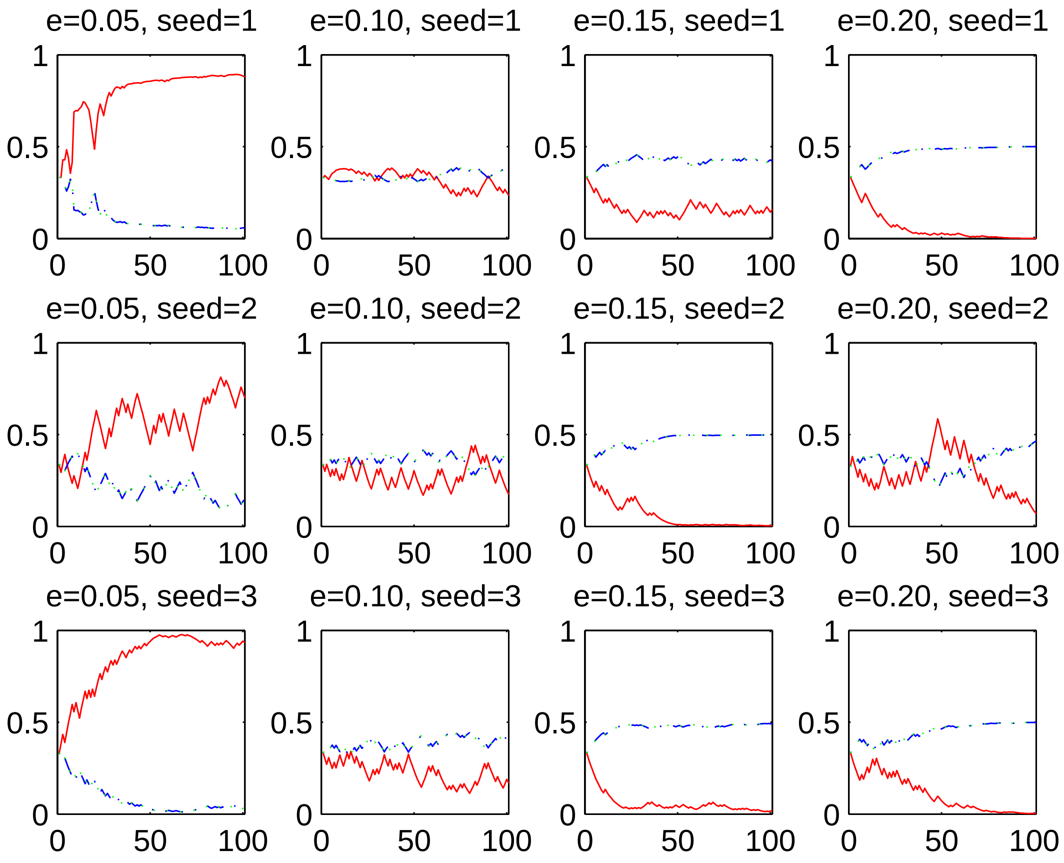
Example of model selection

- Suppose we generate data from $X \to Y$, where $P(X = 0) = P(X = 1) = 0.5$ and $P(Y = 1|X = 0) = 0.5 - \epsilon$, $P(Y = 1|X = 1) = 0.5 + \epsilon$.
- As we increase ϵ, we increase the dependence of Y on X.
- Let us consider 3 hypotheses: $H_0 = X \quad Y$, $H_1 = X \to Y$, $H_2 = Y \leftarrow X$, and use uniform priors.
- We will plot model posteriors vs N for different ϵ and different random trials:

$$P(H_i|D_{1:N}) = \frac{P(D_{1:N}|H_i)P(H_i)}{\sum_j P(D_{1:N}|H_j)P(H_j)}$$

Example of model selection

red $= H_0$ (independence), blue/green $= H_1/H_2$ (dependence).
See `BNT/examples/static/StructLearn/model-select1.m`.



Score equivalence

- $X \rightarrow Y$ and $X \leftarrow Y$ are I-equivalent (have the same likelihood).
- Suppose we use a uniform Dirichlet prior for each node in each graph, with equivalent sample size α (K2-prior):

$$P(\theta_X | H_1) = Dir(\alpha, \alpha), \;\; P(\theta_{X|Y=i} | H_2) = Dir(\alpha, \alpha)$$

- In H_1, the equivalent sample size for X is 2α, but in H_2 it is 4α (since two conditioning contexts). Hence the posterior probabilities are different.
- The BDe (Bayesian Dirichlet likelihood equivalent) prior is to use weights $\alpha_{X_i|X_{\pi_i}} = \alpha P'(X_i, X_{\pi_i})$ where P' could be represented by e.g., a Bayes net.
- The BDeu (uniform) prior is $P'(X_i, X_{\pi_i}) = \frac{1}{|X_i||X_{\pi_i}|}$.
- Using the BDeu prior, the curves for $X \rightarrow Y$ and $X \leftarrow Y$ are indistinguishable. Using the K2 prior, they are not.

Bayesian Occam's razor

- Why is $P(H_0|D)$ higher when then dependence on X and Y is weak (small ϵ)?
- It is not because the prior $P(H_i)$ explicitly favors simpler models (although this is possible).
- It because the evidence $P(D) = \int dw P(D|w)P(w)$, automatically penalizes complex models.
- Occam's razor says "If two models are equally predictive, prefer the simpler one".
- This is an automatic consequence of using Bayesian model selection.
- Maximum likelihood would always pick the most complex model, since it has more parameters, and hence can fit the training data better.
- Good test for a learning algorithm: feed it random noise, see if it "discovers" structure!

Laplace approximation to the evidence

- Consider a large sample approximation, where the parameter posterior becomes peaked.
- Take a second order Taylor expansion around $th\hat{e}ta_{MP}$:

  $$\log P(\theta|D) \approx \log P(\hat{\theta}_{MP}|D) - \frac{1}{2}(\theta - \hat{\theta})^T H (\theta - \hat{\theta})$$

  where

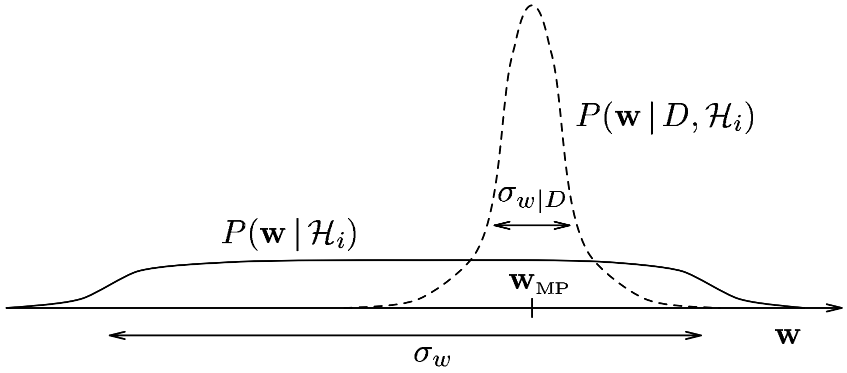
  $$H \overset{\text{def}}{=} -\frac{\partial^2 \log P(\theta|D)}{\partial\theta\partial\theta^T}\,|_{\hat{\theta}_{MP}}$$

  is the Hessian.
- By properties of Gaussian integrals,

  $$\begin{aligned} P(D) &\approx \int d\theta \;\; P(D|\hat{\theta})P(\hat{\theta})e^{-\frac{1}{2}(\theta-\hat{\theta})^T H(\theta-\hat{\theta})} \\ &= \; P(D|\hat{\theta})P(\hat{\theta})(2\pi)^{d/2}|H|^{-\frac{1}{2}} \end{aligned}$$

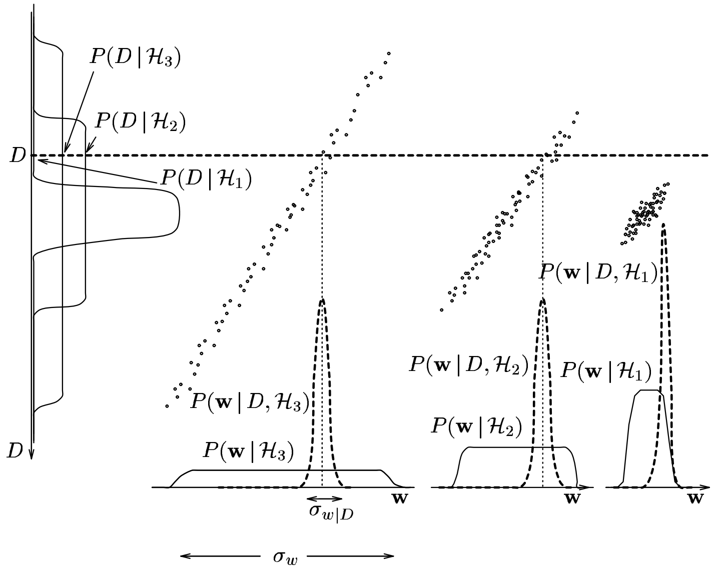
Occam factor

- H is like the precision (inverse covariance) of a Gaussian.
- In the 1d case, $|H|^{-\frac{1}{2}} = \sigma_{\theta|D}$, the width of the posterior.
- Consider a uniform prior with width σ_θ.
  Then $P(D) \approx P(D|\hat{\theta})P(\hat{\theta})|H|^{-\frac{1}{2}} \approx P(D|\hat{\theta})\frac{1}{\sigma_\theta}\sigma_{\theta|D}$
- The ratio of posterior accessible volume of the parameter space to the prior, $\sigma_{\theta|D}/\sigma_\theta$, is called the Occam factor, i.e., the factor by which H_i's hypothesis space collapses when the data arrive.


$P(\mathbf{w}\,|\,D,\mathcal{H}_i)$
$\sigma_{w|D}$
$P(\mathbf{w}\,|\,\mathcal{H}_i)$
$\mathbf{w}_{\text{MP}}$
$\mathbf{w}$
σ_w

Bayesian Occam's razor

- $P(D|H_1)$ is smallest, since it is too simple a model.
- $P(D|H_3)$ is second smallest, since it is too complex, so it spreads its probability mass more thinly over the (D, θ) space (fewer dots on the horizontal line).
- We trust an expert who predicts a few *specific* (and correct!) things more than an expert who predicts many things.


$P(D\,|\,\mathcal{H}_3)$
$P(D\,|\,\mathcal{H}_2)$
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$P(D\,|\,\mathcal{H}_1)$
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$P(\mathbf{w}\,|\,D,\mathcal{H}_2)$
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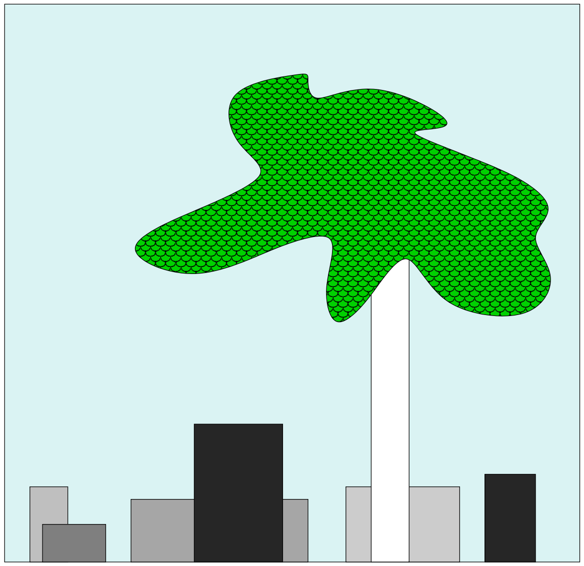
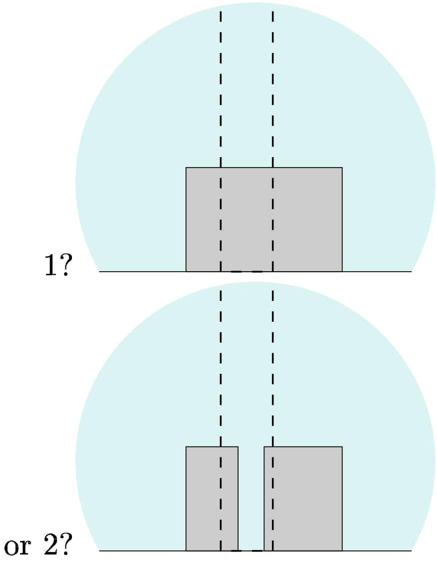
$P(\mathbf{w}\,|\,D,\mathcal{H}_3)$
$P(\mathbf{w}\,|\,\mathcal{H}_2)$
D
$P(\mathbf{w}\,|\,\mathcal{H}_3)$
$\mathbf{w}$
$\mathbf{w}$
$\mathbf{w}$
$\sigma_{w|D}$
σ_w

Bayesian image interpretation

- How many boxes behind the tree?
- The intrepretation that the tree is in front of one box is much more probable than there being 2 boxes which happen to have the same height and color (suspicious coincidence).
- This can be formalized by assuming (uniform) priors on the box parameters, and computing the Occam factors.





Leave one out cross validation (LOOCV)

- The evidence can be evaluated sequentially

$$P(x_{1:N}) = P(x_1)P(x_2|x_1)P(x_3|x_{1:2})\ldots$$

- LOOCV approximates $P(X_t|X_{1:t-1}, \hat{\theta}_{1:t-1})$ under different permutations of the data.
- Advantages of LOOCV
  - Simple (no need to integrate out parameters)
  - Robust (works well even if “truth not in model class”)
- Advantages of LOOCV
  - Slow (in general, must rerun training many times)
  - Does not use all the data

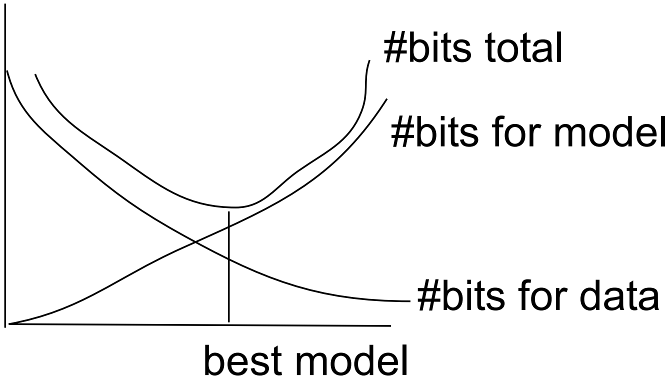
Minimum description length (MDL)

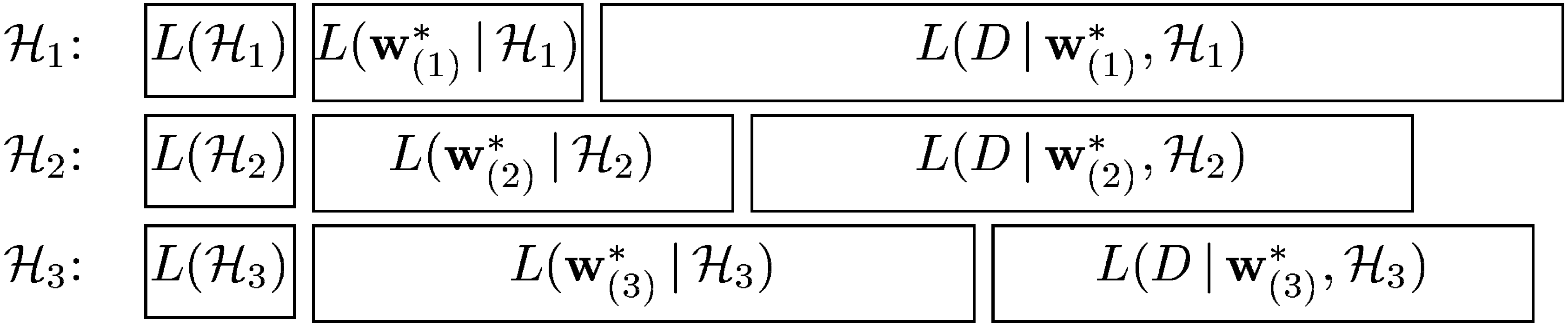
- Another way of thinking about Bayesian Occam's razor is in terms of information theory.
- To losslessly send a message about an event x with probability $P(x)$ takes $L(x) = -\log_2 P(x)$ bits.
- Suppose instead of sending the raw data, you send a model and then the residual errors (the parts of the data not predicted by the model).
- This takes $L(D, H)$ bits:

$$L(D, H) = -\log P(H) - \log(P(D|H)) = -\log P(H|D) + \text{const}$$

- The best model is the one with the overall shortest message.

Minimum description length (MDL)





$\mathcal{H}_1$: $L(\mathcal{H}_1)$ $L(\mathbf{w}^*_{(1)} \,|\, \mathcal{H}_1)$ $L(D \,|\, \mathbf{w}^*_{(1)}, \mathcal{H}_1)$

$\mathcal{H}_2$: $L(\mathcal{H}_2)$ $L(\mathbf{w}^*_{(2)} \,|\, \mathcal{H}_2)$ $L(D \,|\, \mathbf{w}^*_{(2)}, \mathcal{H}_2)$

$\mathcal{H}_3$: $L(\mathcal{H}_3)$ $L(\mathbf{w}^*_{(3)} \,|\, \mathcal{H}_3)$ $L(D \,|\, \mathbf{w}^*_{(3)}, \mathcal{H}_3)$

BIC approximation to the evidence

- Laplace approximation

$$P(D) \approx P(D|\hat{\theta})P(\hat{\theta})(2\pi)^{d/2}|H|^{-\frac{1}{2}}$$

- Taking logs

$$\log P(D) = \log P(D|\hat{\theta}) + \log P(\hat{\theta}) + \frac{d}{2}\log(2\pi) - \frac{1}{2}\log|H|$$

- BIC (Bayesian Information Criterion): drop terms that are independent of N, and approximate $\log|H| \approx d\log N$. So

$$\log P(D) \approx \log P(D|\hat{\theta}_{ML}) - \frac{d}{2}\log N$$

  where d is the number of free parameters.

- AIC (Akaike Information Criterion): derived by minimizing KL divergence independent of N, and approximate $\log|H| \approx d\log N$. So

$$\log P(D) \approx \log P(D|\hat{\theta}_{ML}) - \frac{d}{2}\log N$$

Log-likelihood in information theoretic terms

$$
\begin{aligned}
\frac{1}{N}\ell &= \frac{1}{N}\sum_i \sum_j \sum_k N_{ijk} \log \theta_{ijk} \\
&= \sum_i \sum_j \sum_k \hat{P}(X_i = j, X_{\pi_i} = k) \log P(X_i = j | X_{\pi_i} = k) \\
&= \sum_{ijk} \hat{P}(X_i = j, X_{\pi_i} = k) \log \frac{P(X_i = j, X_{\pi_i} = k) P(X_i = j)}{P(X_{\pi_i} = k) P(X_i = j)} \\
&= \sum_i \sum_{jk} \hat{P}(X_i = j, X_{\pi_i} = k) \log \frac{P(X_i = j, X_{\pi_i} = k)}{P(X_{\pi_i} = k) P(X_i = j)} \\
&\quad + \sum_{ij} (\sum_k \hat{P}(X_i = j, X_{\pi_i} = k)) \log P(X_i = j) \\
&= \sum_i I(X_i, X_{\pi_i}) - H(X_i)
\end{aligned}
$$

BIC in information theoretic terms

$$\begin{aligned}\text{score}_{BIC}(G|D) &= \ell(\hat{\theta}) - \frac{d(G)}{2}\log N(D) \\ &= N\sum_i I(X_i, X_{\pi_i}) - N\sum_i H(X_i) - \frac{d}{2}\log N\end{aligned}$$

- The mutual information term grows linearly in N, the complexity penalty is logarithmic in N.
- So for large datasets, we pay more attention to fitting the data better.
- Also, the structural prior is independent of N, so does not matter very much.

Desirable properties of a scoring function

- Consistency: i.e., if the data is generated by G^*, then G^* and all I-equivalent models maximize the score.
- Decomposability:

  $$\text{score}(G|D) = \sum_i \text{FamScore}(D(X_i, X_{\pi_i}))$$

  which makes it cheap to compare score of G and G' if they only differ in a small number of families.
- Bayesian score (evidence), likelihood and penalized likelihood (BIC) are all decomposable and consistent.

Maximizing the score

- Consider the family of DAGs G_d with maximum fan-in (number of parents) equal to d.
- Theorem 14.4.3: It is NP-hard to find

  $$G^* = \arg\max_{G \in G_d} \mathsf{score}(G, D)$$

  for any $d \geq 2$.
- In general, we need to use heuristic local search.

Maximizing the score: tractable cases

- For $d \leq 1$ (i.e., trees), we can solve the problem in $O(n^2)$ time using max spanning tree (next lecture).
- If we know the ordering of the nodes, we can solve the problem in $O(d \binom{n}{d})$ time (see below).

Known order (K2 algorithm)

- Suppose we a total ordering of the nodes $X_1 \prec X_2 \ldots \prec X_n$ and want to find a DAG consistent with this with maximum score.
- The choice of parents for X_i, from $Pa_i \subseteq \{X_1, \ldots, X_{i-1}\}$, is independent of the choice for X_j: since we obey the ordering, we cannot create a cycle.
- Hence we can pick the best set of parents for each node independently.
- For X_i, we need to search all $\binom{i-1}{d}$ subsets of size up to d for the set which maximizes FamScore.
- We can use greedy techniques for this, c.f., learning a decision tree.

What if order isn't known?

- Search in the space of DAGs.
- Search in the space of orderings, then conditioned on $\prec$, pick best graph using K2 (Rao-Blackwellised sampling).
- Can also search in space of undirected graphs.
- Can also search in space of graphs of variable size, to allow creation of hidden nodes (next lecture).

Searching in DAG space

- Typical search operators:
  - Add an edge
  - Delete an edge
  - Reverse an edge
- We can get from any graph to any other graph in at most $O(n^2)$ moves (the diameter of the search space).
- Moves are reversable.
- Simplest search algorithm: greedy hill climbing.
- We can only apply a search operator o to the current graph G if the resulting graph $o(G)$ satisfies the constraints, e.g., acyclicity, indegree bound, induced treewidth bound ("thin junction trees"), hard prior knowledge.

Cost of evaluating moves

- There are $O(n^2)$ operators we could apply at each step.
- For each operator, we need to check if $o(G)$ is acylic.
- We can check acyclicity in $O(e)$ time, where $e = O(nd)$ is the number of edges.
- For local moves, we can check acyclicity in amortized $O(1)$ time using the ancestor matrix.
- If $o(G)$ is acyclic, we need to evaluate its quality. This requires computing sufficient statistics for every family, which takes $O(Mn)$ time, for M training cases.
- Suppose there are K steps to convergence. (We expect $K \ll n^2$, since the diameter is n^2.)
- Hence total time is $O(K \cdot n^2 \cdot Mn)$.

Exploiting decomposable score

- If the operator is valid, we need to evaluate its quality. Define

$$\delta_G(o) = \mathsf{score}(o(G)|D) - \mathsf{score}(G|D)$$

- If the score is decomposable, and we want to modify an edge involving X and Y, we only need to look at the sufficient statistics for X and Y's families.
- e.g., if $o =$ add $X \rightarrow Y$:

$$\delta_G(o) = \mathsf{FamScore}(Y, Pa(Y, G) \cup X|D) - \mathsf{FamScore}(Y, Pa(Y, G)|D)$$

- So we can evaluate quality in $O(M)$ time by extracting sufficient statistics for the columns related to X, Y and their parents.
- This reduces the time from $O(Kn^3M)$ to $O(Kn^2M)$.

Exploiting decomposable score

- After eg adding $X \rightarrow Y$, we only need to update $\delta(o)$ for the $O(n)$ operators that involve X or Y.
- Also, we can update a heap in $O(n \log n)$ time and thereby find the best o in $O(1)$ time at each step.
- So total cost goes from $O(Kn^2M)$ to $O(K(nM + n \log n))$.
- For large M, we can use fancy data sructures (e.g., kd-trees) to compute sufficient statistics in sub-linear time.

Local maxima

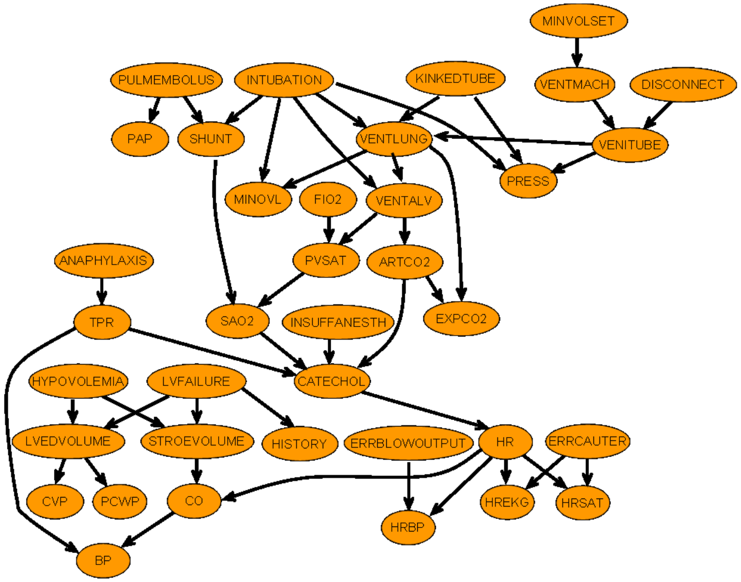
- Greedy hill climbing will stop when it reaches a local maximum or a plateau (a set of neighboring networks that have the same score).
- Unfortunately, plateaux are common, since equivalence classes form contiguous regions of search space (thm 14.4.4), and such classes can be exponentially large.
- Solutions:
  - Random restarts
  - TABU search (prevent the algorithm from undoing an operator applied in the last L steps, thereby forcing it to explore new terrain).
  - Data perturbation (dynamic local search): reweight the data and take step.
  - Simulated annealing: if $\delta(o) > 0$, take move, else accept with probability $e^{\frac{\delta(o)}{t}}$, where t is the temperature. Slow!

Searching in space of equivalence classes

- The space of class PDAGs is smaller.
- We avoid many of the plateux of I-equivalent DAGs.
- Operators are more complicated to implement and evaluate, but can still be done locally (see paper by Max Chickering).
- Cannot exploit causal/ interventional data (which can distinguish members of an equivalence class).
- Currently less common than searching in DAG space.

Learning the ICU-Alarm network with TABU search

- Learned structures often simpler than “true” model (fewer edges), but predict just as well.
- Can only recover structure up to Markov equivalence.
- 10 minutes to learn structure for 100 variables and 5000 cases.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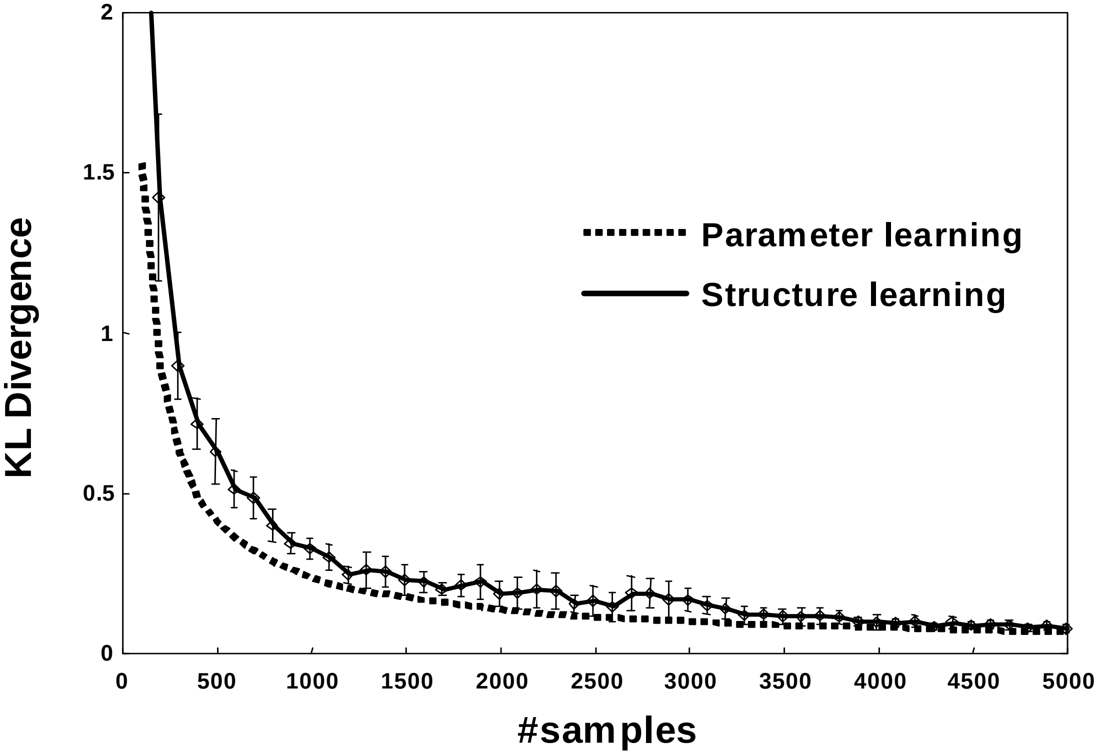
KL Divergence
#samples
Parameter learning
Structure learning