Structure Learning 2

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Structure Scores

- Searching for highest-scoring network structure is intractable
- Need to resort to heuristic search (eg. hillclimbing)
- Need:
  1. Search space
  2. Scoring function
  3. Search procedure

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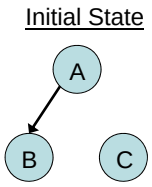
Structure Scores

1. Search space

- Start with initial state (eg. disconnected graph or randomly generated one)



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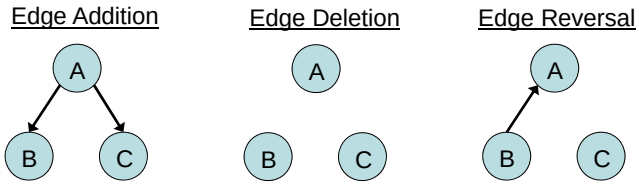
Structure Scores

1. Search space

- Move to a neighboring state by applying an operator:



Can only perform an operator if it doesn't lead to a cycle!

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Structure Scores

2. Scoring function:

- Two general classes of scoring functions:
  1. Likelihood scoring functions
  2. Bayesian scoring functions
- More about this in a bit…assume we have a scoring function for now

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Structure Scores

3. Search procedure

- Greedy search: pick the best scoring neighboring state to move to
- Repeat until convergence
- Converges to a local optimum

Tricks for dealing with this: random restart, simulated annealing, tabu search and data perturbation

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Structure Scores

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Likelihood Scores

$$\max_{\mathcal{G},\boldsymbol{\theta}_{\mathcal{G}}} L(\langle \mathcal{G}, \boldsymbol{\theta}_{\mathcal{G}} \rangle : \mathcal{D})$$
$$= \max_{\mathcal{G}} \left[\max_{\boldsymbol{\theta}_{\mathcal{G}}} L(\langle \mathcal{G}, \boldsymbol{\theta}_{\mathcal{G}} \rangle : \mathcal{D}) \right]$$
$$= \max_{\mathcal{G}} \left[L(\langle \mathcal{G}, \hat{\boldsymbol{\theta}}_{\mathcal{G}} \rangle : \mathcal{D}) \right]$$

Graph structure that maximizes the likelihood

Maximum likelihood estimates of parameters

$$score_L(\mathcal{G} : \mathcal{D}) = l(\hat{\boldsymbol{\theta}}_{\mathcal{G}} : \mathcal{D})$$

Log likelihood

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Likelihood Scores

Let M be the number of samples. We use the notation $M[x]$ to be the count of x in the data.

Let $\hat{P}$ be the empirical distribution observed in the data. Eg.

- $M[x,y] = M \cdot \hat{P}(x,y)$
- $M[y] = M \cdot \hat{P}(y)$

Note that:

- $\hat{\theta}_{y|x} = \hat{P}(y|x)$
- $\hat{\theta}_{y} = \hat{P}(y)$

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Likelihood Scores

Mutual Information

$$\boldsymbol{I}_{\hat{P}}(X;Y) = \sum_{x,y} \hat{P}(x,y) log \frac{\hat{P}(x,y)}{\hat{P}(x)\hat{P}(y)}$$

$$= \frac{1}{M} \sum_{x,y} M[x,y] \, log \left(\frac{M[x,y]}{M[x]M[y]} \right)$$

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Likelihood Scores

Claim:

$$score_L(\mathcal{G}:\mathcal{D}) = M\sum_{i=1}^{n} \boldsymbol{I}_{\hat{P}}(X_i; Parents(X_i,\mathcal{G})) - M\sum_{i=1}^{n} H_{\hat{P}}(X_i)$$

$$= M\sum_{i=1}^{n}\left[\boldsymbol{I}_{\hat{P}}\left(X_i; Parents(X_i,\mathcal{G})\right) - H_{\hat{P}}(X_i)\right]$$

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Likelihood Scores

Proof:

$$l\left(\hat{\theta}_{\mathcal{G}}:\mathcal{D}\right) = \sum_{i=1}^{n}\left[\sum_{\boldsymbol{u}_i \in Val(Parents(X_i,\mathcal{G}))}\sum_{x_i} M[x_i,\boldsymbol{u}_i] log\hat{\theta}_{x_i|\boldsymbol{u}_i}\right]$$

$$= M\sum_{i=1}^{n}\left[\frac{1}{M}\sum_{\boldsymbol{u}_i}\sum_{x_i} M[x_i,\boldsymbol{u}_i] log\hat{\theta}_{x_i|\boldsymbol{u}_i}\right]$$

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Likelihood Scores

$$\frac{1}{M}\sum_{\boldsymbol{u}_i}\sum_{x_i} M[x_i,\boldsymbol{u}_i]log\hat{\theta}_{x_i|\boldsymbol{u}_i}$$
$$=\sum_{\boldsymbol{u}_i}\sum_{x_i}\hat{P}(x_i,\boldsymbol{u}_i)log\hat{P}(x_i|u_i)$$
$$=\sum_{\boldsymbol{u}_i}\sum_{x_i}\hat{P}(x_i,\boldsymbol{u}_i)log\left(\frac{\hat{P}(x_i,\boldsymbol{u}_i)}{\hat{P}(\boldsymbol{u}_i)}\cdot\frac{\hat{P}(x_i)}{\hat{P}(x_i)}\right)$$
$$=\sum_{\boldsymbol{u}_i}\sum_{x_i}\hat{P}(x_i,\boldsymbol{u}_i)log\left(\frac{\hat{P}(x_i,\boldsymbol{u}_i)}{\hat{P}(\boldsymbol{u}_i)\hat{P}(x_i)}\right)+\sum_{x_i}\left(\sum_{\boldsymbol{u}_i}\hat{P}(x_i,\boldsymbol{u}_i)\right)log\hat{P}(x_i)$$
$$=\boldsymbol{I}_{\hat{P}}(X_i;\boldsymbol{U}_i)-\sum_{x_i}\hat{P}(x_i)log\frac{1}{\hat{P}(x_i)}$$
$$=\boldsymbol{I}_{\hat{P}}(X_i;\boldsymbol{U}_i)-\boldsymbol{H}_{\hat{P}}(X_i)$$

Note that if $Parents(X_i,\mathcal{G})=\emptyset$, then $I_{\hat{P}}\big(X_i;Parents(X_i,\mathcal{G})\big)=0$

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Likelihood Scores

What are the implications of

$$\underbrace{\boldsymbol{I}_{\hat{P}}(X_i;\boldsymbol{U}_i)}-\underbrace{\boldsymbol{H}_{\hat{P}}(X_i)}$$

Depends on network structure (because $U_i=\text{Parents}(X_i,\mathcal{G})$). Only need to maximize this.

Does not depend on network structure

The likelihood of a network measures how informative $Parents(X_i)$ are about X_i

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Likelihood Scores

An alternate representation:

$$\frac{1}{M} score_L(\mathcal{G}:\mathcal{D}) = H_{\hat{P}}(X_1, \ldots, X_n) - \sum_{i=1}^{n} I_{\hat{P}}(X_i; \{X_1, \ldots, X_{i-1}\} - Parents(X_i, \mathcal{G}) \mid Parents(X_i, \mathcal{G}))$$

Does not depend on network structure

Depends on network structure

Measures to what extent the Markov properties of the graph are violated in the data (fewer violations ⇒ larger score)

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Problems with Likelihood Score

Never prefers a simpler network over a more complex one eg.

$$score_L(\mathcal{G}_1:\mathcal{D}) \geq score_L(\mathcal{G}_0:\mathcal{D})$$

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Problems with Likelihood Score

- Exhibits a conditional independence only if it holds exactly in the empirical distribution
  - Due to noise, this almost never happens
- Learns a fully connected graph
  - Overfits the training data and does not generalize well to unseen cases
- Needs a penalty for learning overly complex structures

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Bayesian Scoring

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Bayesian Score

- Bayesian philosophy: if you are uncertainty about something, put a distribution over it
- In structure learning, we have uncertainty over the structure and the parameters
- We will have two prior distributions:
  - Structure prior $P(\mathcal{G})$
  - Parameter prior $P(\boldsymbol{\theta}_{\mathcal{G}}|\mathcal{G})$

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Bayesian Score

Recall: $P(\mathcal{G}|D) = \frac{P(\mathcal{D}|\mathcal{G})P(\mathcal{G})}{P(\mathcal{D})} = \alpha P(\mathcal{D}|\mathcal{G})P(\mathcal{G})$

$$score_B(\mathcal{G}:\mathcal{D}) = logP(\mathcal{D} \mid \mathcal{G}) + \log P(\mathcal{G})$$

Marginal Likelihood (dominates the score)

Structure prior

$$P(\mathcal{D}|\mathcal{G}) = \int_{\Theta_{\mathcal{G}}} P\left(D\middle|\boldsymbol{\theta}_{\mathcal{G}},\mathcal{G}\right)P\left(\boldsymbol{\theta}_{\mathcal{G}}|\mathcal{G}\right)d\boldsymbol{\theta}_{\mathcal{G}}$$

"Averages" out $P(\mathcal{D}|\theta_{\mathcal{G}},\mathcal{G})$ over the distribution of $\theta_{\mathcal{G}}$. Contrast this with maximum likelihood which finds the $\theta_{\mathcal{G}}$ that maximizes the likelihood of the data

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Bayesian score

- How does the Bayesian score improve over the likelihood score?
  - By avoiding overfitting
- Likelihood score commits to a single $\hat{\boldsymbol{\theta}}$ value
- Bayesian score works with a distribution of $\boldsymbol{\theta}_{\mathcal{G}}$ and averages $P(\mathcal{D}|\boldsymbol{\theta}_{\mathcal{G}}, \mathcal{G})$ over this distribution
  - Results in an expected likelihood

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Marginal Likelihood (Single Variable case)

- Suppose we have a single binary random variable X
- Let the prior distribution over the parameters of X be $Dirichlet(\alpha_1, \alpha_0)$
- Let the data $\mathcal{D} = \{x[1], \ldots, x[M]\}$ have $M[1]$ heads and $M[0]$ tails
- Maximum likelihood value given D is: $P(\mathcal{D}|\hat{\theta}) = \left(\frac{M[1]}{M}\right)^{M[1]} \cdot \left(\frac{M[0]}{M}\right)^{M[0]}$

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Marginal Likelihood (Single Variable case)

What about the marginal likelihood?

$$P(\mathcal{D}|\mathcal{G}) = \int_{\Theta_\mathcal{G}} P(\mathcal{D}|\boldsymbol{\theta}_\mathcal{G}, \mathcal{G}) P(\boldsymbol{\theta}_\mathcal{G}|\mathcal{G}) d\boldsymbol{\theta}_\mathcal{G}$$

$\left(\frac{M[1]}{M}\right)^{M[1]} \cdot \left(\frac{M[0]}{M}\right)^{M[0]}$ $\quad$ $Dirichlet(\alpha_1, \alpha_0)$

Shorthand: let $p_i = \frac{M[i]}{M}$ and $\alpha = \alpha_0 + \alpha_1$

Marginal Likelihood (Single Variable case)

$$P(\mathcal{D}|\mathcal{G}) = \int_{\Theta_\mathcal{G}} {p_1}^{M[1]} {p_0}^{M[0]} \frac{\Gamma(\alpha_0 + \alpha_1)}{\Gamma(\alpha_0)\Gamma(\alpha_1)} {p_1}^{(\alpha_1 - 1)} {p_0}^{(\alpha_0 - 1)} d\boldsymbol{\theta}_\mathcal{G}$$

$$= \frac{\Gamma(\alpha)}{\Gamma(\alpha_0)\Gamma(\alpha_1)} \int_{\Theta_\mathcal{G}} {p_1}^{(M[1] + \alpha_1 - 1)} {p_0}^{(M[0] + \alpha_0 - 1)} d\boldsymbol{\theta}_\mathcal{G}$$

Note: $\int_{\Theta_\mathcal{G}} Beta(\mathrm{M}[1] + \alpha_1, M[0] + \alpha_0) d\boldsymbol{\theta}_\mathcal{G} = 1$

$$\Rightarrow \int_{\Theta_\mathcal{G}} \frac{\Gamma(\alpha + M)}{\Gamma(M[1] + \alpha_1)\Gamma(M[0] + \alpha_0)} {p_1}^{(M[1] + \alpha_1 - 1)} {p_0}^{(M[0] + \alpha_0 - 1)} d\boldsymbol{\theta}_\mathcal{G} = 1$$

$$\Rightarrow \int_{\Theta_\mathcal{G}} {p_1}^{(M[1] + \alpha_1 - 1)} {p_0}^{(M[0] + \alpha_0 - 1)} d\boldsymbol{\theta}_\mathcal{G} = \frac{\Gamma(\alpha + M)}{\Gamma(M[1] + \alpha_1)\Gamma(M[0] + \alpha_0)}$$

Marginal Likelihood (Single Variable case)

$$P(\mathcal{D}|\mathcal{G}) = \int_{\Theta_\mathcal{G}} {p_1}^{M[1]} {p_0}^{M[0]} \frac{\Gamma(\alpha_0+\alpha_1)}{\Gamma(\alpha_0)\Gamma(\alpha_1)} {p_1}^{(\alpha_1-1)} {p_0}^{(\alpha_0-1)} d\boldsymbol{\theta}_\mathcal{G}$$

$$= \frac{\Gamma(\alpha)}{\Gamma(\alpha_0)\Gamma(\alpha_1)} \int_{\Theta_\mathcal{G}} {p_1}^{(M[1]+\alpha_1-1)} {p_0}^{(M[0]+}$$

Note that the Gamma function is as follows:
$\Gamma(1) = 1$
$\Gamma(x+1) = x\Gamma(x)$

ie. it is a continuous generalization of the factorial:
$\Gamma(n+1) = n!$

Note: $\int_{\Theta_\mathcal{G}} Beta(\mathrm{M}[1]+\alpha_1, M[0]+\alpha_0) d\boldsymbol{\theta}_\mathcal{G} = 1$

$$\Rightarrow \int_{\Theta_\mathcal{G}} \frac{\Gamma(\alpha+M)}{\Gamma(M[1]+\alpha_1)\Gamma(M[0]+\alpha_0)} {p_1}^{(M[1]+\alpha_1-1)} {p_0}^{(M[0]+\alpha_0-1)} d\boldsymbol{\theta}_\mathcal{G} = 1$$

$$\Rightarrow \int_{\Theta_\mathcal{G}} {p_1}^{(M[1]+\alpha_1-1)} {p_0}^{(M[0]+\alpha_0-1)} d\boldsymbol{\theta}_\mathcal{G} = \frac{\Gamma(\alpha+M)}{\Gamma(M[1]+\alpha_1)\Gamma(M[0]+\alpha_0)}$$

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Marginal Likelihood (Single Variable case)

$$= \frac{\Gamma(\alpha)}{\Gamma(\alpha_0)\Gamma(\alpha_1)} \frac{\Gamma(\alpha+M)}{\Gamma(M[1]+\alpha_1)\Gamma(M[0]+\alpha_0)}$$

$$P(\mathcal{D}|\mathcal{G}) = \frac{\Gamma(\alpha)}{\Gamma(\alpha+M)} \cdot \frac{\Gamma(\alpha_1+M)}{\Gamma(\alpha_1)} \cdot \frac{\Gamma(\alpha_0+M)}{\Gamma(\alpha_0)}$$

We can easily generalize to a multinomial distribution over the space of values $x^1, \ldots, x^k$ with a prior $Dirichlet(\alpha_1, \ldots, a_k)$:

$$P(\mathcal{D}|\mathcal{G}) = \frac{\Gamma(\alpha)}{\Gamma(\alpha+M)} \cdot \prod_i^k \frac{\Gamma(\alpha_i+M[x^i])}{\Gamma(\alpha_i)}$$

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Bayesian Scoring

Global parameter independence:

Let $\mathcal{G}$ be a Bayesian network structure with parameters $\boldsymbol{\theta} = (\boldsymbol{\theta}_{X_1|Pa(X_1)}, \ldots, \boldsymbol{\theta}_{X_n|Pa(X_n)})$.

The distribution $P(\boldsymbol{\theta})$ satisfies global parameter independence if it has the form:

$$P(\boldsymbol{\theta}) = \prod_{i=1}^{n} P(\boldsymbol{\theta}_{X_i|Pa(X_i)})$$

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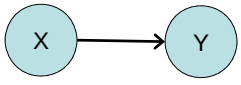
Bayesian Scoring

Local parameter independence:

Let X be a variable with parents $\boldsymbol{U}$. We say that distribution $P(\boldsymbol{\theta}_{X|\boldsymbol{U}})$ satisfies local parameter independence if:

$$P(\boldsymbol{\theta}_{X|\boldsymbol{U}}) = \prod_{\boldsymbol{u}} P(\boldsymbol{\theta}_{X|\boldsymbol{u}})$$

Example:



X	Y	P(Y|X)
0	0	$\theta_{Y\|x^0}$
0	1	
1	0	$\theta_{Y\|x^1}$
1	1	

Only one of the θs applies, depending on the value of x. In other words, the θs don't affect each other

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Bayesian Scoring

Now suppose there are two binary random variables X and Y. Let $\mathcal{G}_0$ be a graph with X and Y and no edges

$$P(\mathcal{D}|\mathcal{G}_0) = \int_{\Theta_X \times \Theta_Y} P(D|\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y, \mathcal{G}_0) P(\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y|\mathcal{G}_0) d[\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y]$$

1. Decompose likelihood in terms of each variable

$$P(D|\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y, \mathcal{G}_0) = \prod_{i=1}^{M} P(x[m]|\theta_X, \mathcal{G}_0)\, P(y[m]|\theta_Y, \mathcal{G}_0)$$

2. Global Parameter Independence: $P(\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y|\mathcal{G}_0) = \mathrm{P}(\boldsymbol{\theta}_X|\mathcal{G}_0) P(\boldsymbol{\theta}_Y|\mathcal{G}_0)$

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Bayesian Scoring

$$P(\mathcal{D}|\mathcal{G}_0) = \int_{\Theta_X \times \Theta_Y} P(D|\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y, \mathcal{G}_0) P(\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y|\mathcal{G}_0) d[\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y]$$

$$= \int_{\Theta_X} \int_{\Theta_Y} \prod_{m=1}^{M} P(x[m]|\boldsymbol{\theta}_X, \mathcal{G}_0)\, P(y[m]|\boldsymbol{\theta}_Y, \mathcal{G}_0) \mathrm{P}(\boldsymbol{\theta}_X|\mathcal{G}_0) P(\boldsymbol{\theta}_Y|\mathcal{G}_0)\; d[\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y]$$

$$= \int_{\Theta_X} \int_{\Theta_Y} \left(\prod_{m=1}^{M} P(x[m]|\boldsymbol{\theta}_X, \mathcal{G}_0) \mathrm{P}(\boldsymbol{\theta}_X|\mathcal{G}_0) \right) \left(\prod_{m=1}^{M} P(y[m]|\boldsymbol{\theta}_Y, \mathcal{G}_0)\, P(\boldsymbol{\theta}_Y|\mathcal{G}_0) \right) d[\boldsymbol{\theta}_X, \boldsymbol{\theta}_Y]$$

Integral of a product of independent functions is the product of integrals:

$$= \left(\int_{\Theta_X} \prod_{m=1}^{M} P(x[m]|\boldsymbol{\theta}_X, \mathcal{G}_0) \mathrm{P}(\boldsymbol{\theta}_X|\mathcal{G}_0)\, d\boldsymbol{\theta}_X \right) \left(\int_{\Theta_Y} \prod_{m=1}^{M} P(y[m]|\boldsymbol{\theta}_Y, \mathcal{G}_0)\, P(\boldsymbol{\theta}_Y|\mathcal{G}_0)\; d\boldsymbol{\theta}_Y \right)$$

Note: decomposes into one term for each random variable

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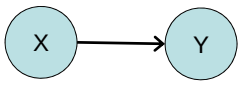
Bayesian Scoring

Now suppose there are two binary random variables X and Y and let $\mathcal{G}_{X\to Y}$ be the graph below:



X	P(X)
0	θ_X
1	

X	Y	P(Y|X)
0	0	$\theta_{Y\|x^0}$
0	1	
1	0	$\theta_{Y\|x^1}$
1	1	

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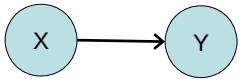
Bayesian Scoring

Now suppose there are two binary random variables X and Y and let $\mathcal{G}_{X\to Y}$ be the graph below:



$$P(\mathcal{D}|\mathcal{G}_{X\to Y}) = \left(\int_{\Theta_X} \prod_{m=1}^{M} P(x[m]|\boldsymbol{\theta}_X, \mathcal{G}_{X\to Y}) \mathrm{P}(\boldsymbol{\theta}_X|\mathcal{G}_{X\to Y})\, d\boldsymbol{\theta}_X\right) \cdot \left(\int_{\Theta_{Y|x^0}} \prod_{m:x[m]=x^0}^{M} P(y[m]|\boldsymbol{\theta}_{Y|x^0}, \mathcal{G}_{X\to Y})\, P(\boldsymbol{\theta}_{Y|x^0}|\mathcal{G}_{X\to Y})\; d\boldsymbol{\theta}_{Y|x^0}\right) \cdot \left(\int_{\Theta_{Y|x^1}} \prod_{m:x[m]=x^1}^{M} P(y[m]|\boldsymbol{\theta}_{Y|x^1}, \mathcal{G}_{X\to Y})\, P(\boldsymbol{\theta}_{Y|x^1}|\mathcal{G}_{X\to Y})\; d\boldsymbol{\theta}_{Y|x^1}\right)$$

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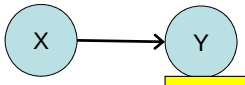
Bayesian Scoring

Now suppose there are two binary random variables X and Y and let $\mathcal{G}_{X\to Y}$ be the graph below:



One term for each parameter family.
Each term has a closed form solution

$$P(\mathcal{D}|\mathcal{G}) = \frac{\Gamma(\alpha)}{\Gamma(\alpha+M)} \cdot \prod_i^k \frac{\Gamma(\alpha_i + M[x^i])}{\Gamma(\alpha_i)}$$

$$P(\mathcal{D}|\mathcal{G}_{X\to Y}) = \left(\int_{\Theta_X} \prod_{m=1}^{M} P(x[m]|\boldsymbol{\theta}_X, \mathcal{G}_{X\to Y}) P(\boldsymbol{\theta}_X|\mathcal{G}_{X\to Y})\, d\boldsymbol{\theta}_X\right) \cdot$$

$$\left(\int_{\Theta_{Y|x^0}} \prod_{m:x[m]=x^0}^{M} P(y[m]|\boldsymbol{\theta}_{Y|x^0}, \mathcal{G}_{X\to Y})\, P(\boldsymbol{\theta}_{Y|x^0}|\mathcal{G}_{X\to Y})\, d\boldsymbol{\theta}_{Y|x^0}\right) \cdot$$

$$\left(\int_{\Theta_{Y|x^1}} \prod_{m:x[m]=x^1}^{M} P(y[m]|\boldsymbol{\theta}_{Y|x^1}, \mathcal{G}_{X\to Y})\, P(\boldsymbol{\theta}_{Y|x^1}|\mathcal{G}_{X\to Y})\, d\boldsymbol{\theta}_{Y|x^1}\right)$$

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Bayesian Scoring

The general case: let $\mathcal{G}$ be a network structure, and let $P(\theta_{\mathcal{G}}|\mathcal{G})$ be a parameter prior satisfying global parameter independence. Then:

$$P(\mathcal{D}|\mathcal{G}) = \prod_{i=1}^{n} \int_{\Theta_{X_i|Pa(X_i)}} \prod_{m=1}^{M} P(x_i[m]|pa(X_i)[m], \boldsymbol{\theta}_{X_i|Pa(X_i)}, \mathcal{G})\, P(\boldsymbol{\theta}_{X_i|Pa(X_i)}|\mathcal{G}) d\boldsymbol{\theta}_{X_i|Pa(X_i)}$$

If $P(\boldsymbol{\theta}_{\mathcal{G}})$ also satisfies local parameter independence, then

$$P(\mathcal{D}|\mathcal{G}) = \prod_{i=1}^{n} \prod_{\boldsymbol{u}_i \in Val(Pa^{\mathcal{G}}(X_i))} \int_{\Theta_{X_i|\boldsymbol{u}_i}} \prod_{m:\, \boldsymbol{u}_i[m]=\boldsymbol{u}_i}^{M} P(x_i[m]|\boldsymbol{u}_i)[m], \boldsymbol{\theta}_{X_i|\boldsymbol{u}_i}, \mathcal{G})\, P(\boldsymbol{\theta}_{X_i|\boldsymbol{u}_i}|\mathcal{G}) d\boldsymbol{\theta}_{X_i|\boldsymbol{u}_i}$$

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Bayesian Scoring

If we have a Bayesian network with Dirichlet priors where $P(\theta_{X_i|pa(X_i)}|\mathcal{G})$ has hyperparameters $\left\{\alpha^{\mathcal{G}}{}_{x^j{}_i|\boldsymbol{u}_i} : j = 1, \ldots, |X_i|\right\}$ then

$$P(\mathcal{D}|\mathcal{G}) = \prod_{i=1}^{n} \prod_{u_i \in Val(Pa^{\mathcal{G}}(X_i))} \frac{\Gamma(\alpha^{\mathcal{G}}{}_{X_i|\boldsymbol{u}_i})}{\Gamma(\alpha^{\mathcal{G}}{}_{X_i|\boldsymbol{u}_i} + M[u_i])} \prod_{x_i{}^j \in Val(X_i)} \left[\frac{\Gamma\left(\alpha^{\mathcal{G}}{}_{x_i{}^j|\boldsymbol{u}_i}\right) + M[x_i{}^j, \boldsymbol{u}_i]}{\Gamma(\alpha^{\mathcal{G}}{}_{x_i{}^j|\boldsymbol{u}_i})}\right]$$

Where:

$$\alpha^{\mathcal{G}}{}_{X_i|\boldsymbol{u}_i} = \sum_j \alpha^{\mathcal{G}}{}_{X_i{}^j|\boldsymbol{u}_i}$$

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Bayesian Scoring

If we have a Bayesian network with Dirichlet priors where $P(\theta_{X_i|pa(X_i)}|\mathcal{G})$ has hyperparameters $\left\{\alpha^{\mathcal{G}}{}_{x^j{}_i|\boldsymbol{u}_i} : j = 1, \ldots, |X_i|\right\}$ then

$$P(\mathcal{D}|\mathcal{G}) = \prod_{i=1}^{n} \prod_{u_i \in Val(Pa^{\mathcal{G}}(X_i))} \frac{\Gamma(\alpha^{\mathcal{G}}{}_{X_i|\boldsymbol{u}_i})}{\Gamma(\alpha^{\mathcal{G}}{}_{X_i|\boldsymbol{u}_i} + M[u_i])} \prod_{x_i{}^j \in Val(X_i)} \left[\frac{\Gamma\left(\alpha^{\mathcal{G}}{}_{x_i{}^j|\boldsymbol{u}_i}\right) + M[x_i{}^j, \boldsymbol{u}_i]}{\Gamma(\alpha^{\mathcal{G}}{}_{x_i{}^j|\boldsymbol{u}_i})}\right]$$

Where:

$$\alpha^{\mathcal{G}}{}_{X_i|\boldsymbol{u}_i} = \sum_j$$

Iterates over # of random variables

Iterates over # of instantiations of parents of X_i

Iterates over # of values of X_i

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Bayesian Scoring

If we use a Dirichlet parameter prior for all parameters in our network, then, because $M \to \infty$ (proof omitted), we have:

$$logP(\mathcal{D}|\mathcal{G}) = l\left(\hat{\theta}_{\mathcal{G}}:\mathcal{D}\right) - \frac{logM}{2} Dim[\mathcal{G}] + O(1)$$

$Dim[\mathcal{G}]$: # of independent parameters in $\mathcal{G}$

This is the Bayesian Information Criterion (BIC) score

Bayesian Scoring

This is the Bayesian Information Criterion (BIC) score:

$$score_{BIC}(\mathcal{G}:\mathcal{D}) = l\left(\hat{\theta}_{\mathcal{G}}:\mathcal{D}\right) - \frac{logM}{2} Dim[\mathcal{G}] + O(1)$$

$l\left(\hat{\theta}_{\mathcal{G}}:\mathcal{D}\right)$: Fit to data

$\frac{logM}{2} Dim[\mathcal{G}]$: Model complexity

Can also interpret this as the # of bits to encode the model and the data given the model (minimum description length)

Bayesian Scoring

$$score_{BIC}(\mathcal{G}:\mathcal{D}) = M\sum_{i=1}^{n} \boldsymbol{I}_{\hat{P}}(X_i; Pa(X_i)) - M\sum_{i=1}^{n} \boldsymbol{H}_{\hat{P}}(X_i) - \frac{logM}{2} Dim[\mathcal{G}]$$

Things to note:

- Entropy term $M\sum_{i=1}^{n} \boldsymbol{H}_{\hat{P}}(X_i)$ can be ignored (doesn't depend on graph structure)
- Trades off fit to data and model complexity
  - The stronger the dependence of a variable on its parents, the higher the score (grows linearly)
  - The more complex the network, the lower the score (grows logarithmically)
- As M grows, the score pays more attention to the data fit

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Bayesian Scoring

Assume that our data are generated by some distribution P^* for which the network $\mathcal{G}^*$ is a perfect map.

We say that a scoring function is consistent if the following properties hold as the amount of data $M \to \infty$, with probability that approaches 1 (over all possible choices of data set $\mathcal{D}$):

- The structure $\mathcal{G}^*$ will maximize the score
- All structures $\mathcal{G}$ that are not I-equivalent to $\mathcal{G}^*$ will have strictly lower score

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Bayesian Scoring

- The BIC score (and the Bayesian score) is consistent [proof omitted]
- In practice though, the BIC score tends to have a very strong preference for simpler structures

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Structure Priors

Recall that

$$score_B(\mathcal{G}:\mathcal{D}) = logP(\mathcal{D} \mid \mathcal{G}) + \log P(\mathcal{G})$$

Grows linearly with the number of examples (dominates the score)

Structure prior (stays constant). Only matters for small sample sizes

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Structure Priors

- Typically assign uniform priors over structures
- If you can provide an informed structure prior, you could penalize edges in the graph:
  - $P(\mathcal{G}) \propto c^{|\mathcal{G}|}$ (where $c < 1$ and $|\mathcal{G}|$ is the number of edges)
- Mathematically convenient to have structure prior with structure modularity:
  - $P(\mathcal{G}) \propto \prod_i P(Pa(X_i) = Pa^{\mathcal{G}}(X_i))$

Uses local properties not global properties of the graph

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