#### Lecture 13

#### **Learning Bayesian Networks from Data**

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http://www.kddresearch.org

http://www.cis.ksu.edu/~bhsu

Readings:

Sections 6.11-6.13, Mitchell

"In Defense of Probability", Cheeseman

"A Tutorial on Learning Bayesian Networks", Heckerman



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#### **Lecture Outline**

- Readings: 6.11-6.13, Mitchell; Pearl; Heckerman Tutorial
- More <u>Bayesian Belief</u> <u>Networks (BBNs</u>)
  - Inference: applying CPTs
  - Learning: CPTs from data, elicitation
  - In-class exercises
    - Hugin, BKD demos
    - CPT elicitation, application
- Learning BBN Structure
  - K2 algorithm
  - Other probabilistic scores and search algorithms
- <u>Causal Discovery</u>: Learning <u>Causality</u> from Observations
- Incomplete Data: Learning and Inference (Expectation-Maximization)
- Next Week: BBNs Concluded; Review for Midterm (11 October 2001)
- After Midterm: EM Algorithm, Unsupervised Learning, Clustering



#### Bayesian Networks: Quick Review

- Recall: Conditional Independence (CI) Assumptions
- Bayesian Network: <u>Digraph Model</u>
  - <u>Vertices</u> (nodes): denote events (each a random variable)
  - Edges (arcs, links): denote conditional dependencies
- Chain Rule for (Exact) Inference in BBNs  $P(X_1, X_2, ..., X_n) = \prod_{i=1}^{n} P(X_i | parents(X_i))$ 
  - Arbitrary Bayesian networks: MP-complete
  - Polytrees: linear time
- Example ("Sprinkler" BBN)



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#### Learning Distributions in BBNs: Quick Review

- Learning Distributions
  - Shortcomings of Naïve Bayes
  - Making judicious Cl assumptions
  - Scaling up to BBNs: need to learn a CPT for all parent sets
  - Goal: generalization
    - Given D (e.g., {1011, 1001, 0100})
    - Would like to know P(schema): e.g.,  $P(11^{**}) \equiv P(x_1 = 1, x_2 = 1)$
- Variants
  - Known or unknown structure
  - Training examples may have missing values
- Gradient Learning Algorithm
  - Weight update rule

$$\boldsymbol{w}_{ijk} \leftarrow \boldsymbol{w}_{ijk} + r \sum_{\boldsymbol{x} \in \boldsymbol{D}} \frac{\boldsymbol{P}_h(\boldsymbol{y}_{ij}, \boldsymbol{u}_{ik} \mid \boldsymbol{x})}{\boldsymbol{w}_{ijk}}$$

- Learns CPTs given data points D





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## **Learning Structure**

- Problem Definition
  - Given: data *D* (tuples or vectors containing observed values of variables)
  - Return: directed graph (*V*, *E*) expressing *target CPTs* (or commitment to acquire)
- Benefits
  - Efficient learning: more accurate models with less data P(A), P(B) vs. P(A, B)
  - Discover <u>structural properties</u> of the domain (causal relationships)
- Acccurate Structure Learning: Issues
  - Superfluous arcs: more parameters to fit; wrong assumptions about causality
  - Missing arcs: cannot compensate using CPT learning; ignorance about causality
- Solution Approaches
  - <u>Constraint-based</u>: enforce <u>consistency of network with observations</u>
  - <u>Score-based</u>: optimize <u>degree of match</u> between network and observations
- Overview: Tutorials
  - [Friedman and Goldszmidt, 1998] http://robotics.Stanford.EDU/people/nir/tutorial/
  - [Heckerman, 1999] <u>http://www.research.microsoft.com/~heckerman</u>



### Learning Structure: Constraints Versus Scores

- Constraint-Based
  - Perform tests of conditional independence
  - Search for network consistent with observed dependencies (or lack thereof)
  - Intuitive; closely follows definition of BBNs
  - Separates construction from form of CI tests
  - Sensitive to errors in individual tests
- Score-Based
  - Define <u>scoring function</u> (*aka* <u>score</u>) that evaluates how well (in)dependencies in a structure match observations
  - Search for structure that maximizes score
  - Statistically and information theoretically motivated
  - Can make compromises
- Common Properties
  - <u>Soundness</u>: with sufficient data and computation, both learn correct structure
  - Both learn structure from observations and *can incorporate knowledge*



## Learning Structure: <u>Maximum Weight Spanning Tree (Chow-Liu)</u>

- Algorithm *Learn-Tree-Structure-I*(*D*)
  - Estimate P(x) and P(x, y) for all single RVs, pairs;  $I(X; Y) = D(P(X, Y) || P(X) \cdot P(Y))$
  - Build *complete* <u>undirected</u> graph: variables as vertices, I(X; Y) as edge weights
  - $T \leftarrow Build-MWST(V \times V, Weights)$  // Chow-Liu algorithm: weight function = I
  - Set directional flow on *T* and place the CPTs on its edges (gradient learning)
  - **RETURN**: tree-structured BBN with CPT values
- Algorithm *Build-MWST-Kruskal* ( $E \subseteq V \times V$ , *Weights*:  $E \rightarrow R^+$ )

| – H ← Build-Heap (E, Weights)   | // aka priority queue                                | O(  <i>E</i>  )                         |
|---|--|---|
| $- E' \leftarrow \emptyset; Forest \leftarrow \{\{v\} \mid v \in V\}$ | // E': <u>set;</u> Forest: union-find                | O(  <i>V</i>  )                         |
| – WHILE Forest.Size > 1 DO  |  | O(  <i>E</i>  )                         |
| • <i>e</i> ← <i>H.Delete-Max</i> ()                                   | // <i>e</i> ≡ new edge from <i>H</i>                 | O(lg   <i>E</i>  )                      |
| • IF $((T_S \leftarrow Forest.Find(e.Start)) \neq (T_B)$              | $ \in Forest.Find(e.End))) THEN $                    | O( <b>Ig</b> <sup>∗</sup>   <i>E</i>  ) |
| E'.Union(e)   | // append edge <i>e</i> ; <i>E</i> '. <i>Size</i> ++ | O(1)                                    |
| Forest.Union (T <sub>S</sub> , T <sub>E</sub> )                       | // Forest.Size                                       | O(1)                                    |
| – RETURN E'   |  | O(1)                                    |

• Running Time:  $O(|E| |g||E|) = O(|V|^2 |g||V|^2) = O(|V|^2 |g||V|) = O(n^2 |g|n)$ 



## Learning Structure: Overfitting Prevention and Avoidance

- "Classic" Issue in Machine Learning
  - h' worse than h on D<sub>train</sub>
  - h' better than h on  $D_{test}$
- Standard Approaches
  - Prevention: restricted hypothesis space H
    - Limits overfitting capability
    - Examples: restrict number of parents, number of parameters
  - Avoidance: <u>Minimum Description Length (MDL)</u>
    - Description length  $MDL(h) = -BIC(h) = -\lg P(D/h) \lg P(h)$  measures complexity
    - Choose model that compactly describes D
  - Avoidance: Bayesian methods (cf. BOC)
    - Average over all possible values of BBN parameters Θ
    - Use prior knowledge
- Other Approaches
  - Holdout, cross-validation (CV), leave-one-out
  - Structural risk minimization: penalize  $H' \subseteq H$  based on their VC dimension



#### Scores for Learning Structure: The Role of Inference

- General-Case BBN Structure Learning: Use Inference to Compute Scores
- Recall: Bayesian Inference aka <u>Bayesian Reasoning</u>
  - Assumption:  $h \in H$  are mutually exclusive and exhaustive
  - Optimal strategy: combine predictions of hypotheses in proportion to likelihood
    - Compute conditional probability of hypothesis *h* given observed data *D*
    - i.e., compute expectation over unknown h for unseen cases
    - Let h = structure, parameters  $\Theta =$  CPTs



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#### Scores for Learning Structure: Prior over Parameters

- Likelihood  $L(\Theta : D)$ 
  - Definition:  $L(\Theta : D) \equiv P(D \mid \Theta) = \prod_{x \in D} P(x \mid \Theta)$
  - General BBN (<u>i.i.d data x</u>):  $L(\Theta : D) \equiv \prod_{x \in D} \prod_i P(x_i | Parents(x_i) \sim \Theta) = \prod_i L(\Theta_i : D)$ 
    - NB: Θ specifies CPTs for *Parents*(*x<sub>i</sub>*)
    - Likelihood decomposes according to the structure of the BBN
- Estimating Prior over Parameters:  $P(\Theta \mid D) \propto P(D) \cdot P(D \mid \Theta) \equiv P(D) \cdot L(\Theta : D)$ 
  - Example: Sprinkler
    - Scenarios D = {(Season(i), Sprinkler(i), Rain(i), Moisture(i), Slipperiness(i))}
    - $P(Su, Off, Dr, Wet, NS) = P(S) \cdot P(O \mid S) \cdot P(D \mid S) \cdot P(W \mid O, D) \cdot P(N \mid W)$
  - MLE for <u>multinomial distribution</u> (e.g., {Spring, Summer, Fall, Winter}):  $\hat{\Theta}_k = \frac{N_k}{\sum N_l}$
  - Likelihood for multinomials  $L(\Theta:D) = \prod_{k=1}^{K} \Theta_k^{N_k}$
  - Binomial case:  $N_1$  = # heads,  $N_2$  = # tails ("frequency is ML estimator")



## Learning Structure: Dirichlet (Bayesian) Score and K2 Algorithm

- Dirichlet Prior
  - Definition: a Dirichlet prior with hyperparameters  $\{\alpha_1, \alpha_2, ..., \alpha_k\}$  is a distribution

$$P(\Theta) \propto \prod_{k=1}^{K} \Theta_k^{\alpha_k - 1}$$
 for legal  $\Theta_k$ 

- Posterior has the same score, with hyperparameters { $\alpha_1 N_1, \alpha_2 N_2, ..., \alpha_k N_k$ }  $P(\Theta / D) \propto P(\Theta) \cdot P(D / \Theta) \propto \prod_{k=1}^{K} \Theta_k^{\alpha_k - 1} \cdot \prod_{k=1}^{K} \Theta_k^{\alpha_k + N_k - 1}$
- <u>Bayesian Score</u> (*aka* <u>Dirichlet Score</u>) for Marginal Likelihood P(D | h)

$$P(D/h) \propto \prod_{i=1}^{n} \left[ \prod_{Pa_{i}^{h}} \frac{\Gamma(\alpha(Pa_{i}^{h}))}{\Gamma(\alpha(Pa_{i}^{h}) + N(Pa_{i}^{h}))} \cdot \prod_{X_{i}=X_{i}} \frac{\Gamma(\alpha(x_{i}, Pa_{i}^{h}) + N(x_{i}, Pa_{i}^{h}))}{\Gamma(\alpha(x_{i}, Pa_{i}^{h}))} \right]$$

where  $x_i \equiv x_{ij} \equiv$  particular value of  $X_i$ ,  $Pa_i^h \equiv Pa_{ik}^h \equiv$  particular value of  $Parents_h(x_i)$ ,  $\Gamma(i) = (i-1)!$  for  $i \in \mathbb{Z}^+$ 

- K2: Algorithm for General Case Structure Learning
  - Greedy, Bayesian score-based
  - See: <u>http://wilma.cs.brown.edu/research/ai/dynamics/tutorial/</u>



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## Learning Structure: *K2* Algorithm and *ALARM*

• Algorithm Learn-BBN-Structure-K2 (D, Max-Parents)

FOR  $i \leftarrow 1$  to n DO// arbitrary ordering of variables { $x_1, x_2, ..., x_n$ }WHILE (Parents[ $x_i$ ].Size < Max-Parents) DO</td>// find best candidate parentBest  $\leftarrow$  argmax<sub>j>i</sub> (P(D |  $x_j \in Parents[x_i]$ )// max Dirichlet scoreIF (Parents[ $x_i$ ] + Best).Score > Parents[ $x_i$ ].Score) THEN Parents[ $x_i$ ] += BestRETURN ({Parents[ $x_i$ ] |  $i \in \{1, 2, ..., n\}$ })

- <u>A Logical Alarm Reduction Mechanism [Beinlich et al, 1989]</u>
  - BBN model for patient monitoring in surgical anesthesia
  - Vertices (37): findings (e.g., *esophageal intubation*), intermediates, observables
  - K2: found BBN different in only 1 edge from gold standard (elicited from expert)





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## Learning Structure: (Score-Based) Hypothesis Space Search

- Learning Structure: Beyond Trees
  - Problem not as easy for more complex networks
  - Example
    - Allow two parents (even <u>singly-connected</u> case, *aka* <u>polytree</u>)
    - Greedy algorithms no longer guaranteed to find optimal network
    - In fact, no efficient algorithm exists
  - <u>Theorem</u>: finding network structure with maximal score, where *H* restricted to BBNs with at most k parents for each variable, is  $\mathcal{MP}$ -hard for k > 1
- Heuristic Search of Search Space H
  - Define *H*: elements denote possible structures, adjacency relation denotes transformation (e.g., arc addition, deletion, reversal)
  - Traverse this space looking for high-scoring structures
  - Algorithms
    - Greedy hill-climbing
    - Best-first search
    - Simulated annealing



## Learning Structure: Causal Discovery

- Learning for Decision Support in Policy-Making
  - Does smoking cause cancer?
  - Does ingestion of lead paint decrease IQ?
  - Do school vouchers improve education?
  - Do Microsoft business practices harm customers?
- <u>Causal Discovery</u>: Inferring Existence, Direction of <u>Causal Relationships</u>
  - Methodology: <u>by experiment</u>
  - Can discover causality from observational data alone?
- What is "Causality" Anyway?
  - Probabilistic question
    - What is *P*(*lung cancer* | *yellow fingers*)?
  - Causal (mechanistic) question
    - What is P(lung cancer | set (yellow fingers))?
- Constraint-Based Methods for Causal Discovery
  - Require: no unexplained correlations, no accidental independencies (cause ^ CI)
  - Find: <u>plausible topologies</u> under <u>local CI tests</u> (cause  $\Leftrightarrow \neg$ CI)



## In-Class Exercise: *Hugin* Demo

- Hugin
  - Commercial product for BBN inference: <u>http://www.hugin.com</u>
  - First developed at University of Aalborg, Denmark
- Applications
  - Popular research tool for inference and learning
  - Used for real-world decision support applications
    - Safety and risk evaluation: <u>http://www.hugin.com/serene/</u>
    - Diagnosis and control in unmanned subs: <u>http://advocate.e-motive.com</u>
    - Customer support automation: <u>http://www.cs.auc.dk/research/DSS/SACSO/</u>
- Capabilities
  - Lauritzen-Spiegelhalter algorithm for inference (clustering aka clique reduction)
  - <u>Object Oriented Bayesian Networks (OOBNs)</u>: structured learning and inference
  - <u>Influence diagrams</u> for decision-theoretic inference (utility + probability)
  - See: <u>http://www.hugin.com/doc.html</u>





## In-Class Exercise: *Hugin* and CPT Elicitation

- Hugin Tutorials
  - Introduction: causal reasoning for diagnosis in decision support (toy problem)
    - http://www.hugin.com/hugintro/bbn\_pane.html
    - Example domain: <u>explaining</u> low yield (drought versus disease)
  - <u>Tutorial 1</u>: constructing a simple BBN in *Hugin* 
    - http://www.hugin.com/hugintro/bbn\_tu\_pane.html
    - Eliciting CPTs (or collecting from data) and entering them
  - Tutorial 2: constructing a simple influence diagram (decision network) in Hugin
    - http://www.hugin.com/hugintro/id tu pane.html
    - Eliciting utilities (or collecting from data) and entering them
- Other Important BBN Resources
  - <u>Microsoft Bayesian Networks: <u>http://www.research.microsoft.com/dtas/msbn/</u>
    </u>
  - XML BN (Interchange Format): <u>http://www.research.microsoft.com/dtas/bnformat/</u>
  - BBN Repository (more data sets) http://www-nt.cs.berkeley.edu/home/nir/public html/Repository/index.html/





# In-Class Exercise: <u>Bayesian Knowledge Discoverer (BKD</u>) Demo

- <u>Bayesian Knowledge Discoverer (BKD)</u>
  - Research product for BBN structure learning: <u>http://kmi.open.ac.uk/projects/bkd/</u>
  - Bayesian Knowledge Discovery Project [Ramoni and Sebastiani, 1997]
    - <u>Knowledge Media Institute (KMI)</u>, Open University, United Kingdom
    - Closed source, beta freely available for educational use
  - Handles missing data
  - Uses <u>Branch and Collapse</u>: Dirichlet score-based BOC approximation algorithm <u>http://kmi.open.ac.uk/techreports/papers/kmi-tr-41.ps.gz</u>
- Sister Product: <u>Robust Bayesian Classifier (RoC</u>)
  - Research product for BBN-based classification with missing data <u>http://kmi.open.ac.uk/projects/bkd/pages/roc.html</u>
  - Uses <u>Robust Bayesian Estimator</u>, a deterministic approximation algorithm <u>http://kmi.open.ac.uk/techreports/papers/kmi-tr-79.ps.gz</u>



#### Learning Structure: Conclusions

- Key Issues
  - Finding a <u>criterion</u> for inclusion or exclusion of an edge in the BBN
  - Each edge
    - "Slice" (axis) of a CPT or a commitment to acquire one
    - Positive statement of conditional dependency
- Other Techniques
  - Focus today: <u>constructive</u> (score-based) view of BBN structure learning
  - Other score-based algorithms
    - Heuristic search over space of addition, deletion, reversal operations
    - Other criteria (information theoretic, coding theoretic)
  - Constraint-based algorithms: *incorporating knowledge into causal discovery*
- Augmented Techniques
  - <u>Model averaging</u>: optimal Bayesian inference (integrate over <u>structures</u>)
  - <u>Hybrid BBN/DT models</u>: use a decision tree to record P(x | Parents(x))
- Other Structures: e.g., <u>Belief Propagation with Cycles</u>



## **Bayesian Network Learning: Related Fields and References**

- ANNs: BBNs as Connectionist Models
- GAs: BBN Inference, Learning as Genetic Optimization, Programming
- Hybrid Systems (Symbolic / Numerical Al)
- Conferences
  - General (with respect to machine learning)
    - International Conference on Machine Learning (ICML)
    - <u>American Association for Artificial Intelligence (AAAI)</u>
    - <u>International Joint Conference on Artificial Intelligence (IJCAI</u>, biennial)
  - Specialty
    - International Joint Conference on Neural Networks (IJCNN)
    - <u>Genetic and Evolutionary Computation Conference (GECCO)</u>
    - <u>Neural Information Processing Systems (NIPS)</u>
    - <u>Uncertainty in Artificial Intelligence (UAI)</u>
    - <u>Computational Learning Theory (COLT)</u>
- Journals
  - General: <u>Artificial Intelligence</u>, Machine Learning, <u>Journal of AI Research</u>
  - Specialty: Neural Networks, Evolutionary Computation, etc.



## Learning Bayesian Networks: Missing Observations

- Problem Definition
  - <u>Given</u>: data (*n*-tuples) with <u>missing values</u>, *aka* <u>partially observable</u> (PO) data
  - Kinds of missing values
    - <u>Undefined</u>, <u>unknown</u> (possible *new*)
    - Missing, corrupted (not properly collected)
  - Second case ("truly missing"): want to fill in ? with expected value
- Solution Approaches
  - Expected = distribution over possible values
  - Use "best guess" BBN to estimate distribution
  - <u>Expectation-Maximization (EM)</u> algorithm can be used here
- Intuitive Idea
  - Want to find  $h_{ML}$  in PO case ( $D \equiv$  unobserved variables ° observed variables)
  - Estimation step: calculate E[unobserved variables | h], assuming current h
  - <u>Maximization step</u>: update  $w_{ijk}$  to maximize  $E[\lg P(D | h)], D \equiv all variables$



# **Expectation-Maximization (EM)**

- Intuitive Idea
  - In fully observable case:  $h_{ML} = \arg \max_{h \in H} \frac{\# \text{ data cases with } \vec{n}, \vec{e}}{\# \text{ data cases with } \vec{e}} = \arg \max_{h \in H} \frac{\sum_{j} I_{\vec{N} = \vec{n}, \vec{E} = \vec{e}}(\vec{X}_{j})}{\sum_{j} I_{\vec{E} = \vec{e}}(\vec{X}_{j})}$
  - $h \equiv BBN$  parameters ( $\Theta$ ),  $N_i \equiv$  unobserved variable,  $E_i \equiv$  observed variable

$$- I_{E_i=e_i}(\vec{X}_j) = \delta(e_i, X_{ji})$$
$$= \begin{cases} 1 \text{ if } (X_{ji} \equiv E_i) = e_i \text{ in data case } \vec{X}_j \\ 0 \text{ otherwise} \end{cases}$$

- Partially Observable Case
  - / is unknown
  - Best estimate for *I*:  $\hat{I}(\vec{n},\vec{e} \mid \vec{x}) = P(\vec{n},\vec{e} \mid \vec{x}, h_{ML}), h_{ML} \equiv \Theta_{ML}$  unknown!
- Incomplete Data: Learning and Inference
  - <u>Missing values</u>: to be filled in given <u>partial observations</u>
  - <u>Expectation-Maximization (EM)</u>: <u>iterative refinement</u> algorithm
    - Estimation step: use current parameters  $\Theta$  to estimate missing  $\{N_i\}$
    - Maximization (<u>re-estimation</u>) step: update  $\Theta$  to maximize  $P(N_i, E_i | D)$



## Continuing Research on Learning Bayesian Networks from Data

- Advanced Topics (Not Covered)
  - Continuous variables and hybrid (discrete/continuous) BBNs
  - Induction of <u>hidden variables</u>
  - Local structure: localized constraints and assumptions, e.g., <u>Noisy-OR</u> BBNs
  - Online learning
    - Incrementality (aka lifelong, situated, in vivo learning)
    - Ability to change network structure during inferential process
  - Structural EM
  - Polytree structure learning (tree decomposition): alternatives to Chow-Liu MWST
  - Hybrid <u>quantitative</u> and <u>qualitative</u> Inference ("<u>simulation</u>")
  - Complexity of learning, inference in restricted classes of BBNs
- Topics to Be Covered Later
  - Decision theoretic models: <u>decision networks</u> aka <u>influence diagrams</u> (briefly)
  - Control and prediction models: <u>POMDPs</u> (for <u>reinforcement learning</u>)
  - Some temporal models: <u>Dynamic Bayesian Networks (DBNs</u>)



# Terminology

- Bayesian Networks: Quick Review on Learning, Inference
  - <u>Structure learning</u>: determining the best <u>topology</u> for a graphical model from data
    - <u>Constraint-based</u> methods
    - <u>Score-based</u> methods: statistical or information-theoretic degree of match
    - Both can be global or local, exact or approximate
  - Elicitation of subjective probabilities
- Causal Modeling
  - <u>Causality</u>: "direction" from cause to effect among events (observable or not)
  - <u>Causal discovery</u>: learning causality from observations
- Incomplete Data: Learning and Inference
  - <u>Missing values</u>: to be filled in given <u>partial observations</u>
  - <u>Expectation-Maximization (EM)</u>: <u>iterative refinement</u> clustering algorithm
    - Estimation step: use current parameters  $\Theta$  to estimate missing  $\{N_i\}$
    - <u>Maximization</u> (re-estimation) step: update  $\Theta$  to maximize  $P(N_i, E_i | D)$



## **Summary Points**

- Bayesian Networks: Quick Review on Learning, Inference
  - Learning, eliciting, applying CPTs
  - In-class exercise: *Hugin* demo; CPT elicitation, application
  - Learning BBN structure: <u>constraint-based</u> versus <u>score-based</u> approaches
  - K2, other scores and search algorithms
- Causal Modeling and Discovery: Learning Causality from Observations
- Incomplete Data: Learning and Inference (Expectation-Maximization)
- Tutorials on Bayesian Networks
  - Breese and Koller (AAAI '97, BBN intro): <u>http://robotics.Stanford.EDU/~koller</u>
  - Friedman and Goldszmidt (AAAI '98, Learning BBNs from Data): <u>http://robotics.Stanford.EDU/people/nir/tutorial/</u>
  - Heckerman (various UAI/IJCAI/ICML 1996-1999, Learning BBNs from Data): <u>http://www.research.microsoft.com/~heckerman</u>
- Next Week: BBNs Concluded; Review for Midterm (Thu 17 October 2002)
- After Midterm: More EM, Clustering, Exploratory Data Analysis

