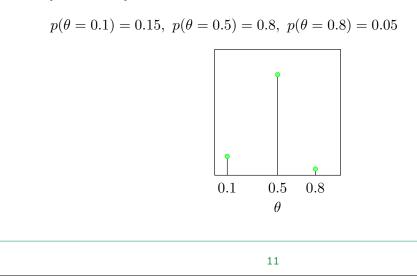


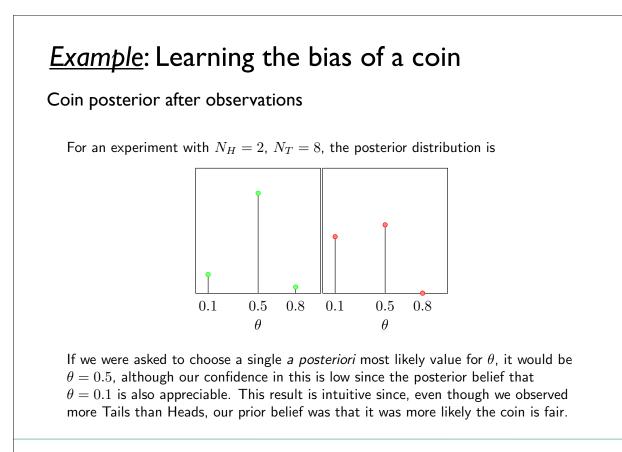
Example: Learning the bias of a coin The posterior $p(\theta|v^{1},...,v^{N}) \propto p(\theta) \prod_{n=1}^{N} p(v^{n}|\theta)$ $= p(\theta) \prod_{n=1}^{N} \theta^{\mathbb{I}[v^{n}=1]} (1-\theta)^{\mathbb{I}[v^{n}=0]}$ $\propto p(\theta) \theta^{\sum_{n=1}^{N} \mathbb{I}[v^{n}=1]} (1-\theta)^{\sum_{n=1}^{N} \mathbb{I}[v^{n}=0]}$ Hence $p(\theta|v^{1},...,v^{N}) \propto p(\theta) \theta^{N_{H}} (1-\theta)^{N_{T}}$ $N_{H} = \sum_{n=1}^{N} \mathbb{I}[v^{n}=1] \text{ is the number of occurrences of heads.}$ $N_{T} = \sum_{n=1}^{N} \mathbb{I}[v^{n}=0] \text{ is the number of tails.}$

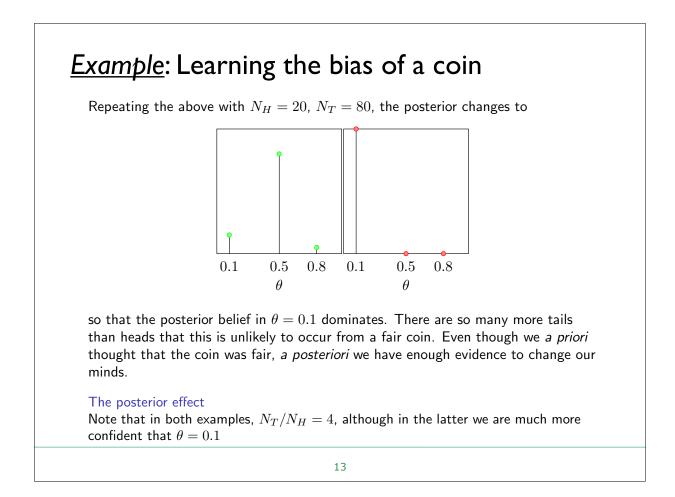
Example: Learning the bias of a coin

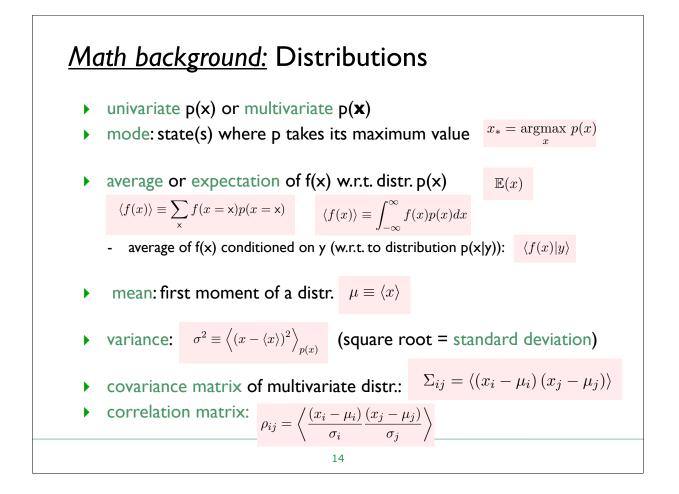
The prior

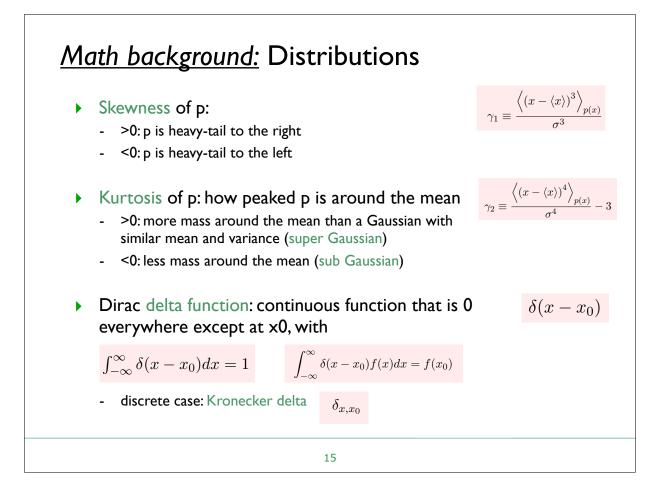
We still need to fully specify the prior $p(\theta)$. To avoid complexities resulting from continuous variables, we'll consider a discrete θ with only three possible states, $\theta \in \{0.1, 0.5, 0.8\}$. Specifically, we assume

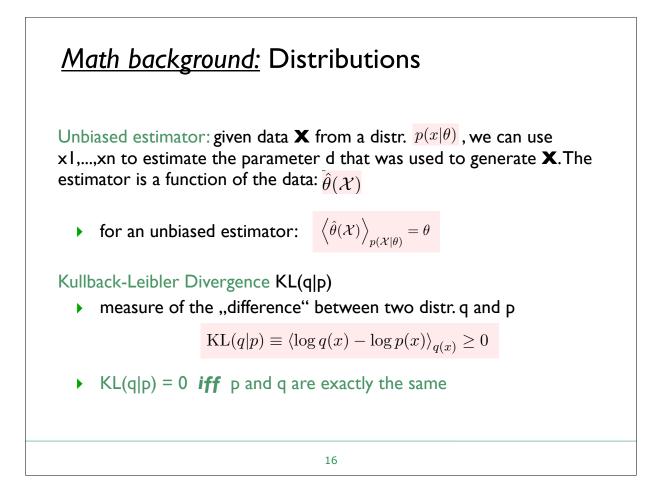


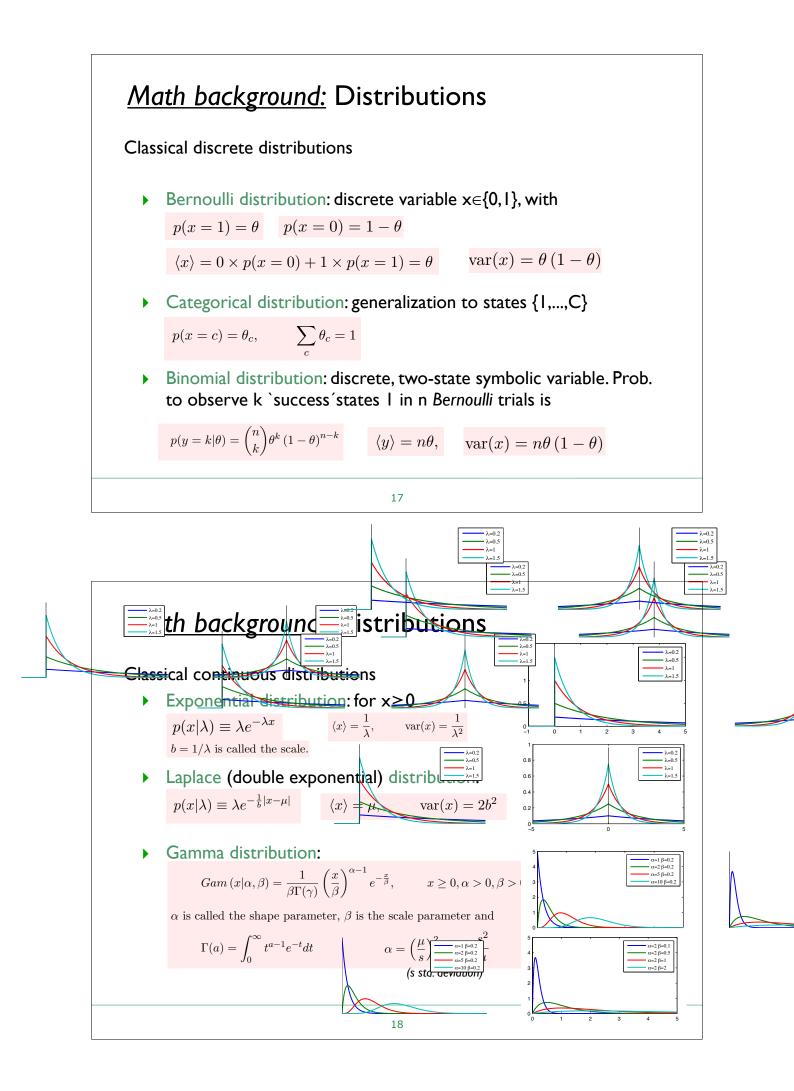


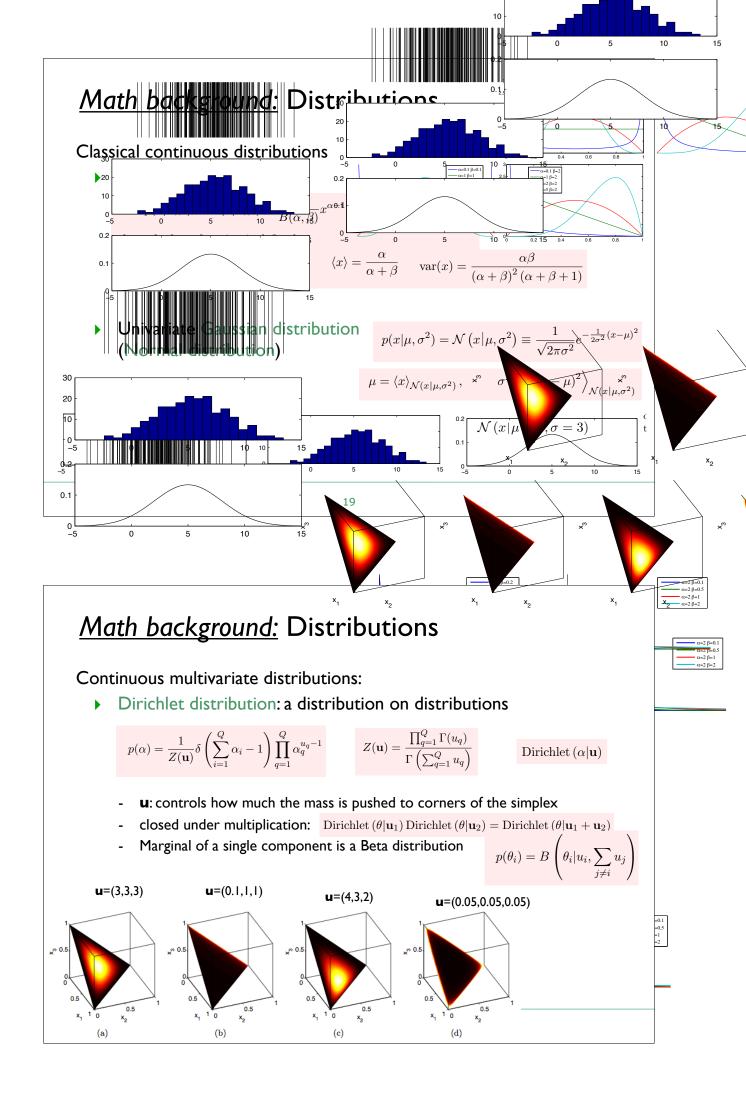


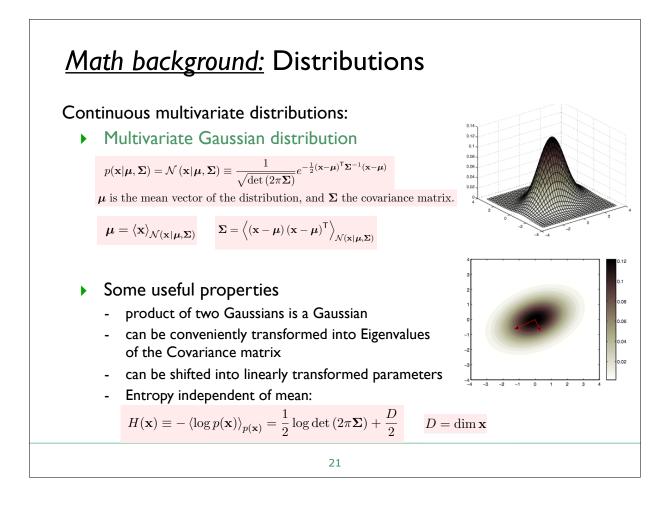












Learning distributions

For a distribution $p(x|\theta)$ and data $X = \{x \mid \dots, xN\}$, learning corresponds to <u>inferring</u> the parameter θ that best explains data X. Using Bayes: posterior $p(\theta|X) =$ likelihood $p(X|\theta) *$ prior $p(\theta) /$ evidence p(X)

- Bayesian methods: examine posterior p(θ|x) ∝ p(X|θ) p(θ). This gives rise to a distribution over θ.
- Maximum a posteriori: $\theta^{MAP} = \operatorname{argmax}_{\theta} p(\theta | \mathbf{X})$
- Maximum likelihood: Under a flat prior p(θ)=const., the MAP solution is equivalent to setting θ to the value that maximizes the likelihood of observing the data: θ^{ML}=argmax_θ p(**X**|θ)

Learning distributions

Often, a numerical optimization is required to single out the best parameter value. Thus it is important to find a good model that makes computation feasible, or to find good approximations.

Often, the distributions are also conditioned on the model M

- $\mathsf{p}(\theta | \mathbf{X}, M) = \mathsf{p}(\mathbf{X} | \theta, M) \mathsf{p}(\theta | M) / \mathsf{p}(\mathbf{X} | M)$
 - model likelihood p(X|M)

For a set of observations x1,...,xN, conditioned on θ , we say the **X** are independent and identically distributed (i.i.d.) if there is no dependence between the observations: $p(\mathbf{X}|\theta) = \prod p(xi|\theta)$

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Maximum likelihood estimation (MLE)

With i.i.d. data samples $D=\{x[m]\}, m=1...N$, what are the parameters Θ that makes sampling x from $p(x|\Theta)$ as likely as possible?

Maximize

$$\mathsf{P}(\mathsf{D} \mid \theta) = \prod_{\mathsf{m}} \mathsf{P}(\mathsf{x}[\mathsf{m}] \mid \theta)$$

Direct approach:

- maximize the log likelihood: $log(L) = \sum_{m} log p(x[m]|\Theta)$
- \blacktriangleright write down derivative dL/d Θ with respect to each parameter and solve for 0

In practice, one is often interested in (assumed) certain distributions, whose parameter(s) should be learned

Maximum likelihood learning

Given a set of training data $\mathcal{X} = \{\mathbf{x}^1, \dots, \mathbf{x}^N\}$, drawn from a Gaussian $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma})$ with unknown mean $\boldsymbol{\mu}$ and covariance $\boldsymbol{\Sigma}$, how can we find these parameters? Assuming the data are drawn i.i.d. the log likelihood is

$$L(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \equiv \sum_{n=1}^{N} \log p(x|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = -\frac{1}{2} \sum_{n=1}^{N} (\mathbf{x}^{n} - \boldsymbol{\mu})^{\mathsf{T}} \boldsymbol{\Sigma}^{-1} (\mathbf{x}^{n} - \boldsymbol{\mu}) - \frac{N}{2} \log \det (2\pi \boldsymbol{\Sigma})$$
(8.6.37)

Direct approach:

• optimal mean: search for zero vector derivative

$$\nabla_{\boldsymbol{\mu}} L(\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \sum_{n=1}^{N} \boldsymbol{\Sigma}^{-1} \left(\mathbf{x}^{n} - \boldsymbol{\mu} \right) \qquad \qquad \sum_{n=1}^{N} \boldsymbol{\Sigma}^{-1} \mathbf{x}^{n} = N \boldsymbol{\mu} \boldsymbol{\Sigma}^{-1} \qquad \qquad \boldsymbol{\mu} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}^{n}$$

• optimal covariance: setting derivative w.r.t. the covariance matrix to zero gives $\Sigma = \frac{1}{N} \sum_{n=1}^{N} (\mathbf{x}^n - \boldsymbol{\mu}) (\mathbf{x}^n - \boldsymbol{\mu})^{\mathsf{T}}$

 \rightarrow max. likelihood solution for training data X simply sets parameters to sample statistics of the empirical distribution, i.e. we can count.

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Example

Consider the following model of the relationship between exposure to asbestos (a), being a smoker (s) and the incidence of lung cancer (c)

p(a, s, c) = p(c|a, s)p(a)p(s)

Each variable is binary, $dom(a) = \{0, 1\}$, $dom(s) = \{0, 1\}$, $dom(c) = \{0, 1\}$. Furthermore, we assume that we have a list of patient records, where each row represents a patient's data.

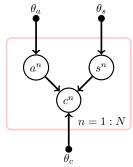
а	S	с	
1	1	1	
1	0	0	
0	1	1	
0	1	0	
1	1	1	
0	0	0	
1	0	1	

A database containing information about the Asbestos exposure (1 signifies exposure), being a Smoker (1 signifies the individual is a smoker), and lung Cancer (1 signifies the individual has lung Cancer). Each row contains the information for an individual, so that there are 7 individuals in the database.

Example

Choosing a structure and learning the table

а	S	с
1	1	1
1	0	0
0	1	1
0	1	0
1	1	1
0	0	0
1	0	1



To learn the table entries p(c|a, s) we can do so by counting the number of c is in state 1 for each of the 4 parental states of a and s:

 $\begin{array}{ll} p(c=1|a=0,s=0)=0, & p(c=1|a=0,s=1)=0.5\\ p(c=1|a=1,s=0)=0.5 & p(c=1|a=1,s=1)=1 \end{array} \end{array}$

Similarly, based on counting, p(a = 1) = 4/7, and p(s = 1) = 4/7. These three CPTs then complete the full distribution specification.

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Maximum likelihood learning

Maximum likelihood and KL divergence

Let q be the empirical distribution:

$$q(x) = \frac{1}{N}\sum_{n=1}^{N}\mathbb{I}\left[x = x^{n}\right]$$

Then

$$\begin{split} \mathrm{KL}(q|p(x|\theta)) &= \langle \log q(x) \rangle_{q(x)} - \langle \log p(x|\theta) \rangle_{q(x)} \\ &= -\frac{1}{N} \sum_{n=1}^{N} \log p(x^n|\theta) + \mathsf{const.} \end{split}$$

Hence setting parameters of p that maximise the likelihood is equivalent to setting parameters of p that minimise the KL divergence between p and the empirical distribution.

Maximum likelihood learning

Maximum likelihood BN training and counting

A BN takes the form:

$$p(x) = \prod_{i=1}^{K} p(x_i | \operatorname{pa}(x_i))$$

For the BN $p(\boldsymbol{x}),$ and empirical distribution $q(\boldsymbol{x})$ we have

$$\begin{split} \mathrm{KL}(q|p) &= -\left\langle \sum_{i=1}^{K} \log p\left(x_{i}|\mathrm{pa}\left(x_{i}\right)\right) \right\rangle_{q(x)} + \mathrm{const.} \\ &= -\sum_{i=1}^{K} \left\langle \log p\left(x_{i}|\mathrm{pa}\left(x_{i}\right)\right) \right\rangle_{q(x_{i},\mathrm{pa}(x_{i}))} + \mathrm{const.} \\ &= \sum_{i=1}^{K} \left[\left\langle \log q(x_{i}|\mathrm{pa}\left(x_{i}\right)\right) \right\rangle_{q(x_{i},\mathrm{pa}(x_{i}))} - \left\langle \log p\left(x_{i}|\mathrm{pa}\left(x_{i}\right)\right) \right\rangle_{q(x_{i},\mathrm{pa}(x_{i}))} \right] + \\ &= \sum_{i=1}^{K} \left\langle \mathrm{KL}(q(x_{i}|\mathrm{pa}\left(x_{i}\right))|p(x_{i}|\mathrm{pa}\left(x_{i}\right))) \right\rangle_{q(\mathrm{pa}(x_{i}))} + \mathrm{const.} \end{split}$$

Maximum likelihood learning

Maximum likelihood BN training and counting

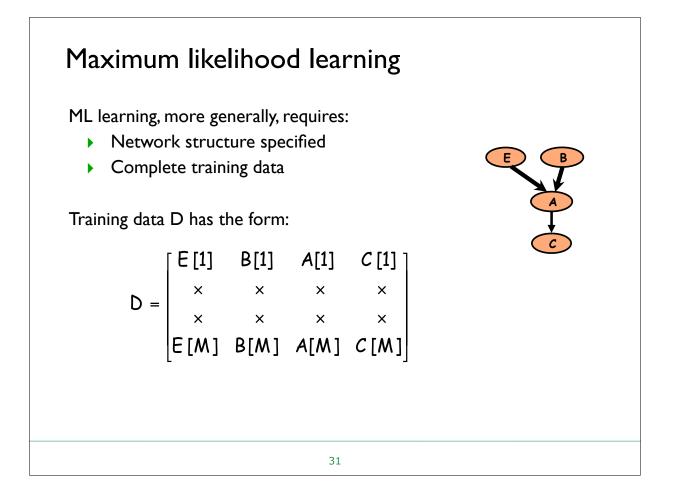
The minimal Kullback-Leibler setting, and that which corresponds to Maximum Likelihood, is therefore

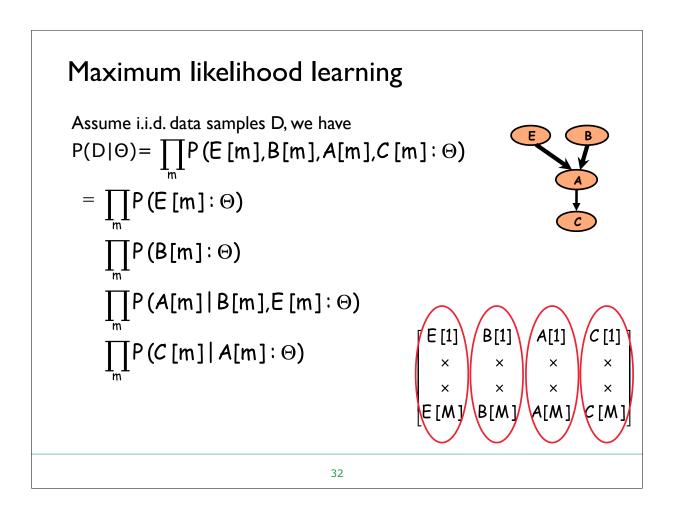
$$p(x_i | \operatorname{pa}(x_i)) = q(x_i | \operatorname{pa}(x_i))$$

In terms of the original data, this is

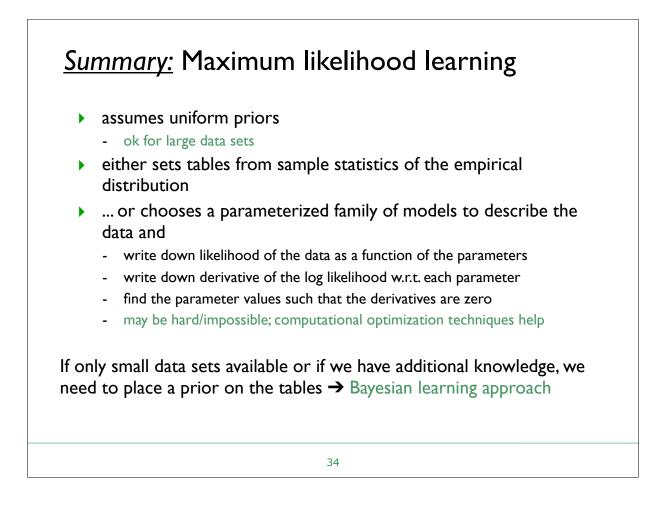
$$p(x_i = \mathsf{s}|\mathrm{pa}\,(x_i) = \mathsf{t}) \propto \sum_{n=1}^{N} \mathbb{I}\left[x_i^n = \mathsf{s}\right] \prod_{x_j \in \mathrm{pa}(x_i)} \mathbb{I}\left[x_j^n = \mathsf{t}^j\right]$$

The table entry $p(x_i|pa(x_i))$ can be set by counting the number of times the state $\{x_i = s, pa(x_i) = t\}$ occurs in the dataset (where t is a vector of parental states). The table is then given by the relative number of counts of being in state s compared to the other states s', for fixed joint parental state t.





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Bayesian Belief Net training

We continue with the Asbestos, Smoking, Cancer scenario,

$$p(a, c, s) = p(c|a, s)p(a)p(s)$$

and a set of visible observations, $\mathcal{V}=\{(a^n,s^n,c^n)\,,n=1,\ldots,N\}.$ With all variables binary we have parameters such as

$$p(a = 1|\theta_a) = \theta_a, \quad p(c = 1|a = 0, s = 1, \theta_c) = \theta_c^{0,1}$$

The parameters are

$$\theta_a, \theta_s, \underbrace{\theta_c^{0,0}, \theta_c^{0,1}, \theta_c^{1,0}, \theta_c^{1,1}}_{\theta_c}$$

In Bayesian learning of BNs, we need to specify a prior on the joint table entries. Since in general dealing with multi-dimensional continuous distributions is computationally problematic, it is useful to specify only uni-variate distributions in the prior. As we show below, this has a pleasing consequence that for i.i.d. data the posterior also factorises into uni-variate distributions.

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Global parameter independence

A convenient assumption is that the prior factorises over parameters. For our Asbestos, Smoking, Cancer example, we assume

$$p(\theta_a, \theta_s, \theta_c) = p(\theta_a)p(\theta_s)p(\theta_c)$$

Assuming the data is i.i.d., we then have the joint model

$$p(\theta_a, \theta_s, \theta_c, \mathcal{V}) = p(\theta_a)p(\theta_s)p(\theta_c)\prod_n p(a^n|\theta_a)p(s^n|\theta_s)p(c^n|s^n, a^n, \theta_c)$$

Learning then corresponds to inference of

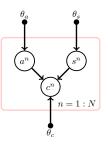
$$p(\theta_a, \theta_s, \theta_c | \mathcal{V}) = \frac{p(\mathcal{V} | \theta_a, \theta_s, \theta_c) p(\theta_a, \theta_s, \theta_c)}{p(\mathcal{V})} = \frac{p(\mathcal{V} | \theta_a, \theta_s, \theta_c) p(\theta_a) p(\theta_s) p(\theta_c)}{p(\mathcal{V})}$$

The posterior also factorises, since

$$p(\theta_a, \theta_s, \theta_c | \mathcal{V}) \propto p(\theta_a, \theta_s, \theta_c, \mathcal{V})$$

$$= \left\{ p(\theta_a) \prod_n p(a^n | \theta_a) \right\} \left\{ p(\theta_s) \prod_n p(s^n | \theta_s) \right\} \left\{ p(\theta_c) \prod_n p(c^n | s^n, a^n, \theta_c) \right\}$$

$$\propto p(\theta_a | \mathcal{V}_a) p(\theta_s | \mathcal{V}_s) p(\theta_c | \mathcal{V}_c)$$



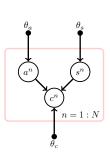
Local parameter independence

If we further assume that the prior for the table factorises over all states a, c:

$$p(\theta_c) = p(\theta_c^{0,0}) p(\theta_c^{1,0}) p(\theta_c^{0,1}) p(\theta_c^{1,1})$$

then the posterior

$$p(\theta_{c}|\mathcal{V}_{c}) \propto p(\mathcal{V}_{c}|\theta_{c})p(\theta_{c}^{0,0})p(\theta_{c}^{1,0})p(\theta_{c}^{0,1})p(\theta_{c}^{1,1}) \\ = \underbrace{\left[\theta_{c}^{0,0}\right]^{\sharp(a=0,s=0)} p(\theta_{c}^{0,0})}_{\propto p(\theta_{c}^{0,0}|\mathcal{V}_{c})} \underbrace{\left[\theta_{c}^{0,1}\right]^{\sharp(a=0,s=1)} p(\theta_{c}^{0,1})}_{\propto p(\theta_{c}^{0,1}|\mathcal{V}_{c})} \\ \times \underbrace{\left[\theta_{c}^{1,0}\right]^{\sharp(a=1,s=0)} p(\theta_{c}^{1,0})}_{\propto p(\theta_{c}^{1,0}|\mathcal{V}_{c})} \underbrace{\left[\theta_{c}^{1,1}\right]^{\sharp(a=1,s=1)} p(\theta_{c}^{1,1})}_{\propto p(\theta_{c}^{1,1}|\mathcal{V}_{c})}$$



so that the posterior also factorises over the parental states of the local conditional table.

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Using a Beta prior

$$p(\theta_a) = B\left(\theta_a | \alpha_a, \beta_a\right) = \frac{1}{B(\alpha_a, \beta_a)} \theta_a^{\alpha_a - 1} \left(1 - \theta_a\right)^{\beta_a - 1}$$

for which the posterior is also a Beta distribution:

$$p(\theta_a | \mathcal{V}_a) = B\left(\theta_a | \alpha_a + \sharp \left(a = 1\right), \beta_a + \sharp \left(a = 0\right)\right)$$

The marginal table is given by

$$p(a=1|\mathcal{V}_a) = \int_{\theta_a} p(\theta_a|\mathcal{V}_a)\theta_a = \frac{\alpha_a + \sharp (a=1)}{\alpha_a + \sharp (a=1) + \beta_a + \sharp (a=0)}$$

Corresponds in this case to adding 'pseudo counts' to the data.

hyperparameters

The prior parameters α_a,β_a are called hyperparameters. If one had no preference, one would set $\alpha_a=\beta_b=1.$

<u>Summary</u> : Learning Parameters				
Estimation relies on sufficient statistics				
Maximum-likelihood (estimation) (ML/MLE)				
 standard (non-bayesian) statistical learning 				
 useful for large data sets, where priors get irrelevant 				
Bayesian parameter learning				
 Include prior probabilities, useful when data sets smaller 				
 Prediction is standard Bayesian inference 				
MLE vs. Bayesian learning				
 Both are asymptotically equivalent and consistent 				
 Both can be implemented in an on-line manner by accumulating sufficient statistics 				
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Outlook

Next week:

Learning with missing data (hidden variables)

Expectation Maximization

Learning network structure

- PC (local search)
- scoring (global search)