Exploiting Structure in Probability Distributions

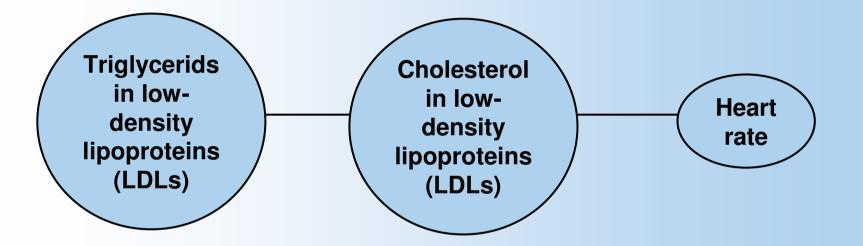
Irit Gat-Viks

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

General References:

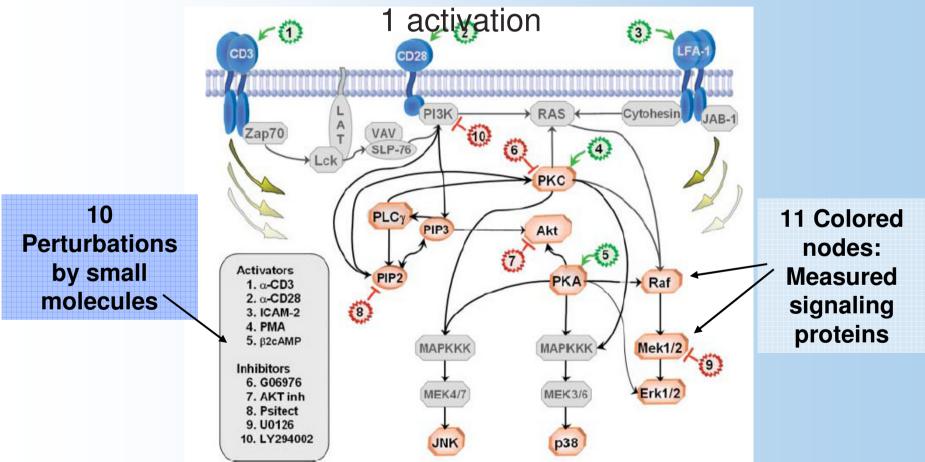
- D. Koller and N. Friedman, probabilistic graphical models
- Pearl, Probabilistic Reasoning in Intelligent Systems
- Jensen, An Introduction to Bayesian Networks
- Heckerman, A tutorial on learning with Bayesian networks



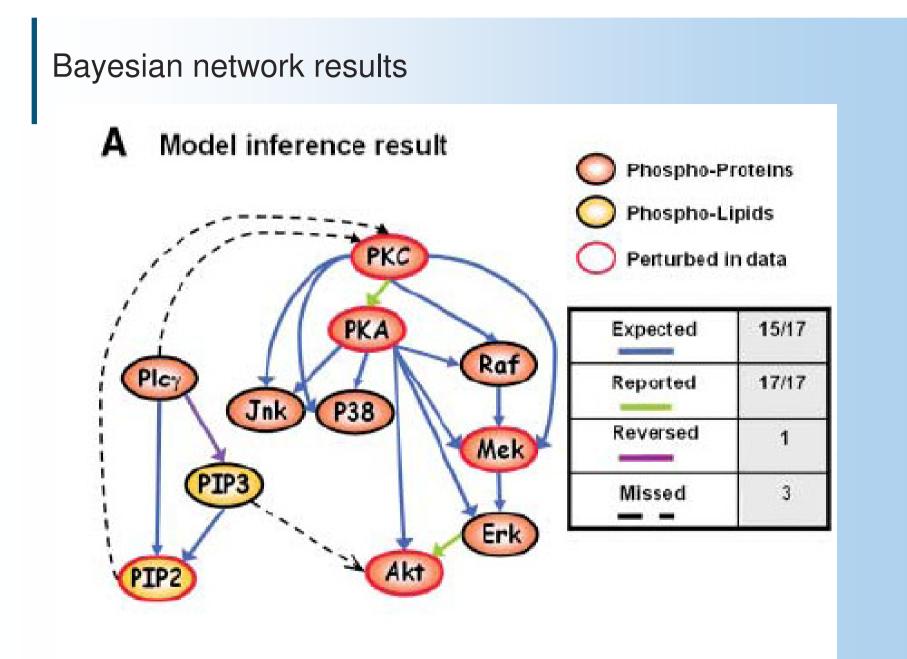


Example II

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

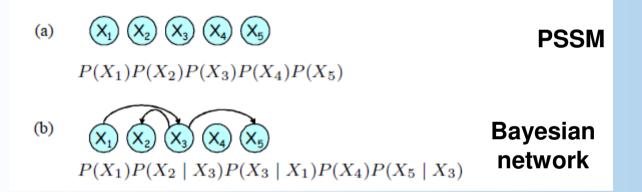


Causal Protein-Signaling Networks Derived from Multiparameter Single-Cell Data. Karen Sachs, et al. 2005.

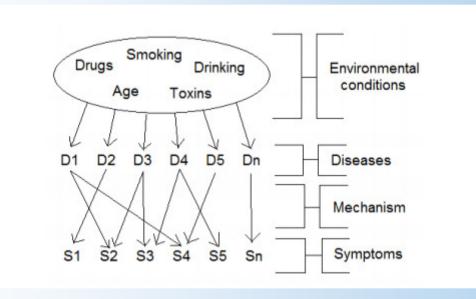


- PKC->PKA was validated experimentally.
- Akt was not affected by Erk in additional experiments

Example III: Bayesian network models for a transcription factor-DNA binding motif with 5 positions



Example IV: Diagnostic Bayesian network model



Basic Probability Definitions

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

$$P(A) = \sum_{i=1}^{n} P(A, B_i) = \sum_{i=1}^{n} P(B_i) * P(A | B_i)$$

Basic Probability Definitions

◆Bayes Rule:

 $P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)}$

$$P(A \mid B, C) = \frac{P(B \mid A, C) \cdot P(A \mid C)}{P(B \mid C)}$$

Chain Rule:

 $P(X_1, ..., X_n) =$ $P(X_1 | X_2, ..., X_n) \cdot P(X_2 | X_3, ..., X_n) \cdot P(X_3 | X_4, ..., X_n) \cdot ... P(X_{n-1} | X_n) \cdot P(X_n)$

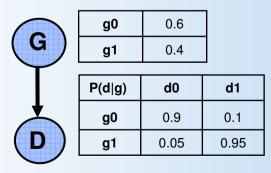
Exploiting Independence Property

G: whether the woman is pregnant
D: whether the doctor's test is positive
<u>The joint distribution representation P(g,d)</u>:

G	D	P(G,D)
0	0	0.54
0	1	0.06
1	0	0.02
1	1	0.38

Factorial representation

Using conditional probability: $P(g,d)=P(g)^*P(d|g)$. The distribution of P(g), P(d|g):

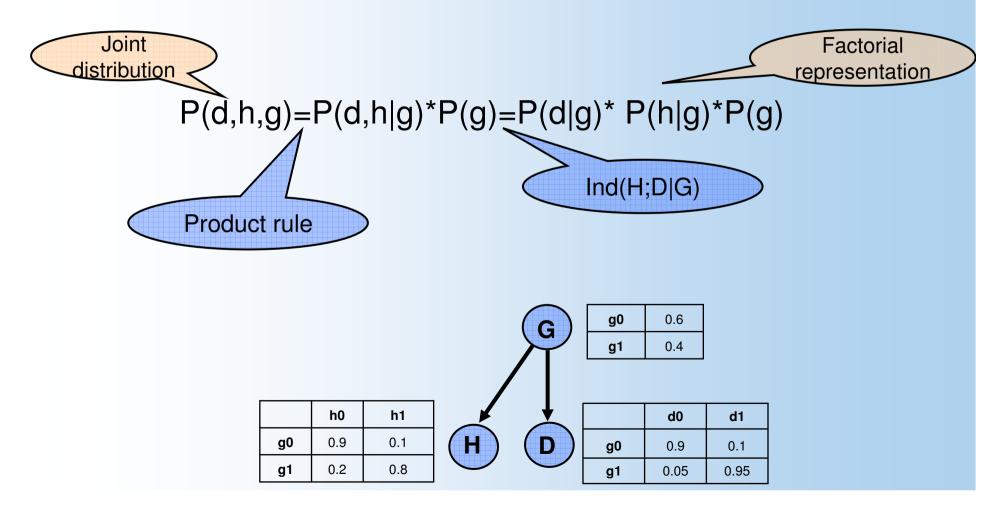


Example: P(g0,d1)=0.06 vs. P(g0)*P(d1|g0)=0.6*0.1=0.06

Exploiting Independence Property

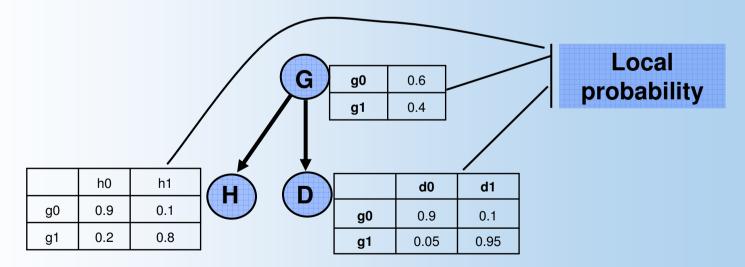
♦H: home test

◆Independence assumption: Ind(H;D|G) (i.e., given G, H is independent of D).



Exploiting Independence Property

	representation of P(d,g,h)		
	joint distribution	factored distribution	
No. of parameters	7	5	
Adding new variable H	changing the distribution entirely	Modularity : reuse the local probability model. (Only new 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 25=32 parameters

maybe...

Radio

Burglar

Alarm

Call

- An expert system for monitoring intensive care patients
 - Specify joint distribution over 37 variables with (at least) 2³⁷ parameters

no way!!!

Probabilistic Independence: a Key for Representation and Reasoning

• Recall that if X and Y are **independent** given Z then P(X | Z, Y) = P(X | 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

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

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

Need a language to represent independence statements

Markov Assumption

Y₁

Descendent

Y₂

X

Ancestor

Parent

Non-descendent

Descendent

Generalizing:

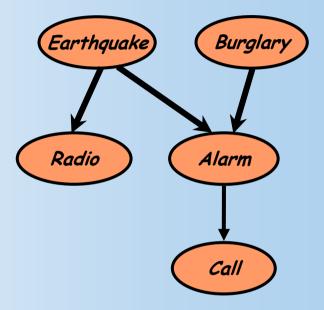
A child is conditionally independent from its non-descendents, given the value of its parents.

Ind(Xi; NonDescendantXi | PaXi

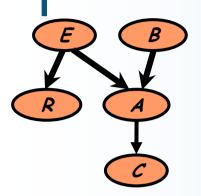
It is a natural assumption for many causal processes

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, linear Gaussian)

Unique joint distribution over domain

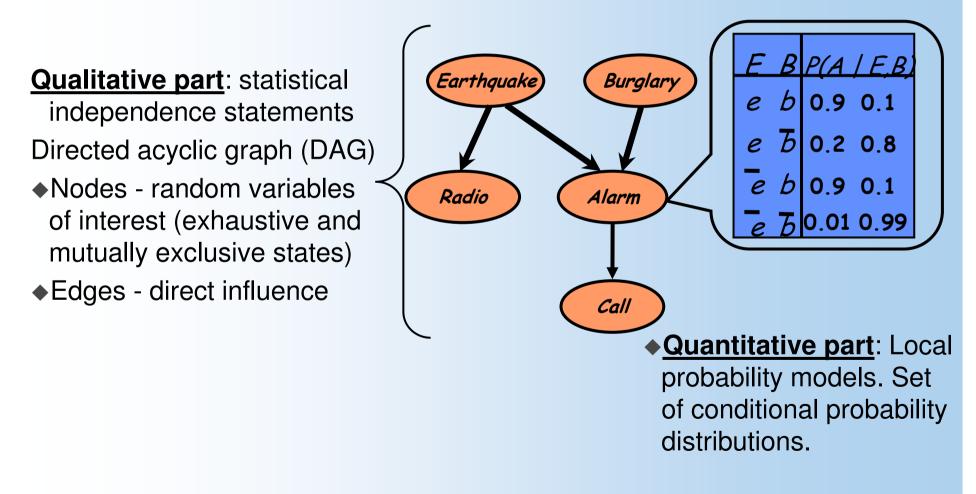
Compact & efficient representation:

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

P(C,A,R,E,B) = P(B)*P(E|B)*P(R|E,B)*P(A|R,B,E)*P(C|A,R,B,E) versus P(C,A,R,E,B) = P(B)*P(E) * P(R|E) * P(A|B,E) * P(C|A) → In general: $P(x_1,...,x_n) = \prod_{i=1,...,n} P(x_i | Pa_{x_i})$

Bayesian networks

Efficient representation of probability distributions via conditional independence



Outline

Introduction

Bayesian Networks

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- Learning Bayesian networks

Inference in Bayesian networks

- A Bayesian network represents a probability distribution.
- Can we answer queries about this distribution?

Examples:

- P(Y|Z=z)
- •Most probable estimation $MPE(W | Z = z) = \arg \max_{w} P(w, z)$
- •Maximum a posteriori $MAP(Y | Z = z) = \arg \max_{y} P(y | z)$

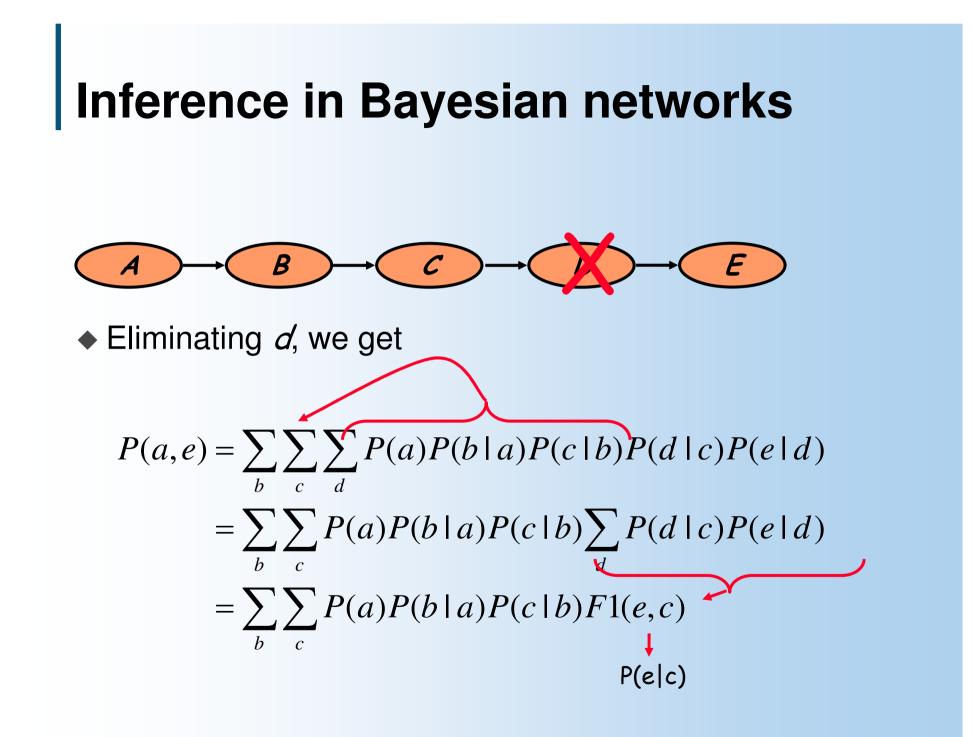
Inference in Bayesian networks

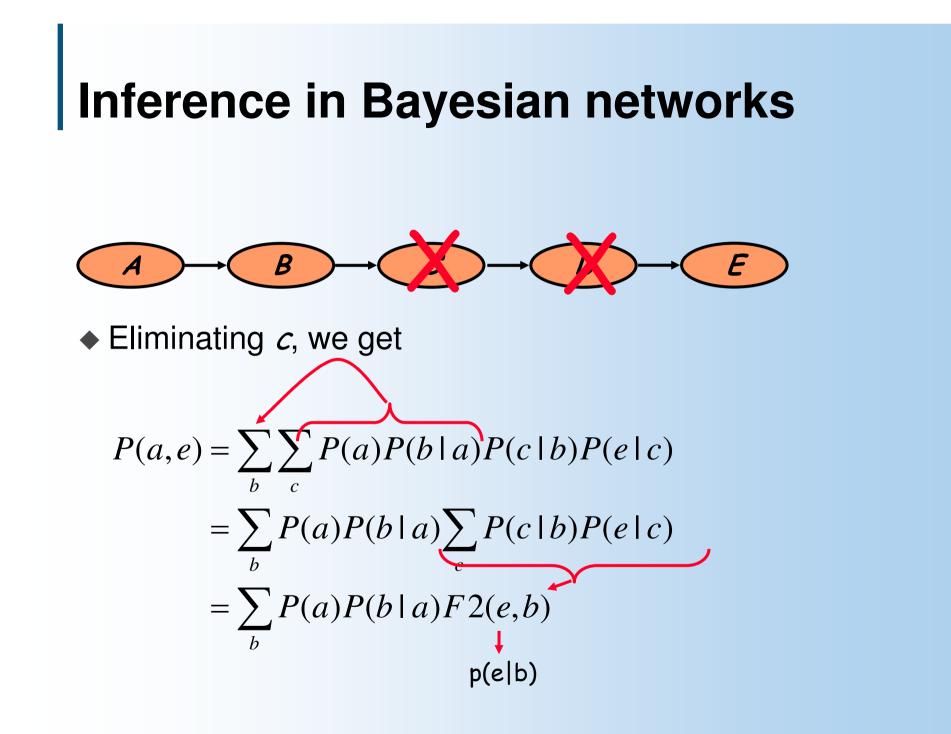
♦ Goal: compute P(E=e,A=a) in the following Bayesian network:



Using definition of probability, we have

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





Inference in Bayesian networks



◆ Finally, we eliminate *b*

$$P(a,e) = \sum_{b} P(a)P(b \mid a) p(e \mid b)$$

= $P(a)\sum_{b} P(b \mid a) p(e \mid b)$
= $P(a)F3(e,a)$
(e|a)

Variable Elimination Algorithm

General idea:

Write query in the form

$$P(x_1) = \sum_{x_k} \cdots \sum_{x_3} \sum_{x_2} \prod_i P(x_i \mid pa_i)$$

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 $P(x_1 | \text{evidence } x_j)$, use: $P(x_i | x_j) = P(x_i, x_j) / P(x_j)$

Complexity of inference

Naïve exact inference

exponential in the number of variables in the network <u>Variable elimination complexity</u>

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).

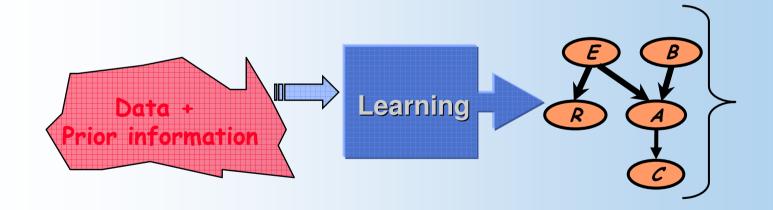
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 - Structure Learning

Learning

Process

- Input: <u>dataset</u> and <u>prior information</u>
- Output: <u>Bayesian</u> <u>network</u>



The Learning Problem

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

•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

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

m

 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

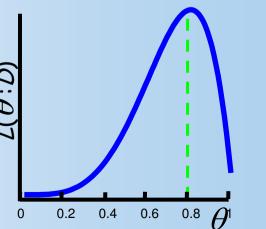
MLE principle for Binomial Data

• Data: *H*, *H*, *T*, *H*, *H*. Θ 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]...x[M], we want to estimate the probability P(H)= θ and P(T)=1-θ.
- MLE principle: choose parameter that maximize the likelihood function.
- Applying the MLE principle we get

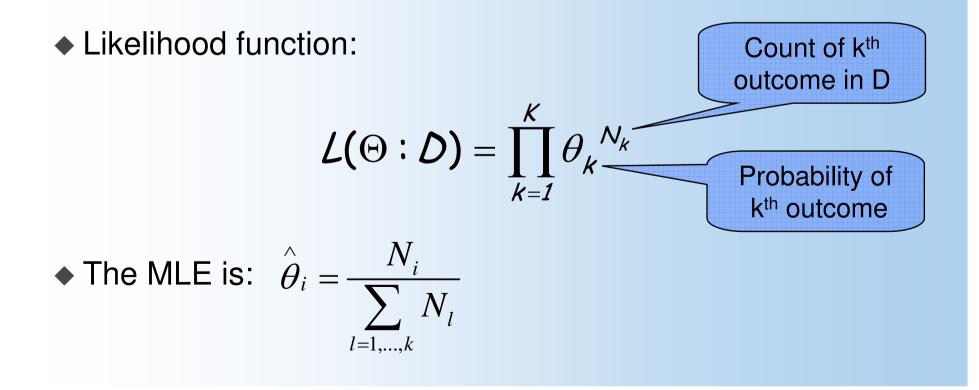
$$\hat{\theta} = \frac{N_H}{N_H + N_T}$$

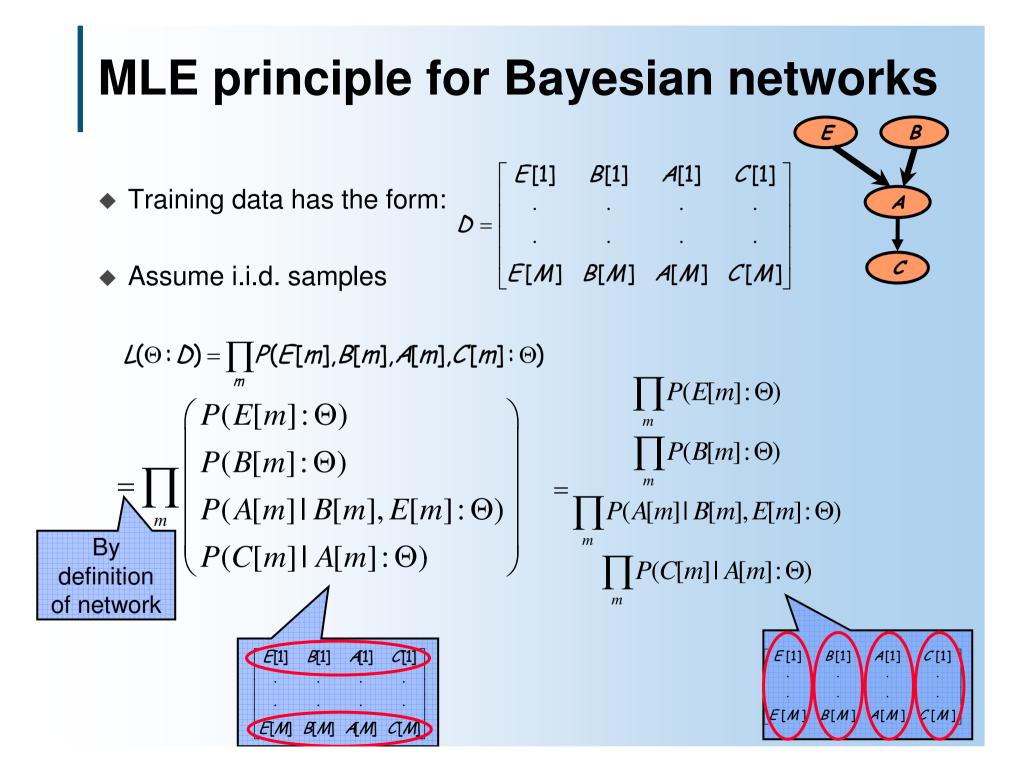
•MLE for P(X = H) is 4/5 = 0.8



MLE principle for Multinomial Data

- Suppose X can have the values 1,2,...,k.
- We want to learn the parameters $\theta_1, \ldots, \theta_{k}$.
- N₁,...,N_k The number of times each outcome is observed.





MLE principle for Bayesian networks

• Generalizing for any Bayesian network: $L(\Theta:D) = \prod_{i} \prod_{m} P(x_{i}[m] | Pa_{i}[m]:\Theta_{i}) = \prod_{i} L_{i}(\Theta_{i}:D)$

$$L_{i}(\theta_{i}:D) = \prod_{m} P(x_{i}[m] | Pa_{i}[m]:\theta_{i})$$
$$= \prod_{pa_{i}} \prod_{x_{i}} P(x_{i} | pa_{i}:\theta_{i})^{N(x_{i,pa_{i}})} = \prod_{pa_{i}} \prod_{x_{i}} \theta_{x_{i}|pa_{i}}^{N(x_{i,pa_{i}})}$$

- The likelihood decomposes according to the network structure.
- Decomposition ⇒ 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
$$\hat{\theta}_{x_i|pa_i} = \frac{N(x_i, pa_i)}{N(pa_i)}$$

Continuous (Gaussian) variables

Discrete X

$$X \rightarrow Y Y | X \sim N(\mu, \sigma^2)$$

 $L(\Theta:D) = \prod_{i} \prod_{m} P(x_{i}[m] | Pa_{i}[m]:\Theta_{i}) = \prod_{i} L_{i}(\Theta_{i}:D)$

 $L_i(\theta_i:D) = \prod_m P(x_i[m] | Pa_i[m]:\theta_i)$

$$X_i \mid Pa_i \sim N(\mu_{i,Pa_i}, \sigma^{2}_{i,Pa_i})$$

- The likelihood decomposes according to the network structure.
- Decomposition ⇒ 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

$$\hat{\sigma}_{i,Pa_{i}}^{n} = \frac{\sum_{m:Pa_{i}[m]=pa_{i}} x_{i}[m]}{N(pa_{i})}$$

$$\hat{\sigma}_{i,Pa_{i}}^{2} = \frac{\sum_{m:Pa_{i}[m]=pa_{i}} (x_{i}[m] - \mu_{i,Pa_{i}}^{n})^{2}}{N(pa_{i})}$$

Continuous (Gaussian) variables $X \sim N(\mu, \sigma_X^2)$ $X \rightarrow Y$ $Y \mid X \sim N(ax+b, \sigma^2)$ $Pa_i \sim N(\mu_{Pa_i}, \sigma_{Pa_i}^2)$ $A \rightarrow X_i \mid Pa_i \sim N(a \cdot pa_i + b, \sigma^2)$

$$L(\Theta:D) = \prod_{i} \prod_{m} P(x_{i}[m] | Pa_{i}[m]:\Theta_{i}) = \prod_{i} L_{i}(\Theta_{i}:D)$$

$$L_i(\theta_i:D) = \prod_m P(x_i[m] | Pa_i[m]:\theta_i)$$

 The likelihood decomposes ⇒ Independent estimation problems The MLE is

$$X_i \mid Pa_i \sim N(a \cdot pa_i + b, \sigma^2)$$

Statistical background - regression

Assume Y = aX + b + Z, where $Z \sim N(0, \sigma_z^2)$, Ind(X,Z). σ_x^2, μ_x are population variance and mean of X. Thus: 1. $\mu_y = a\mu_x + b$

2. $Y \mid X \sim N(aX + b, \sigma_z^2)$.

Using least - squares estimation of a and b :

$$\hat{a}, \hat{b} = \arg\min\sum_{i} (y_i - (ax_i + b))^2$$

Solving max likelihood estimation of Y | X :

 $\hat{a}, \hat{b} = \arg \max \log L(Y | X)$ = $\arg \max \frac{n}{2} \ln \frac{1}{2\pi\sigma^2} - \sum_i (y_i - (ax_i + b))^2 / 2\sigma^2$ = $\arg \min \sum_i (y_i - (ax_i + b))^2$

Statistical background - regression

$$\hat{a}, \hat{b} = \arg\min\sum_{i} (y_i - (ax_i + b))^2$$
$$\hat{a} = \frac{\cos(X, Y)}{\sigma_x^2} = \frac{\rho_{xy}\sigma_x\sigma_y}{\sigma_x^2} = \frac{\rho_{xy}\sigma_y}{\sigma_x}$$
$$\hat{b} = E(Y) - \hat{a}E(X) = \mu_y - \hat{a}\mu_x$$

Express Y | X using population parameters $\mu_y \mu_x \sigma_y^2 \sigma_x^2 \rho_{xy}$

$$E(Y \mid X) = \hat{a} X + \hat{b} = \hat{a} X + \mu_{y} - \hat{a} \mu_{x} = \mu_{y} + \hat{a}(X - \mu_{x}) = \mu_{y} + \frac{\rho_{xy}\sigma_{y}}{\sigma_{x}}(X - \mu_{x})$$
$$Var(Y \mid X) = \dots = \sigma_{y}^{2}(1 - \rho_{xy}^{2})$$

Continuous (Gaussian) variables $X \sim N(\mu, \sigma_X^2)$ $X \rightarrow Y$ $Y \mid X \sim N(ax+b, \sigma^2)$

 $E(Y \mid X) = \mu_{y} + \frac{\rho_{xy}\sigma_{y}}{\sigma_{x}}(X - \mu_{x})$ $Var(Y \mid X) = \sigma_{y}^{2}(1 - \rho_{xy}^{2})$

$$Pa_i \sim N(\mu_{Pa_i}, \sigma_{Pa_i}^2)$$
 $(a \cdot pa_i \rightarrow X_i) X_i \mid Pa_i \sim N(a \cdot pa_i + b, \sigma^2)$

$$E(X_{i} | Pa_{i}) = \mu_{X_{i}} + \frac{\rho_{Pa_{i}X_{i}}\sigma_{X_{i}}}{\sigma_{Pa_{i}}}(Pa_{i} - \mu_{Pa_{i}})$$
$$Var(X_{i} | Pa_{i}) = \sigma_{X_{i}}^{2}(1 - \rho_{Pa_{i}X_{i}}^{2})$$

Learning Parameters

Key concept: the likelihood function

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

m

 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!

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

Bayesian approach for Binomial Data

♦ P(H)= *θ*.

• **<u>Prior</u>**: uniform for θ in [0,1]. (therefore, P(θ)=1)

- MLE for P(X = H) is $N_{H'}(N_{H+}N_{T})=4/5 = 0.8$
- Bayesian prediction is:

$$P(x[M+1] = H \mid D) = \frac{\int \theta P(\theta) P(D \mid \theta) d\theta}{\int P(\theta) P(D \mid \theta) d\theta} = \frac{\int \theta (\theta) P(D \mid \theta) d\theta}{\int \theta (1 - \theta)^{N_T} d\theta} = \dots = \frac{5}{7} = 0.7142\dots$$

0.2

0

0.4

0.6

0.8

Bayesian approach for Multinomial Data

Recall that the likelihood function is

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

• **Dirichlet prior** with hyperparameters $\alpha_1, \ldots, \alpha_K$

$$P(\Theta) = \frac{(\sum_{j=1}^{k} \alpha_j - 1)!}{(\alpha_1 - 1)!(\alpha_2 - 1)!\dots(\alpha_k - 1)!} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1}$$

 \Rightarrow the posterior: **Dirichlet** with hyperparameters $\alpha_1 + N_1, \dots, \alpha_K + N_K$

$$P(\Theta \mid D) = \frac{P(\Theta)P(D \mid \Theta)}{P(D)} = \frac{c(\alpha)}{P(D)} \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} \prod_{k=1}^{K} \theta_k^{N_k} = \frac{\sum_{j=1}^{k} \alpha_j + N_j - 1}{(\alpha_1 + N_1 - 1)!(\alpha_2 + N_2 - 1)!\dots(\alpha_k + N_k - 1)!} \prod_{k=1}^{K} \theta_k^{\alpha_k + N_k - 1}$$

Bayesian approach for Multinomial Data

• If $P(\Theta)$ is Dirichlet with hyperparameters $\alpha_1, \ldots, \alpha_K$

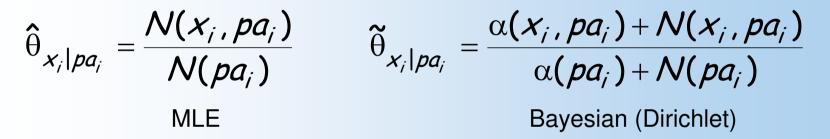
The posterior is also Dirichlet:

 $P(\Theta|D)$ is Dirichlet with hyperparameters $\alpha_1 + N_1 \dots, \alpha_k + N_k$ and thus we get

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

Learning Parameters for Bayesian networks : Summary

- For multinomials: counts N(x_i, pa_i)
- Parameter estimation

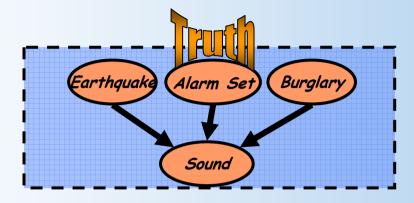


 Both can be implemented in an on-line manner by accumulating counts.

Outline

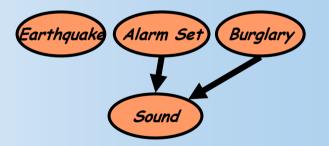
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Learning Structure: Motivation



Adding an arc

Earthquake Alarm Set Burglary Sound 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

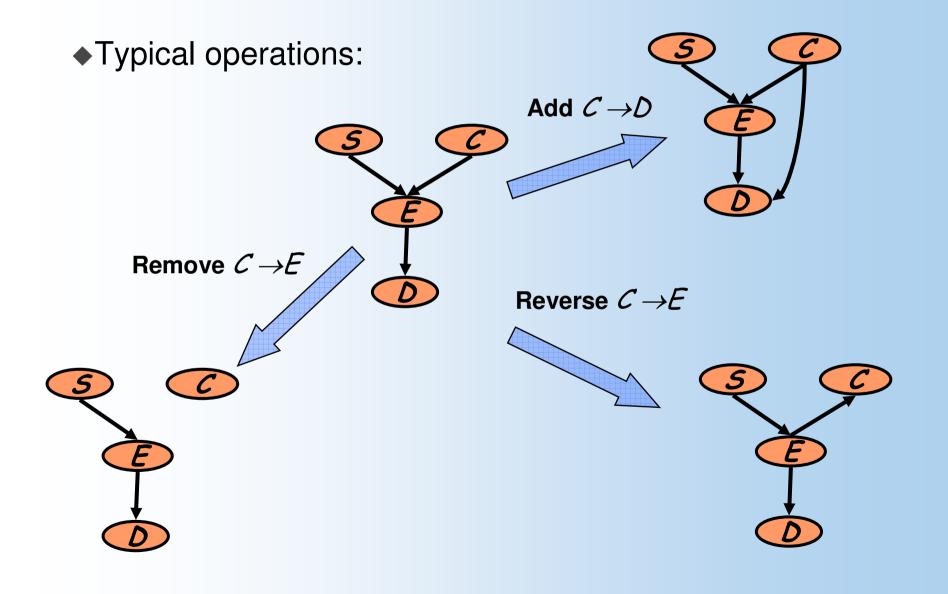
For example. The BDE score:

$$Score(G:D) = P(G \mid D) \propto P(D \mid G)P(G)$$
$$= \int P(D \mid G, \theta)P(\theta \mid G)d\theta P(G)$$

When the data is complete, the score is **decomposable**:

$$Score(G:D) = \sum_{i} Score(X_{i} | Pa_{i}^{G}:D)$$

Heuristic Search (cont.)



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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Introduction

Bayesian Networks

- Representation & Semantics
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- Conclusion

Applications