Probabilistic Graphical Models

Parameter learning in Bayesian networks

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Learning objectives

- likelihood function and MLE
- role of the sufficient statistics
- MLE for parameter learning in directed models
    - why is it easy?
- conjugate priors and Bayesian parameter learning

Likelihood function through an example

a thumbtack with unknown prob. of heads & tails

Bernoulli dist. $p(x;\theta) = \theta^x (1-\theta)^{(1-x)}$

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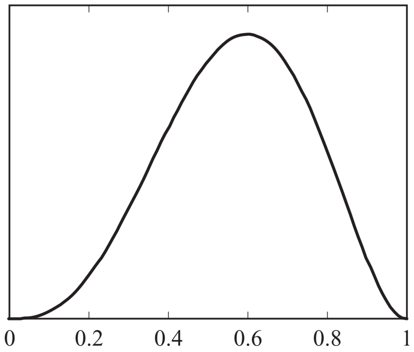
IID observations $\mathcal{D} = \{1,0,0,1,1\}$

likelihood of θ is $L(\theta;\mathcal{D}) = \prod_{x\in\mathcal{D}} P(x;\theta) = \theta^3(1-\theta)^2$



likelihood function θ

not a pdf (it does not integrate to 1)

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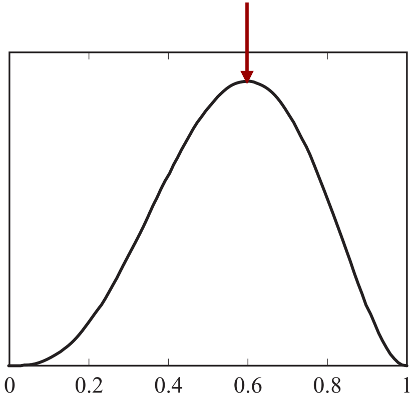
log-likelihood: $\log L(\theta;\mathcal{D}) = 3\log\theta + 2\log(1-\theta)$

maximizing the log-likelihood (M-projection of $P_{\mathcal{D}}$)

$$\frac{\partial}{\partial\theta}\left(3\log\theta + 2\log(1-\theta)\right) = \frac{3}{\theta} - \frac{2}{1-\theta} = \frac{3-5\theta}{\theta(1-\theta)} = 0 \Rightarrow \hat{\theta} = \frac{3}{5}$$

max-likelihood estimate (MLE)



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Sufficient statistics through an example

IID observations $\mathcal{D} = \{1, 0, 0, 1, 1\}$

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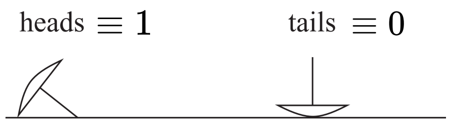

all we needed to know about the data:

- number of heads and tails

given a distribution $P(x; \theta)$

- its sufficient statistics is function $\phi = [\phi_1, \ldots, \phi_K]$ such that

$$\mathbb{E}_{\mathcal{D}}[\phi(x)] = \mathbb{E}_{\mathcal{D}'}[\phi(x')] \quad \Rightarrow \quad \frac{1}{|\mathcal{D}|} L(\theta, \mathcal{D}) = \frac{1}{|\mathcal{D}'|} L(\theta, \mathcal{D}') \quad \forall \mathcal{D}, \mathcal{D}', \theta$$

sufficient statistics of the dataset is all that matters about the data

Revisiting exponential family

given a distribution $P(x;\theta)$

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$L(\theta, \mathcal{D}) = \prod_{x \in \mathcal{D}} p(x; \theta)$

the (linear) exponential family: $p(x) \propto \exp(\langle \theta, \phi(x) \rangle)$

- max-entropy distribution subject to $\mathbb{E}_p[\phi(x)] = \mu$

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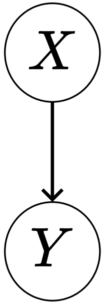
- max-entropy distribution subject to $\mathbb{E}_p[\phi(x)] = \mu$
- if $\phi_1, \ldots, \phi_k$ are linearly independent, then $\theta \leftrightarrow \mu$

MLE for Bayesian networks an example

a simple network $p(x, y; \theta) = p(x; \theta_X)p(y|x; \theta_{Y|X})$



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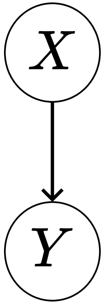

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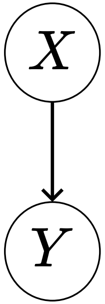

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for discrete vars.

number of times $x = \ell$ in the dataset

number of times $x = \ell, y = \ell'$ in the dataset

$$L(\mathcal{D}; \theta) = \left(\prod_{\ell \in Val(X)} \theta_{X,\ell}^{N(x=\ell)}\right) \left(\prod_{\ell, \ell' \in Val(X) \times Val(Y)} \theta_{Y|X,\ell,\ell'}^{N(x=\ell, y=\ell')}\right)$$

$\theta_{X,\ell} \rightarrow p(X = \ell)$

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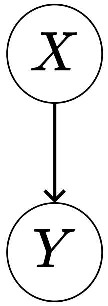

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$\theta_{X,\ell} \to p(X = \ell)$

$\theta_{Y|X,\ell,\ell'} \to p(X = \ell \mid Y = \ell')$

MLE : maximize local likelihood terms individually

$$\theta_{X,\ell} = \frac{N(x=\ell)}{|\mathcal{D}|} \quad \theta_{Y|X,\ell,\ell'} = \frac{N(x=\ell,y=\ell')}{|\mathcal{D}|}$$

MLE for Bayesian networks general case

Bayes-net $$p(x;\theta) = \prod_i p(x_i \mid Pa_{x_i}; \theta_{X_i|Pa_{X_i}})$$

likelihood $$L(\mathcal{D};\theta) = \prod_{x \in \mathcal{D}} \prod_i p(x_i \mid Pa_{x_i}; \theta_{i|Pa_i})$$

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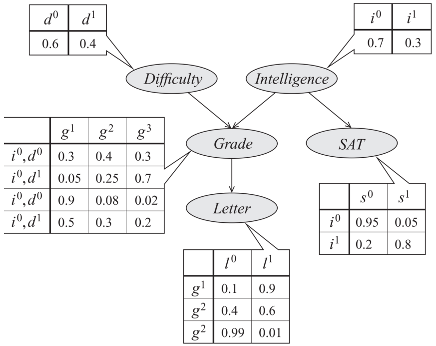

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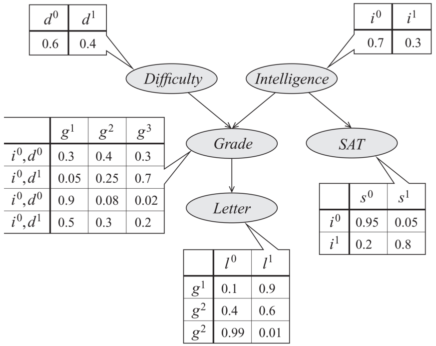

maximizing the conditional likelihood for each node

- similar to solving individual prediction problems

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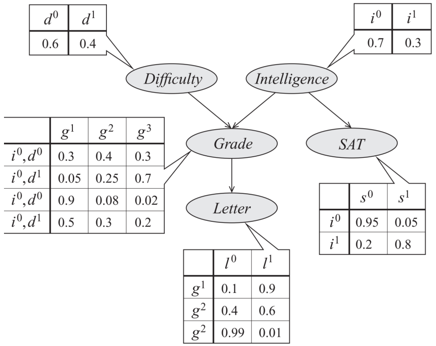

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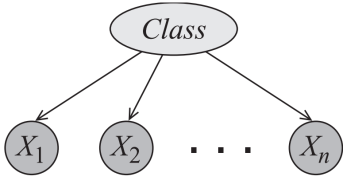
Example how to learn a naive Bayes?



Bayesian parameter estimation

max-likelihood is the same $\hat{\theta} = \frac{1}{3}$ for

case 1. $N(x=1) = 1, N(x=0) = 2$

case 2. $N(x=1) = 100, N(x=0) = 200$

Example

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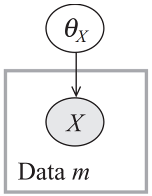
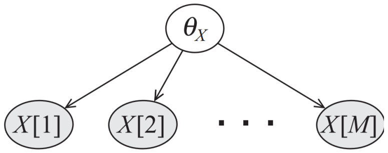
Example

need to model our uncertainty

Bayesian approach:

- assume a prior $p(\theta)$
- estimate the posterior





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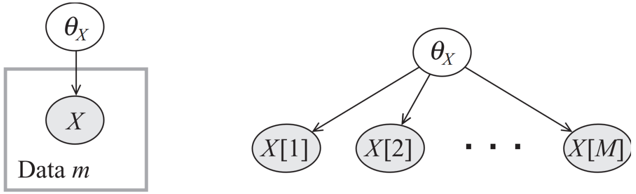
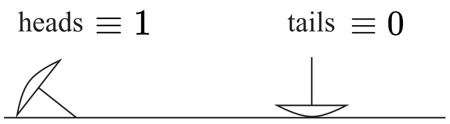
$$p(\theta \mid \mathcal{D}) = \frac{p(\theta)p(\mathcal{D}|\theta)}{p(\mathcal{D})} \propto p(\theta)p(\mathcal{D} \mid \theta)$$

posterior; prior: $p(\theta)$; likelihood: $p(\mathcal{D} \mid \theta) \rightarrow \prod_{x \in \mathcal{D}} p(x|\theta)$; marginal likelihood: $p(\mathcal{D})$



Bayesian parameter estimation

assuming a uniform prior $p(\theta) = \begin{cases} 1 & 0 \leq \theta \leq 1 \\ 0 & o.w. \end{cases}$



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posterior predictive: predicting heads/tails using the posterior

rather than a single MLE value

$$p(x \mid \mathcal{D}) = \int_0^1 p(\theta|\mathcal{D})p(x|\theta)\mathrm{d}\theta$$

$\propto \theta^{N(1)}(1-\theta)^{N(0)}$ $\theta^{x}(1-\theta)^{(1-x)}$

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(and normalize)

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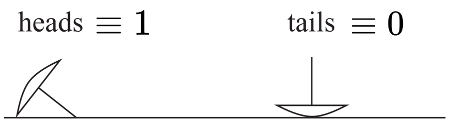

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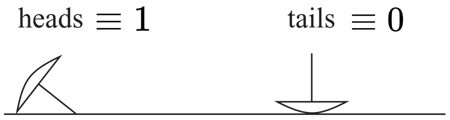
compare with prediction using MLE $p(x=1 \mid \mathcal{D}) = \frac{N(1)}{N(0)+N(1)}$

Conjugate priors



how about non-uniform priors? E.g., more likely to see heads

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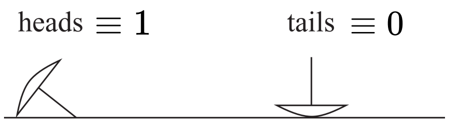

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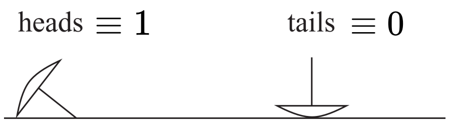

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conjugate prior to the Bernoulli likelihood is the Beta distribution

$$p(\mathcal{D}|\theta) \propto \theta^{N(1)}(1-\theta)^{N(0)}$$

$$p(\theta;\alpha,\beta) = \gamma\theta^{\alpha-1}(1-\theta)^{\beta-1}$$

$$\gamma = \frac{\Gamma(\alpha+\beta)}{\Gamma(\alpha)\Gamma(\beta)}$$

Conjugate priors: Beta-Bernoulli

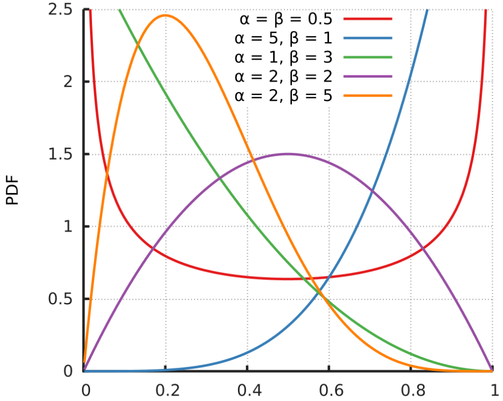

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image: wikipedia

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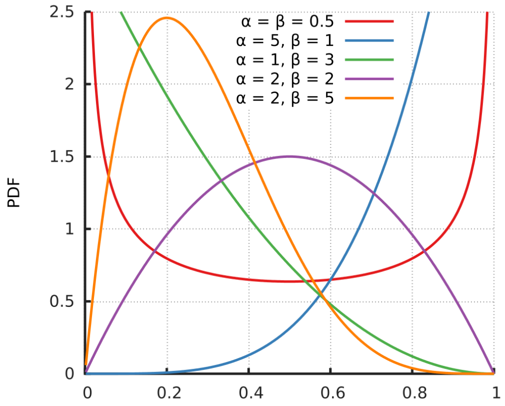

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extension of factorial function $\Gamma(n+1) = n!$

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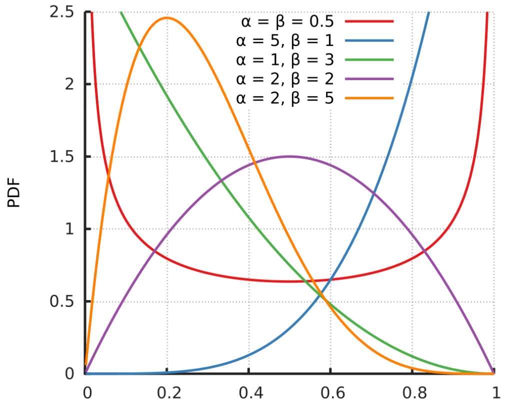

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hyper-parameters: can be interpreted as # **imaginary** heads & tails

prior predictive: $p(x=1 \mid \mathcal{D}=\emptyset) = \int_\theta p(x=1 \mid \theta) p(\theta; \alpha, \beta) \mathrm{d}\theta = \frac{\alpha}{\alpha+\beta}$

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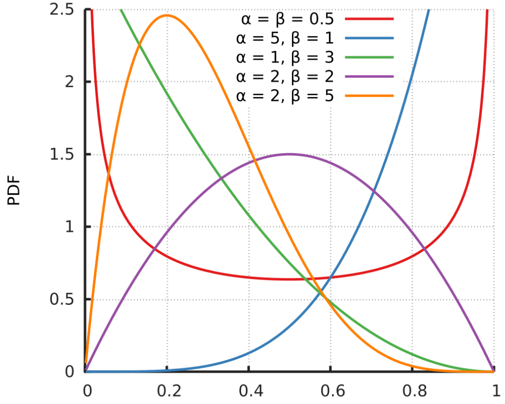

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posterior: $p(\theta \mid \mathcal{D}) \propto p(\theta) P(\mathcal{D} \mid \theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1} \theta^{N(1)}(1-\theta)^{N(0)} = \theta^{\alpha-1+N(1)}(1-\theta)^{\beta-1+N(0)}$

if the prior is $p(\theta;\alpha,\beta)$, the posterior is $p(\theta;\alpha+N(1),\beta+N(0))$

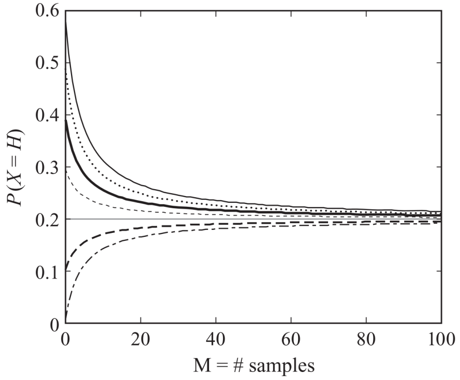
image: wikipedia

Beta-Bernoulli: Example

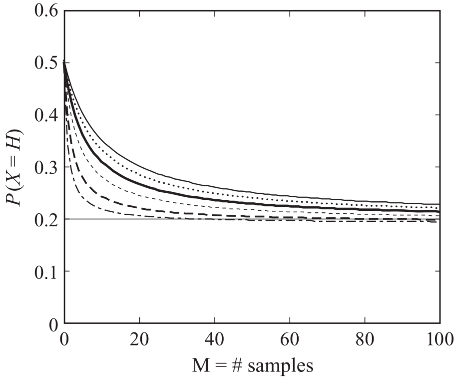
$p(x = 1) = .2$ ←

posterior for different priors and sample sizes

different prior means $\frac{\alpha}{\alpha+\beta}$



different prior strength $\alpha + \beta$



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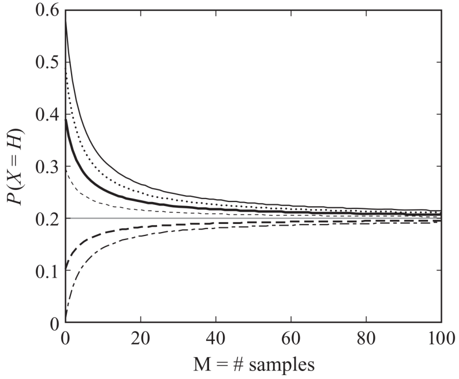

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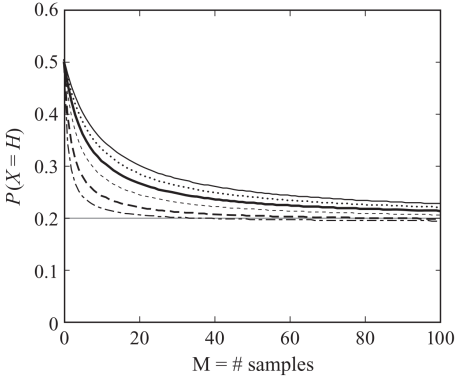
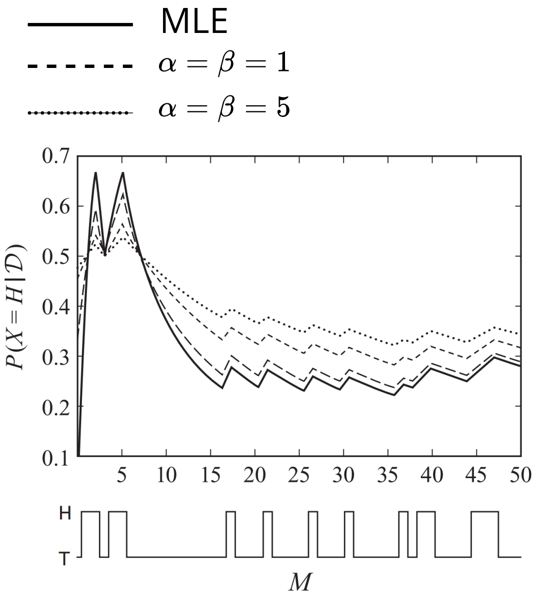
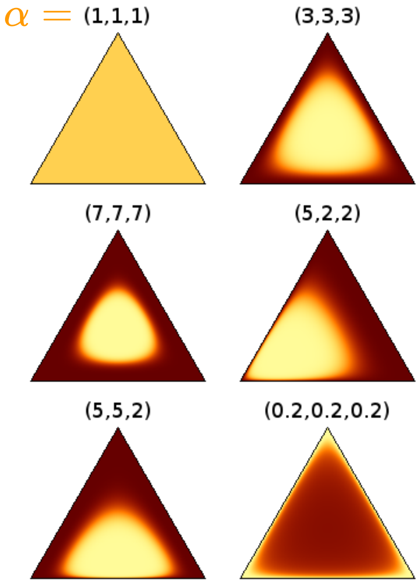
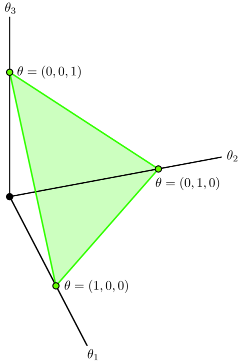


posterior predictive for online setting



Conjugate priors: Dirichlet-categorical





Bernoulli → Beta

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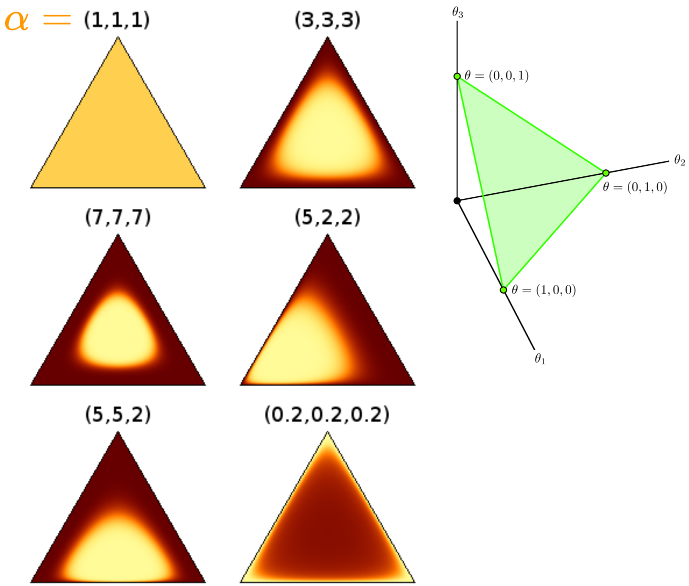

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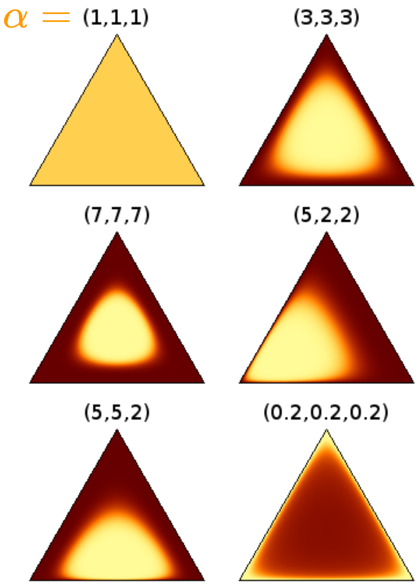

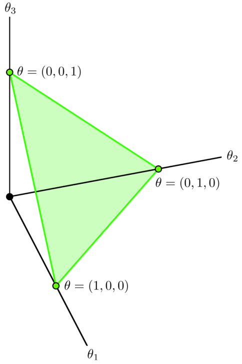

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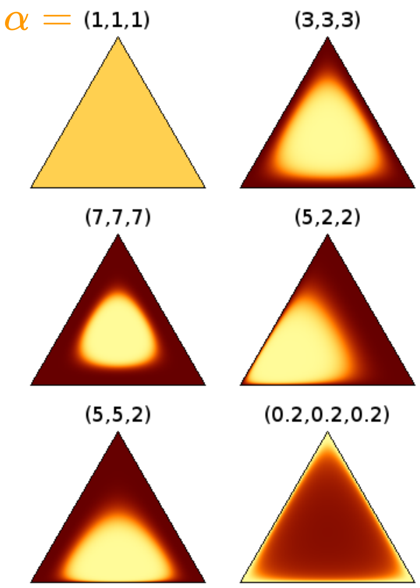

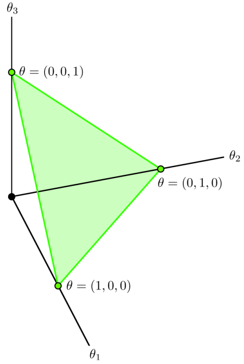

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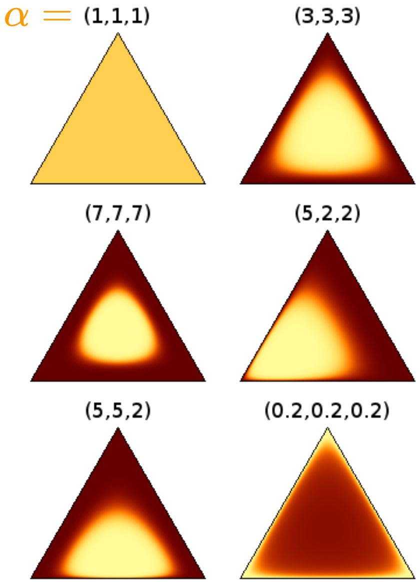

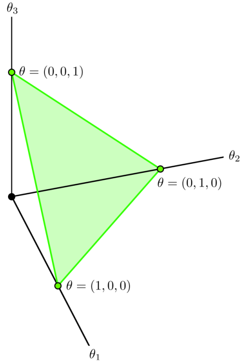

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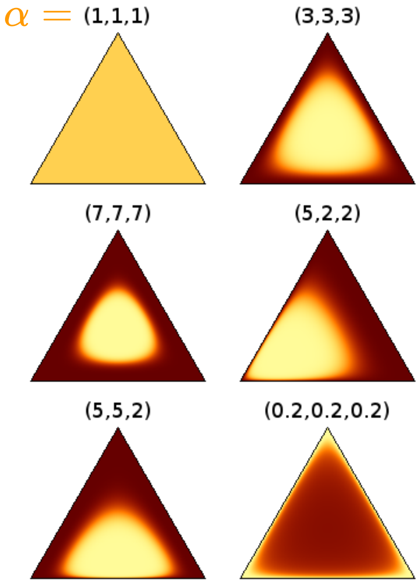

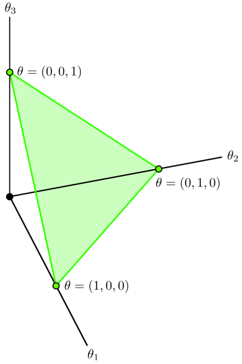

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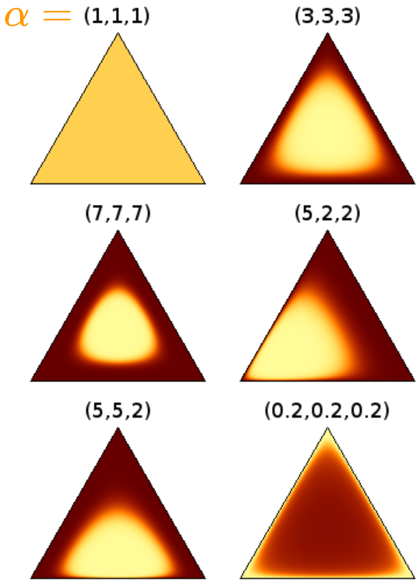

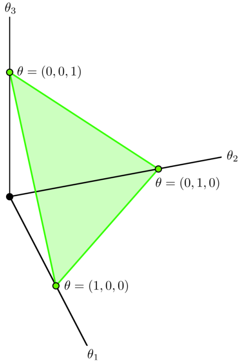

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Marginal likelihood vs. maximum likelihood

$$\mathcal{D} = \{1, 0, 0, 1, 1\}$$

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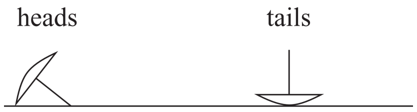

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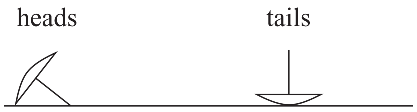

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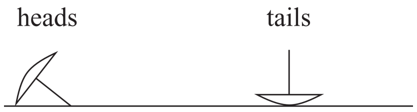

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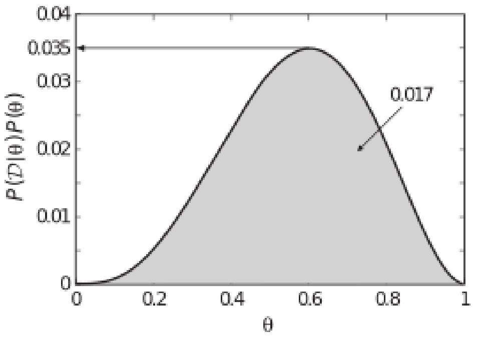

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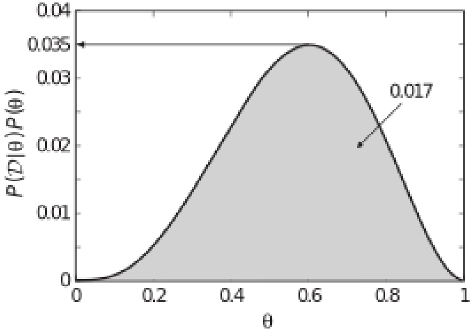

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marginal likelihood for Dirichlet $P(\mathcal{D}) = \frac{\Gamma(\alpha)}{\Gamma(\alpha+|\mathcal{D}|)} \prod_i \frac{\Gamma(\alpha_i + |\mathcal{D}| p_{\mathcal{D}}(i))}{\Gamma(\alpha_i)}$

Conjugate priors: exponential family

for the likelihood function: $p(x \mid \theta) = \exp(\langle \phi(x), \theta \rangle - A(\theta))$

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imaginary expected sufficient statistics

imaginary counts

posterior: $p(\theta \mid \mathcal{D}; \eta, \nu) = \exp\left(\langle \nu\eta + \sum_{x \in \mathcal{D}} \phi(x), \theta \rangle - (\nu + N) A(\theta)\right)$

Bayesian learning for Bayes-nets

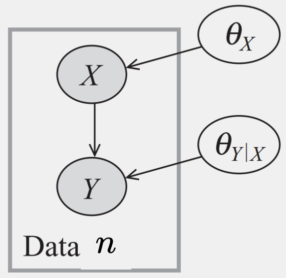
assumption

- global parameter independence: prior decomposes $p(\theta) = \prod_i p(\theta_{X_i|Pa_{X_i}})$

conclusion

- posterior also decomposes $p(\theta \mid \mathcal{D}) = \prod_i p(\theta_{X_i|Pa_{X_i}} \mid \mathcal{D})$

example



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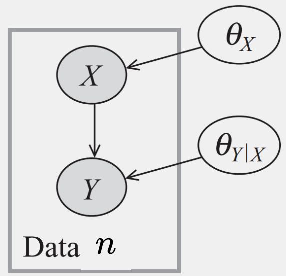

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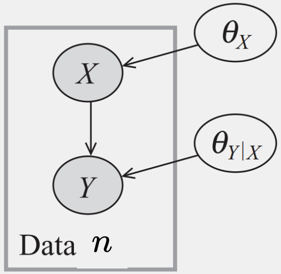

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individual posteriors

- we can apply Bayesian learning to individual conditional distributions

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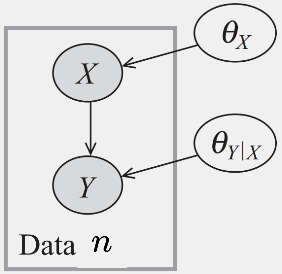

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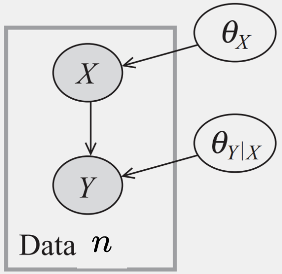

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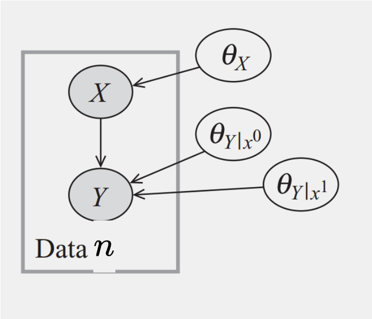
- posterior predictive also decomposes: $p(x' \mid \mathcal{D}) = \prod_i p(x'_i \mid \mathcal{D})$

$$p(x'_i \mid \mathcal{D}) \rightarrow \int_\theta p(\theta_{X_i|Pa_{X_i}} \mid \mathcal{D}) p(x'_i|Pa_{x'_i}; \theta_{X_i|Pa_{X_i}}) \mathrm{d}\theta_{X_i|Pa_{X_i}}$$

Bayesian learning for Bayes-nets

discrete case: conditional probability tables (CPTs)

we can further decompose the prior & posterior



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Bayesian learning for Bayes-nets

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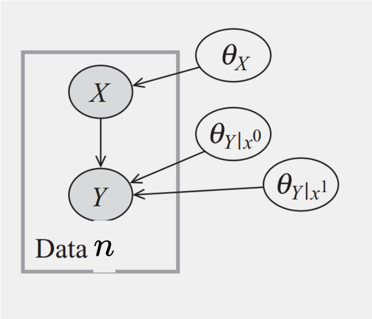

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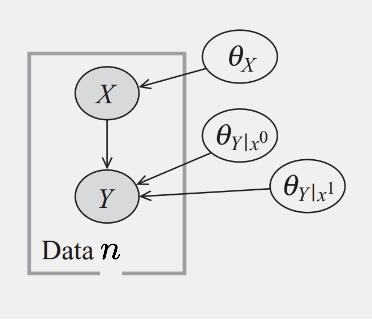
$$p(\theta_{Y|x^0}) \prod_{(x^0,y)\in\mathcal{D}} p(y|x^0;\theta_{Y|x^0})$$

Bayesian learning for Bayes-nets

discrete case: conditional probability tables (CPTs)

In practice this means:

- keep a vector of *pseudo-counts* for each node
- after observing N samples:
  - update these based on the frequency of different (x,y) values



K2 prior $\alpha_{Y|x^0} = \alpha_{Y|x^1} = [1, \ldots, 1]$

similar to Laplace smoothing

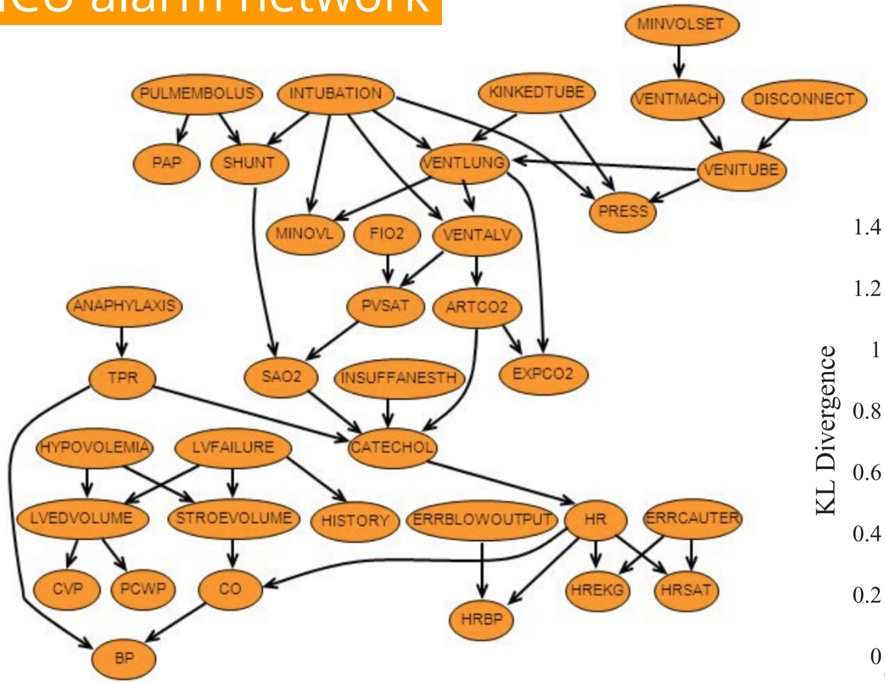
BDe prior use a second Bayes-net to
- keep frequencies $P'(x_i, pa_{X_i})$
- keep a total pseudo-count α

then $\alpha_{x_i|pa_{X_i}} = \alpha P'(x_i, pa_{X_i})$

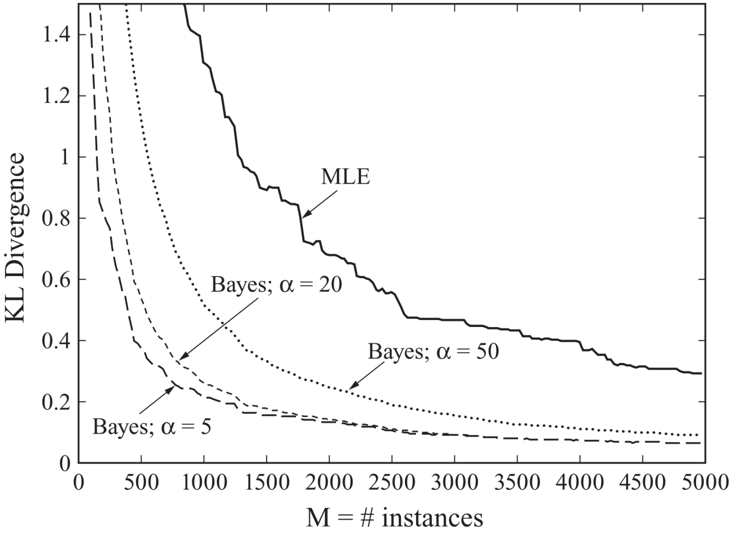
Bayesian learning for Bayes-nets

example

ICU alarm network



Bayesian learning vs MLE



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In Bayes-nets:

- both MLE and Bayesian learning is easy
  - they have a decomposed form