CMSC828G Principles of Data Mining Lecture #15

- Readings:
  - handouts
- Today's Lecture:
  - Inference
  - Learning BNs
  - slides courtesy of Nir Friedman
- Upcoming Dates:
  - Midterm Thursday

Inference in Bayesian Networks

Variable Elimination

General idea:

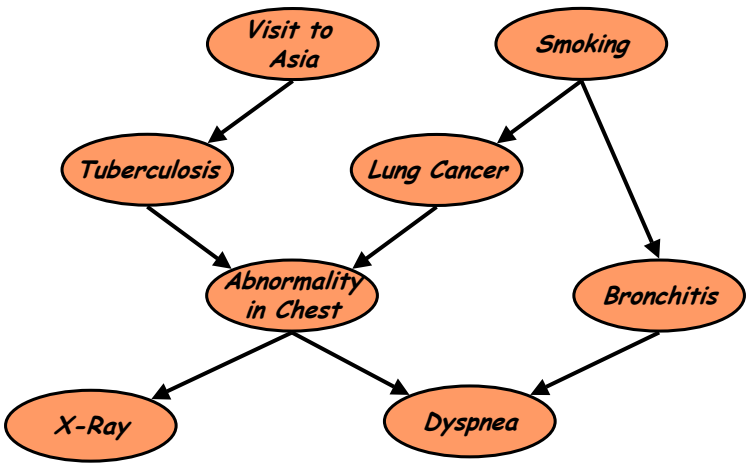
- Write query in the form

$$P(X_n, \boldsymbol{e}) = \sum_{x_k} \cdots \sum_{x_3} \sum_{x_2} \prod_i P(x_i \mid pa_i)$$

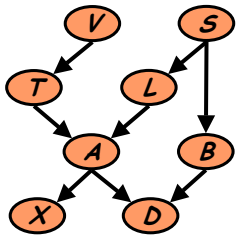
- Iteratively
  - Move all irrelevant terms outside of innermost sum
  - Perform innermost sum, getting a new term
  - Insert the new term into the product

A More Complex Example

- "Asia" network:



- We want to compute $P(d)$
- Need to eliminate: v,s,x,t,l,a,b



Initial factors

$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

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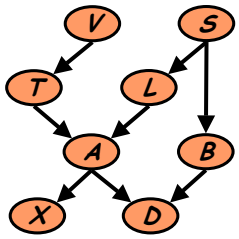


Initial factors

$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Eliminate: v

Compute: $$f_v(t) = \sum_v P(v)P(t \mid v)$$

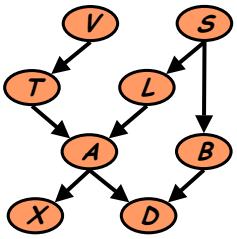
$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Note: $f_v(t) = P(t)$

In general, result of elimination is not necessarily a probability term

- We want to compute *P(d)*
- Need to eliminate: *s,x,t,l,a,b*

- Initial factors



$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$
$$\Rightarrow f_v(t)P(s)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Eliminate: *s*

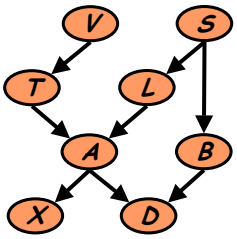
Compute: $f_s(b,l) = \sum_s P(s)P(b \mid s)P(l \mid s)$

$$\Rightarrow f_v(t)f_s(b,l)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Summing on *s* results in a factor with two arguments $f_s(b,l)$
In general, result of elimination may be a function of several variables

- We want to compute *P(d)*
- Need to eliminate: *x,t,l,a,b*

- Initial factors



$$P(v)P(s)P(t \mid v)P(l \mid s)P(b \mid s)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$
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$$\Rightarrow f_v(t)f_s(b,l)P(a \mid t,l)P(x \mid a)P(d \mid a,b)$$

Eliminate: *x*

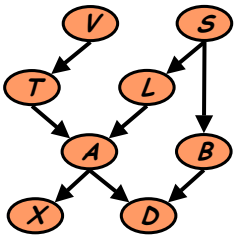
Compute: $f_x(a) = \sum_x P(x \mid a)$

$$\Rightarrow f_v(t)f_s(b,l)f_x(a)P(a \mid t,l)P(d \mid a,b)$$

Note: $f_x(a) = 1$ for all values of *a* !!

- We want to compute $P(d)$
- Need to eliminate: t,l,a,b

- Initial factors



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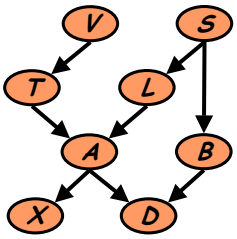
Eliminate: t

Compute: $f_t(a,l) = \sum_t f_v(t)P(a \mid t,l)$

$$\Rightarrow f_s(b,l)f_x(a)f_t(a,l)P(d \mid a,b)$$

- We want to compute $P(d)$
- Need to eliminate: l,a,b

- Initial factors



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$$\Rightarrow f_s(b,l)f_x(a)f_t(a,l)P(d \mid a,b)$$

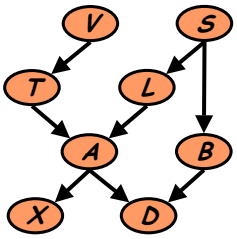
Eliminate: l

Compute: $f_l(a,b) = \sum_l f_s(b,l)f_t(a,l)$

$$\Rightarrow f_l(a,b)f_x(a)P(d \mid a,b)$$

- We want to compute $P(d)$
- Need to eliminate: b

- Initial factors



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$$\Rightarrow f_s(b,l)f_x(a)f_t(a,l)P(d \mid a,b)$$
$$\Rightarrow \underline{f_l(a,b)f_x(a)P(d \mid a,b)} \Rightarrow \underline{f_a(b,d)} \Rightarrow \underline{f_b(d)}$$

Eliminate: a,b

Compute:

$$f_a(b,d) = \sum_a f_l(a,b)f_x(a)p(d \mid a,b) \qquad f_b(d) = \sum_b f_a(b,d)$$

Variable Elimination

- We now understand variable elimination as a sequence of **rewriting** operations
- Actual computation is done in elimination step
- Exactly the same computation procedure applies to Markov networks
- Computation depends on order of elimination

Complexity of variable elimination

- Suppose in one elimination step we compute

$$f_x(y_1,\ldots,y_k) = \sum_x f'_x(x,y_1,\ldots,y_k)$$

$$f'_x(x,y_1,\ldots,y_k) = \prod_{i=1}^{m} f_i(x,y_{1,1},\ldots,y_{1,l_i})$$

This requires

- $m \cdot |\mathrm{Val}(X)| \cdot \prod_i |\mathrm{Val}(Y_i)|$ multiplications
  - For each value for $x, y_1, \ldots, y_k$, we do m multiplications
- $|\mathrm{Val}(X)| \cdot \prod_i |\mathrm{Val}(Y_i)|$ additions
  - For each value of $y_1, \ldots, y_k$, we do $|Val(X)|$ additions

Complexity is exponential in number of variables in the intermediate factor!

Understanding Variable Elimination

- We want to select "good" elimination orderings that reduce complexity
- We start by attempting to understand variable elimination via the graph we are working with
- This will reduce the problem of finding good ordering to graph-theoretic operation that is well-understood

Undirected graph representation

- At each stage of the procedure, we have an algebraic term that we need to evaluate
- In general this term is of the form:

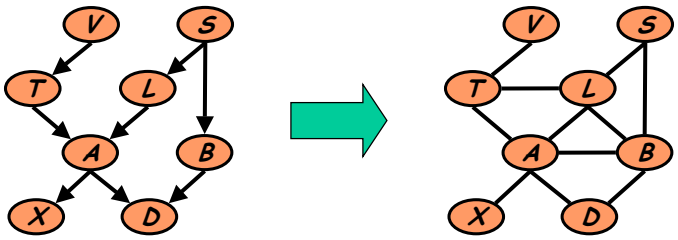
$$P(x_1,\ldots,x_k) = \sum_{y_1}\cdots\sum_{y_n}\prod_i f_i(\boldsymbol{Z}_i)$$

where $\boldsymbol{Z}_i$ are sets of variables

- We now plot a graph where there is undirected edge X--Y if X,Y are arguments of some factor
  - that is, if X,Y are in some $\boldsymbol{Z}_i$
- Note: this is the Markov network that describes the probability on the variables we did not eliminate yet

Chordal Graphs

- elimination ordering ⇒ undirected chordal graph



Graph:

- Maximal cliques are factors in elimination
- Factors in elimination are cliques in the graph
- Complexity is exponential in size of the largest clique in graph

Induced Width

- The size of the largest clique in the induced graph is thus an indicator for the complexity of variable elimination
- This quantity is called the **induced width** of a graph according to the specified ordering
- Finding a good ordering for a graph is equivalent to finding the minimal induced width of the graph

General Networks

- From graph theory:

Thm:

- Finding an ordering that minimizes the induced width is NP-Hard

However,

- There are reasonable heuristic for finding "relatively" good ordering
- There are provable approximations to the best induced width
- If the graph has a small induced width, there are algorithms that find it in polynomial time

Elimination on Trees

- Formally, for any tree, there is an elimination ordering with induced width = 1

Thm

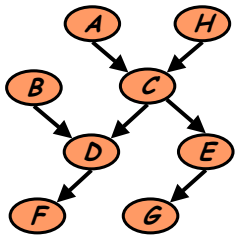
- Inference on trees is linear in number of variables

PolyTrees

- A polytree is a network where there is at most one path from one variable to another

Thm:

- Inference in a polytree is linear in the representation size of the network
  - This assumes tabular CPT representation



Approaches to inference

- Exact inference
  - Inference in Simple Chains
  - Variable elimination
  - Clustering / join tree algorithms
- **Approximate inference**
  - Stochastic simulation / sampling methods
  - Markov chain Monte Carlo methods
  - Mean field theory

Stochastic simulation

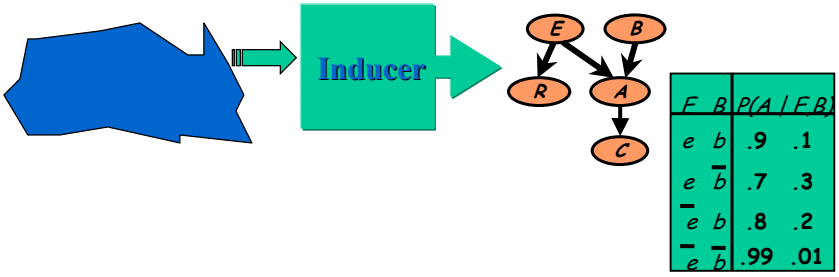
- Suppose you are given values for some subset of the variables, G, and want to infer values for unknown variables, U
- Randomly generate a very large number of instantiations from the BN
  - Generate instantiations for **all** variables – start at root variables and work your way "forward"
- Only keep those instantiations that are consistent with the values for G
- Use the frequency of values for U to get estimated probabilities
- Accuracy of the results depends on the size of the sample (asymptotically approaches exact results)

Markov chain Monte Carlo methods

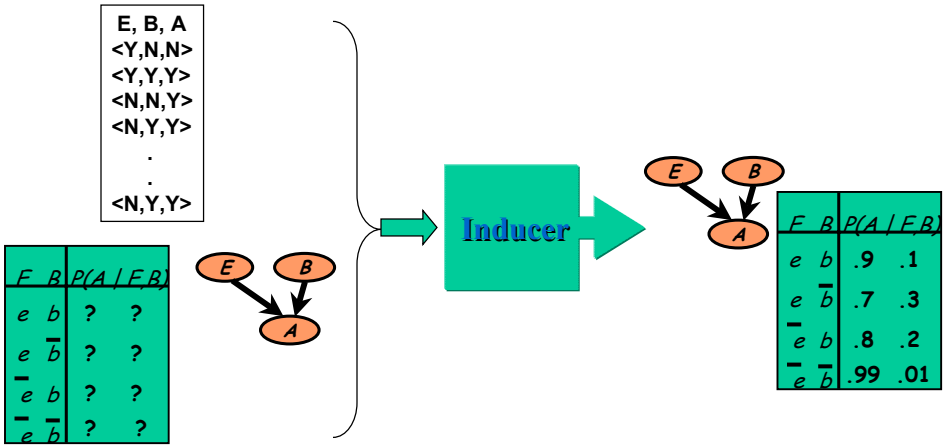
- So called because
  - Markov chain – each instance generated in the sample is dependent on the previous instance
  - Monte Carlo – statistical sampling method
- Perform a random walk through variable assignment space, collecting statistics as you go
  - Start with a random instantiation, consistent with evidence variables
  - At each step, for some nonevidence variable, randomly sample its value, consistent with the other current assignments
- Given enough samples, MCMC gives an accurate estimate of the true distribution of values

Learning Bayesian Networks

Learning Bayesian networks

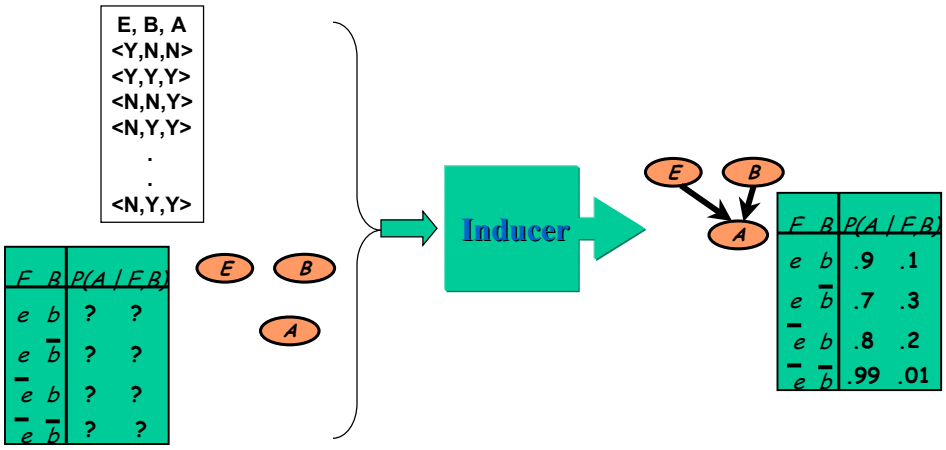


Known Structure -- Complete Data



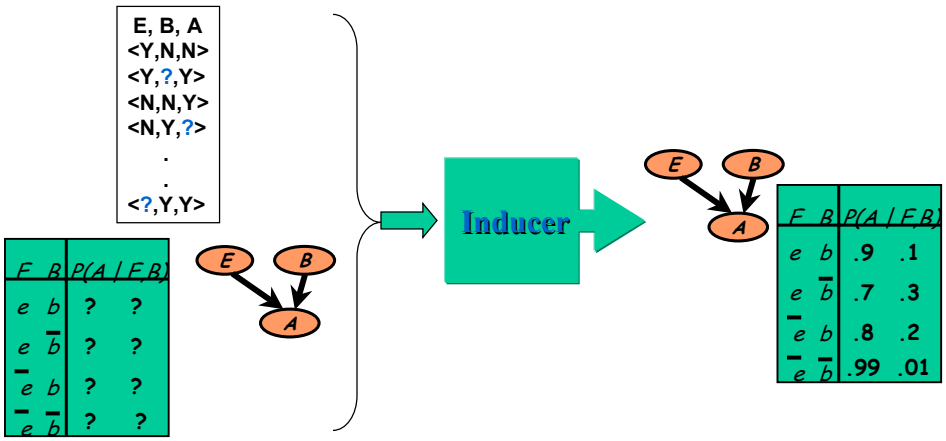
- Network structure is specified
  - Inducer needs to estimate parameters
- Data does not contain missing values

Unknown Structure -- Complete Data



- Network structure is not specified
  - Inducer needs to select arcs & estimate parameters
- Data does not contain missing values

Known Structure -- Incomplete Data



- Network structure is specified
- Data contains missing values
  - We consider assignments to missing values

Known Structure / Complete Data

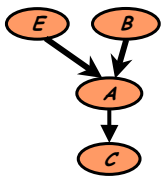
- Given a network structure G
  - And choice of parametric family for $P(X_i|Pa_i)$
- Learn parameters for network

Goal

- Construct a network that is "closest" to probability that generated the data

Learning Parameters for a Bayesian Network

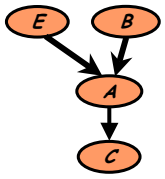
- Training data has the form:



$$D = \begin{bmatrix} E[1] & B[1] & A[1] & C[1] \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ E[M] & B[M] & A[M] & C[M] \end{bmatrix}$$

Learning Parameters for a Bayesian Network

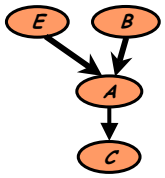
- Since we assume i.i.d. samples, likelihood function is



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

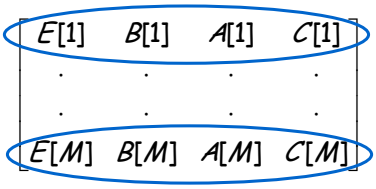
Learning Parameters for a Bayesian Network

- By definition of network, we get



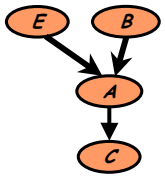
$$L(\Theta : D) = \prod_m P(E[m], B[m], A[m], C[m] : \Theta)$$

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



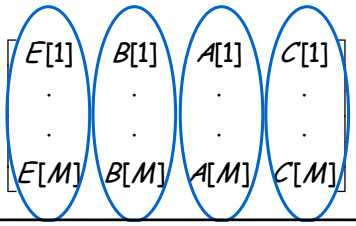
Learning Parameters for a Bayesian Network

- Rewriting terms, we get



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

$$= \prod_m P(E[m] : \Theta) \prod_m P(B[m] : \Theta) \prod_m P(A[m] \mid B[m], E[m] : \Theta) \prod_m P(C[m] \mid A[m] : \Theta)$$



General Bayesian Networks

Generalizing for any Bayesian network**:**

$$L(\Theta : D) = \prod_m P(x_1[m], \ldots, x_n[m] : \Theta)$$

i.i.d. samples

$$= \prod_m \prod_i P(x_i[m] \mid Pa_i[m] : \Theta_i)$$

Network factorization

$$= \prod_i \prod_m P(x_i[m] \mid Pa_i[m] : \Theta_i)$$

$$= \prod_i L_i(\Theta_i : D)$$

- The likelihood **decomposes** according to the structure of the network.

General Bayesian Networks (Cont.)

Decomposition

$\Rightarrow$ **Independent Estimation Problems**

If the parameters for each family are not related, then they can be estimated independently of each other.

From Binomial to Multinomial

- For example, suppose X can have the values $1,2,\ldots,K$
- We want to learn the parameters $\theta_1, \theta_2, \ldots, \theta_K$

Sufficient statistics:

- $N_1, N_2, \ldots, N_K$ - the number of times each outcome is observed

Likelihood function:

$$L(\theta : D) = \prod_{k=1}^{K} \theta_k^{N_k}$$

MLE:

$$\hat{\theta}_k = \frac{N_k}{\sum_{\ell} N_\ell}$$

Likelihood for Multinomial Networks

- When we assume that $P(X_i \mid Pa_i)$ is multinomial, we get further decomposition:

$$L_i(\Theta_i : D) = \prod_m P(x_i[m] \mid Pa_i[m] : \Theta_i)$$
$$= \prod_{pa_i} \prod_{m, Pa_i[m]=pa_i} P(x_i[m] \mid pa_i : \Theta_i)$$
$$\equiv \prod_{pa_i} \prod_{x_i} P(x_i \mid pa_i : \Theta_i)^{N(x_i, pa_i)}$$
$$= \prod_{pa_i} \prod_{x_i} \theta_{x_i \mid pa_i}^{N(x_i, pa_i)}$$

Likelihood for Multinomial Networks

- When we assume that $P(X_i \mid Pa_i)$ is multinomial, we get further decomposition:

$$L_i(\Theta_i : D) = \prod_{pa_i} \prod_{x_i} \theta_{x_i \mid pa_i}^{N(x_i, pa_i)}$$

- For each value pa_i of the parents of X_i we get an independent multinomial problem

- The MLE is

$$\hat{\theta}_{x_i \mid pa_i} = \frac{N(x_i, pa_i)}{N(pa_i)}$$

Maximum Likelihood Estimation

Consistency

- Estimate converges to best possible value as the number of examples grow
- To make this formal, we need to introduce some definitions

KL-Divergence

- Let P and Q be two distributions over X
- A measure of distance between P and Q is the Kullback-Leibler Divergence

$$KL(P \,||\, Q) = \sum_x P(x) \log \frac{P(x)}{Q(x)}$$

- $KL(P||Q) = 1$ (when logs are in base 2) =
  - The probability P assigns to an instance is, on average, half the probability Q assigns to it
- $KL(P||Q) \geq 0$
- $KL(P||Q) = 0$ iff are P and Q equal

Consistency

- Let $P(X|\theta)$ be a parametric family
  - We need to make various regularity condition we won't go into now
- Let $P^*(X)$ be the distribution that generates the data
- Let $\hat{\theta}_D$ be the MLE estimate given a dataset D

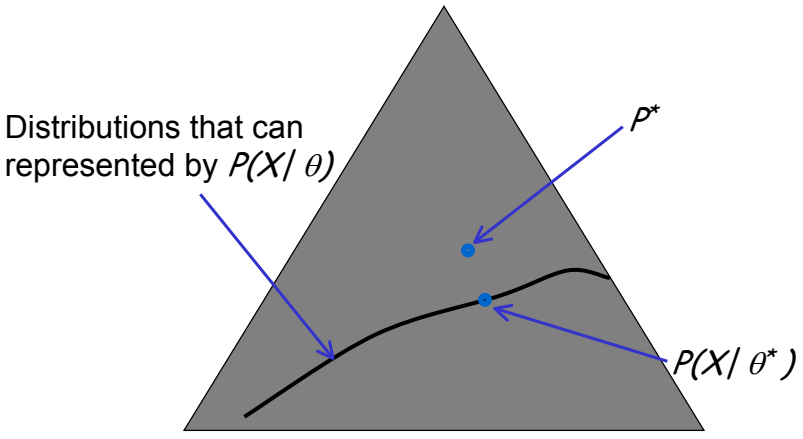
Thm

- As $N \to \infty$, $\hat{\theta}_D \to \theta^*$ where

with probability 1

$$\theta^* = \arg\min_\theta KL(P^*(X)||P(X:\theta))$$

Consistency -- Geometric Interpretation



Bayesian Inference

Frequentist Approach:

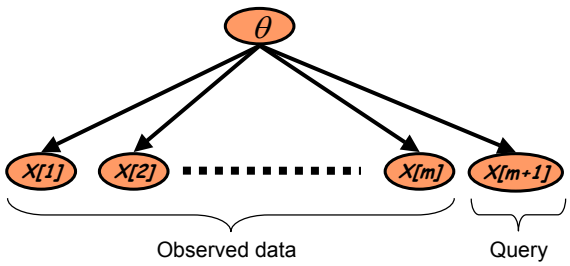
- Assumes there is an unknown but fixed parameter θ
- Estimates θ with some confidence
- Prediction by using the estimated parameter value

Bayesian Approach:

- Represents uncertainty about the unknown parameter
- Uses probability to quantify this uncertainty:
  - Unknown parameters as **random variables**
- Prediction follows from the rules of probability:
  - Expectation over the unknown parameters

Bayesian Inference (cont.)

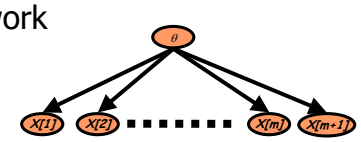
- We can represent our uncertainty about the sampling process using a Bayesian network



- The values of X are independent given θ
- The conditional probabilities, $P(x[m] \mid \theta)$, are the parameters in the model
- Prediction is now inference in this network

Bayesian Inference (cont.)

Prediction as **inference** in this network



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

where

Likelihood

Prior

$$P(\theta \mid x[1],\ldots x[M]) = \frac{P(x[1],\ldots x[M] \mid \theta) P(\theta)}{P(x[1],\ldots x[M])}$$

Posterior

Probability of data

Dirichlet Priors

- Recall that the likelihood function is $L(\Theta : D) = \prod_{k=1}^{K} \theta_k^{N_k}$
- A **Dirichlet** prior with hyperparameters $\alpha_1,\ldots,\alpha_K$ is defined as

$$P(\Theta) \propto \prod_{k=1}^{K} \theta_k^{\alpha_k - 1}$$ for legal $\theta_1,\ldots, \theta_K$

Then the posterior has the same form, with hyperparameters $\alpha_1+N_1,\ldots,\alpha_K+N_K$

$$P(\Theta \mid D) \propto P(\Theta) P(D \mid \Theta) \propto \prod_{k=1}^{K} \theta_k^{\alpha_k - 1} \prod_{k=1}^{K} \theta_k^{N_k} = \prod_{k=1}^{K} \theta_k^{\alpha_k + N_k - 1}$$

Dirichlet Priors (cont.)

- We can compute the prediction on a new event in closed form:
- If $P(\Theta)$ is Dirichlet with hyperparameters $\alpha_1,\ldots,\alpha_K$ then

$$P(X[1] = k) = \int \theta_k \, P(\Theta) d\Theta = \frac{\alpha_k}{\sum_\ell \alpha_\ell}$$

- Since the posterior is also Dirichlet, we get

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

Prior Knowledge

- The hyperparameters $\alpha_1,\ldots,\alpha_K$ can be thought of as "imaginary" counts from our prior experience
- Equivalent sample size = $\alpha_1+\ldots+\alpha_K$
- The larger the **equivalent sample size** the more confident we are in our prior

Bayesian Prediction(cont.)

- Given these observations, we can compute the posterior for each multinomial θ_{X_i / pa_i} independently
  - The posterior is Dirichlet with parameters
    $\alpha(X_i=1/pa_i)+N(X_i=1/pa_i),\ldots, \alpha(X_i=k/pa_i)+N(X_i=k/pa_i)$
- The predictive distribution is then represented by the parameters

$$\tilde{\theta}_{x_i|pa_i} = \frac{\alpha(x_i, pa_i) + N(x_i, pa_i)}{\alpha(pa_i) + N(pa_i)}$$

Learning Parameters: Summary

- Estimation relies on **sufficient statistics**
  - For multinomial these are of the form $N(x_i,pa_i)$
  - Parameter estimation

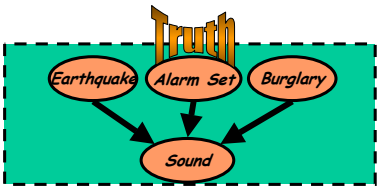
$$\hat{\theta}_{x_i|pa_i} = \frac{N(x_i, pa_i)}{N(pa_i)} \qquad \tilde{\theta}_{x_i|pa_i} = \frac{\alpha(x_i, pa_i) + N(x_i, pa_i)}{\alpha(pa_i) + N(pa_i)}$$

MLE Bayesian (Dirichlet)

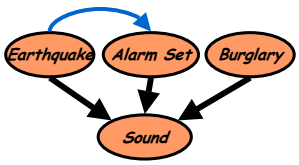
- Bayesian methods also require choice of priors
- Both MLE and Bayesian are asymptotically equivalent and consistent
- Both can be implemented in an **on-line** manner by accumulating sufficient statistics

Learning Structure from Complete Data

Why Struggle for Accurate Structure?

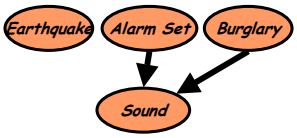


Adding an arc



- Increases the number of parameters to be fitted
- Wrong assumptions about causality and domain structure

Missing an arc



- Cannot be compensated by accurate fitting of parameters
- Also misses causality and domain structure

Approaches to Learning Structure

- **Constraint based**
  - Perform tests of conditional independence
  - Search for a network that is consistent with the observed dependencies and independencies
- **Pros & Cons**
  - \+ Intuitive, follows closely the construction of BNs
  - \+ Separates structure learning from the form of the independence tests
  - – Sensitive to errors in individual tests

Approaches to Learning Structure

- **Score based**
  - Define a score that evaluates how well the (in)dependencies in a structure match the observations
  - Search for a structure that maximizes the score
- **Pros & Cons**
  - \+ Statistically motivated
  - \+ Can make compromises
  - \+ Takes the structure of conditional probabilities into account
  - – Computationally hard

Likelihood Score for Structures

First cut approach:

- Use likelihood function

- Recall, the likelihood score for a network structure and parameters is

$$L(G, \Theta_G : D) = \prod_m P(x_1[m], \ldots, x_n[m] : G, \Theta_G)$$

$$= \prod_m \prod_i P(x_i[m] \mid Pa_i^G[m] : G, \Theta_{G,i})$$

- Since we know how to maximize parameters from now we assume

$$L(G : D) = \max_{\Theta_G} L(G, \Theta_G : D)$$

Avoiding Overfitting

"Classic" issue in learning.

Approaches:

- **Restricting the hypotheses space**
  - Limits the overfitting capability of the learner
  - Example: restrict # of parents or # of parameters
- **Minimum description length**
  - Description length measures complexity
  - Prefer models that compactly describes the training data
- **Bayesian methods**
  - Average over all possible parameter values
  - Use prior knowledge

Bayesian Inference

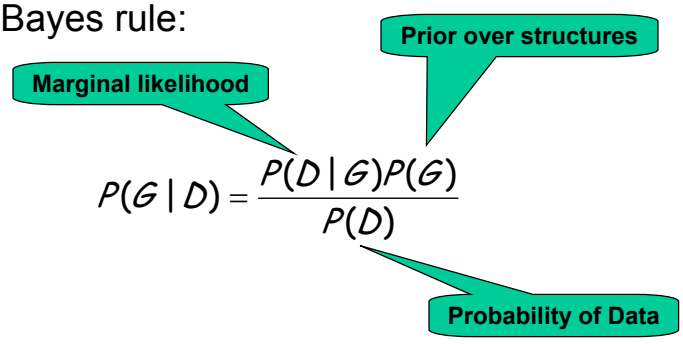
- Bayesian Reasoning---compute expectation over unknown *G*

$$P(x[M+1] \mid D) = \sum_G P(x[M+1] \mid D, G) P(G \mid D)$$

- **Assumption**: *G*s are mutually exclusive and exhaustive
- We know how to compute *P(x[M+1]|G,D)*
  - Same as prediction with fixed structure
- How do we compute *P(G|D)*?

Posterior Score

Using Bayes rule:



P(D) is the same for all structures G

Can be ignored when comparing structures

Marginal Likelihood

- By introduction of variables, we have that

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

Likelihood

Prior over parameters

- This integral measures sensitivity to choice of parameters

Marginal Likelihood: Multinomials

The same argument generalizes to multinomials with Dirichlet prior

- $P(\Theta)$ is Dirichlet with hyperparameters $\alpha_1, \ldots, \alpha_K$
- D is a dataset with sufficient statistics $N_1, \ldots, N_K$

Then

$$P(D) = \frac{\Gamma\left(\sum_\ell \alpha_\ell\right)}{\Gamma\left(\sum_\ell (\alpha_\ell + N_\ell)\right)} \prod_\ell \frac{\Gamma(\alpha_\ell + N_\ell)}{\Gamma(\alpha_\ell)}$$

Marginal Likelihood for General Network

The marginal likelihood has the form:

$$P(D \mid G) = \prod_i \prod_{pa_i^G} \underbrace{\frac{\Gamma\left(\alpha(pa_i^G)\right)}{\Gamma\left(\alpha(pa_i^G) + N(pa_i^G)\right)} \prod_{x_i} \frac{\Gamma(\alpha(x_i, pa_i^G) + N(x_i, pa_i^G))}{\Gamma(\alpha(x_i, pa_i^G))}}_{\text{Dirichlet Marginal Likelihood}}$$

For the sequence of values of X_i when X_is parents have a particular value

where

- $N(..)$ are the counts from the data
- $\alpha(..)$ are the hyperparameters for each family **given** G

Priors

- We need: prior counts $\alpha(..)$ for each network structure G
- This can be a formidable task
  - There are exponentially many structures…

BDe Score

Possible solution: The **BDe prior**

- Represent prior using two elements M_0, B_0
  - M_0 - **equivalent sample size**
  - B_0 - network representing the prior probability of events

BDe Score

Intuition: M_0 prior examples distributed by B_0

- Set $\alpha(x_i, pa_i^{\mathcal{G}}) = M_0 P(x_i, pa_i^{\mathcal{G}} \mid B_0)$
  - Note that $pa_i^{\mathcal{G}}$ are not the same as the parents of X_i in B_0.
  - Compute $P(x_i, pa_i^{\mathcal{G}} \mid B_0)$ using standard inference procedures
- Such priors have desirable theoretical properties
  - Equivalent networks are assigned the same score

Bayesian Score: Asymptotic Behavior

Theorem: If the prior $P(\Theta \mid G)$ is "well-behaved", then

$$\log P(D \mid G) = l(G : D) - \frac{\log M}{2} \dim(G) + O(1)$$

Asymptotic Behavior: Consequences

$$\log P(D \mid G) = l(G : D) - \frac{\log M}{2} \dim(G) + O(1)$$

- Bayesian score is **consistent**
  - As $M \to \infty$ the "true" structure G^* maximizes the score (almost surely)
  - For sufficiently large M, the maximal scoring structures are **equivalent** to G^*
- Observed data eventually overrides prior information
  - Assuming that the prior assigns positive probability to all cases

Asymptotic Behavior

$$\text{Score}(G : D) = I(G : D) - \frac{\log M}{2}\dim(G)$$

- This score can also be justified by the **Minimal Description Length (MDL)** principle
- This equation explicitly shows the tradeoff between
  - Fitness to data --- likelihood term
  - Penalty for complexity --- regularization term

Scores -- Summary

- Likelihood, MDL, (log) BDe have the form

$$Score(G : D) = \sum_i Score(X_i \mid Pa_i^G : N(X_i, Pa_i))$$

- BDe requires assessing prior network.
  It can naturally incorporate prior knowledge and previous experience
- BDe is consistent and asymptotically equivalent (up to a constant) to MDL
- All are **score-equivalent**
  - G equivalent to $G' \Rightarrow$ $Score(G) = Score(G')$

Optimization Problem

Input:

- Training data
- Scoring function (including priors, if needed)
- Set of possible structures
  - Including prior knowledge about structure

Output:

- A network (or networks) that maximize the score

Key Property:

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

Difficulty

Theorem: Finding maximal scoring network structure with at most k parents for each variables is NP-hard for $k > 1$

Heuristic Search

We address the problem by using heuristic search

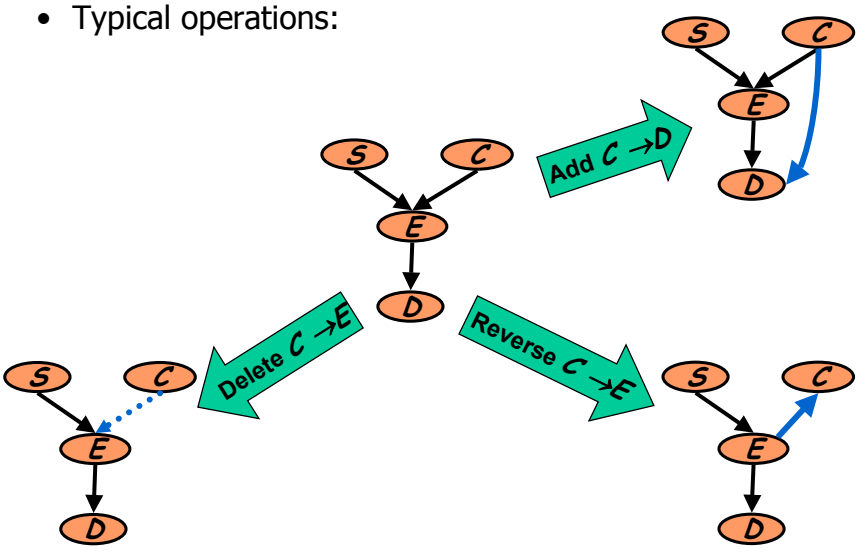
- Define a search space:
  - nodes are possible structures
  - edges denote adjacency of structures
- Traverse this space looking for high-scoring structures

Search techniques:

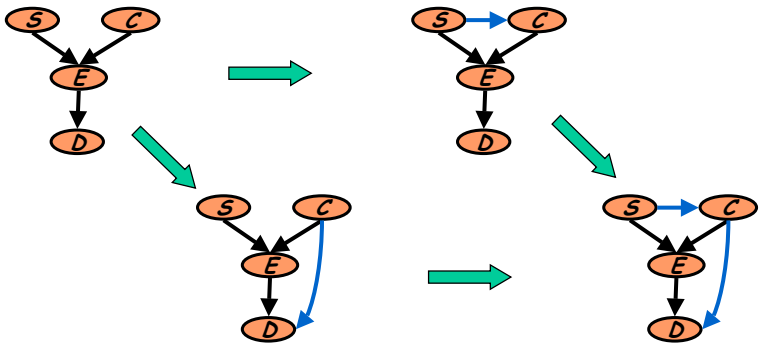
- Greedy hill-climbing
- Best first search
- Simulated Annealing
- ...

Heuristic Search (cont.)

- Typical operations:



Exploiting Decomposability in Local Search



- **Caching:** To update the score of after a local change, we only need to re-score the families that were changed in the last move

Greedy Hill-Climbing

- Simplest heuristic local search
  - Start with a given network
    - empty network
    - best tree
    - a random network
  - At each iteration
    - Evaluate all possible changes
    - Apply change that leads to best improvement in score
    - Reiterate
  - Stop when no modification improves score
- Each step requires evaluating approximately n new changes

Greedy Hill-Climbing: Possible Pitfalls

- Greedy Hill-Climbing can get struck in:
  - **Local Maxima:**
    - All one-edge changes reduce the score
  - **Plateaus:**
    - Some one-edge changes leave the score unchanged
    - Happens because equivalent networks received the same score and are neighbors in the search space
- Both occur during structure search
- Standard heuristics can escape both
  - Random restarts
  - TABU search

Model Selection

- So far, we focused on single model
  - Find best scoring model
  - Use it to predict next example
- Implicit assumption:
  - Best scoring model dominates the weighted sum
- **Pros:**
  - We get a single structure
  - Allows for efficient use in our tasks
- **Cons:**
  - We are committing to the independencies of a particular structure
  - Other structures might be as probable given the data

Model Averaging

- Recall, Bayesian analysis started with

$$P(x[M+1] \mid D) = \sum_{G} P(x[M+1] \mid D, G) P(G \mid D)$$

  - This requires us to average over all possible models

Model Averaging (cont.)

- **Full Averaging**
  - Sum over all structures
  - Usually intractable---there are exponentially many structures
- **Approximate Averaging**
  - Find K largest scoring structures
  - Approximate the sum by averaging over their prediction
  - Weight of each structure determined by the **Bayes Factor**

$$\frac{P(G \mid D)}{P(G' \mid D)} = \frac{P(G) P(D \mid G)}{P(G') P(D \mid G')} \cdot \frac{P(D)}{P(D)}$$

The actual score we compute

Search: Summary

- Discrete optimization problem
- In general, NP-Hard
  - Need to resort to heuristic search
  - In practice, search is relatively fast (~100 vars in ~10 min):
    - Decomposability
    - Sufficient statistics
- In some cases, we can reduce the search problem to an easy optimization problem
  - Example: learning trees

References

- *Principles of Data Mining*, Hand, Mannila, Smyth. MIT Press, 2001.
- Nir Friedman's excellent lecture notes, http://www.cs.huji.ac.il/~pmai/