Readings:
K&F: 15.1, 15.2, 15.3, 15.4, 15.5
K&F: 7 (overview of inference)
K&F: 8.1, 8.2 (Variable Elimination)

Structure Learning in BNs 3:

(the good, the bad,) and, finally, the ugly

Inference

we now get to use the BNs!!

Graphical Models – 10708
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October 6th, 2006

Bayesian, a decomposable score

$$\log P(D \mid \mathcal{G}) = \log \int_{\theta_{\mathcal{G}}} P(D \mid \mathcal{G}, \theta_{\mathcal{G}}) P(\theta_{\mathcal{G}} \mid \mathcal{G}) d\theta_{\mathcal{G}}$$

- As with last lecture, assume:
  - Local and global parameter independence

$\theta_{Y|X} \perp \theta_X$

- Also, prior satisfies **parameter modularity**:
  - If X_i has same parents in G and G', then parameters have same prior

G: $A \rightarrow X_i \leftarrow B$, $X_i \rightarrow C$ $\quad G'$: $C \rightarrow A$, $A \rightarrow X_i \leftarrow B$

$\theta_{X_i|Pa_{X_i}}$

- Finally, structure prior P(*G*) satisfies **structure modularity**
  - Product of terms over families
  - E.g., P(*G*) $\propto c^{|G|}$

$P(G) \propto \prod_i P(E(X_i, Pa_{X_i}))$

$|G|$ = number edges

$c < 1$

like fewer edges

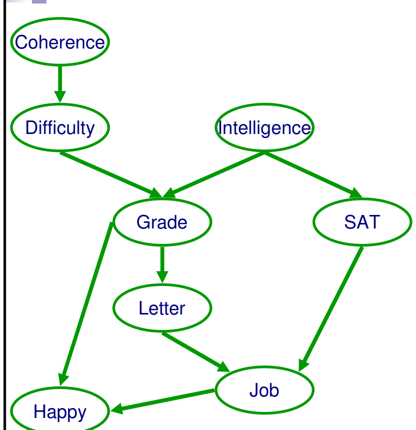
- Bayesian score decomposes along families!

$$\log P(G \mid D) \propto \sum_i \text{Score Fam}(X_i \mid Pa_{X_i} : D)$$

Structure learning for general graphs

- In a tree, a node only has one parent
- **Theorem**:
  - The problem of learning a BN structure with at most d parents is NP-hard for any (fixed) $d \geq 2$
- Most structure learning approaches use heuristics
  - Exploit score decomposition
  - (Quickly) Describe two heuristics that exploit decomposition in different ways

Understanding score decomposition



Fixed variable order 1

- Pick a variable order $\prec$
  - e.g., $X_1,\ldots,X_n$
- X_i can only pick parents in $\{X_1,\ldots,X_{i-1}\}$
  - Any subset
  - Acyclicity guaranteed!
- Total score = sum score of each node

Fixed variable order 2

- Fix max number of parents to k
- For each *i* in order $\prec$
  - Pick $\mathbf{Pa}_{Xi} \subseteq \{X_1,\ldots,X_{i-1}\}$
    - Exhaustively search through all possible subsets
    - $\mathbf{Pa}_{Xi}$ is maximum $\mathbf{U} \subseteq \{X_1,\ldots,X_{i-1}\}$ FamScore($X_i|\mathbf{U}$: D)
- Optimal BN for each order!!!
- Greedy search through space of orders:
  - E.g., try switching pairs of variables in order
  - If neighboring vars in order are switch, only need to recompute score for this pair
    - O(n) speed up per iteration
    - Local moves may be worse

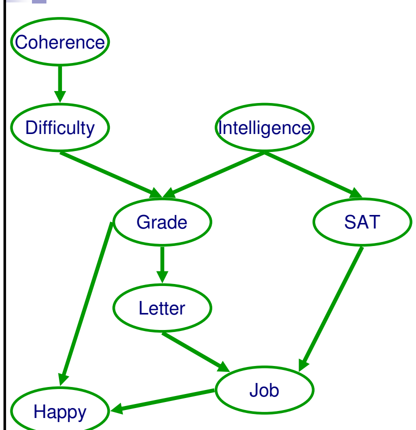
Learn BN structure using local search

Starting from Chow-Liu tree

Local search,
possible moves:
Only if acyclic!!!
• Add edge
• Delete edge
• Invert edge

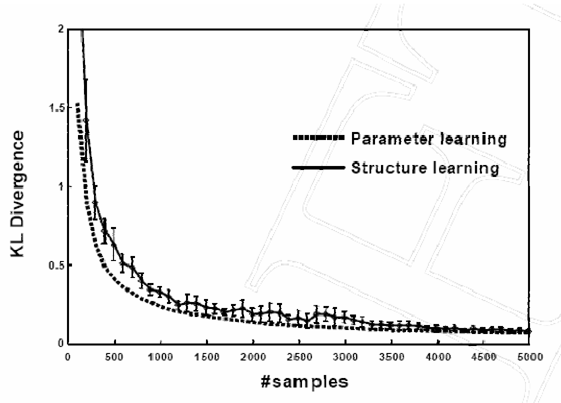
Select using favorite score

Exploit score decomposition in local search



- Add edge and delete edge:
  - Only rescore one family!
- Reverse edge
  - Rescore only two families

Some experiments



Alarm network

Order search versus graph search

- Order search advantages
  - For fixed order, optimal BN – more "global" optimization
  - Space of orders much smaller than space of graphs
- Graph search advantages
  - Not restricted to k parents
    - Especially if exploiting CPD structure, such as CSI
  - Cheaper per iteration
  - Finer moves within a graph

Bayesian model averaging

- So far, we have selected a single structure
- But, if you are really Bayesian, must average over structures
  - Similar to averaging over parameters

$$\log P(D \mid \mathcal{G}) = \log \int_{\theta_{\mathcal{G}}} P(D \mid \mathcal{G}, \theta_{\mathcal{G}}) P(\theta_{\mathcal{G}} | \mathcal{G}) d\theta_{\mathcal{G}}$$

- Inference for structure averaging is very hard!!!
  - Clever tricks in reading

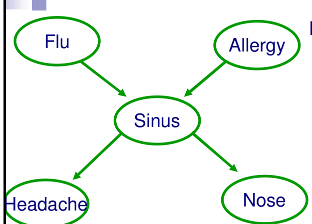
What you need to know about learning BN structures

- Decomposable scores
  - Data likelihood
  - Information theoretic interpretation
  - Bayesian
  - BIC approximation
- Priors
  - Structure and parameter assumptions
  - BDe if and only if score equivalence
- Best tree (Chow-Liu)
- Best TAN
- Nearly best k-treewidth (in $O(N^{k+1})$)
- Search techniques
  - Search through orders
  - Search through structures
- Bayesian model averaging

Announcements

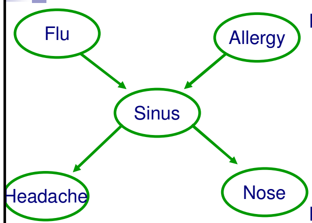
- Don't forget project proposals due this Wednesday
- Special recitation on advanced topic:
  - Ajit Singh on Optimal Structure Learning
  - On Monday Oct 9, 5:30-7:00pm in Wean Hall 4615A

Inference in graphical models: Typical queries 1



- Conditional probabilities
  - Distribution of some var(s). given evidence

Inference in graphical models: Typical queries 2 – Maximization



- Most probable explanation (MPE)
  - Most likely assignment to all hidden vars given evidence
- Maximum a posteriori (MAP)
  - Most likely assignment to some var(s) given evidence

Are MPE and MAP Consistent?

$P(S=t)=0.4$
$P(S=f)=0.6$

$P(N|S)$

- Most probable explanation (MPE)
  - Most likely assignment to all hidden vars given evidence
- Maximum a posteriori (MAP)
  - Most likely assignment to some var(s) given evidence

Complexity of conditional probability queries 1

- How hard is it to compute P(X|**E**=**e**)?

Reduction – 3-SAT

$$(\overline{X}_1 \vee X_2 \vee X_3) \wedge (\overline{X}_2 \vee X_3 \vee X_4) \wedge \ldots$$

Complexity of conditional probability queries 2

- How hard is it to compute P(X|**E**=**e**)?
  - At least NP-hard, but even harder!

Inference is #P-hard, hopeless?

- Exploit structure!
- Inference is hard in general, but easy for many (real-world relevant) BN structures

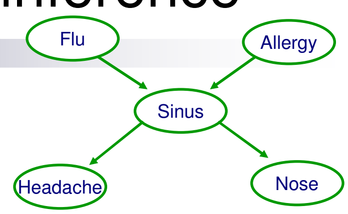
Complexity for other inference questions

- Probabilistic inference
  - general graphs:
  - poly-trees and low tree-width:
- Approximate probabilistic inference
  - Absolute error:
  - Relative error:
- Most probable explanation (MPE)
  - general graphs:
  - poly-trees and low tree-width:
- Maximum a posteriori (MAP)
  - general graphs:
  - poly-trees and low tree-width:

Inference in BNs hopeless?

- In general, yes!
  - Even approximate!
- In practice
  - Exploit structure
  - Many effective approximation algorithms (some with guarantees)
- For now, we'll talk about exact inference
  - Approximate inference later this semester

General probabilistic inference



- Query: $P(X \mid e)$
- Using def. of cond. prob.:

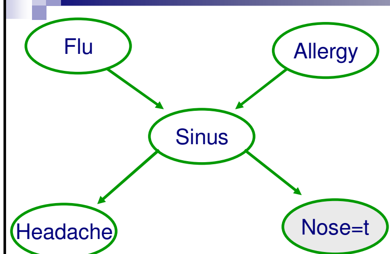
$$P(X \mid e) = \frac{P(X, e)}{P(e)}$$

- Normalization:

$$P(X \mid e) \propto P(X, e)$$

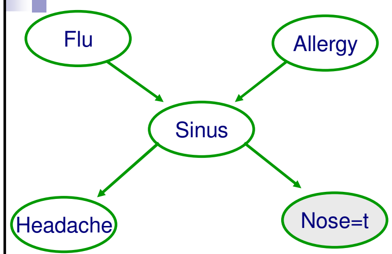
Marginalization

Probabilistic inference example



Inference seems exponential in number of variables!

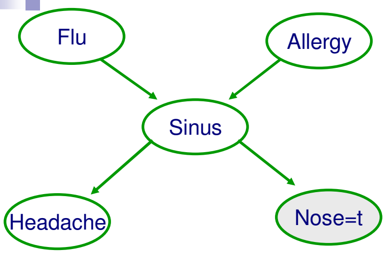
Fast probabilistic inference example – Variable elimination



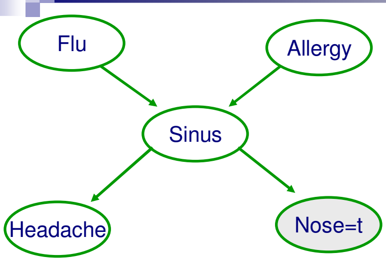
(Potential for) Exponential reduction in computation!

Understanding variable elimination – Exploiting distributivity

Understanding variable elimination – Order can make a HUGE difference

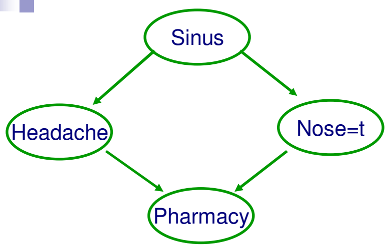


Understanding variable elimination – Intermediate results

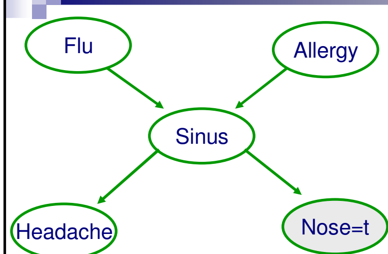


Intermediate results are probability distributions

Understanding variable elimination – Another example



Pruning irrelevant variables



Prune all non-ancestors of query variables
More generally: Prune all nodes not on active trail between evidence and query vars

Variable elimination algorithm

- Given a BN and a query $P(X|e) \propto P(X,e)$
- Instantiate evidence **e**
- Prune non-active vars for {X,**e**}

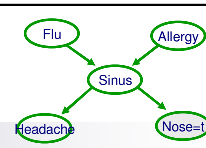
IMPORTANT!!!

- Choose an ordering on variables, e.g., $X_1, \ldots, X_n$
- Initial *factors* $\{f_1,\ldots,f_n\}$: $f_i = P(X_i|\mathbf{Pa}_{X_i})$ (CPT for X_i)
- For i = 1 to n, If $X_i \notin \{X,\mathbf{E}\}$
  - Collect factors $f_1,\ldots,f_k$ that include X_i
  - Generate a new factor by eliminating X_i from these factors

$$g = \sum_{X_i} \prod_{j=1}^{k} f_j$$

  - Variable X_i has been eliminated!
- Normalize $P(X,\mathbf{e})$ to obtain $P(X|\mathbf{e})$

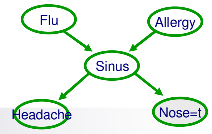
Operations on factors



$$g = \sum_{X_i} \prod_{j=1}^{k} f_j$$

Multiplication:

Operations on factors



$$g = \sum_{X_i} \prod_{j=1}^{k} f_j$$

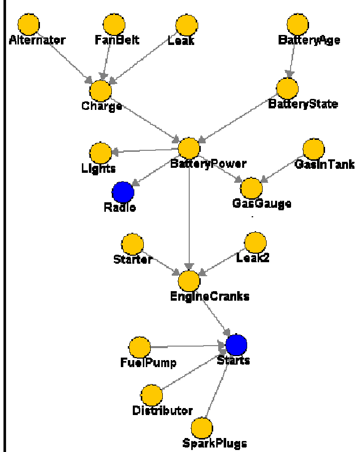
Marginalization:

Complexity of VE – First analysis

- Number of multiplications:

- Number of additions:

Complexity of variable elimination – (Poly)-tree graphs



Variable elimination order:
Start from "leaves" inwards:
- Start from skeleton!
- Choose a "root", any node
- Find topological order for root
- Eliminate variables in reverse order

Linear in CPT sizes!!! (versus exponential)

What you need to know about inference thus far

- Types of queries
  - probabilistic inference
  - most probable explanation (MPE)
  - maximum a posteriori (MAP)
    - MPE and MAP are truly different (don't give the same answer)
- Hardness of inference
  - Exact and approximate inference are NP-hard
  - MPE is NP-complete
  - MAP is much harder (NP^{PP}-complete)
- Variable elimination algorithm
  - Eliminate a variable:
    - Combine factors that include this var into single factor
    - Marginalize var from new factor
  - Efficient algorithm ("only" exponential in induced-width, not number of variables)
    - If you hear: "Exact inference only efficient in tree graphical models"
    - You say: "No!!! Any graph with low induced width"
    - And then you say: "And even some with very large induced-width" (next week with context-specific independence)
- Elimination order is important!
  - NP-complete problem
  - Many good heuristics