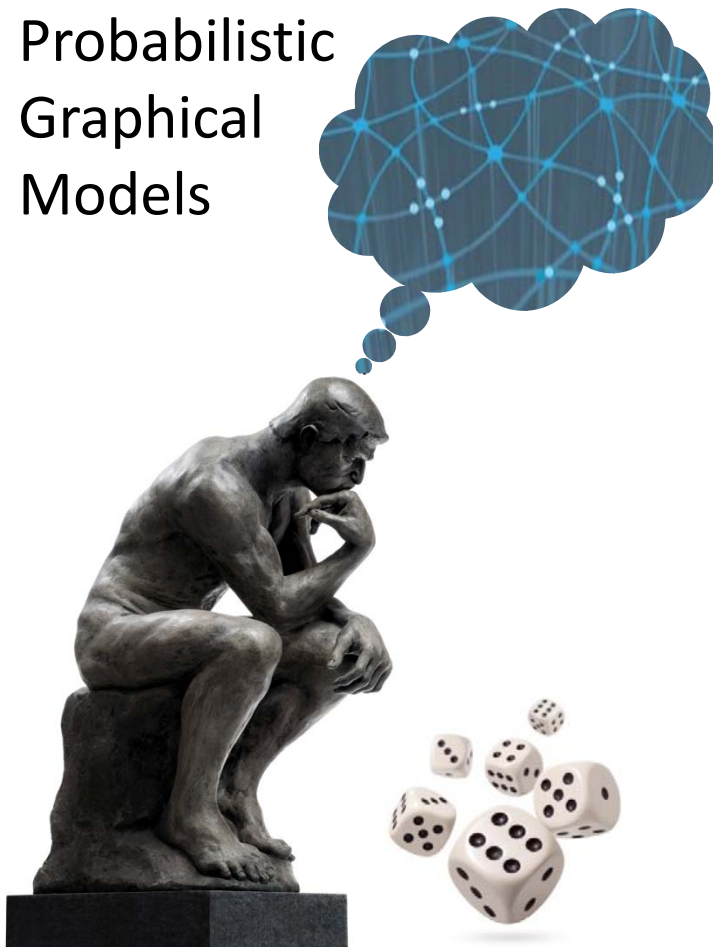


Probabilistic
Graphical
Models

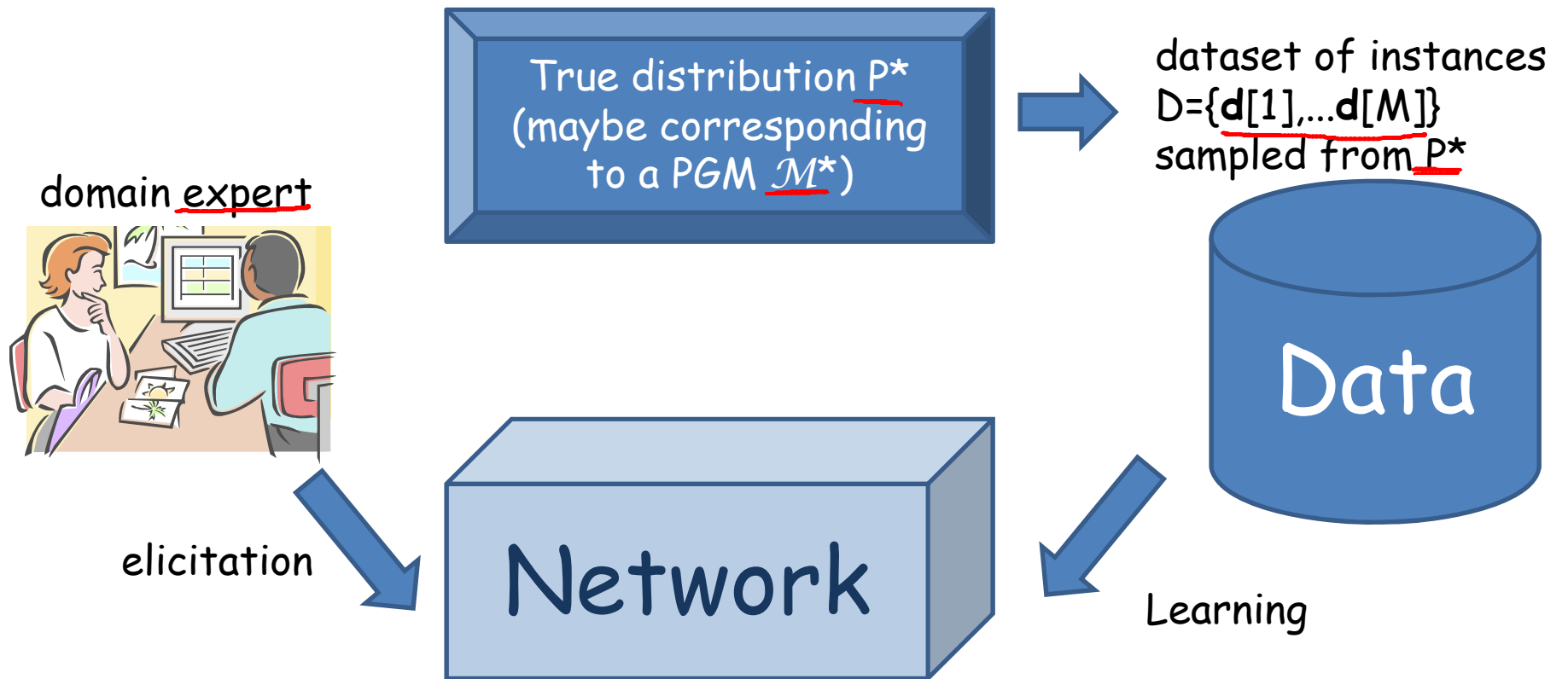


Learning

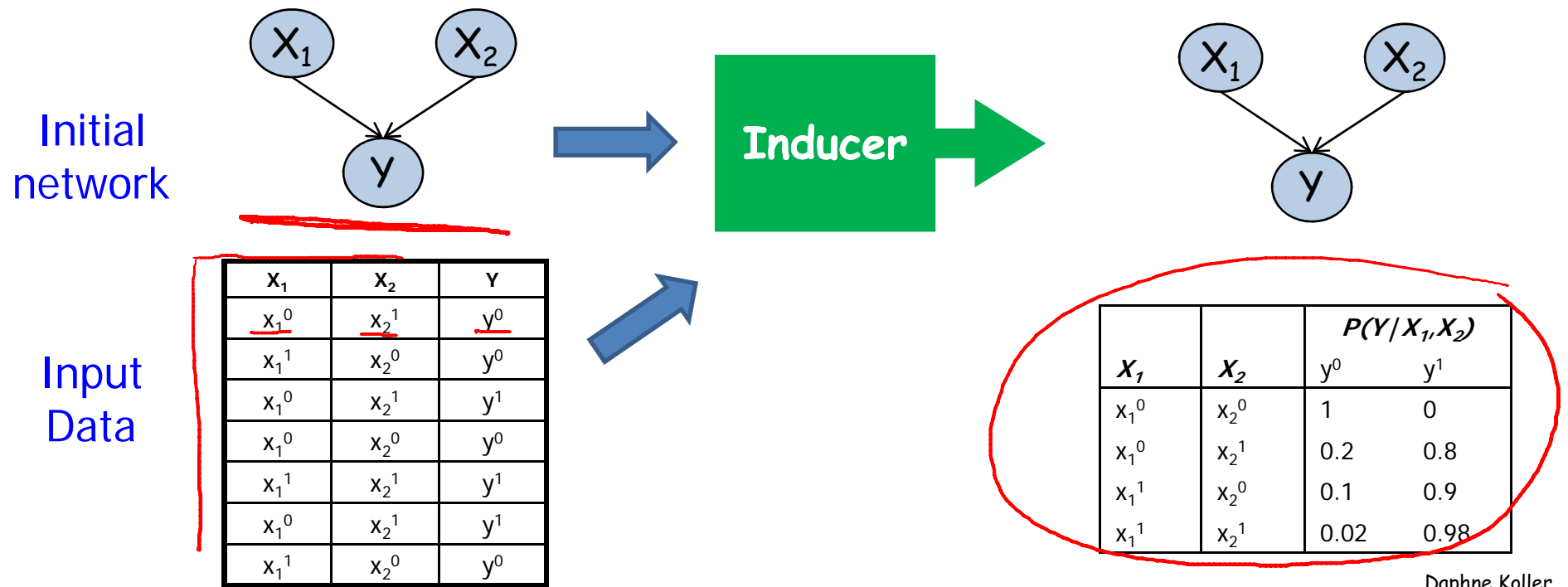
Overview

PGM Learning Tasks and Metrics

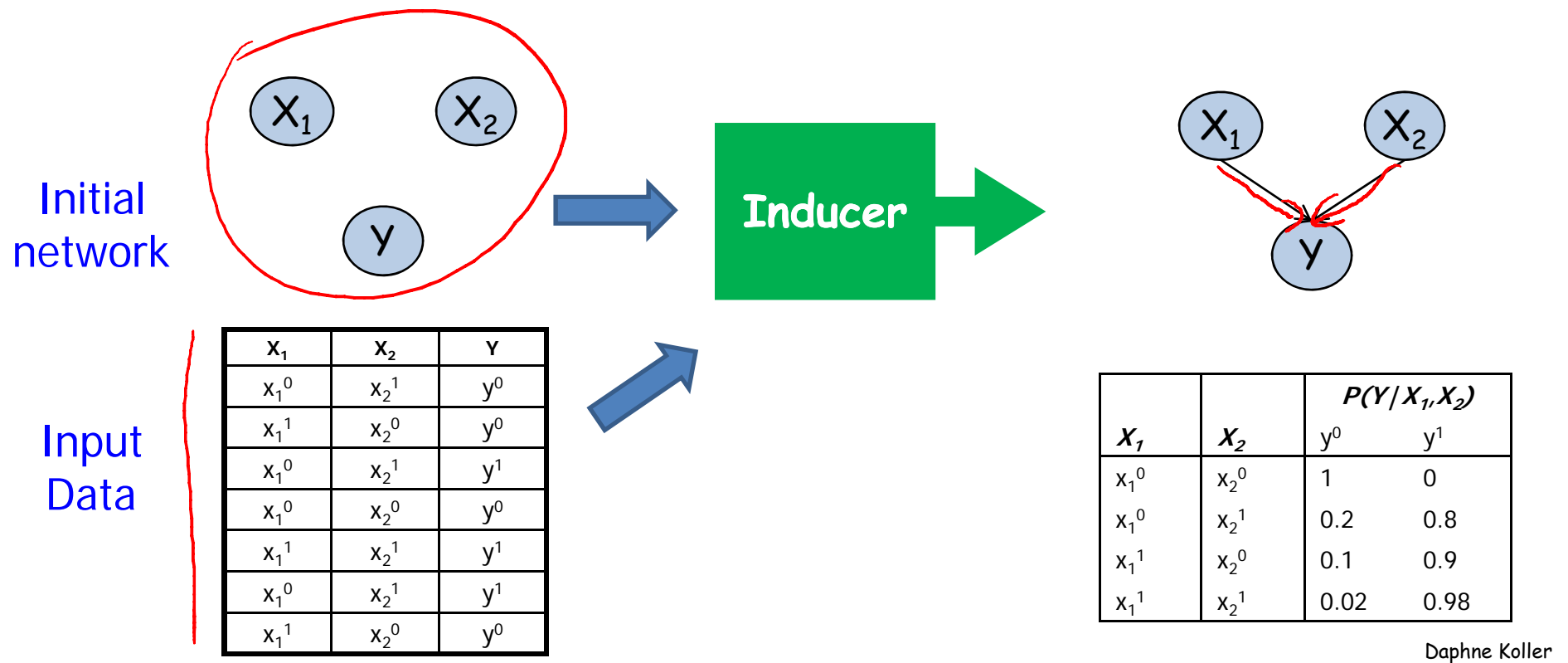
Learning



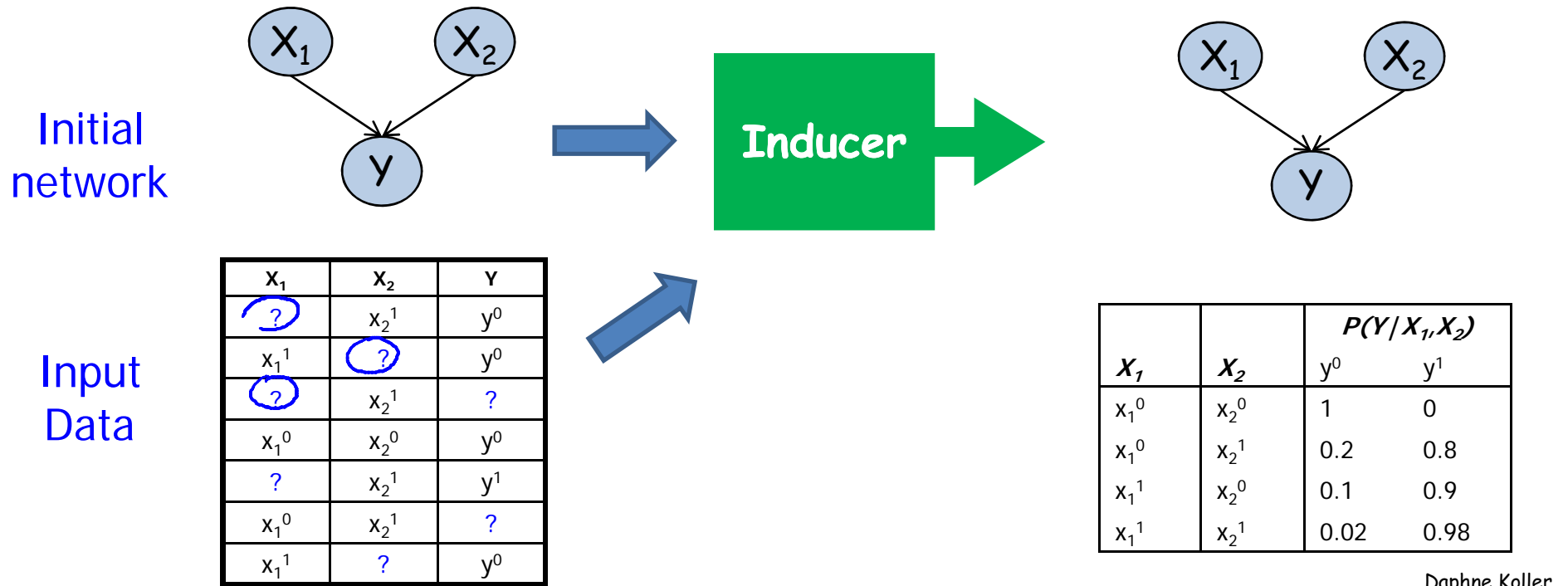
Known Structure, Complete Data



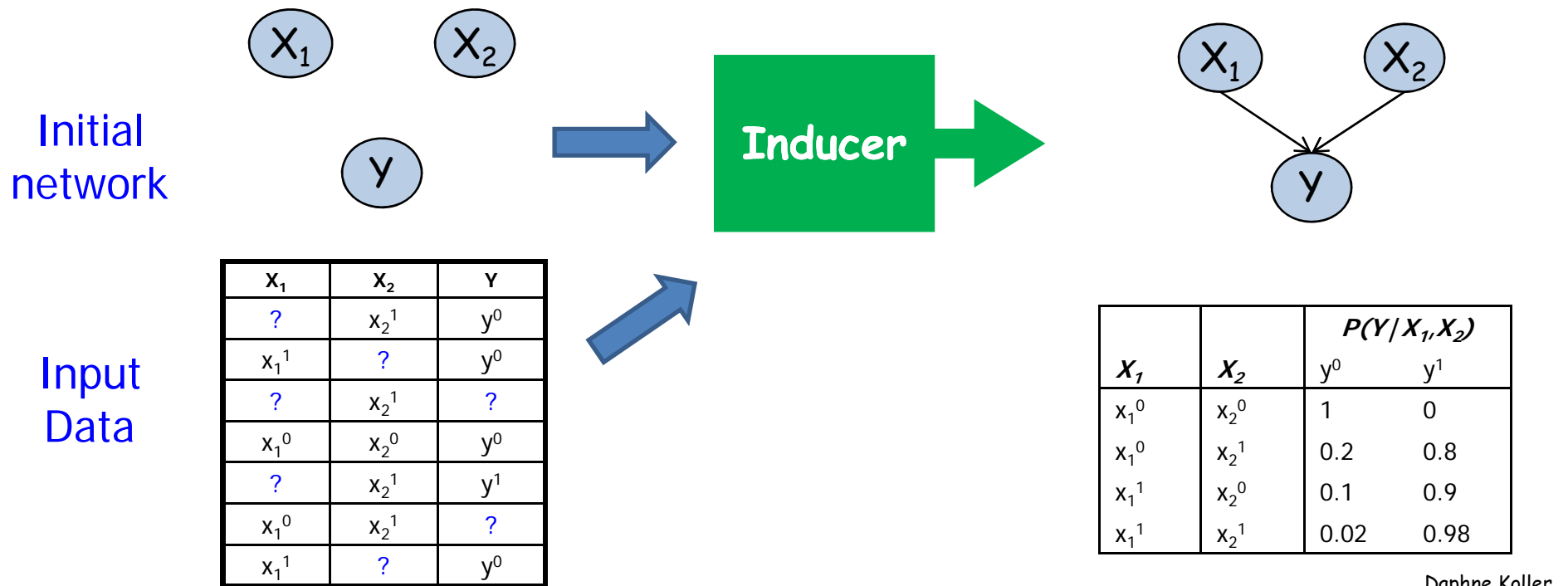
Unknown Structure, Complete Data



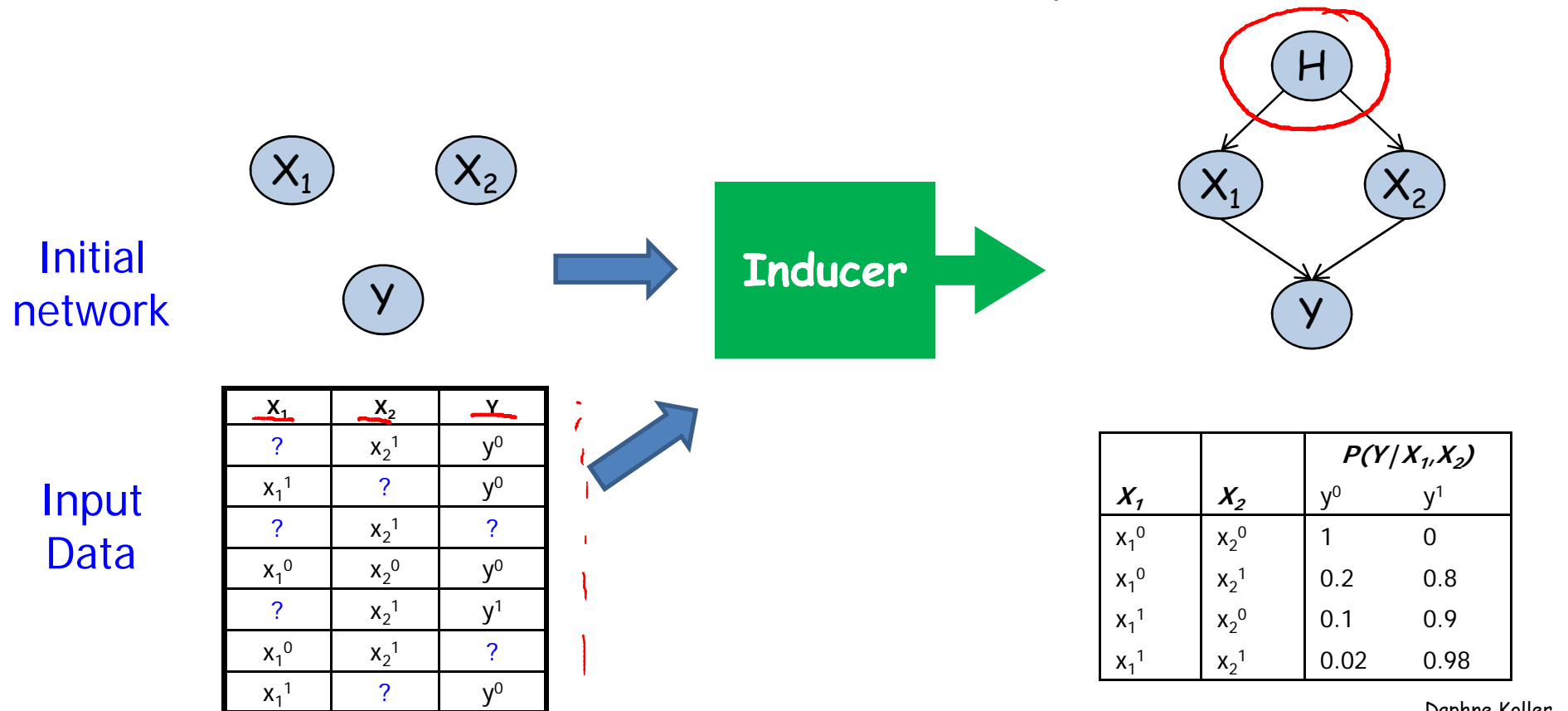
Known Structure, Incomplete Data



Unknown Structure, Incomplete Data



Latent Variables, Incomplete Data



PGM Learning Tasks I

- Goal: Answer general probabilistic queries about new instances
- Simple metric: Training set likelihood
 - $P(\overset{\text{data}}{\mathcal{D}} : \mathcal{M}) = \prod_m P(\underline{d[m]} : \mathcal{M})$ (ILD)
- But we really care about new data
 - Evaluate on test set likelihood - $P(\mathcal{D}' : \mathcal{M})$
generalization performance

PGM Learning Tasks II

- Goal: Specific prediction task on new instances
 - Predict target variables y from observed variables x
 - E.g., image segmentation, speech recognition
- Often care about specialized objective
 - E.g., pixel-level segmentation accuracy
- Often convenient to select model to optimize
 - likelihood $\prod_m P(\mathbf{d}[m] : \mathcal{M})$ or
 - conditional likelihood $\prod_m P(\mathbf{y}[m] | \mathbf{x}[m] : \mathcal{M})$
- Model evaluated on "true" objective over test data

PGM Learning Tasks III



- Goal: Knowledge discovery of \mathcal{M}^*
 - Distinguish direct vs indirect dependencies
 - Possibly directionality of edges
 - Presence and location of hidden variables
- Often train using likelihood
 - Poor surrogate for structural accuracy
- Evaluate by comparing to prior knowledge

Avoiding Overfitting

- Selecting \mathcal{M} to optimize training set likelihood overfits to statistical noise
- Parameter overfitting
 - Parameters fit random noise in training data
 - Use regularization / parameter priors
- Structure overfitting
 - Training likelihood always increases for more complex structures
 - Bound or penalize model complexity

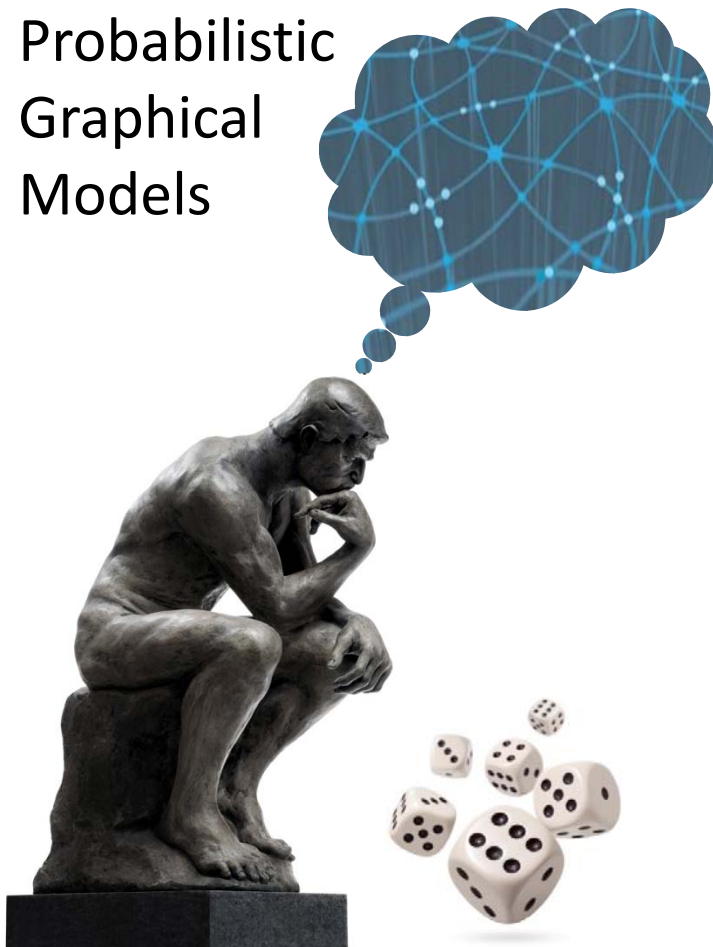
Selecting Hyperparameters

- Regularization for overfitting involves hyperparameters:
 - Parameter priors (regularization)
 - Complexity penalty
- Choice of hyperparameters makes a big difference to performance
- Must be selected on validation set ~~training test~~ (cross-validation)

Why PGM Learning

- Predictions of structured objects
(sequences, graphs, trees)
 - Exploit correlations between several predicted variables
- Can incorporate prior knowledge into model
- Learning single model for multiple tasks
- Framework for knowledge discovery

Probabilistic
Graphical
Models



Learning

Parameter Estimation

Maximum
Likelihood
Estimation

Biased Coin Example

P is a Bernoulli distribution:

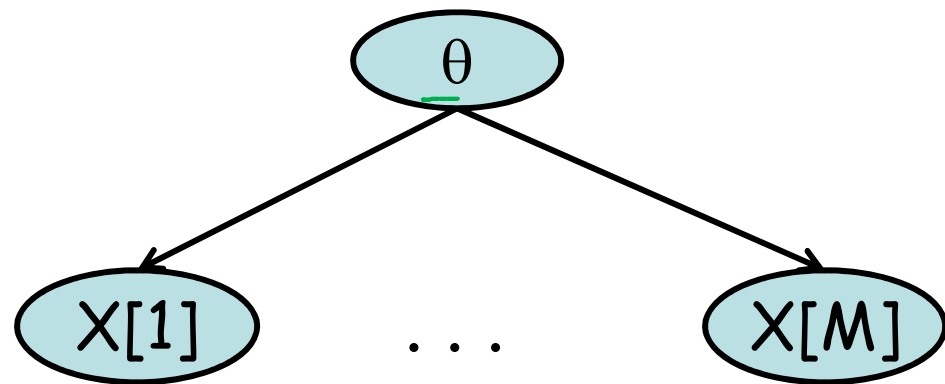
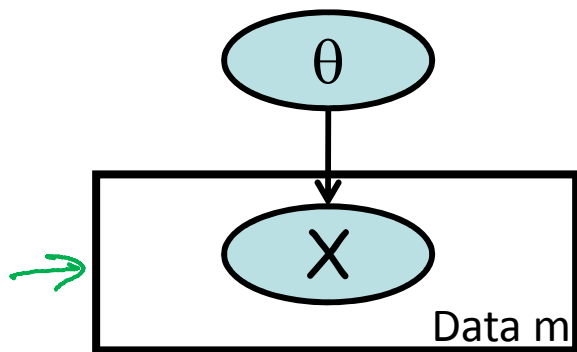
$$P(\underline{X}=1) = \underline{\theta}, P(\underline{X}=0) = \underline{1-\theta}$$



$\underline{\mathcal{D}} = \{x[1], \dots, x[M]\}$ sampled IID from P

- Tosses are independent of each other
- Tosses are sampled from the same distribution (identically distributed)

IID as a PGM



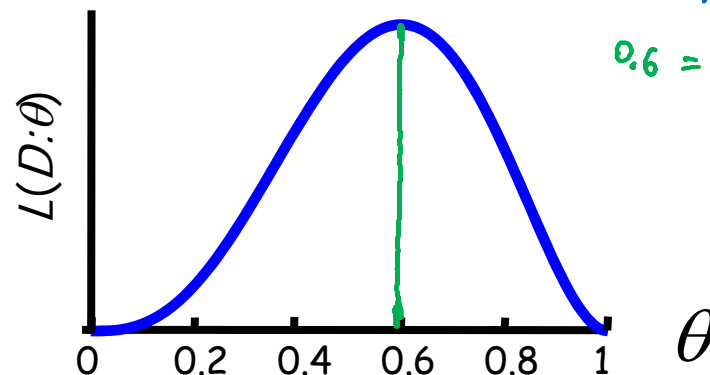
$$\underline{P(x[m] | \theta)} = \begin{cases} \underline{\theta} & x[m] = \underline{x^1} \\ \underline{1 - \theta} & x[m] = \underline{x^0} \end{cases}$$

Maximum Likelihood Estimation

- **Goal:** find $\theta \in [0,1]$ that predicts D well
- **Prediction quality = likelihood of D given θ**

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

$L(\theta : \langle H, T, T, H, H \rangle) = \underbrace{P(H|\theta)}_{\theta} \cdot \underbrace{P(T|\theta)}_{(1-\theta)} \cdot \underbrace{P(T|\theta)}_{(1-\theta)} \cdot \underbrace{P(H|\theta)}_{\theta} \cdot \underbrace{P(H|\theta)}_{\theta} = \theta^3(1-\theta)^2$



Maximum Likelihood Estimator

- Observations: M_H heads and M_T tails
- Find θ maximizing likelihood

- Equivalent to maximizing log-likelihood

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

- Differentiating the log-likelihood and solving for θ :

$$\hat{\theta} = \frac{M_H}{M_H + M_T}$$

Sufficient Statistics

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

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

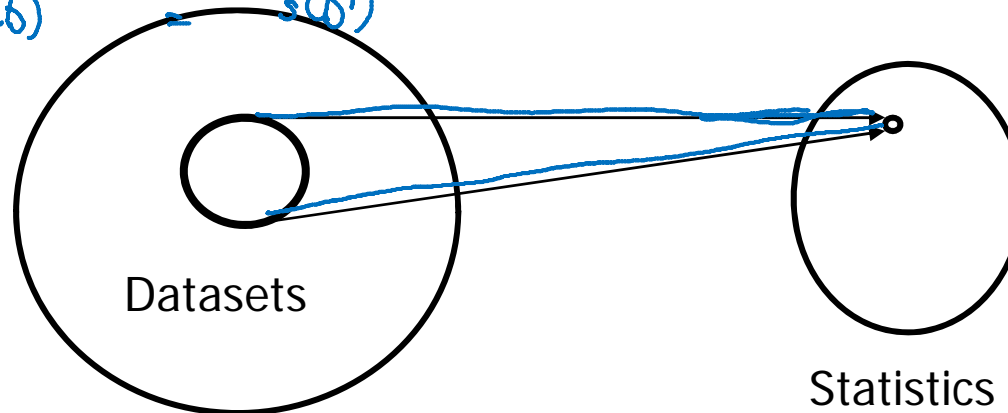
- $\rightarrow M_H$ and M_T are sufficient statistics

Sufficient Statistics

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

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

$\underbrace{\sum_{x[i] \in D} s(x[i])}_{s(D)} = \underbrace{\sum_{x[i] \in D'} s(x[i])}_{s(D')}$



Sufficient Statistic for Multinomial

- For a dataset D over variable X with k values, the sufficient statistics are counts $\langle \bar{M}_1, \dots, \bar{M}_k \rangle$ where M_i is the # of times that $X[m]=x^i$ in D
- Sufficient statistic $s(x)$ is a tuple of dimension k
 - $s(x^i) = (0, \dots, 0, 1, 0, \dots, 0)$ $\sum_n s(x[m]) = \{M_1, M_2, \dots, M_k\}$

$$L(\theta : D) = \prod_{i=1}^k \theta_i^{M_i} \quad \text{where } \theta_i \text{ is param for } x=x^i$$

Sufficient Statistic for Gaussian

- Gaussian distribution:

$$P(X) \sim N(\underline{\mu}, \underline{\sigma^2}) \quad \text{if} \quad p(X) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

- Rewrite as

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

- Sufficient statistics for Gaussian:

$$s(x) = \langle 1, x, x^2 \rangle \quad s(D) = \left(\sum_n x[n]^2, \sum_n x[n], n \right)$$

Maximum Likelihood Estimation

- MLE Principle: Choose θ to maximize $L(D;\Theta)$

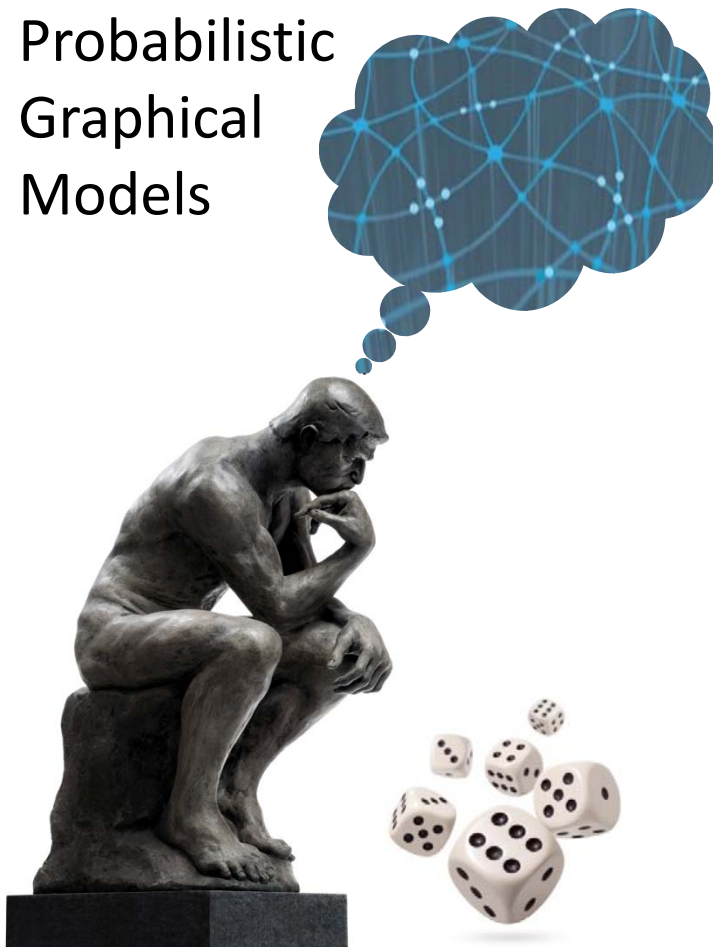
- Multinomial MLE: $\hat{\theta}^i = \frac{M_i}{\sum_{i=1}^m M_i}$ *fraction of x_i in data*

- Gaussian MLE:
 $\hat{\mu} = \frac{1}{M} \sum_m x[m]$ *empirical mean*
 $\hat{\sigma} = \sqrt{\frac{1}{M} \sum_m (x[m] - \hat{\mu})^2}$ *empirical st dev*

Summary

- Maximum likelihood estimation is a simple principle for parameter selection given D
- Likelihood function uniquely determined by sufficient statistics that summarize D
- MLE has closed form solution for many parametric distributions

Probabilistic
Graphical
Models



Learning

Parameter Estimation

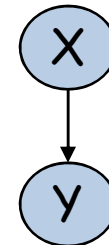
Max-Likelihood for BNs

MLE for Bayesian Networks

- Parameters: $\rightarrow \theta_{x^0}, \theta_{x^1}$
 $\theta_{y^0|x^0}, \theta_{y^1|x^0}, \theta_{y^0|x^1}, \theta_{y^1|x^1}$
- Data instances: $\langle x[m], y[m] \rangle$

x	
x^0	x^1
0.7	0.3

$P(x)$

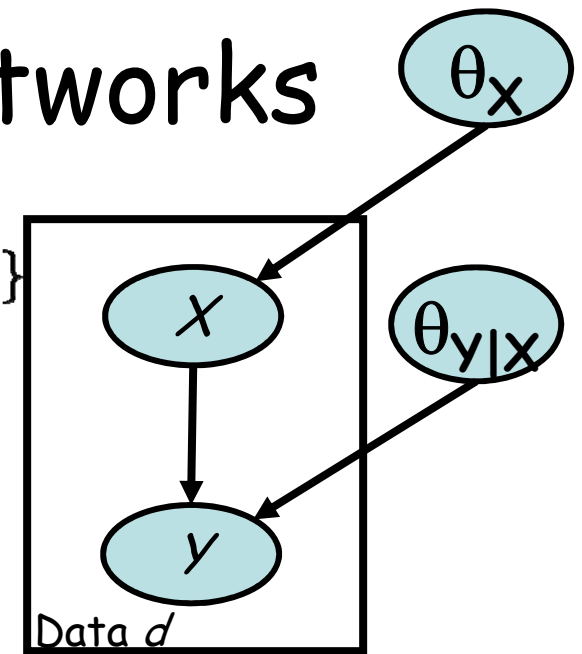


x	y	
	y^0	y^1
x^0	0.95	0.05
x^1	0.2	0.8

$P(y|x)$

MLE for Bayesian Networks

- Parameters: $\{\theta_x : x \in \text{Val}(X)\}$
 $\{\theta_{y|x} : x \in \text{Val}(X), y \in \text{Val}(Y)\}$



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

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

// chain rule for BNs

$$= \left(\prod_{m=1}^M P(x[m] : \theta) \right) \left(\prod_{m=1}^M P(y[m] | x[m] : \theta) \right)$$

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

*product of two
local likelihood*

MLE for Bayesian Networks

- Likelihood for Bayesian network

$$\begin{aligned}
 L(\Theta : D) &= \prod_m P(x[m] : \Theta) \\
 &= \prod_m \prod_i P(x_i[m] | \underline{U_i[m]} : \Theta_i) \\
 &= \prod_m \prod_i P(x_i[m] | U_i[m] : \Theta_i) \\
 &\stackrel{\text{local likelihood}}{\Rightarrow} \prod_i \underbrace{\prod_m P(x_i[m] | U_i[m] : \Theta_i)}_{L_i(\Theta_i : D)}
 \end{aligned}$$

parents of X_i (points to U_i)
chain rule (points to the product over m)
local likelihood (points to the final expression)
 $L_i(\Theta_i : D)$ (points to the term in the final product)

\Rightarrow if $\theta_{X_i|U_i}$ are disjoint, then MLE can be computed by maximizing each local likelihood separately

MLE for Table CPDs

$$\prod_{m=1}^M P(x[m] | u[m] : \theta) = \prod_{m=1}^M P(x[m] | u[m] : \theta_{x|u})$$

$$= \prod_{x,u} \left(\prod_{m: x[m]=x, u[m]=u} P(x[m] | u[m] : \theta_{x|u}) \right)$$

$P(x[m]=x | u[m]=u : \theta_{x|u}) = \theta_{x|u}$

$$= \prod_{x,u} \left(\prod_{m: x[m]=x, u[m]=u} \theta_{x|u} \right)$$

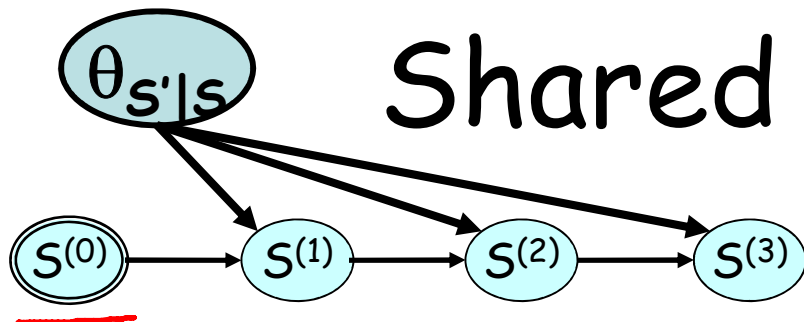
$$= \prod_{x,u} \frac{\theta_{x|u}^{M[x,u]}}{p(x|u)}$$

$p(x|u)$

fraction of $X=x$ among u 's where $\bar{u}=u$

$$\theta_{x|u} = \frac{M[x, u]}{\sum_{x'} M[x', u]} = \frac{M[x, u]}{M[u]}$$

Shared Parameters



$$L(\theta : S^{(0:T)}) = \prod_{t=1}^T P(S^{(t)} | S^{(t-1)} : \theta)$$

$$= \prod_{i,j} \prod_{t: S^{(t)}=s^i, S^{(t+1)}=s^j} P(S^{(t+1)} | S^{(t)} : \theta_{s^i|s^j})$$

$$= \prod_{i,j} \prod_{t: S^{(t)}=s^i, S^{(t+1)}=s^j} \theta_{s^i \rightarrow s^j}$$

$$= \prod_{i,j} \theta_{s^i \rightarrow s^j}^{M[s^i \rightarrow s^j]}$$

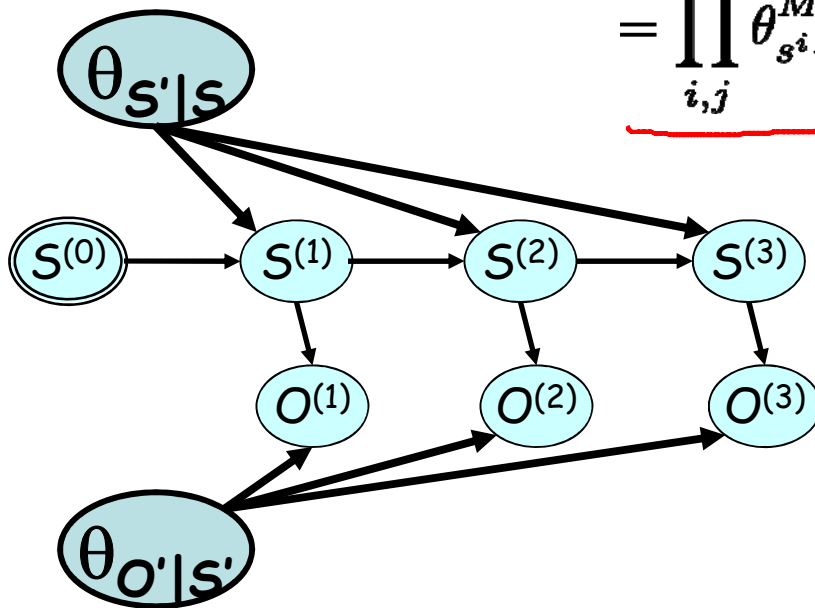
$$\hat{\theta}_{s^i \rightarrow s^j} = \frac{M[s^i \rightarrow s^j]}{M[s^i]}$$

$$M[s^i \rightarrow s^j] = |\{t : S^{(t)} = s^i, S^{(t+1)} = s^j\}|$$

Shared Parameters

$$L(\Theta : S^{(0:T)}, O^{(0:T)}) = \prod_{t=1}^T P(S^{(t)} | S^{(t-1)} : \theta_{S'|S}) \prod_{t=1}^T P(O^{(t)} | S^{(t)} : \theta_{O'|S'})$$

$$= \prod_{i,j} \theta_{S^i \rightarrow S^j}^{M[S^i \rightarrow S^j]} \prod_{i,k} \theta_{O^k | S^i}^{M[o^k, s^i]}$$



$$M[s^i \rightarrow s^j] = |\{t : S^{(t)} = s^i, S^{(t+1)} = s^j\}|$$

$$M[o^k, s^i] = |\{t : S^{(t)} = \underline{s^i}, O^{(t)} = \underline{o^k}\}|$$

Summary

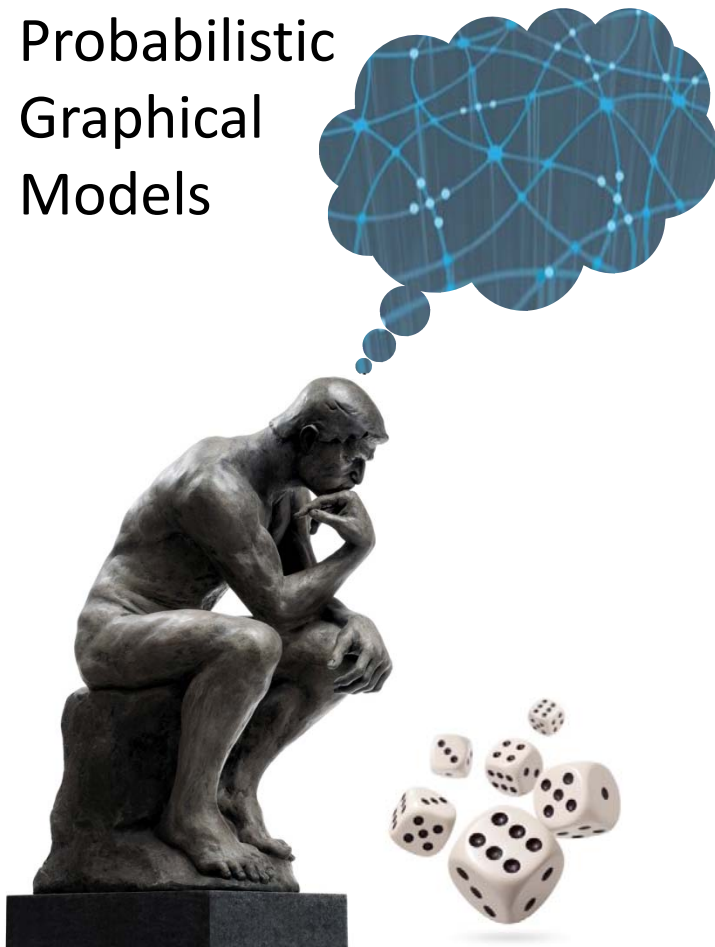
- For BN with disjoint sets of parameters in CPDs, likelihood decomposes as product of local likelihood functions, one per variable
- For table CPDs, local likelihood further decomposes as product of likelihood for multinomials, one for each parent combination
- For networks with shared CPDs, sufficient statistics accumulate over all uses of CPD

Fragmentation & Overfitting

$$\theta_{x|u} = \frac{M[x, u]}{\sum_{x'} M[x', u]} = \frac{M[x, u]}{M[u]}$$

- # of "buckets" increases exponentially with $|U|$
- For large $|U|$, most "buckets" will have very few instances
 \Rightarrow **very poor parameter estimates**
- **With limited data, we often get better generalization with simpler structures**
even when wrong

Probabilistic
Graphical
Models



Learning

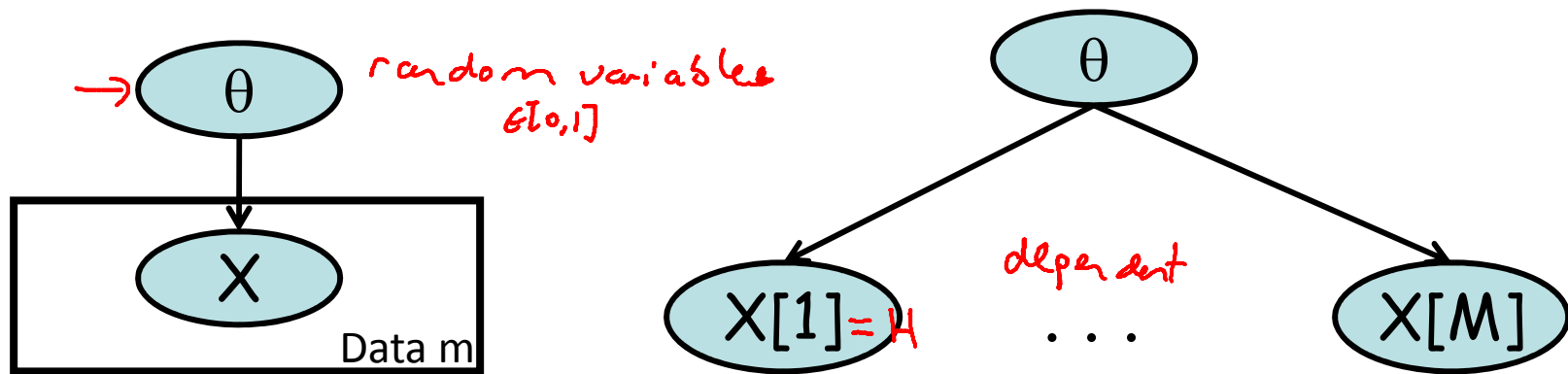
Parameter Estimation

Bayesian Estimation

Limitations of MLE

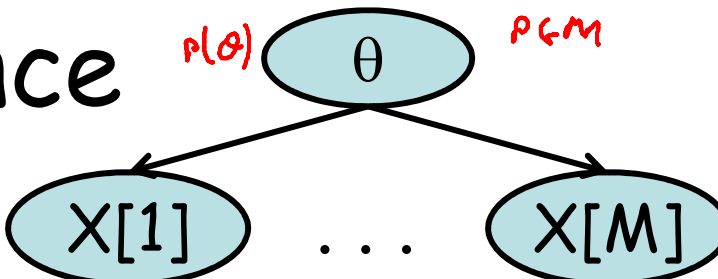
- Two teams play 10 times, and the first wins 7 of the 10 matches
 - ⇒ Probability of first team winning = 0.7
- A coin is tossed 10 times, and comes out 'heads' 7 of the 10 tosses
 - ⇒ Probability of heads = 0.7
- A coin is tossed 10000 times, and comes out 'heads' 7000 of the 10000 tosses
 - ⇒ Probability of heads = 0.7

Parameter Estimation as a PGM



- Given a fixed θ , tosses are independent
- If θ is unknown, tosses are not marginally independent
 - each toss tells us something about θ

Bayesian Inference

- Joint probabilistic model 

$$\underline{P(x[1], \dots, x[M], \theta)} = \underline{P(x[1], \dots, x[M] | \theta)} \underline{P(\theta)}$$

$$= P(\theta) \prod_{i=1}^M P(x[i] | \theta)$$

$$= \underline{P(\theta)} \underbrace{\theta^{M_H} (1 - \theta)^{M_T}}_{\text{likelihood function}} \leftarrow \text{likelihood function}$$

$$\underline{P(\theta | x[1], \dots, x[M])} = \frac{\underbrace{P(x[1], \dots, x[M] | \theta)}_{\text{likelihood}} \underbrace{P(\theta)}_{\text{prior}}}{\underbrace{P(x[1], \dots, x[M])}_{\text{constant relative to } \theta} \underbrace{\theta}_{\text{data } D}}$$

Dirichlet Distribution

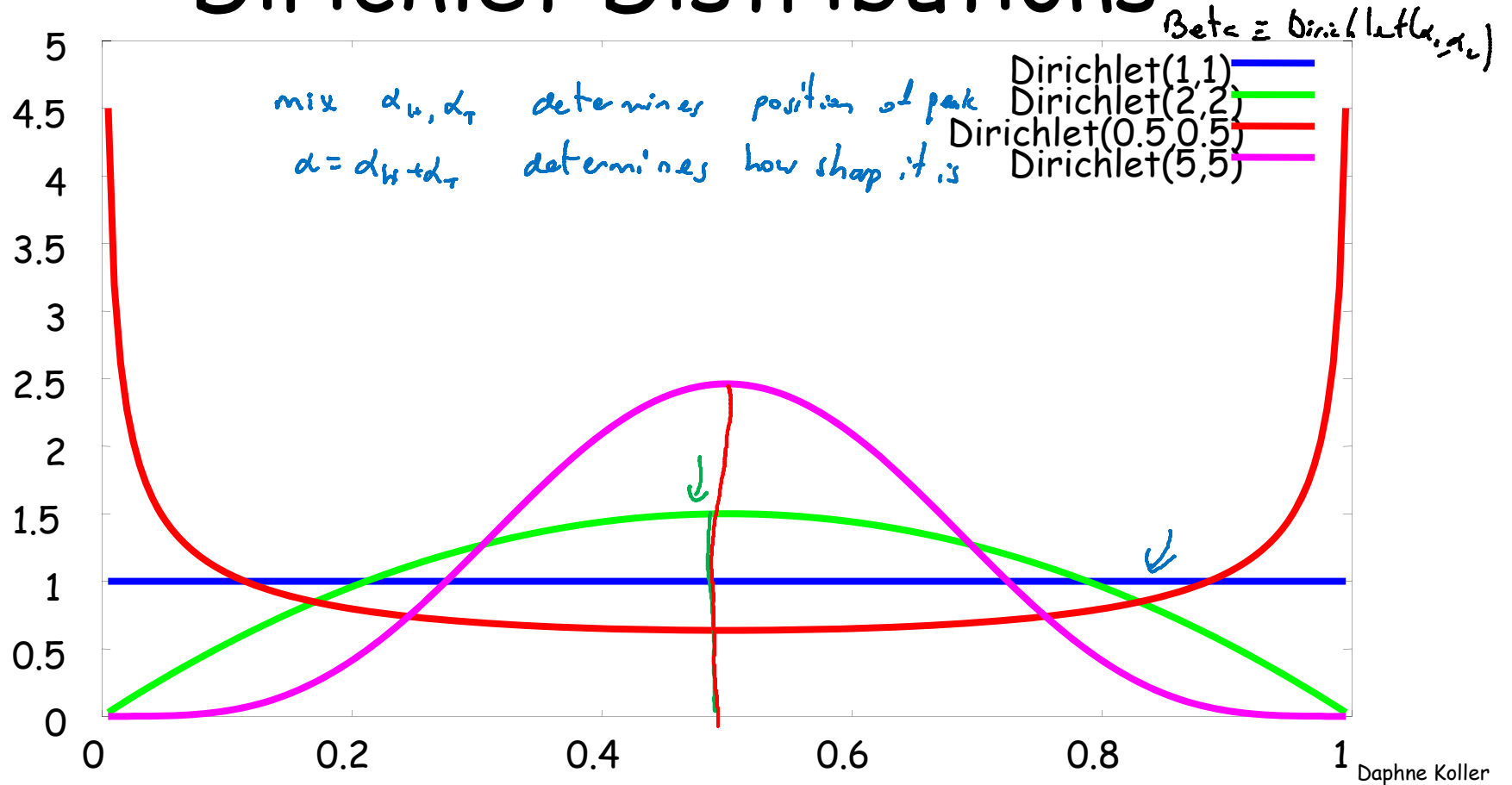
- θ is a multinomial distribution over k values
- Dirichlet distribution $\theta \sim \text{Dirichlet}(\alpha_1, \dots, \alpha_k)$

– where $P(\theta)$ = $\frac{1}{Z} \prod_{i=1}^k \theta_i^{\alpha_i - 1}$ and $Z = \frac{\prod_{i=1}^k \Gamma(\alpha_i)}{\Gamma(\sum_{i=1}^k \alpha_i)}$ $\Gamma(x) = \int_0^\infty t^{x-1} e^{-t} dt$

Handwritten notes: A red arrow points from the α_i in the Dirichlet distribution to the α_i in the probability formula. A blue box encloses the product term in the probability formula. A blue box encloses the gamma function ratio in the normalization constant. A red bracket under the $\alpha_1, \dots, \alpha_k$ in the Dirichlet distribution is labeled "hyperparameters". A red α_i is written above the word "hyperparameters".

- Intuitively, hyperparameters correspond to the number of samples we have seen

Dirichlet Distributions



Dirichlet Priors & Posteriors

$$\overbrace{P(\theta | D)}^{\text{posterior}} \propto \overbrace{P(D | \theta)}^{\text{likelihood}} \overbrace{P(\theta)}^{\text{prior}}$$

$$m_i = \# \text{ instances with } x_i \quad \overbrace{P(D | \theta)}^{\text{multinomial } \theta} = \prod_{i=1}^k \underbrace{\theta_i^{M_i}}_{\theta_i^{m_i + \alpha_i - 1}} \quad P(\theta) \propto \prod_{i=1}^k \underbrace{\theta_i^{\alpha_i - 1}}$$

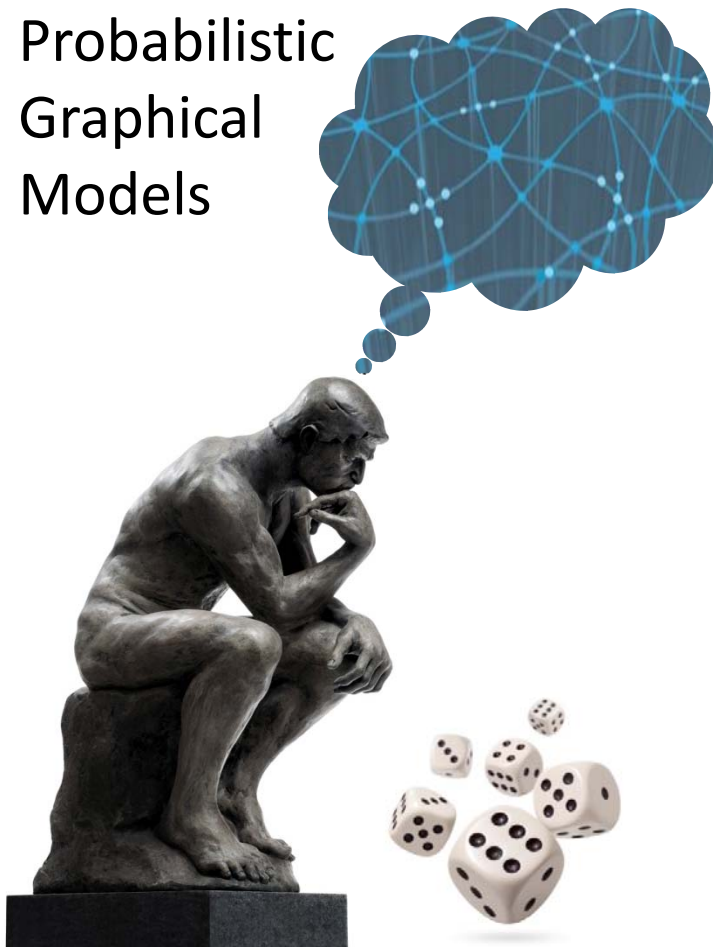
- If $P(\theta)$ is Dirichlet and the likelihood is multinomial, then the posterior is also Dirichlet
 - Prior is $\text{Dir}(\alpha_1, \dots, \alpha_k)$
 - Data counts are M_1, \dots, M_k
 - Posterior is $\text{Dir}(\alpha_1 + M_1, \dots, \alpha_k + M_k)$
- Dirichlet is a conjugate prior for the multinomial

prior, posterior have the same form

Summary

- Bayesian learning treats parameters as random variables
 - Learning is then a special case of inference
- Dirichlet distribution is conjugate to multinomial
 - Posterior has same form as prior
 - Can be updated in closed form using sufficient statistics from data

Probabilistic
Graphical
Models

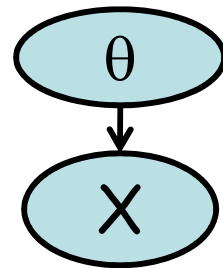


Learning

Parameter Estimation

Bayesian Prediction

Bayesian Prediction



$\sim \text{Dirichlet}(\alpha_1, \dots, \alpha_k)$

$$\underline{P(X)} = \int_{\theta} \underline{P(X | \theta)} \underline{P(\theta)} d\theta$$

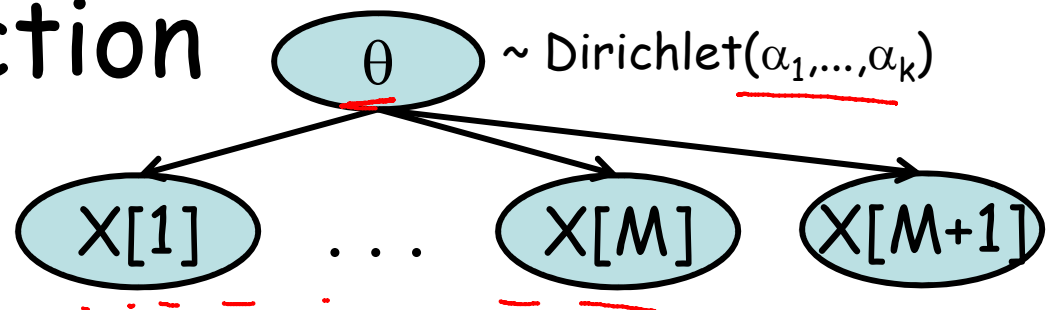
← marginalizing over θ

$$\begin{aligned} \underline{P(X = \underline{x}^i | \theta)} &= \frac{1}{Z} \int_{\theta} \theta_i \cdot \underbrace{\prod_j \theta^{\alpha_j - 1}}_{\text{prior}} d\theta \\ &= \frac{\alpha_i}{\sum_j \alpha_j = \alpha} \end{aligned}$$

fraction of instances we've seen where x^i

- Dirichlet hyperparameters correspond to the number of samples we have seen

Bayesian Prediction



$$P(\underline{x[M+1]} | \underline{x[1]}, \dots, \underline{x[M]})$$

$$= \int_{\theta} P(\underline{x[M+1]} | \underline{x[1]}, \dots, \underline{x[M]}, \theta) P(\theta | \underline{x[1]}, \dots, \underline{x[M]}) d\theta$$

$$= \int_{\theta} \underline{P(x[M+1] | \theta)} \boxed{P(\theta | \underline{x[1]}, \dots, \underline{x[M]})} d\theta$$

~ Dirichlet($\alpha_1 + M_1, \dots, \alpha_k + M_k$)
Posterior over θ given D

$$P(X[M+1] = \underline{x^i} | \theta, x[1], \dots, x[M]) = \frac{\alpha_i + M_i}{\underline{\alpha + M}}$$

$\alpha = \sum \alpha_i$
 $M = \sum M_i$

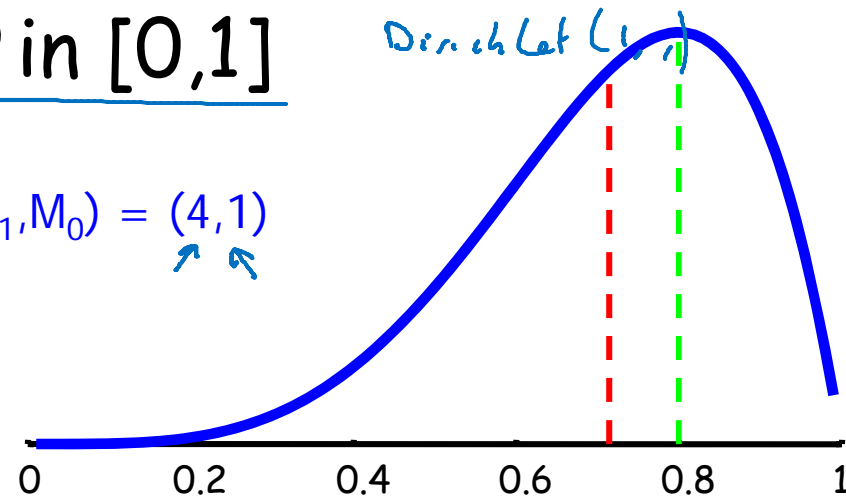
- Equivalent sample size $\alpha = \alpha_1 + \dots + \alpha_k$
 - Larger $\alpha \Rightarrow$ more confidence in our prior

Example: Binomial Data

- Prior: uniform for θ in $[0,1]$

$$P(\theta) = \frac{1}{Z} \prod_k \theta^{\alpha_k - 1}$$

$$(M_1, M_0) = (4, 1)$$

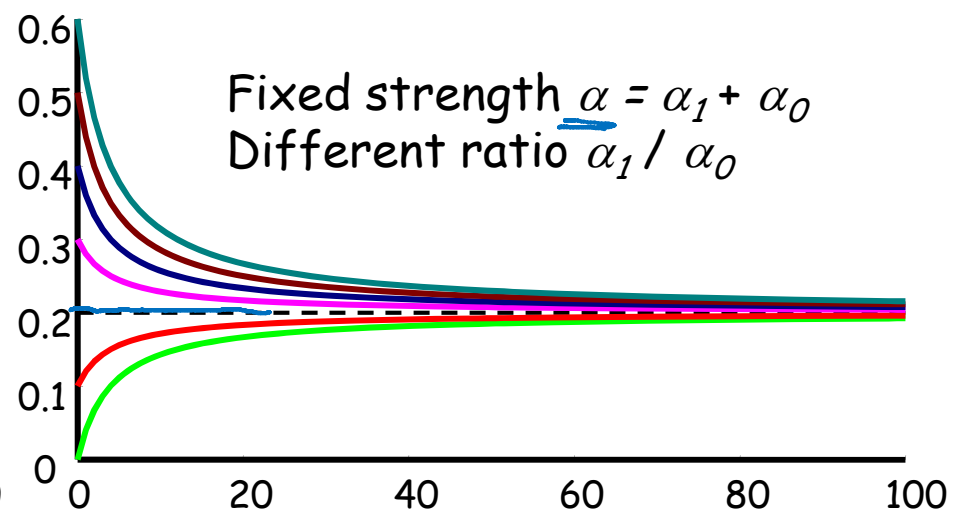
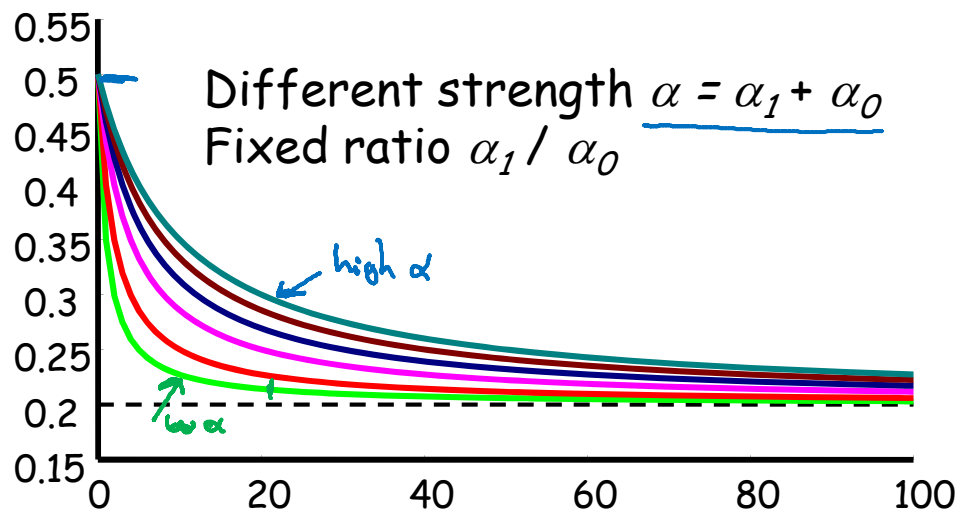


- MLE for $P(X[6]=1)=4/5$
- Bayesian prediction is $5/7$

$$\frac{\alpha_1 + m_1}{\alpha + m} = \frac{1 + 4}{2 + 5}$$

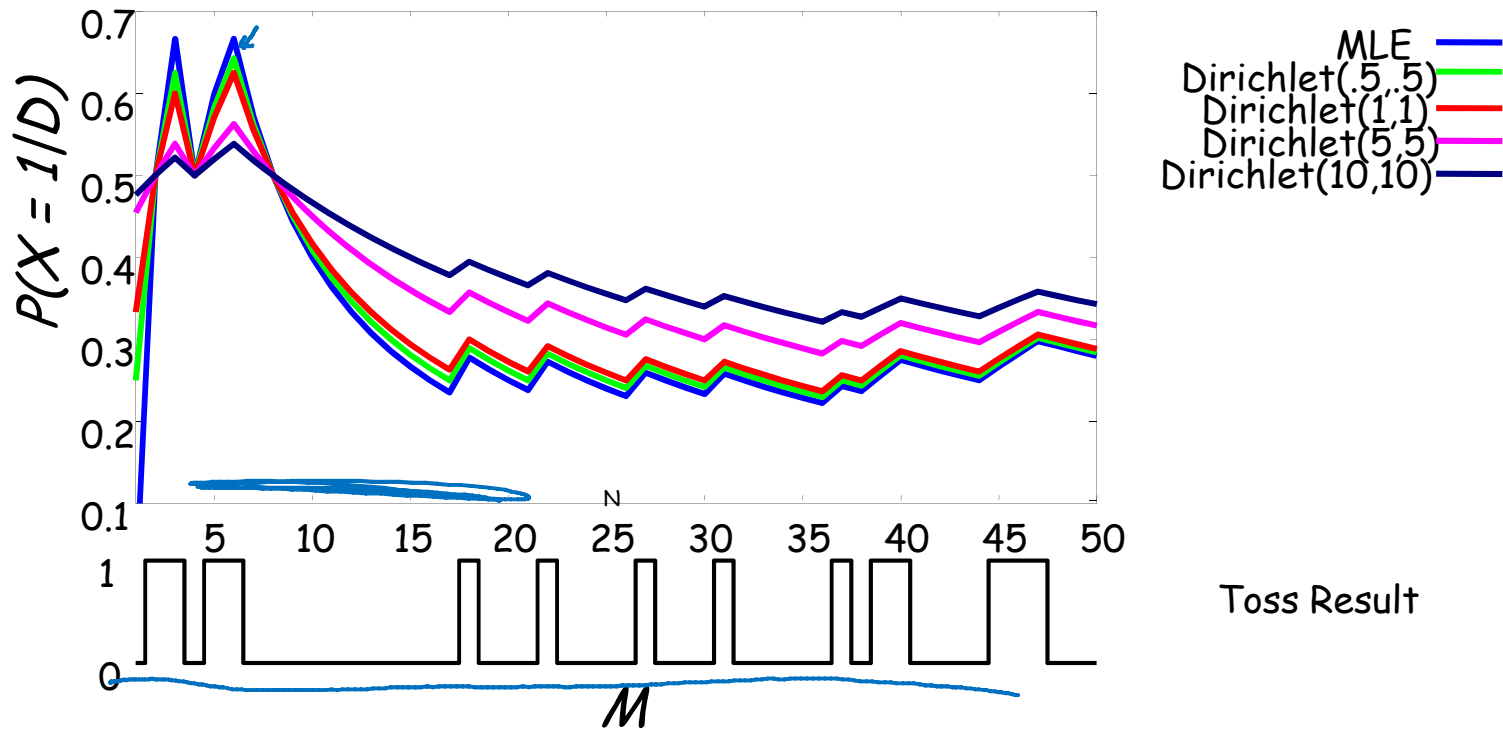
Effect of Priors

- Prediction of $P(X=1)$ after seeing data with $M_1 = \frac{1}{4}M_0$ as a function of sample size M



Effect of Priors

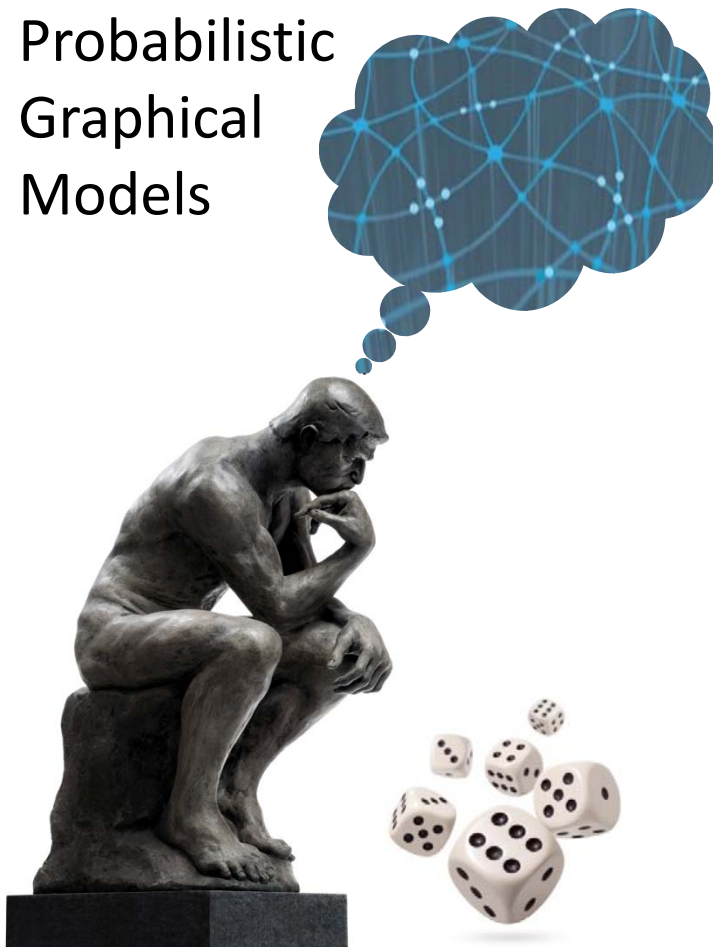
- In real data, Bayesian estimates are less sensitive to noise in the data



Summary

- Bayesian prediction combines sufficient statistics from imaginary Dirichlet samples and real data samples
- Asymptotically the same as MLE
- But Dirichlet hyperparameters determine both the prior beliefs and their strength

Probabilistic
Graphical
Models

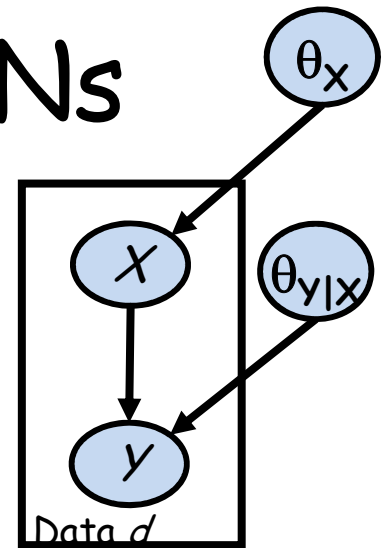
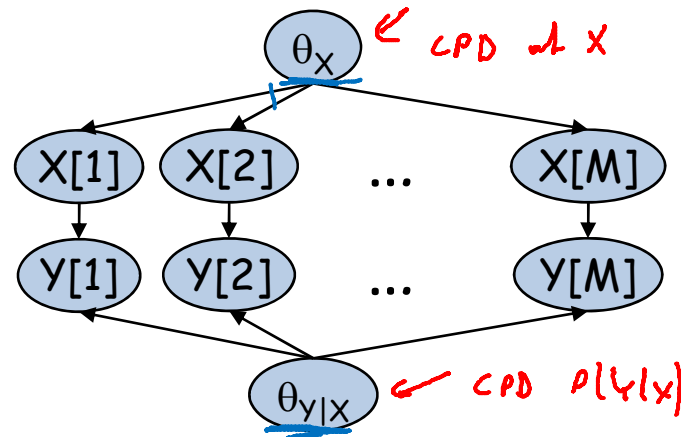


Learning

Parameter Estimation

Bayesian Estimation for BNs

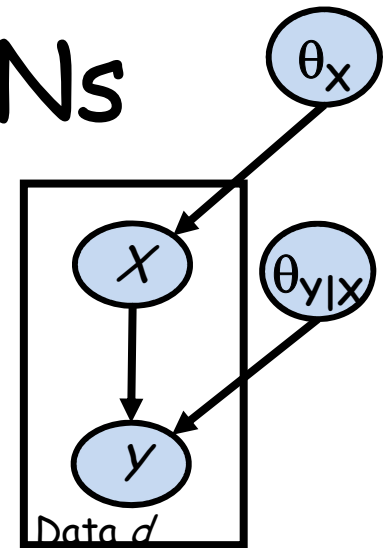
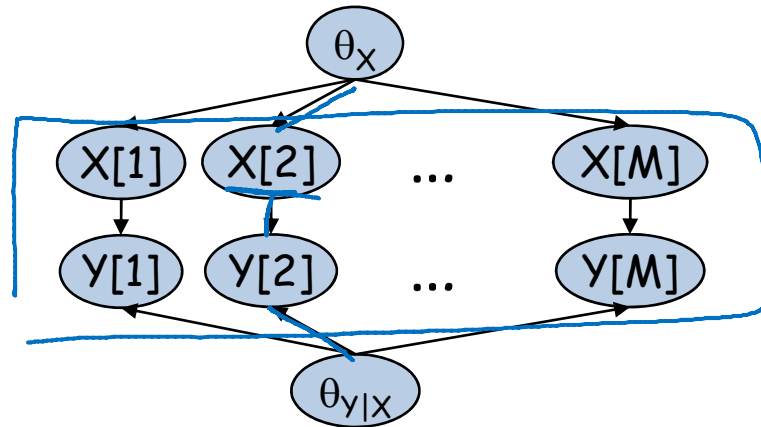
Bayesian Estimation in BNs



- Instances are independent given the parameters
 - $(X[m'], Y[m'])$ are d-separated from $(X[m], Y[m])$ given θ
- Parameters for individual variables are independent a priori

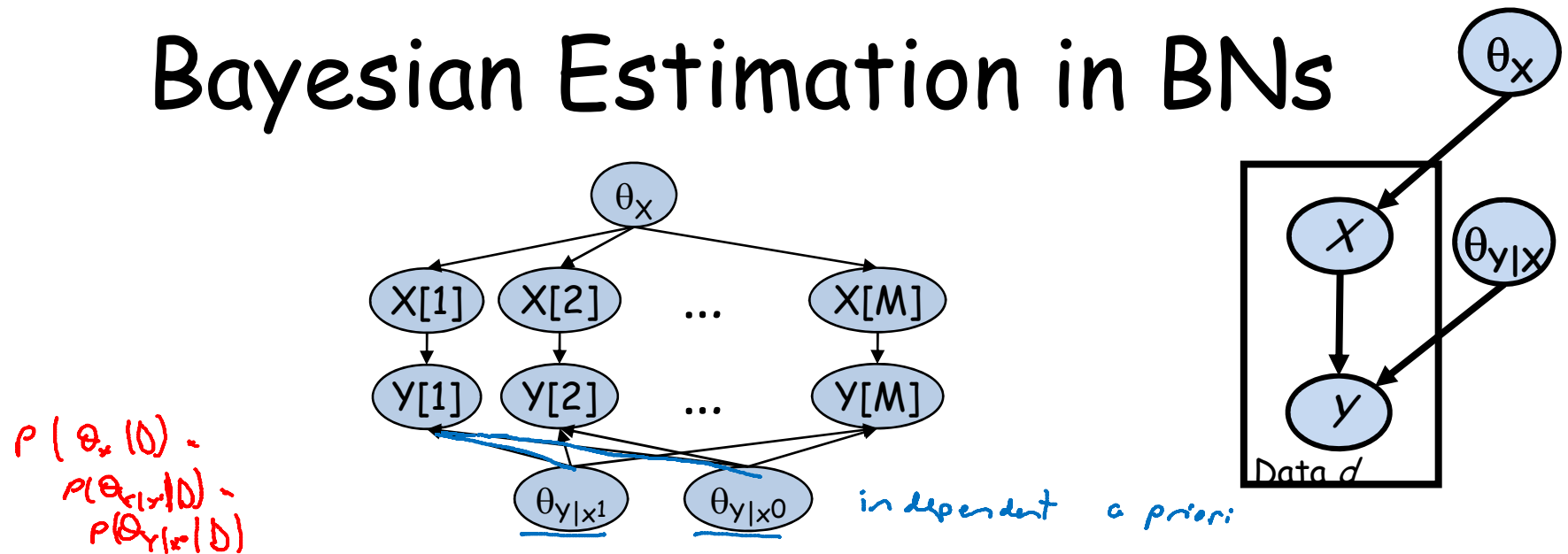
$$P(\theta) = \prod_i P(\theta_{X_i | Pa(X_i)})$$

Bayesian Estimation in BNs



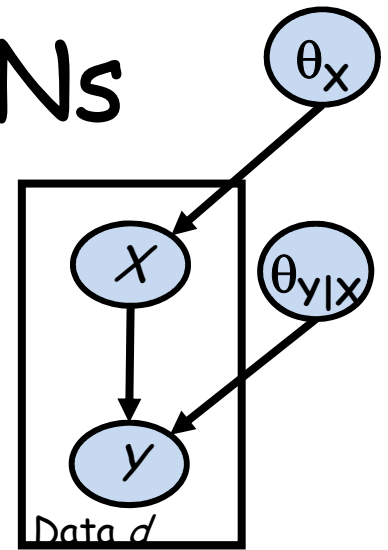
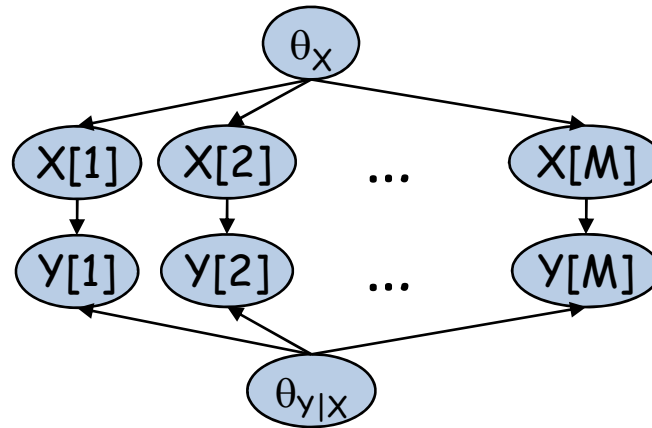
- Posteriors of θ are independent given complete data
 - Complete data d -separates parameters for different CPDs
 - $P(\theta_x, \theta_{y|x} | D) = P(\theta_x | D)P(\theta_{y|x} | D)$
 - As in MLE, we can solve each estimation problem separately

Bayesian Estimation in BNs



- Posteriors of θ are independent given complete data
 - Also holds for parameters within families
 - Note **context specific independence** between $\theta_{y|x1}$ and $\theta_{y|x0}$ when given both X 's and Y 's

Bayesian Estimation in BNs



- Posteriors of θ can be computed independently
 - For multinomial $\theta_{x|u}$ ^{assignment to x 's parents u} if prior is $\text{Dirichlet}(\alpha_{x^1|u}, \dots, \alpha_{x^k|u})$
 - posterior is $\text{Dirichlet}(\alpha_{x^1|u} + M[x^1, u], \dots, \alpha_{x^k|u} + M[x^k, u])$

Assessing Priors for BNs

- We need hyperparameter $\alpha_{x|u}$ for each node X , value x , and parent assignment u
 - Prior network with parameters Θ_0
 - Equivalent sample size parameter α
 - $\alpha_{x|u} := \alpha \cdot P(x, u | \Theta_0)$ $X=y, \bar{u}=\bar{u}$

\textcircled{X} Θ_0 uniform

\textcircled{Y}

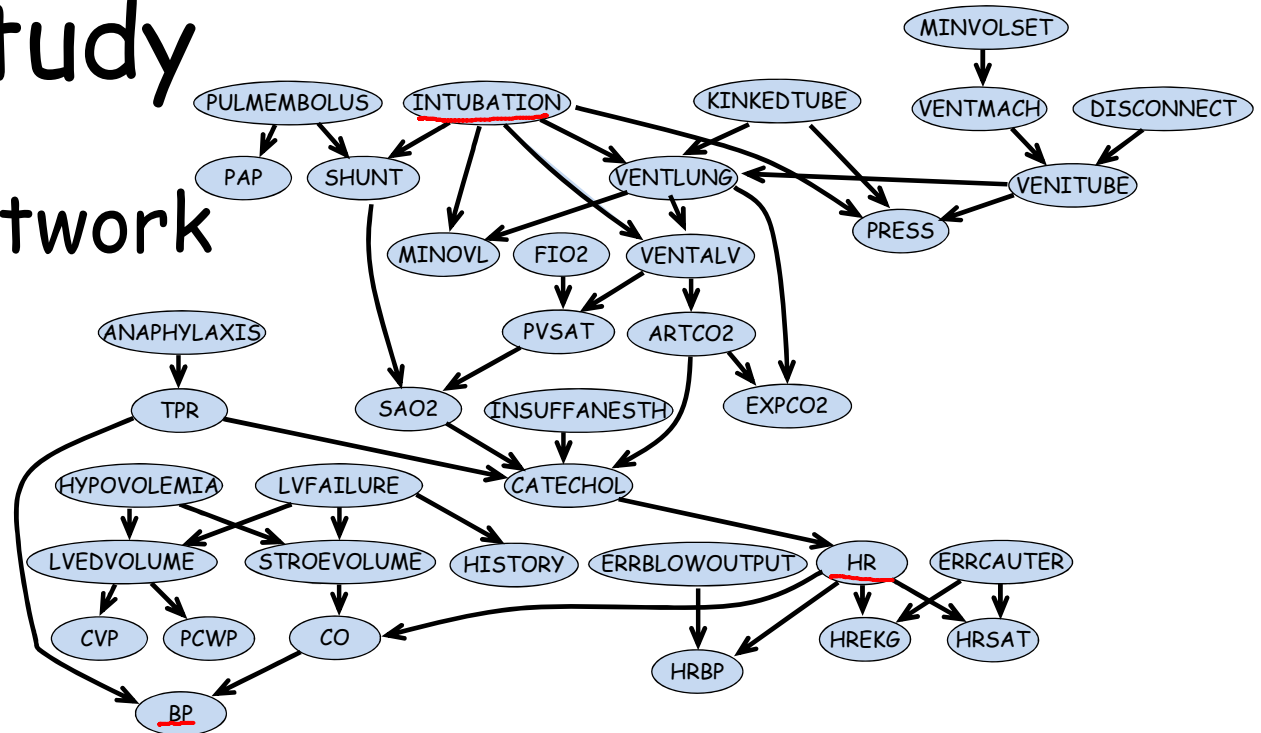
$\textcircled{X} \sim \text{Dirichlet}(\frac{\alpha}{2}, \frac{\alpha}{2})$

$\textcircled{Y} \sim \text{Dirichlet}(\frac{\alpha}{4}, \frac{\alpha}{4})$
 $\rightarrow \Theta_{y|u} \sim \text{Dirichlet}(\frac{\alpha}{4}, \frac{\alpha}{4})$

Case Study

- ICU-Alarm network

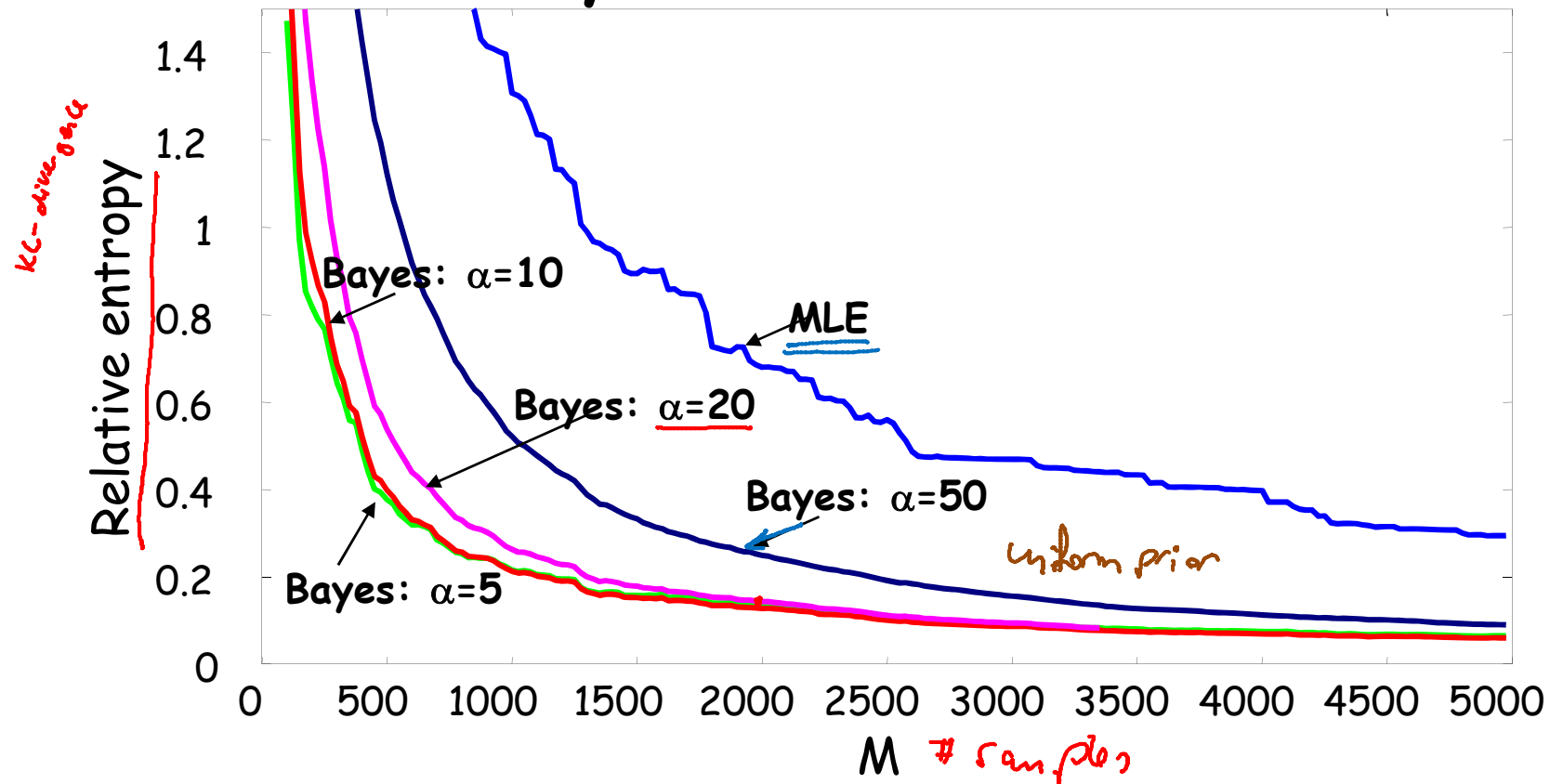
- 37 variables
- 504 params



- Experiment

- Sample instances from network
- Relearn parameters

Case Study: ICU Alarm Network



Summary

- In Bayesian networks, if parameters are independent a priori, then also independent in the posterior
- For multinomial BNs, estimation uses sufficient statistics $M[x, u]$

$$\hat{\theta}_{x|u} = \frac{M[x, u]}{M[u]}$$

MLE

$$P(x | u, D) = \frac{\alpha_{x,u} + M[x, u]}{\alpha_u + M[u]}$$

Bayesian (Dirichlet)

- Bayesian methods require choice of prior
 - can be elicited as prior network and equivalent sample size α