# Exploiting Structure in Probability Distributions 

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Based on presentation and lecture notes of Nir Friedman, Hebrew University

## General References:

$\bullet$ D. Koller and N. Friedman, probabilistic graphical models
-Pearl, Probabilistic Reasoning in Intelligent Systems

- Jensen, An Introduction to Bayesian Networks
$\bullet$ Heckerman, A tutorial on learning with Bayesian networks


## Example I <br> Relationships in obesity



## Example II

The currently accepted consensus network of human primary CD4 T cells, downstream of CD3, CD28, and LFA-


Causal Protein-Signaling Networks Derived from Multiparameter Single-Cell Data. Karen Sachs, et al. 2005.

## Bayesian network results

A Model inference result

Phospho-Proteins
Phospho-LipidsPerturbed in data

| Expected | $15 / 17$ |
| :---: | :---: |
| Reperted | $17 / 17$ |
| Reversed <br>  <br> Missed | 1 |

- PKC->PKA was validated experimentally.
- Akt was not affected by Erk in additional experiments

Example III: Bayesian network models for a transcription factor-DNA binding motif with 5 positions
(a) $\left.\times_{1}\right) \times_{2} \times_{3} \times_{3} \times_{3}$
$P\left(X_{1}\right) P\left(X_{2}\right) P\left(X_{3}\right) P\left(X_{4}\right) P\left(X_{5}\right)$
(b)


Bayesian network

## Example IV: Diagnostic Bayesian network model



## Basic Probability Definitions

- Product Rule: $\mathrm{P}(\mathrm{A}, \mathrm{B})=\mathrm{P}(\mathrm{A} \mid \mathrm{B})^{*} \mathrm{P}(\mathrm{B})=\mathrm{P}(\mathrm{B} \mid \mathrm{A})^{*} \mathrm{P}(\mathrm{A})$
- Independence between $A$ and $B: P(A, B)=P(A)^{*} P(B)$, or alternatively: $P(A \mid B)=P(A), P(B \mid A)=P(B)$.
$\bullet$ Total probability theorem: $\bigcup_{i=1}^{n} B_{i}=\Omega, \forall i \neq j \quad B_{i} \bigcap B_{j}=\phi$

$$
P(A)=\sum_{i=1}^{n} P\left(A, B_{i}\right)=\sum_{i=1}^{n} P\left(B_{i}\right) * P\left(A \mid B_{i}\right)
$$

## Basic Probability Definitions

-Bayes Rule:

$$
\begin{aligned}
& P(A \mid B)=\frac{P(B \mid A) \cdot P(A)}{P(B)} \\
& P(A \mid B, C)=\frac{P(B \mid A, C) \cdot P(A \mid C)}{P(B \mid C)}
\end{aligned}
$$

-Chain Rule:

$$
\begin{aligned}
& P\left(X_{1}, \ldots, X_{n}\right)= \\
& P\left(X_{1} \mid X_{2}, \ldots, X_{n}\right) \cdot P\left(X_{2} \mid X_{3}, \ldots, X_{n}\right) \cdot P\left(X_{3} \mid X_{4}, \ldots, X_{n}\right) \cdot \ldots P\left(X_{n-1} \mid X_{n}\right) \cdot P\left(X_{n}\right)
\end{aligned}
$$

## Exploiting Independence Property

-G: whether the woman is pregnant
$\bullet$ D: whether the doctor's test is positive
The joint distribution representation $\mathrm{P}(\mathrm{g}, \mathrm{d})$ :

| $\mathbf{G}$ | $\mathbf{D}$ | $\mathbf{P}(\mathbf{G}, \mathbf{D})$ |
| :---: | :---: | :---: |
| 0 | 0 | 0.54 |
| 0 | 1 | 0.06 |
| 1 | 0 | 0.02 |
| 1 | 1 | 0.38 |

## Factorial representation

Using conditional probability: $\mathrm{P}(\mathrm{g}, \mathrm{d})=\mathrm{P}(\mathrm{g}){ }^{\star} \mathrm{P}(\mathrm{d} \mid \mathrm{g})$.
The distribution of $\mathrm{P}(\mathrm{g}), \mathrm{P}(\mathrm{d} \mid \mathrm{g})$ :


Example: $\mathrm{P}(\mathrm{g} 0, \mathrm{~d} 1)=0.06$ vs. $\mathrm{P}(\mathrm{g} 0)^{*} \mathrm{P}(\mathrm{d} 1 \mid \mathrm{g} 0)=0.6^{*} 0.1=0.06$

## Exploiting Independence Property

- H: home test
- Independence assumption: $\operatorname{Ind}(\mathrm{H} ; \mathrm{D} \mid \mathrm{G})$ (i.e., given $\mathrm{G}, \mathrm{H}$ is independent of D$)$.

$P(d, h, g)=P(d, h \mid g)^{*} P(g)=P(d \mid g)^{*} P(h \mid g)^{*} P(g)$ $\operatorname{Ind}(H ; \mathrm{D} \mid \mathrm{G})$


## Product rule



## Exploiting Independence Property

|  | representation of $\mathbf{P ( d , g , h})$ |  |
| :--- | :---: | :---: |
|  | joint distribution | factored distribution |
| No. of <br> parameters | 7 | 5 |
| Adding new <br> variable H | changing the distribution <br> entirely | Modularity: reuse the local <br> probability model. (Only new <br> local probability model for H.) |


=> Bayesian networks: Exploiting independence properties of the distribution in order to allow a compact and natural representation.

## Outline

- Introduction
-Bayesian Networks
" Representation \& Semantics
- Inference in Bayesian networks
- Learning Bayesian networks


## Representing the Uncertainty

- A story with five random variables:
- Burglary, Earthquake, Alarm, Neighbor Call, Radio Announcement
- Specify joint distribution with $2^{5}=32$ parameters maybe...
$\bullet$ An expert system for monitoring intensive care patients
- Specify joint distribution over 37 variables with (at least) $2^{37}$ parameters


## Probabilistic Independence: a Key for Representation and Reasoning

Recall that if X and Y are independent given Z then

$$
P(X \mid Z, Y)=P(X \mid Y)
$$

- In our story...if
- burglary and earthquake are independent
- alarm sound and radio are independent given earthquake
- burglary and radio are independent given earthquake
-then instead of 15 parameters we need 8

$$
P(A, R, E, B)=P(A \mid R, E, B) \cdot P(R \mid E, B) \cdot P(E \mid B) \cdot P(B)
$$

versus

$$
P(A, R, E, B)=P(A \mid E, B) \cdot P(R \mid E) \cdot P(E) \cdot P(B)
$$

Need a language to represent independence statements

## Markov Assumption

Generalizing:
A child is conditionally independent from its non-descendents, given the value of its parents.
Ind(Xi ; NonDescendantXi | PaXi)

- It is a natural assumption for many causal processes


## Markov Assumption (cont.)

- Examples:
- $R$ is independent of $A, B, C$, given $E$
- $A$ is independent of $R$, given $B$ and $E$
- $C$ is independent of $B, E, R$, given $A$



## Bayesian Network Semantics



## Qualitative part conditional independence statements in BN structure

Quantitative part local probability Models (e.g., multinomial, $=$ distribution over domain
-Compact \& efficient representation:

- nodes have $\leq k$ parents $\Rightarrow O\left(2^{k} n\right)$ vs. $O\left(2^{n}\right)$ params
- parameters pertain to local interactions

```
\(P(C, A, R, E, B)=P(B)^{\star} P(E \mid B)^{\star} P(R \mid E, B)^{\star} P(A \mid R, B, E)^{\star P}(C \mid A, R, B, E)\)
I
\(P(C, A, R, E, B)=P(B) * P(E) * P(R \mid E) * P(A \mid B, E) * P(C \mid A)\)
\(\rightarrow\) In general: \(P\left(x_{1}, \ldots, x_{n}\right)=\prod P\left(x_{i} \mid P a_{x i}\right)\)
```


## Bayesian networks

## Efficient representation of probability distributions via conditional independence

Qualitative part: statistical independence statements Directed acyclic graph (DAG) - Nodes - random variables of interest (exhaustive and mutually exclusive states)
-Edges - direct influence


Quantitative part: Local probability models. Set of conditional probability distributions.

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## Inference in Bayesian networks

- A Bayesian network represents a probability distribution.
-Can we answer queries about this distribution?
Examples:
- $\mathrm{P}(\mathrm{Y} \mid \mathrm{Z}=\mathrm{z})$
- Most probable estimation $M P E(W \mid Z=z)=\arg \max _{w} P(w, z)$
$\bullet$ Maximum a posteriori $M A P(Y \mid Z=z)=\arg \max _{y} P(y \mid z)$


## Inference in Bayesian networks

- Goal: compute $\mathrm{P}(\mathrm{E}=e, \mathrm{~A}=\mathrm{a})$ in the following Bayesian network:
$A \rightarrow B$
- Using definition of probability, we have

$$
\begin{aligned}
P(a, e) & =\sum_{b} \sum_{c} \sum_{d} P(a, b, c, d, e) \\
& =\sum_{b} \sum_{c} \sum_{d} P(a) P(b \mid a) P(c \mid b) P(d \mid c) P(e \mid d)
\end{aligned}
$$

## Inference in Bayesian networks



- Eliminating d, we get

$$
\begin{aligned}
P(a, e) & =\sum_{b} \sum_{c} \sum_{d} P(a) P(b \mid a) P(c \mid b) P(d \mid c) P(e \mid d) \\
& =\sum_{b} \sum_{c} P(a) P(b \mid a) P(c \mid b) \sum_{c} P(d \mid c) P(e \mid d) \\
& =\sum_{b} \sum_{c} P(a) P(b \mid a) P(c \mid b) F 1(e, c)
\end{aligned}
$$

## Inference in Bayesian networks



- Eliminating $c$, we get

$$
\begin{aligned}
P(a, e) & =\sum_{b}^{b} \sum_{c} P(a) P(b \mid a) P(c \mid b) P(e \mid c) \\
& =\sum_{b} P(a) P(b \mid a) \sum_{\substack{ \\
p \\
p(e \mid b)}} P(c \mid b) P(e \mid c) \\
& =\sum_{b} P(a) P(b \mid a) F 2(e, b)
\end{aligned}
$$

## Inference in Bayesian networks



Finally, we eliminate $b$

$$
\begin{aligned}
& P(a, e)=\sum_{b} P(a) P(b \mid a) p(e \mid b) \\
&=P(a) \sum_{b} P(b \mid a) p(e \mid b) \\
&=P(a) F 3(e, a) \\
& \downarrow \\
& p(e \mid a)
\end{aligned}
$$

## Variable Elimination Algorithm

General idea:

- Write query in the form

$$
P\left(x_{1}\right)=\sum_{x_{k}} \cdots \sum_{x_{3}} \sum_{x_{2}} \prod_{i} P\left(x_{i} \mid p a_{i}\right)
$$

- Iteratively
- Move all irrelevant terms outside of innermost sum
- Perform innermost sum, getting a new term
- Insert the new term into the product
- In case of evidence $\mathrm{P}\left(\mathrm{x}_{1} \mid\right.$ evidence $\left.\mathrm{x}_{\mathrm{j}}\right)$, use: $P\left(x_{i} \mid x_{j}\right)=P\left(x_{i}, x_{j}\right) / P\left(x_{j}\right)$


## Complexity of inference

Naïve exact inference
exponential in the number of variables in the network
Variable elimination complexity
exponential in the size of largest factor
polynomial in the number of variables in the network

- Variable elimination computation depend on order of elimination (many heuristics, e.g., clique tree algorithm).


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- Parameter Learning

Structure Learning
-Process

- Input: dataset and prior information
- Output: Bayesian network



## The Learning Problem

|  | Known Structure | Unknown Structure |
| :--- | :---: | :---: |
| Complete Data | Statistical <br> parametric <br> estimation <br> (closed-form eq.) | Discrete optimization <br> over structures <br> (discrete search) |
| Incomplete Data | Parametric <br> optimization <br> (EM, gradient <br> descent...) | Combined <br> (Structural EM, mixture <br> models...) |
|  |  |  |

$\bullet$ We will focus on complete data for the rest of the talk

- The situation with incomplete data is more involved


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## Learning Parameters

-Key concept: the likelihood function

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

- measures how the probability of the data changes when we change parameters
-Estimation:
- MLE: choose parameters that maximize likelihood
- Bayesian: treat parameters as an unknown quantity, and marginalize over it


## MLE principle for Binomial Data

$\rightarrow$ Data: $H, H, T, H, H . \Theta$ is the unknown probability $P(H)$. Likelihood function: $L(\Theta: D)=\prod_{k=0,1} \theta_{k}^{N_{k}}$

$$
L(\theta: D)=\theta \cdot \theta \cdot(1-\theta) \cdot \theta \cdot \theta
$$

Estimation task: Given a sequence of samples $x[1]$, $x[2] \ldots x[M]$, we want to estimate the probability $P(H)=\theta$ and $P(T)=1-\theta$.
$\star$ MLE principle: choose parameter that maximize the likelihood function.

- Applying the MLE principle we get

$$
\hat{\theta}=\frac{N_{H}}{N_{H}+N_{T}}
$$

$\rightarrow$ MLE for $P(X=H)$ is $4 / 5=0.8$


## MLE principle for Multinomial Data

- Suppose $X$ can have the values $1,2, \ldots, k$.
- We want to learn the parameters $\theta_{1}, \ldots, \theta_{k}$.
$-\mathrm{N}_{1}, \ldots, \mathrm{~N}_{\mathrm{k}}$ - The number of times each outcome is observed.
- Likelihood function:

$$
L(\Theta: D)=\prod_{k=1}^{K} \theta_{k} \frac{\text { outcome in D }}{\begin{array}{c}
\text { Probability of } \\
k_{k}^{\text {th }} \text { outcome }
\end{array}}
$$

The MLE is: $\hat{\theta}_{i}=\frac{N_{i}}{\sum_{l=1, \ldots, k} N_{l}}$

## MLE principle for Bayesian networks

- Training data has the form: $D=\left[\begin{array}{cccc}E[1] & B[1] & A[1] & C[1] \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ E[M] & B[M] & A[M] & C[M]\end{array}\right]$


$$
L(\Theta: D)=\prod_{m} P(E[m], B[m], A[m], C[m]: \Theta)
$$


$\left(\begin{array}{l}P(E[m]: \Theta) \\ P(B[m]: \Theta) \\ P(A[m] \mid B[m], E[m]: \Theta) \\ P(C[m] \mid A[m]: \Theta)\end{array}\right)$

$$
\prod_{m} P(E[m]: \Theta)
$$

$$
=\begin{gathered}
\prod_{m}^{m} P(B[m]: \Theta) \\
\prod_{m} P(A[m] \mid B[m], E[m]: \Theta) \\
\prod_{m} P(C[m] \mid A[m]: \Theta)
\end{gathered}
$$



## MLE principle for Bayesian networks

- Generalizing for any Bayesian network:

$$
\begin{aligned}
& L(\Theta: D)=\prod_{i} \prod_{m} P\left(x_{i}[m] \mid P a_{i}[m]: \Theta_{i}\right)=\prod_{i} L_{i}\left(\Theta_{i}: D\right) \\
& L_{i}\left(\theta_{i}: D\right)=\prod_{m} P\left(x_{i}[m] \mid P a_{i}[m]: \theta_{i}\right) \\
& \quad=\prod_{p a_{i}} \prod_{x_{i}} P\left(x_{i} \mid p a_{i}: \theta_{i}\right)^{N\left(x_{i, p e}\right)}=\prod_{p a_{i}} \prod_{x_{i}} \theta_{x_{i} \mid a_{i}}^{N\left(x_{i}, p q_{i}\right)}
\end{aligned}
$$

- The likelihood decomposes according to the network structure.
- Decomposition $\Rightarrow$ Independent estimation problems (If the parameters for each family are not related)
- For each value pai of the parent of Xi we get independent multinomial problem.
- The MLE is $\hat{\theta}_{x_{i} \mid p a_{i}}=\frac{N\left(x_{i}, p a_{i}\right)}{N\left(p a_{i}\right)}$


## Continuous (Gaussian) variables

$$
\begin{gathered}
\text { Discrete } \mathrm{X} \text { X Y Y X } ~
\end{gathered}
$$

- The likelihood decomposes according to the network structure.
- Decomposition $\Rightarrow$ Independent estimation problems (If the parameters for each family are not related)
- For each value pai of the parent of Xi we get independent maximization problem.
- The MLE is

$$
\begin{array}{|l}
\hat{\mu}_{i, p p_{i}}=\frac{\sum_{m: P a_{i}[m]=p a_{i}} x_{i}[m]}{N\left(p a_{i}\right)} \\
\hat{\sigma}^{2}{ }_{i, p a_{i}}=\frac{\sum_{m: P a_{i}[m]=p a_{i}}\left(x_{i}[m]-\mu_{i, P a_{i}}\right)^{2}}{N\left(p a_{i}\right)}
\end{array}
$$

## Continuous (Gaussian) variables

$$
\begin{gathered}
X \sim N\left(\mu, \sigma_{X}^{2}\right) X Y \rightarrow X \sim N\left(a x+b, \sigma^{2}\right) \\
P a_{i} \sim N\left(\mu_{P a_{i}}, \sigma_{P a_{i}}^{2}\right) \\
L(\Theta: D)=\prod_{i} \prod_{m} P\left(x_{i}[m] \mid P a_{i}[m]: \Theta_{i}\right)=\prod_{i} L_{i}\left(\Theta_{i}: D\right) \\
L_{i}\left(\theta_{i}: D\right)=\prod_{m} P\left(x_{i}[m] \mid P a_{i}[m]: \theta_{i}\right)
\end{gathered}
$$

- The likelihood decomposes $\Rightarrow$ Independent estimation problems The MLE is

$$
X_{i} \mid P a_{i} \sim N\left(a \cdot p a_{i}+b, \sigma^{2}\right)
$$

## Statistical background - regression

Assume $Y=a X+b+Z$, where $Z \sim N\left(0, \sigma_{z}^{2}\right), \quad \operatorname{Ind}(\mathrm{X}, \mathrm{Z})$.
$\sigma_{x}^{2}, \mu_{x}$ are population variance and mean of X.
Thus:

1. $\mu_{y}=a \mu_{x}+b$
2. $Y \mid X \sim N\left(a X+b, \sigma_{z}^{2}\right)$.

Using least - squares estimation of a and b :
$\hat{a}, \hat{b}=\arg \min \sum_{i}\left(y_{i}-\left(a x_{i}+b\right)\right)^{2}$
Solving max likelihood estimation of $\mathrm{Y} \mid \mathrm{X}$ :
$\hat{a}, \hat{b}=\arg \max \log \mathrm{L}(\mathrm{Y} \mid \mathrm{X})$

$$
\begin{aligned}
& =\arg \max \frac{n}{2} \ln \frac{1}{2 \pi \sigma^{2}}-\sum_{i}\left(y_{i}-\left(a x_{i}+b\right)\right)^{2} / 2 \sigma^{2} \\
& =\arg \min \sum_{i}\left(y_{i}-\left(a x_{i}+b\right)\right)^{2}
\end{aligned}
$$

## Statistical background - regression

$\hat{a}, \hat{b}=\arg \min \sum_{i}\left(y_{i}-\left(a x_{i}+b\right)\right)^{2}$
$\hat{a}=\frac{\operatorname{cov}(X, Y)}{\sigma_{x}^{2}}=\frac{\rho_{x y} \sigma_{x} \sigma_{y}}{\sigma_{x}^{2}}=\frac{\rho_{x y} \sigma_{y}}{\sigma_{x}}$
$\hat{b}=\mathrm{E}(\mathrm{Y})-\hat{a} \mathrm{E}(\mathrm{X})=\mu_{y}-\hat{a} \mu_{x}$

Express YIX using population parameters $\mu_{y} \mu_{x} \sigma_{y}^{2} \sigma_{x}^{2} \rho_{x y}$
$\mathrm{E}(Y \mid X)=\hat{a} X+\hat{b}=\hat{a} X+\mu_{y}-\hat{a} \mu_{x}=\mu_{y}+\hat{a}\left(X-\mu_{x}\right)=\mu_{y}+\frac{\rho_{x y} \sigma_{y}}{\sigma_{x}}\left(X-\mu_{x}\right)$
$\operatorname{Var}(Y \mid X)=\ldots=\sigma_{y}^{2}\left(1-\rho_{x y}^{2}\right)$

## Continuous (Gaussian) variables

$$
X \sim N\left(\mu, \sigma_{X}^{2}\right) ญ \rightarrow Y \mid X \sim N\left(a x+b, \sigma^{2}\right)
$$

$$
\begin{aligned}
& \mathrm{E}(Y \mid X)=\mu_{y}+\frac{\rho_{x y} \sigma_{y}}{\sigma_{x}}\left(X-\mu_{x}\right) \\
& \operatorname{Var}(Y \mid X)=\sigma_{y}^{2}\left(1-\rho_{x y}^{2}\right)
\end{aligned}
$$

$$
P a_{i} \sim N\left(\mu_{P a_{i}}, \sigma_{P a_{i}}^{2}\right) \text { 人ai } \rightarrow X_{i} \mid P a_{i} \sim N\left(a \cdot p a_{i}+b, \sigma^{2}\right)
$$

$$
\begin{aligned}
& \mathrm{E}\left(X_{i} \mid P a_{i}\right)=\mu_{X_{i}}+\frac{\rho_{P a_{i} X_{i}}}{\sigma_{X_{X_{i}}}}\left(P a_{i}-\mu_{P a_{i}}\right) \\
& \operatorname{Var}\left(X_{i} \mid P a_{i}\right)=\sigma_{X_{i}}^{2}\left(1-\rho_{P a_{i} X_{i}}^{2}\right)
\end{aligned}
$$

## Learning Parameters

-Key concept: the likelihood function

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

- measures how the probability of the data changes when we change parameters
-Estimation:
- MLE: choose parameters that maximize likelihood
- Bayesian: treat parameters as an unknown quantity, and marginalize over it


## The Bayesian Approach to learning

- Find the posterior!

$$
\begin{aligned}
& P(X[M+1]=H \mid D)=\int P(X[M+1]=H \mid \theta, D) P(\theta \mid D) d \theta= \\
& =\int P(X[M+1]=H \mid \theta) P(\theta \mid D) d \theta= \\
& \int P(X[M+1]=H \mid \theta) \frac{P(\theta) P(D \mid \theta)}{P(D)} d \theta= \\
& \frac{\int P(X[M+1]=H \mid \theta) P(\theta) P(D \mid \theta) d \theta}{\int P(\theta) P(D \mid \theta) d \theta}= \\
& \frac{\int \theta P(\theta) P(D \mid \theta) d \theta}{\int P(\theta) P(D \mid \theta) d \theta}
\end{aligned}
$$

## Bayesian approach for Binomial Data

$-\mathrm{P}(\mathrm{H})=\theta$.

- Prior: uniform for $\theta$ in $[0,1]$. (therefore, $P(\theta)=1$ )
- Data: $\left(N_{H}, N_{T}\right)=(4,1)$
- MLE for $P(X=H)$ is $N_{H}\left(N_{H+} N_{T}\right)=4 / 5=0.8$
- Bayesian prediction is:


$$
\begin{aligned}
& P(x[M+1]=H \mid D)=\frac{\int \theta P(\theta) P(D \mid \theta) d \theta}{\int P(\theta) P(D \mid \theta) d \theta}= \\
& \frac{\int \theta \cdot 1 \cdot \theta^{N_{H}}(1-\theta)^{N_{T}} d \theta}{\int 1 \cdot \theta^{N_{H}}(1-\theta)^{N_{T}} d \theta}=\cdots=\frac{5}{7}=0.7142 \ldots
\end{aligned}
$$

## Bayesian approach for Multinomial Data

- Recall that the likelihood function is

$$
L(\Theta: D)=\prod_{k=1}^{K} \theta_{k}^{N_{k}}
$$

$\bullet$ Dirichlet prior with hyperparameters $\alpha_{1}, \ldots, \alpha_{K}$

$$
P(\Theta)=\frac{\left(\sum_{j=1}^{k} \alpha_{j}-1\right)!}{\left(\alpha_{1}-1\right)!\left(\alpha_{2}-1\right)!\ldots .\left(\alpha_{k}-1\right)!} \prod_{k=1}^{K} \theta_{k}^{\alpha_{k}-1}
$$

$\Rightarrow$ the posterior: Dirichlet with hyperparameters $\alpha_{1}+N_{1, \ldots, \alpha_{K}}+N_{K}$

$$
\begin{aligned}
& P(\Theta \mid D)=\frac{P(\Theta) P(D \mid \Theta)}{P(D)}=\frac{c(\alpha)}{P(D)} \prod_{k=1}^{K} \theta_{k}^{\alpha_{k}-1} \prod_{k=1}^{K} \theta_{k}^{N_{k}}= \\
& \frac{\left(\sum_{j=1}^{k} \alpha_{j}+N_{j}-1\right)!}{\left(\alpha_{1}+N_{1}-1\right)!\left(\alpha_{2}+N_{2}-1\right)!\ldots .\left(\alpha_{k}+N_{k}-1\right)!} \prod_{k=1}^{K} \theta_{k}^{\alpha_{k}+N_{k}-1}
\end{aligned}
$$

## Bayesian approach for Multinomial Data

- If $P(\Theta)$ is Dirichlet with hyperparameters $\alpha_{1}, \ldots, \alpha_{K}$
- The posterior is also Dirichlet:
$P(\Theta / D)$ is Dirichlet with hyperparameters $\alpha_{1}+N_{1} \ldots, \alpha_{K}+N_{k}$ and thus we get

$$
P(X[M+1]=k \mid D)=\int \theta_{k} \cdot P(\theta \mid D) d \theta=\frac{\alpha_{k}+N_{k}}{\sum_{\ell}\left(\alpha_{\ell}+N_{\ell}\right)}
$$

## Learning Parameters for Bayesian networks : Summary

- For multinomials: counts $N\left(x_{i,}, p a_{i}\right)$
- Parameter estimation

$$
\begin{gathered}
\hat{\theta}_{x_{i} \mid p a_{i}}=\frac{N\left(x_{i}, p a_{i}\right)}{N\left(p a_{i}\right)} \\
\text { MLE }
\end{gathered} \quad \tilde{\theta}_{x_{i} \mid p a_{i}}=\frac{\alpha\left(x_{i}, p a_{i}\right)+N\left(x_{i}, p a_{i}\right)}{\alpha\left(p a_{i}\right)+N\left(p a_{i}\right)}
$$

- Both can be implemented in an on-line manner by accumulating counts.


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## Learning Structure: Motivation



Adding an arc


Missing an arc


## Optimization Problem

## Input:

- Training data
- Scoring function (including priors)
- Set of possible structures


## Output:

- A network (or networks) that maximize the score

Key Property:

- Decomposability: the score of a network is a sum of terms.


## Scores

For example. The BDE score:

$$
\begin{aligned}
\operatorname{Score}(G & : D)=P(G \mid D) \propto P(D \mid G) P(G) \\
& =\int P(D \mid G, \theta) P(\theta \mid G) d \theta P(G)
\end{aligned}
$$

When the data is complete, the score is decomposable:

$$
\operatorname{Score}(G: D)=\sum_{i} \operatorname{Score}\left(X_{i} \mid P a_{i}^{G}: D\right)
$$

## Heuristic Search (cont.)

-Typical operations:


## Heuristic Search

-We address the problem by using heuristic search

- Traverse the space of possible networks, looking for high-scoring structures
-Search techniques:
- Greedy hill-climbing
- Simulated Annealing
- ...


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- Representation \& Semantics
- Inference in Bayesian networks
- Learning Bayesian networks
- Conclusion
- Applications

