Parameter Estimation

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Slides adapted from Profs. Suin Lee & Eran Segal

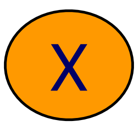
Key ideas:

- Sufficient Statistics
- MLE for Bayesian Networks
- Conjugate Prior for Table CPDs

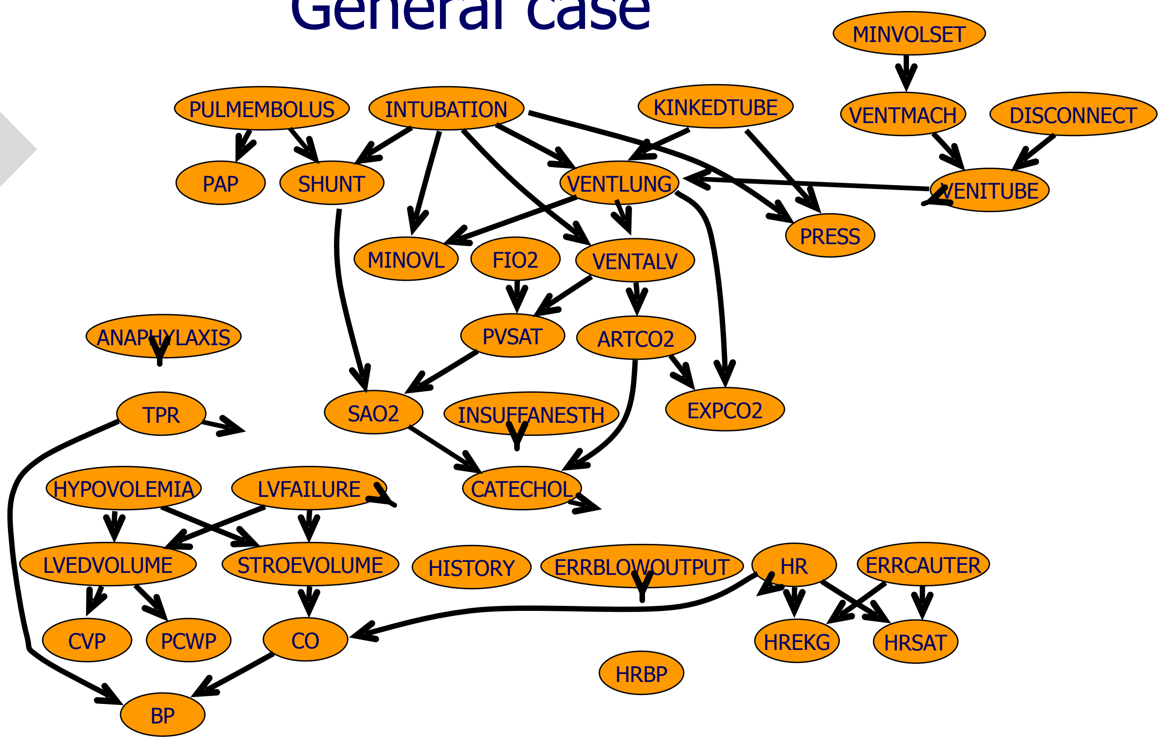
Parameter estimation

- Maximum likelihood estimation (MLE)
  - Parameter estimation based on observations
- Bayesian approach
  - Incorporate our prior knowledge

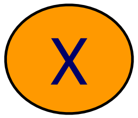
A single variable Bayesian network



General case



Maximum Likelihood Estimator: Review



- The Coin example – general case
  - X: result of a coin toss (head or tail)
  - Training data (instances) D=<x[1],...x[m]> (M_H heads and M_T tails)
  - Parameters: P(X=h)= θ
- Goal: find the model ($\theta \in [0,1]$) that describes the data well
  - "describes the data well" = likelihood of the data given θ

$$L(\theta : D) = P(D : \theta) = P(x[1], \ldots, x[m] : \theta)$$

  - MLE: Find θ maximizing likelihood

$$L(\theta : D) = \prod_{i=1}^{m} P(x[i] \mid x[1], \ldots, x[i-1], \theta) = \prod_{i=1}^{m} P(x[i] \mid \theta) = \theta^{M_H} (1-\theta)^{M_T}$$

  - Equivalent to maximizing log-likelihood

$$l(\theta : D) = \log P(D : \theta) = M_H \log \theta + M_T \log(1-\theta)$$

  - Differentiating the log-likelihood and solving for θ, we get that the maximum likelihood parameter:

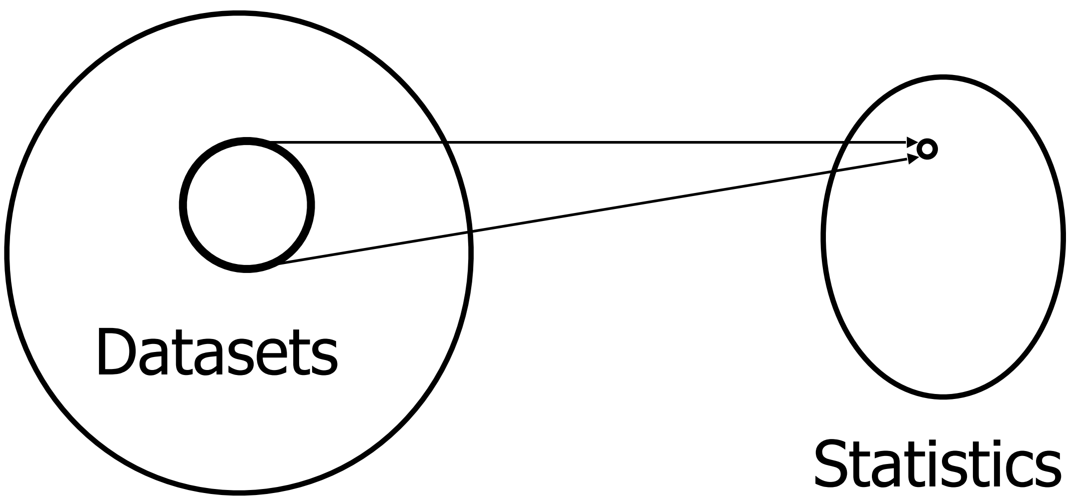
$$\theta_{mle} = \arg\max l(\theta : D) = \frac{M_H}{M_H + M_T}$$

Sufficient Statistics

- For computing the parameter θ of the coin toss example, we only needed M_H and M_T since

$$L(\theta : D) = P(D : \theta) = \theta^{M_H} (1-\theta)^{M_T}$$

→ M_H and M_T are sufficient statistics



Intuitive Definition: Sufficient Statistics

A statistic is *sufficient* with respect to a statistical model and its associated unknown parameter if "no other statistic that can be calculated from the same sample provides any additional information as to the value of the parameter"

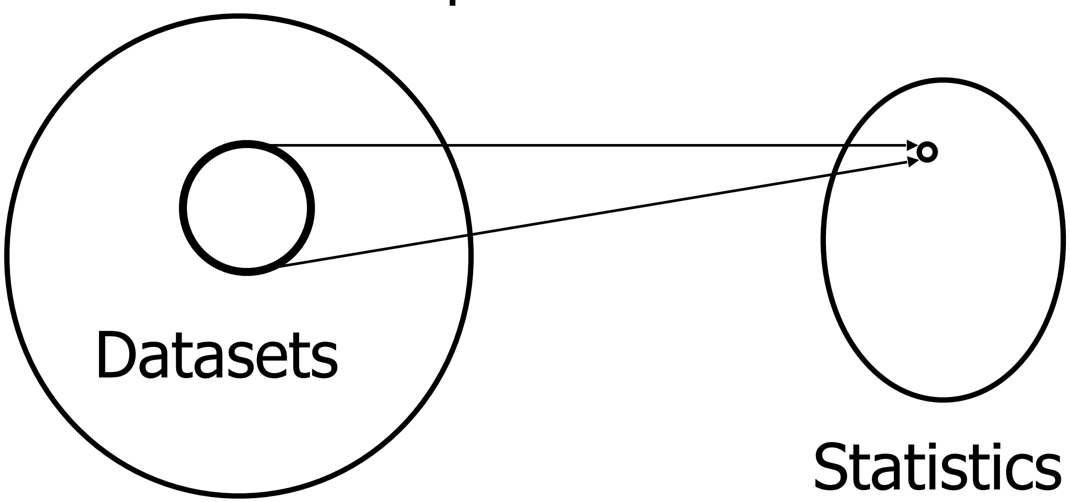
Sufficient Statistics

- A function s(D) is a sufficient statistic from instances to a vector in $\Re^k$ if, for any two datasets D and D' and any $\theta \in \Theta$, we have

$$\sum_{x[i] \in D} s(x[i]) = \sum_{x[i] \in D'} s(x[i]) \quad \Rightarrow \quad L(D:\theta) = L(D':\theta)$$

- We often refer to the tuple $\sum_{x[i] \in D} s(x[i])$ as the sufficient statistics of the data set D.
  - In coin toss experiment, M_H and M_T are sufficient statistics

"Many-to-one" relationship between datasets and statistics



Sufficient Statistics for Multinomial

- Y: multinomial, k values (e.g. result of a dice throw)

- A sufficient statistics for a dataset D over Y is the tuple of counts $<M_1,...M_k>$ such that M_i is the number of times that the $Y=y^i$ in D

- Likelihood function: $L(D:\theta) = \prod_{i=1}^{k} \theta_i^{M_i}$ where $\theta_i = P(Y = y^i)$

- MLE Principle: Choose Θ that maximize $L(D:\Theta)$

- Multinomial MLE: $$\theta^i = \frac{M_i}{\sum_{i=1}^{m} M_i}$$

Sufficient Statistic for Gaussian

- Gaussian distribution: $X \sim N(\mu, \sigma^2)$
  - Probability density function (pdf): $p(X) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$

- Rewrite as $p(X) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-x^2 \frac{1}{2\sigma^2} + x\frac{\mu}{\sigma^2} - \frac{\mu^2}{\sigma^2} \right)$

→ sufficient statistics for Gaussian: <M,Σ_mx[m], Σ_mx[m]^2>

- MLE Principle: Choose Θ that maximize L(D:Θ)

- Multinomial MLE:

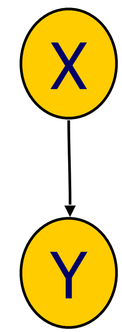
$$\mu = \frac{1}{M}\sum_m x[m]$$

$$\sigma = \sqrt{\frac{1}{M}\sum_m (x[m]-\mu)^2}$$

MLE for Bayesian Networks

- Parameters
  - $\theta_{x^0}, \theta_{x^1}$
  - $\theta_{y^0|x^0}, \theta_{y^1|x^0}, \theta_{y^0|x^1}, \theta_{y^1|x^1}$
- Training data:
  - tuples <x[m],y[m]> m=1,…,M
- Likelihood function:

X	
x^0	x^1
0.7	0.3



	Y	
X	y^0	y^1
x^0	0.95	0.05
x^1	0.2	0.8

→ Likelihood decomposes into two separate terms, one for each variable ("decomposability of the likelihood function")

MLE for Bayesian Networks

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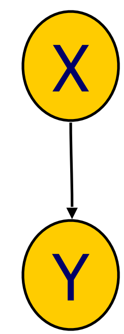


X	Y: y^0	y^1
x^0	0.95	0.05
x^1	0.2	0.8

$$L(D:\theta) = \prod_{m=1}^{M} P(x[m], y[m]:\theta)$$

$$= \prod_{m=1}^{M} P(x[m]:\theta_X) P(y[m] \mid x[m]:\theta_{Y|X})$$

$$= \left(\prod_{m=1}^{M} P(x[m]:\theta_X) \right) \left(\prod_{m=1}^{M} P(y[m] \mid x[m]:\theta_{Y|X}) \right)$$

→ Likelihood decomposes into two separate terms, one for each variable ("decomposability of the likelihood function")

MLE for Bayesian Networks

- Terms further decompose by CPDs:

$$\prod_{m=1}^{M} P(y[m] \mid x[m] : \theta) = \prod_{m:x[m]=x^0} P(y[m] \mid x[m] : \theta_{Y|X}) \prod_{m:x[m]=x^1} P(y[m] \mid x[m] : \theta_{Y|X})$$
$$= \prod_{m:x[m]=x^0} P(y[m] \mid x[m] : \theta_{Y|x^0}) \prod_{m:x[m]=x^1} P(y[m] \mid x[m] : \theta_{Y|x^1})$$

- By sufficient statistics

$$\prod_{m:x[m]=x^1} P(y[m] \mid x[m] : \theta_{Y|x^1}) = \theta_{y^0|x^1}^{M[x^1,y^0]} \cdot \theta_{y^1|x^1}^{M[x^1,y^1]}$$

where $M[x^1,y^1]$ is the number of data instances in which X takes the value x^1 and Y takes the value y^1

- MLE

$$\theta_{y^0|x^1} = \frac{M[x^1,y^0]}{M[x^1,y^0]+M[x^1,y^1]} = \frac{M[x^1,y^0]}{M[x^1]}$$

MLE for Bayesian Networks

- Likelihood for Bayesian network

$$
\begin{aligned}
L(\Theta : D) &= \prod_m P(x[m] : \Theta) \\
&= \prod_m \prod_i P(x_i[m] \mid Pa_i[m] : \Theta_i) \\
&= \prod_i \left[\prod_m P(x_i[m] \mid Pa_i[m] : \Theta_i) \right] \\
&= \prod_i L_i(\boldsymbol{\theta}_{x_i \mid Px_i} : X_i, Pa_i)
\end{aligned}
$$

Conditional likelihood or "Local likelihood"

→ if $\theta_{X_i|Pa(X_i)}$ are disjoint then MLE can be computed by maximizing each local likelihood separately

MLE for Table CPD BayesNets

- Multinomial CPD

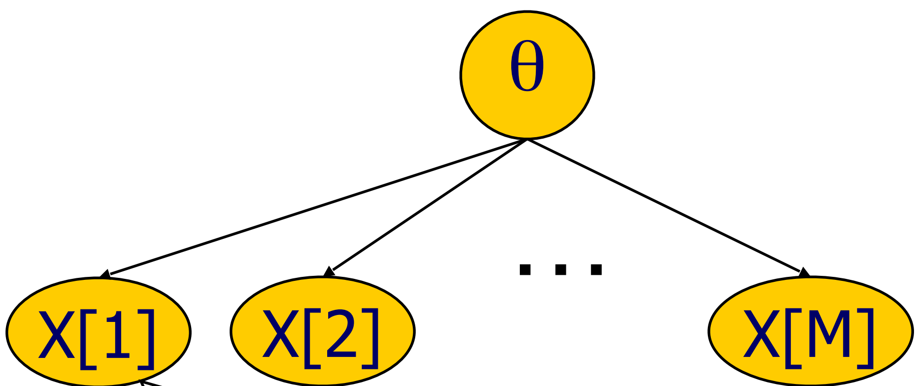
$$
\begin{aligned}
L_Y(D:\theta_{Y|\mathbf{X}}) &= \prod_m \theta_{y[m]|\mathbf{X}[m]} \\
&= \prod_{\mathbf{x}\in Val(\mathbf{X})} \left[\prod_{y\in Val(Y)} \theta_{y|\mathbf{x}}{}^{M[\mathbf{x},y]} \right]
\end{aligned}
$$

- For each value **x**∈**X** we get an independent multinomial problem where the MLE is

$$
\theta_{y^i|\boldsymbol{x}} = \frac{M[\boldsymbol{x}, y^i]}{M[\boldsymbol{x}]}
$$

Bayesian Inference in Graphical Notation: Coin toss example

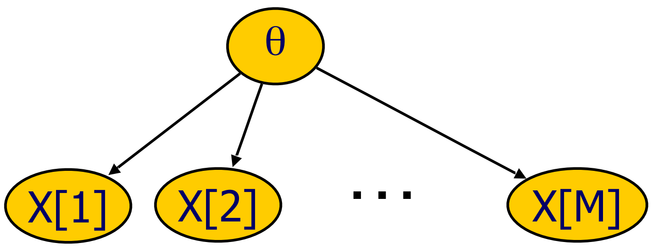
- Assumptions
  - Given a fixed θ tosses are independent
  - If θ is unknown tosses are not marginally independent – each toss tells us something about θ
- The following network captures our assumptions



$$P(x[m] \mid \theta) = \begin{cases} \theta & x[m] = x^1 \\ 1-\theta & x[m] = x^0 \end{cases}$$

Reminder: Bayesian Inference

- Joint probabilistic model



$$
\begin{aligned}
P(x[1],\ldots,x[M],\theta) &= P(x[1],\ldots,x[M] \mid \theta)P(\theta) \\
&= P(\theta)\prod_{i=1}^{M} P(x[i] \mid \theta) \\
&= P(\theta)\theta^{M_H}(1-\theta)^{M_T}
\end{aligned}
$$

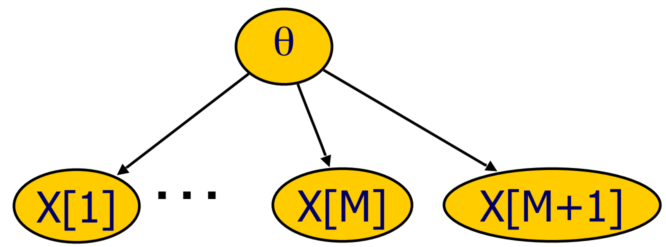
- Posterior probability over θ

$$
P(\theta \mid x[1],\ldots,x[M]) = \frac{\overbrace{P(x[1],\ldots,x[M] \mid \theta)}^{\text{Likelihood}}\overbrace{P(\theta)}^{\text{Prior}}}{\underbrace{P(x[1],\ldots,x[M])}_{\text{Normalizing factor}}}
$$

For a uniform prior, posterior is the normalized likelihood

Reminder: Bayesian Prediction

- Predict the data instance from the previous ones



$$P(x[M+1] \mid x[1],\ldots,x[M])$$

$$= \int_\theta P(x[M+1],\theta \mid x[1],\ldots,x[M])d\theta$$

$$= \int_\theta P(x[M+1] \mid x[1],\ldots,x[M],\theta)P(\theta \mid x[1],\ldots,x[M])d\theta$$

$$= \int_\theta P(x[M+1] \mid \theta)P(\theta \mid x[1],\ldots,x[M])d\theta$$

- Solve for uniform prior P(θ)=1 (for 0≤θ≤1) and binomial variable

$$P(x[M+1]=x^1 \mid x[1],\ldots,x[M]) = \frac{1}{P(x[1],\ldots,x[M])}\int_\theta \theta \cdot \theta^{M_H} \cdot (1-\theta)^{M_T}$$

"Bayesian estimate"

$$= \frac{M_H+1}{M_H+M_T+2}$$

"Imaginary counts"

Reminder: General Formulation

- Joint distribution over D,θ

$$P(D,\theta) = P(D \mid \theta)P(\theta)$$

- Posterior distribution over parameters

$$P(\theta \mid D) = \frac{P(D \mid \theta)P(\theta)}{P(D)}$$

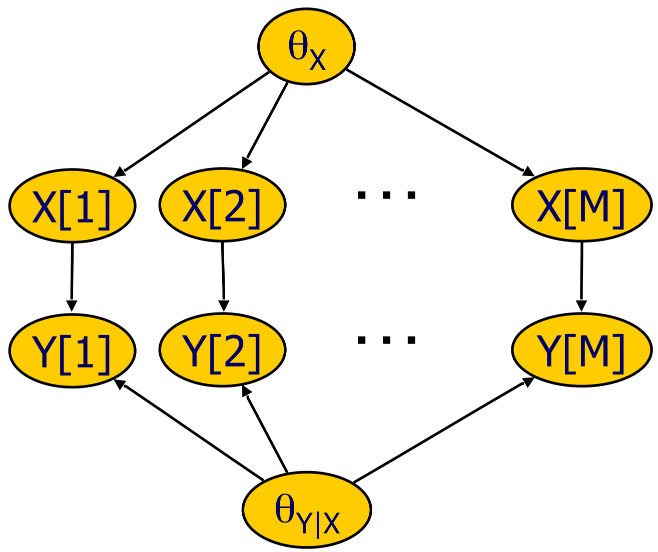
- P(D) is the marginal likelihood of the data

$$P(D) = \int_{\theta} P(D \mid \theta)P(\theta)d\theta$$

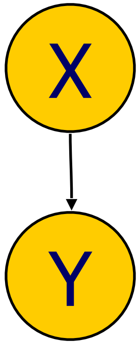
- Likelihood can be described compactly using sufficient statistics
- We want conditions in which posterior is also compact

Bayesian Estimation in BayesNets: Graphical Notation

Bayesian network for parameter estimation



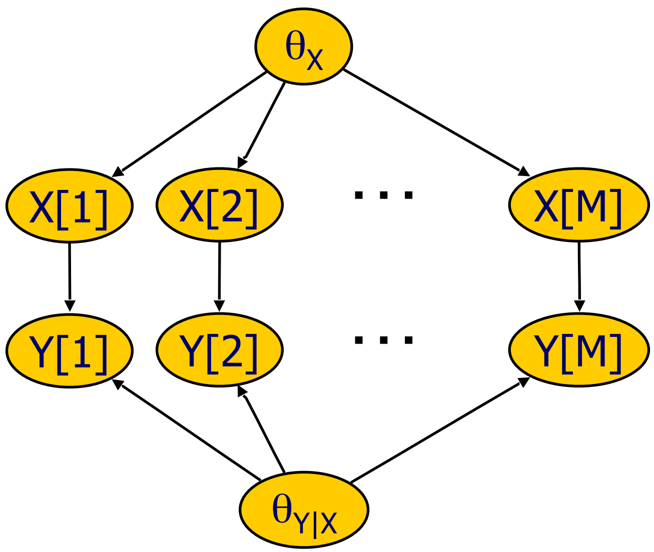
Bayesian network



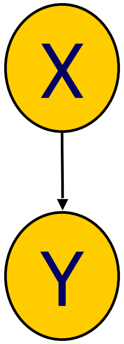
- Instances are independent given the parameters
  - (x[m′],y[m′]) are d-separated from (x[m],y[m]) given θ
- Priors for individual variables are a priori independent
  - Global independence of parameters $P(\theta) = \prod_i P(\theta_{X_i|Pa(X_i)})$

Bayesian Estimation in BayesNets

Bayesian network for parameter estimation



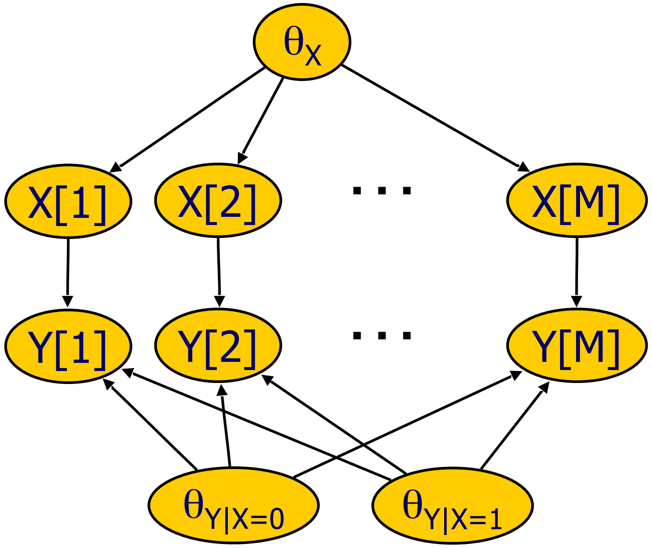
Bayesian network



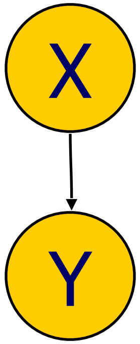
- Posteriors of θ are independent given complete data
  - Complete data d-separates parameters for different CPDs
  - $P(\theta_X, \theta_{Y|X} \mid D) = P(\theta_X \mid D) P(\theta_{Y|X} \mid D)$
  - As in MLE, we can solve each estimation problem separately

Bayesian Estimation in BayesNets

Bayesian network for parameter estimation



Bayesian network



- Posteriors of θ are independent given complete data
  - Also holds for parameters within families
  - V-structure is deceptive! Note context specific independence between $\theta_{Y|X=0}$ and $\theta_{Y|X=1}$ when given both X and Y

Reminder: Conjugate Families

- A family of priors $P(\theta:\alpha)$ is conjugate to a model $P(\xi|\theta)$ if for any possible dataset D of i.i.d samples from $P(\xi|\theta)$ and choice of hyperparameters α for the prior over θ, there are hyperparameters α' that describe the posterior, i.e., $P(\theta:\alpha') \propto P(D|\theta)P(\theta:\alpha)$
  - Posterior has the same parametric form as the prior
  - Dirichlet prior is a conjugate family for the multinomial likelihood
- Conjugate families are useful since:
  - Many distributions can be represented with hyperparameters
  - They allow for sequential update within the same representation
  - In many cases we have closed-form solutions for prediction

Conjugate Prior for Table CPDs: Dirichlet Priors

- A Dirichlet prior is specified by a set of (non-negative) hyper-parameters $\alpha_1, \ldots \alpha_k$ so that

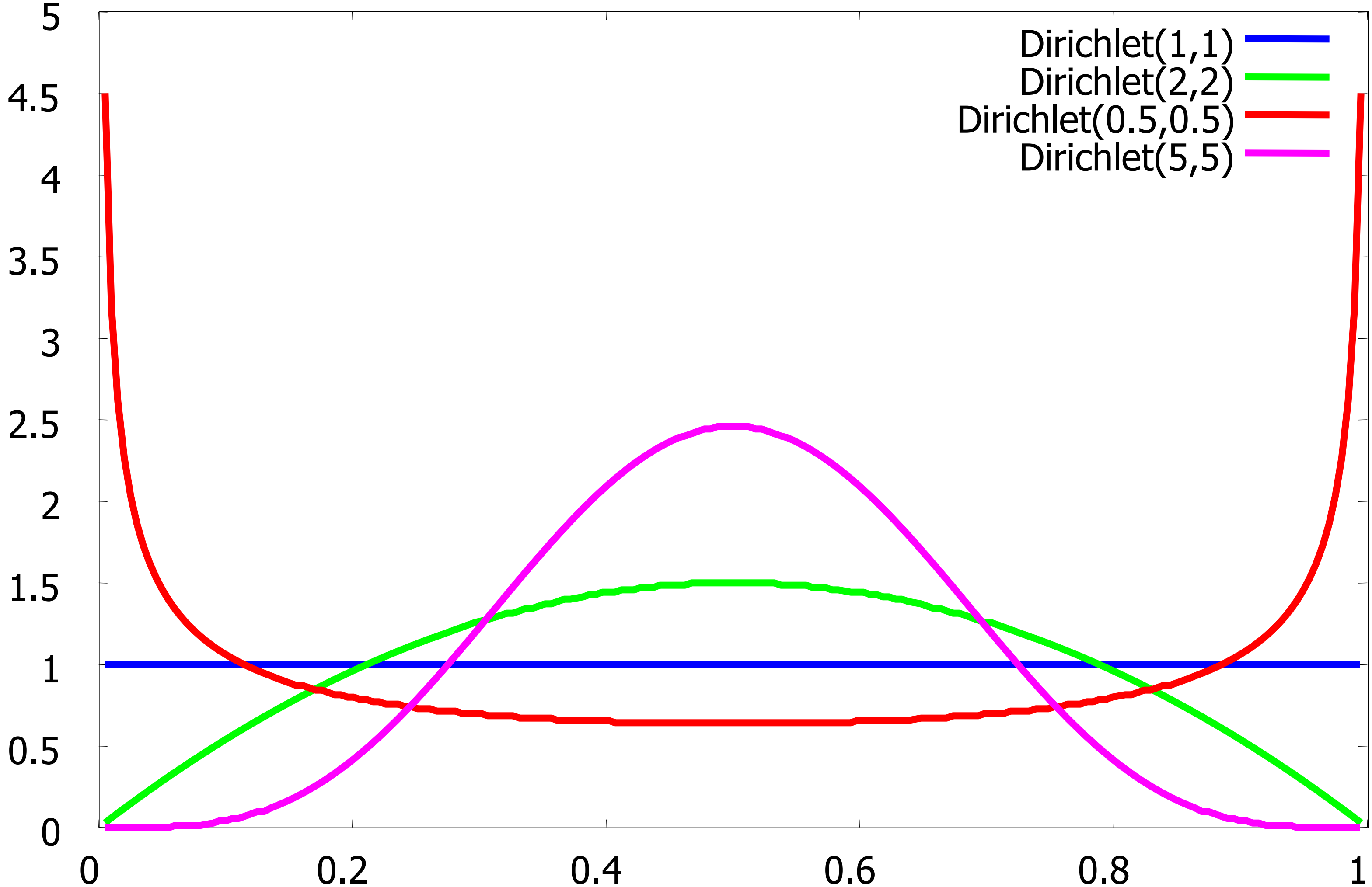
  $\theta = [\theta_1, \ldots, \theta_k] \sim \text{Dirichlet}(\alpha_1, \ldots \alpha_k)$ if

  - $$p(\theta) = \frac{1}{Z} \prod_k \theta_k^{\alpha_k - 1} \quad \text{where} \quad \sum_k \theta_k = 1, \quad \Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$$

    and $$Z = \frac{\prod_{i=1}^{k} \Gamma(\alpha_i)}{\Gamma(\sum_{i=1}^{k} \alpha_i)}.$$

  - Intuitively, hyper-parameters correspond to the number of imaginary counts before starting the coin toss experiment

Dirichlet Priors – Example



Dirichlet Priors

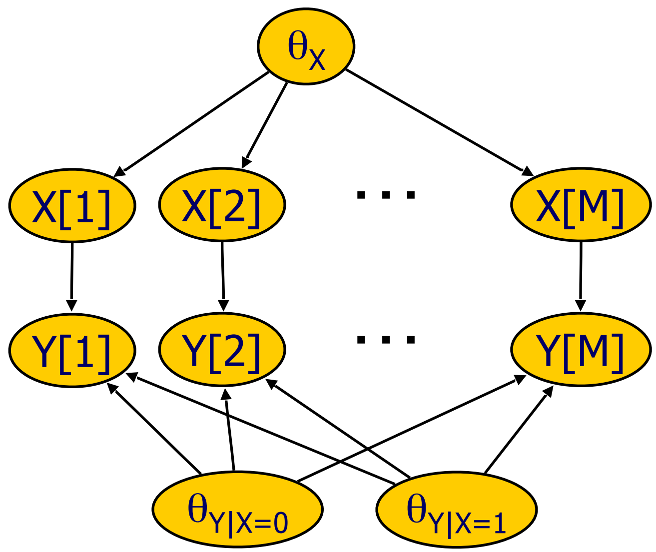
- Dirichlet priors have the property that the posterior is also Dirichlet
  - Prior is Dir(α_1,...α_k) $$p(\theta) = \frac{1}{Z}\prod_k \theta_k^{\alpha_k - 1}$$
  - Data counts are M_1,...,M_k
  - Posterior is Dir(α_1+M_1,...α_k+M_k) $$p(\theta \mid D) = \frac{1}{Z'}\prod_k \theta_k^{\alpha_k + M_k - 1}$$

- The hyperparameters α_1,…,α_K can be thought of as "imaginary" counts from our prior experience

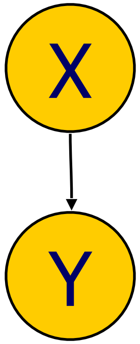
- Equivalent sample size = α_1+…+α_K
  - The larger the equivalent sample size the more confident we are in our prior

Bayesian Estimation in BayesNets

Bayesian network for parameter estimation



Bayesian network



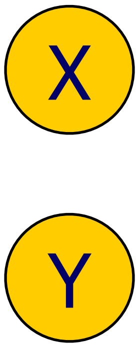
- Posteriors of θ can be computed independently
  - For multinomial $\theta_{X_i|pa_i}$ posterior is Dirichlet with parameters $(\alpha_{X_i=1|pa_i}+M[X_i=1|pa_i]),\ldots,(\alpha_{X_i=k|pa_i}+M[X_i=k|pa_i])$
  - $$P(X_i[M+1]=x_i \mid Pa_i[M+1]=pa_i, D) = \frac{\alpha_{x_i|pa_i}+M[x_i,pa_i]}{\sum_i \alpha_{x_i|pa_i}+M[x_i,pa_i]}$$

Assessing Priors for BayesNets

- We need the $\alpha(x_i, pa_i)$ for each node x_i

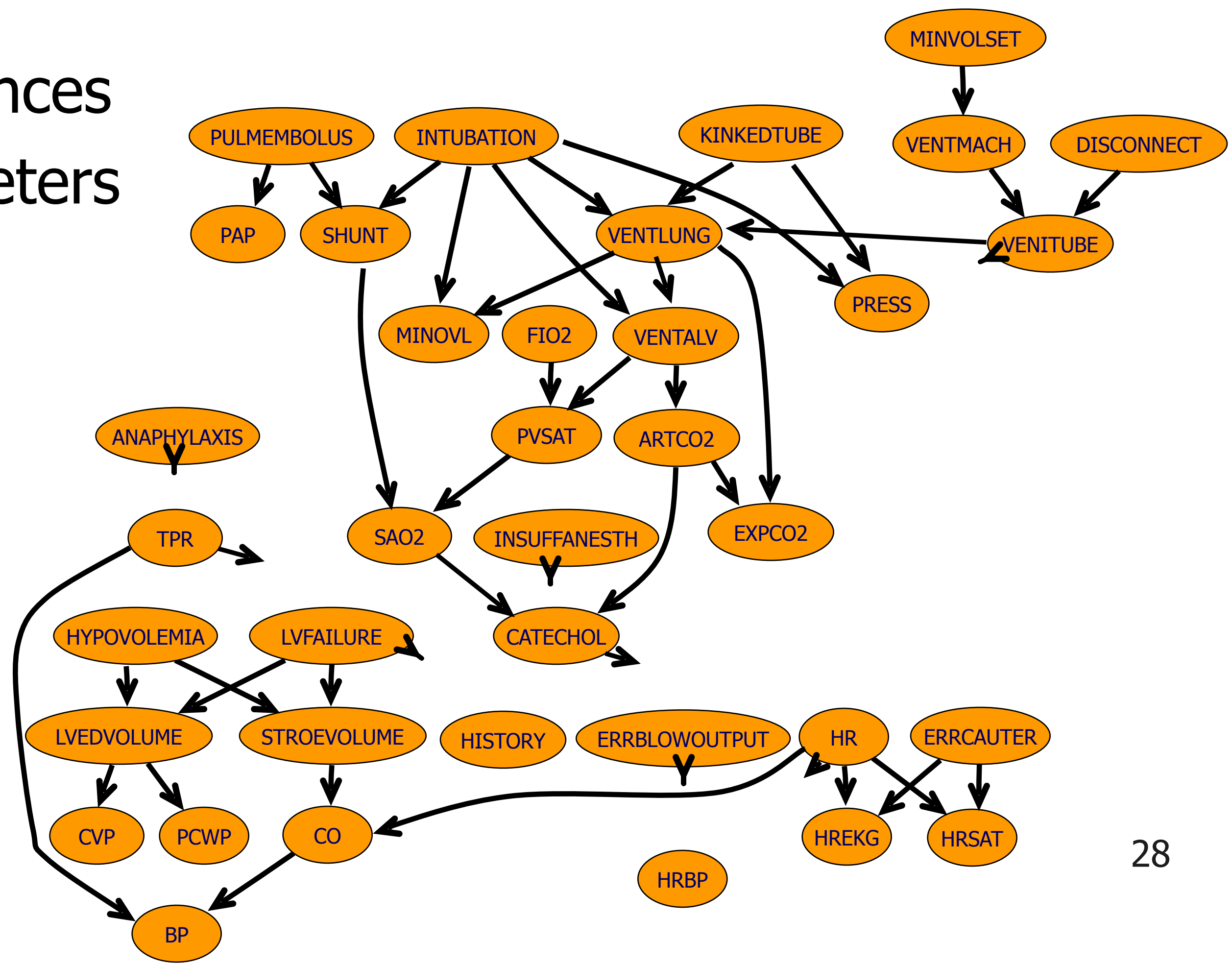
- We can use initial parameters Θ_0 as prior information
  - Need also an equivalent sample size parameter M′
  - Then, we let $\alpha(x_i, pa_i) = M' \cdot P(x_i, pa_i | \Theta_0)$

- This allows to update a network using new data
  - Example network for priors
    - $P(X=0)=P(X=1)=0.5$
    - $P(Y=0)=P(Y=1)=0.5$
    - $M'=1$
    - Note: $\alpha(x_0)=0.5$ $\alpha(x_0, y_0)=0.25$



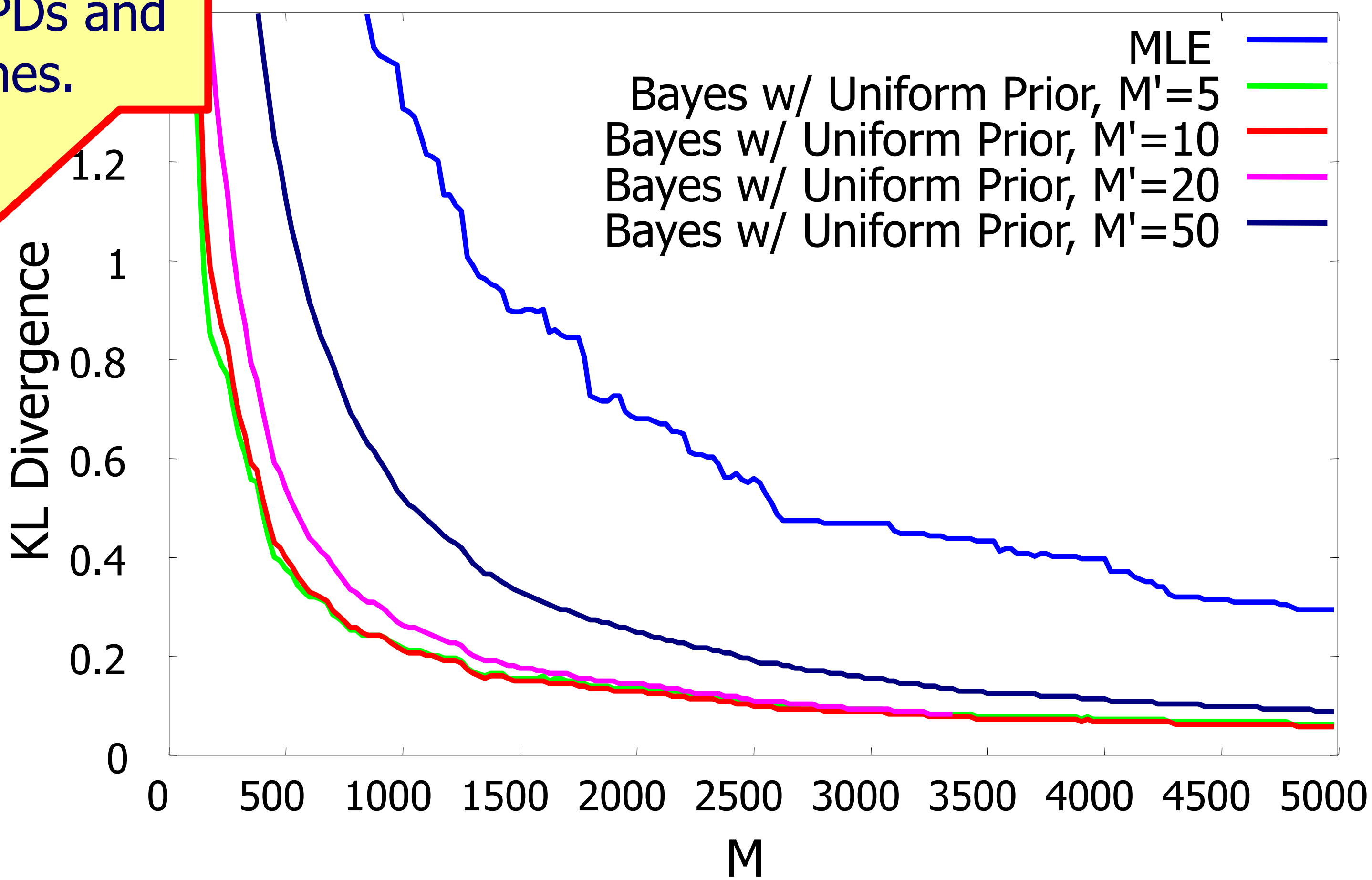
Case Study: ICU Alarm Network

- The "Alarm" network
  - 37 variables
- Experiment
  - Sample instances
  - Learn parameters
    - MLE
    - Bayesian



Case Study: ICU Alarm Network

The distance between the original CPDs and the learned ones.



- MLE performs worst
- Prior M'=5 provides best smoothing

Parameter Estimation Summary

- Estimation relies on sufficient statistics
  - For multinomials these are of the form $M[x_i,pa_i]$
  - Parameter estimation

$$\hat{\theta}_{x_i|pa_i} = \frac{M[x_i, pa_i]}{M[pa_i]}$$

MLE

$$P(x_i \mid pa_i, D) = \frac{\alpha_{x_i, pa_i} + M[x_i, pa_i]}{\alpha_{pa_i} + M[pa_i]}$$

Bayesian (Dirichlet)

- Bayesian methods also require choice of priors
- MLE and Bayesian are asymptotically equivalent
- Both can be implemented in an online manner by accumulating sufficient statistics