# **Tutorial on Graphical Models**

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# **Graphical Model**

A graphical representation of a (typically highly multivariate) set of joint distributions

- Intuitive interface for modeling
- Modular: Useful tool for managing complexity
- Useful data structure for applying Bayes rule efficiently
- Common formalism for many models
  - Facilitates transfer of ideas between communities
  - Facilitates design of new systems

# Overview

- Introduction to graphical models
- Applications without data: Expert systems
- Learning from data
- Applications of learning
- Influence diagrams: Graphical models for decision making and causal reasoning

Two popular classes of graphical models

Undirected Graph (UG; MRF; Markov Network)



Directed acyclic graph (DAG; Bayesian Network)



# Other types of graphical models

Chain graphs:



Directed cyclic graphs:

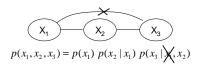


# **Graphical Model**

Assumption for intro: Joint distribution known with certainty

- Domain:  $X = (X_1,...,X_n)$
- Graphical model = structure + collection of local distributions
- Structure:
  - Nodes ~ variables
  - Missing arcs ~ conditional independence
- Independencies + local distributions => joint distribution ("modularity")

Directed Acyclic Graphs e.g. Wright, 1921; Good, 1961; Howard & Matheson 1981; Pearl 1988



# **Directed Acyclic Graphs**

The DAG structure encodes those independencies that permits the factorization:

$$p(\mathbf{x}) = \prod_{i} p(x_i \mid \mathbf{pa}_i)$$
 \(\geq \text{parents of } x\_i

Namely, for any total ordering of the variables consistent with the DAG:

$$p(x_i | x_1,...,x_{i-1}) = p(x_i | \mathbf{pa}_i)$$

Equivalently, each variable is independent of its non-descendants given its parents (Howard & Matheson 1981).

# **Directed Acyclic Graphs**

Thus, independencies + local distributions yield joint:

$$p(\mathbf{x}) = \prod_{i} p(x_i \mid \mathbf{pa}_i)$$
local distributions

Caveat: Local distributions may exist but joint does not.

# **Undirected Graphs**

e.g. Darroch, Lauritzen, & Speed 1980; Whittaker, 1990

Assumption to simplify presentation: p(x) is positive.

$$X_1$$
  $X_2$   $X_3$   $X_3$ 

# **Undirected Graphs**

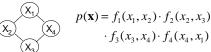
Each variable is independent of all other variables given its neighbors in the graph.

If p(x) is positive, then (Hammersly-Clifford-Besag):

$$p(\mathbf{x}) = \prod_{i} f_{i}(\mathbf{x}_{c_{i}})$$
maximal cliques of the graph

of the graph

Example:



# **Undirected Graphs**

$$p(\mathbf{x}) = \prod_{i} f_i(\mathbf{x}_{c_i})$$

When working with contingency tables or the case where p(x) is a multivariate Gaussian:

Can generate joint from clique marginals p(x<sub>ci</sub>) using Iterative Proportional Scaling (Deming and Stephan 1940).

Note:  $p(x_{ci})$  are local distributions.

# **Iterative Proportional Scaling**

E.g., for contingency table:

- Intialize  $\boldsymbol{p}_{old}(\boldsymbol{x})$  to be uniform
- Iterate, cycling over cliques ci:

$$p_{new}(\mathbf{x}) \leftarrow p_{old}(\mathbf{x}) \frac{p(\mathbf{x}_{c_i})}{p_{old}(\mathbf{x}_{c_i})}$$

# **Undirected Graphs – Alternate Form**

e.g., Levy 1948, Besag 1974

Each variable is independent of all other variables given its neighbors in the graph.

Use "local distributions" p(x<sub>i</sub>|neighbors<sub>i</sub>)



# **Undirected Graphs - Alternate Form**

Each variable is independent of all other variables given its neighbors in the graph.

Use "local distributions"  $p(x_i|neighbors_i)$ 



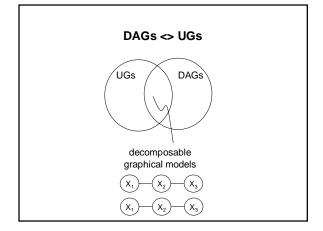
Generate p(x) via Gibbs sampling (Heckerman, Chickering, Meek, Rounthwaite, and Kadie 2000)

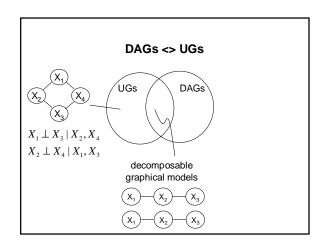
 $p(x_i | \text{neighbors}_i) = p(x_i | x \setminus x_i)$ 

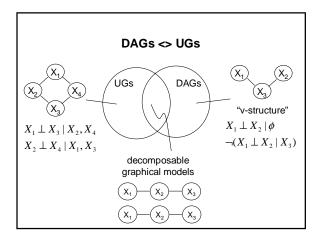
# **Summary**

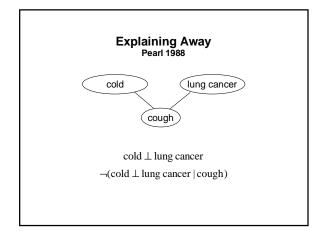
 $\begin{array}{ll} \underline{\text{Model}} & \underline{\text{Local distrbns}} \\ \text{DAG} & p(x_i|pa_i) & \underline{\text{multiplication}} \\ \\ \text{UG}_{\text{IPS}} & p(x_{\text{ci}}) & \text{IPS} \\ \end{array}$ 

 $UG_{MC}$   $p(x_i|n_i)$  Gibbs sampling

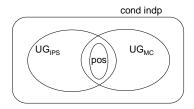








# **UGs and non-positive distributions**



 $UG_{IPS}$ : Those distributions encoded by  $p(\mathbf{x}) = \prod_i f(\mathbf{x}_{c_i})$  $UG_{MC}$ : Those distributions encoded by irreducible MC

# "Inference" in graphical models



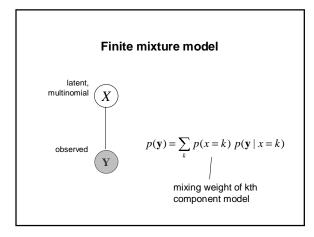
 $p(x_n) = \sum_{x_1, \dots, x_{n-1}} p(x_1) \ p(x_2 \mid x_1) \cdots p(x_n \mid x_{n-1})$ =  $\sum_{x_1} p(x_1) \sum_{x_2} p(x_2 \mid x_1) \cdots \sum_{x_{n-1}} p(x_{n-1} \mid x_{n-2}) p(x_n \mid x_{n-1})$ 

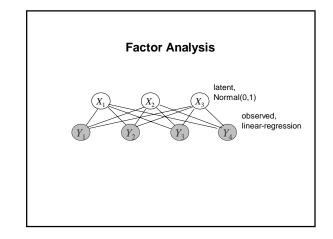
# Inference in graphical models

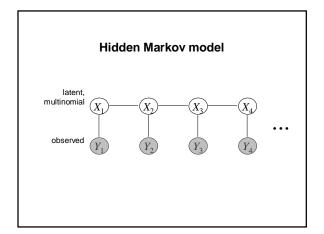
- Exact methods that exploit UG/DAG structure e.g., Laurtizen and Spiegelhalter 1988
  - Convert to triangulated (decomposable) UG
  - Create tree of cliques (running int property)
  - Perform tree version of dynamic programming
- Approximation methods needed when largest cliques contains too many variables
  - MCMC (e.g., Geman and Geman 1984)
  - Variational methods (e.g., Jordan et al. 1999)
  - Loopy propagation (e.g., Murphy et al. 1999)

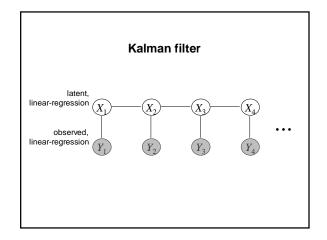
# Graphical models are a common representation for many models

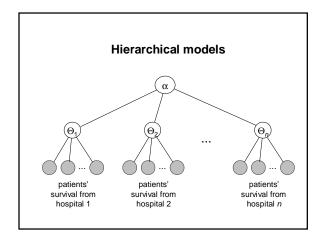
- Finite mixture models
- Factor analysis
- Hidden Markov model
- Kalman filter
- Hierarchical models

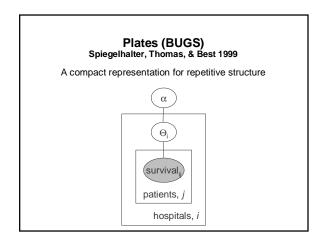






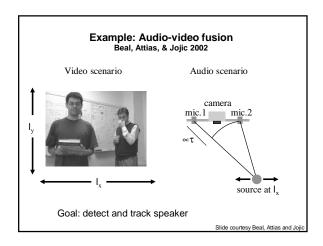


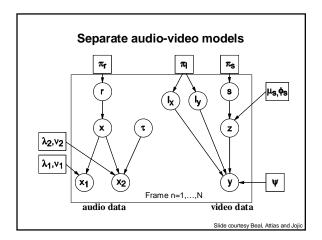


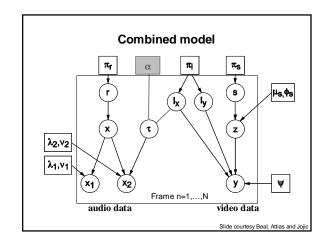


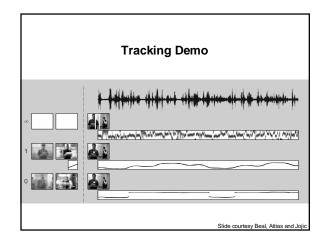
# Advantages of common representation

- Transfer ideas between research communities
- Design new models









# Applications of graphical models DAGs and UGs: Density estimation Classification and regression Clustering (finite mixture models) UGs: Acausal models Spatial processes DAGs: Acausal and causal models Expert systems

# DAGs or "Bayesian Networks" and expert systems

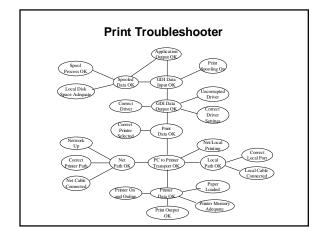
Early competitors to representing uncertainty in expert systems (late 70s, early 80s)

- MYCIN certainty-factor model (rule-based systems)
- Dempster-Shafer theory
- Fuzzy set theory
- Bayesian probability

Bayesian probability dominant by 1987 (in large part due to Bayesian Networks)

# **Examples of expert systems**

- MUNIN: Neuromuscular diagnosis Andreassen, Woldbye, Falck, and Andersen 1987
- Pathfinder: Lymph-node pathology diagnosis Heckerman, Horvitz, & Nathwani 1989
- QMR-DT: Internal medicine diagnosis Shwe et al. 1991
- Microsoft Windows Troubleshooters Heckerman et al. 1995



# So simple, a child could do it...

Teenager Designs Award-Winning Science Project

.. For her science project, which she called "Dr. Sigmund Microchip," Tovar wanted to create a computer program to diagnose the probability of certain personality types. With only answers from a few questions, the program was able to accurately diagnose the correct personality type 90 percent of the time



marginal likelihood

# **Software**

http://www.cs.berkeley.edu/~murphyk/Bayes/bnsoft.html

# Learning graphical models from data

Uncertainty in parameters:  $p(\theta | \mathbf{m})$  (assumed smooth)

Uncertainty in model:  $p(\mathbf{m})$ 

Given finite sample of inf exchangeable data  $\mathbf{d} = (\mathbf{x}_1, ..., \mathbf{x}_N)$ :

$$p(q | \mathbf{d}) = \sum_{\mathbf{m}} p(\mathbf{m} | \mathbf{d}) \int p(q | \theta, \mathbf{m}) \ p(\theta | \mathbf{d}, \mathbf{m}) \ d\theta$$

$$p(\mathbf{m} | \mathbf{d}) \propto p(\mathbf{m}) \int p(\mathbf{d} | \theta, \mathbf{m}) \ p(\theta | \mathbf{m}) \ d\theta$$

# Marginal parameter prior is not smooth

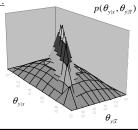
$$p(\theta) = p(\theta \mid \mathbf{m}_1) p(\mathbf{m}_1) + p(\theta \mid \mathbf{m}_2) p(\mathbf{m}_2)$$

# Example for binary X, Y:





 $\theta_{v} = \theta_{v|x} = \theta_{v}$ 



# Methods and approximations

### Only parameters uncertain:

- Bayesian MCMC (e.g., BUGS)
- MAP/ML EM (e.g., NIPS community)

## Both parameters and structure uncertain:

- Bayesian RJMCMC (Green 1995); MC<sup>3</sup> (Madigan and York 1995)
- Bayesian model selection for complete data (e.g., Cooper and Herskovits 1992; Spiegelhalter et al. 1993; Buntine 1994; Heckerman et al. 1995)
- Approx Bayesian model selection for incomplete data (e.g. Friedman 1997; Attias 2000)
- Constraint-based methods (Spirtes et al. 2001, Pearl 2000)

# Computationally attractive paremeter priors for DAG models

Geiger and Heckerman 1997, 2002

Challenge: The number of DAG models for n variables grows super exponentially with n

- Want priors for all DAG models for X to come from a small number of assessments
- Want closed form for marginal likelihood

Solution: A set of assumptions

Extension of Dawid and Lautitzen's (1993) priors for decomposable models

# **Assumptions**

For eligible local distribution families:

- Parameter independence
- (Conjugate priors)
- Complete data
- Equivalent graphs have equivalent priors
- Parameter modularity

# Eligible local distribution families

**u**  $X=(X_1,...,X_n)$  discrete (finite):  $p(x_i|pa_i,\theta_i)$  is "full table"

$$p(x_i | \mathbf{pa}_i = j, \theta_i, \mathbf{m}) \text{ is } mult(\theta_{x_i^1 | pa_i^j}, \dots, \theta_{x_i^{n_i} | pa_i^j})$$

$$\boldsymbol{\theta}_{ij} = (\boldsymbol{\theta}_{\boldsymbol{x}_i^1 \mid pa_i^j}, \dots, \boldsymbol{\theta}_{\boldsymbol{x}_i^n \mid pa_i^j})$$

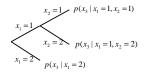
■ X continuous: p(x<sub>i</sub>|pa<sub>i</sub>,θ<sub>i</sub>) is linear regression

$$p(x_i | \mathbf{pa}_i, \theta_i, \mathbf{m}) = m_i + \sum_{x_j \in \mathbf{pa}_i} b_{ji} x_j + N(0, \sigma_i^2)$$

$$\theta_i = (m_i, \mathbf{b_i}, \sigma_i^2)$$
 Note:  $p(\mathbf{x}|\theta)$  is m.v. Gaussian

# Other eligible distribution families

■ X=(X<sub>1</sub>,...,X<sub>n</sub>) discrete: p(x<sub>i</sub>|pa<sub>i</sub>,θ<sub>i</sub>) a (probabilistic) decision tree



■ X<sub>i</sub> continuous: p(x<sub>i</sub>|pa<sub>i</sub>,θ<sub>i</sub>) is a linear regression for each configuration of the discrete parents of X<sub>i</sub>;

 $X_i$  discrete:  $p(x_i|pa_i,\theta_i)$  is full table (cont parents not allowed);  $p(x|\theta)$  is conditional Gaussian (Lauritzen 1992)

# First Assumption: Parameter independence Speigelhalter and Lauritzen 1990

X discrete:

$$p(\theta) = \prod_{i} \prod_{j} p(\theta_{ij})$$

X continuous:

$$p(\theta) = \prod_{i} p(\theta_i)$$

# Second assumption: Conjugate priors

When  $p(x_i|pa_i,\theta_i)$  is a full table:

$$p(\theta_{ij}) = Dir(\alpha_{ij1}, \dots, \alpha_{ijr_i})$$

When p(x<sub>i</sub>|pa<sub>i</sub>,θ<sub>i</sub>) is a linear regression

$$p(\theta_i) = \text{Normal - gamma}$$

# Third assumption: Complete data

Yields fast-to-compute, closed-form formula E.g., when p(x,|pa,θ) is a full table (Cooper and Herskovits 1992):

$$p(\mathbf{d} \mid \mathbf{m}) = \prod_{i=1}^{n} \prod_{j=1} \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + N_{ij})} \prod_{k=1} \frac{\Gamma(\alpha_{ijk} + N_{ijk})}{\Gamma(\alpha_{ijk})}$$

 $N_{ijk}$ :# cases where  $X_i = x_i^k$  and  $\mathbf{Pa}_i = \mathbf{pa}_i^j$ 

$$\alpha_{ij} = \sum_{k=1}^{\infty} \alpha_{ijk} N_{ij} = \sum_{k=1}^{\infty} N_{ijk}$$

## Problem with equivalent models

Two DAGs for X are equivalent if they encode the same sets of distributions for X.

If each  $p(x_i|pa_i,\theta_i)$  is full table or linear regression, then two DAGs for X are equivalent iff they encode the same independencies.

Example: Three discrete variables; full tables

$$\begin{array}{c}
(X_1) - (X_2) - (X_3) \\
(X_1) - (X_2) - (X_3)
\end{array}$$

$$X_1 \perp X_3 \mid X_2$$

# Complete network structures encode no independence







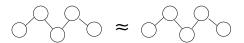
$$(X_3)$$
  $(X_2)$   $(X_1)$ 

# General test for equivalence

Verma & Pearl 1990: Two DAGs for X encode the same independencies iff

- They have the same skeleton
- They have the same v-structures





Problem: Equivalent graphs have different priors (for almost all hyperparameter values)

Example: X and Y binary; full tables

$$\begin{split} \mathbf{m}_{1} &: \underbrace{\mathbf{Y}} & \underbrace{\mathbf{Y}} & \mathbf{m}_{2} &: \underbrace{\mathbf{Y}} & \underbrace{\mathbf{Y}} \\ \theta_{x} & \theta_{y|x}, \theta_{y|\overline{x}} & \theta_{y} &= \theta_{x} \theta_{y|x} + (1 - \theta_{x}) \theta_{y|\overline{x}} \\ & \text{etc.} \end{split}$$

If each multinomial (bernoulli) has a Dir(1,1) prior, then

$$p(\boldsymbol{\theta}_{m2} \mid \mathbf{m}_{2}) \neq \left| \frac{\partial \boldsymbol{\theta}_{m1}}{\partial \boldsymbol{\theta}_{m2}} \right| p(\boldsymbol{\theta}_{m1} \mid \mathbf{m}_{1})$$

# Fourth assumption

Equivalent (complete) graphs have equivalent priors, and hence equal marginal likelihoods

$$\mathbf{m}_1$$
:  $\mathbf{x}$   $\mathbf{m}_2$ :  $\mathbf{x}$   $\mathbf{Y}$ 

$$p(\boldsymbol{\theta}_{m2} \mid \mathbf{m}_{2}) = \left| \frac{\partial \boldsymbol{\theta}_{m1}}{\partial \boldsymbol{\theta}_{m2}} \right| p(\boldsymbol{\theta}_{m1} \mid \mathbf{m}_{1})$$

## Independence + Equivalence => Conjugacy Geiger and Heckerman 1997, 2002

- Parameter independence
- Equivalent complete graphs have equivalent priors
- Technical conditions



parameters have conjugate distributions

# **Example: Two binary variables**





parameter independence equivalence property

$$\frac{f(\theta_x) g(\theta_{y|x}) h(\theta_{y|\overline{x}})}{\theta_x (1 - \theta_x)} = \frac{i(\theta_y) j(\theta_{x|y}) k(\theta_{x|\overline{y}})}{\theta_y (1 - \theta_y)}$$

$$\downarrow$$

positivity

$$p(\theta_{\mathbf{x}}) = p(\theta_{xy}, \theta_{x\bar{y}}, \theta_{\bar{x}y}, \theta_{\bar{x}y}, \theta_{\bar{x}\bar{y}}) \propto \theta_{xy}^a \theta_{x\bar{y}}^b \theta_{\bar{x}y}^c \theta_{\bar{x}\bar{y}}^b \theta_{\bar{x}\bar{y}}^d$$

# General discrete case

- Parameter independence
- Equivalent complete graphs have equivalent priors
- p(θ) strictly positive

$$\downarrow$$

$$\mathbf{X} \sim mult; \quad p(\theta_{\mathbf{x}} \mid \mathbf{m}_{\text{complete}}) = \text{Dir}(\alpha_{1}, ..., \alpha_{|\mathbf{x}|})$$
"hyper Dirichlet"

# **Characterization of the Dirichlet**

- Parameter independence
- Equivalent complete graphs have equivalent priors
- p(θ) strictly positive

$$\mathbf{X} \sim mult; \quad p(\theta_{\mathbf{x}} \mid \mathbf{m}_{\text{complete}}) = \text{Dir}(\alpha_1, \dots, \alpha_{|\mathbf{x}|})$$
"hyper Dirichlet"

# **Characterization of Normal-Wishart**

- Parameter independence
- Equivalent complete graphs have equivalent priors
- n>2; no element of ∑-1 is zero



 $\mathbf{X} \sim m.v.Gaussian; \quad p(\theta_{\mathbf{x}} \mid \mathbf{m}_{complete}) = \text{NW}(\boldsymbol{\mu}, \boldsymbol{\Sigma}^{-1})$ 

"hyper Normal-Wishart"

# Hyperparameters are highly constrained

E.g., discrete case:

$$p(\theta_{\mathbf{x}} \mid \mathbf{m}_{\text{complete}}) = \text{Dir}(\alpha_1, \dots, \alpha_{|\mathbf{x}|}), \ \alpha_i = \alpha \cdot p(\mathbf{x} = i)$$



 $p(\theta_{x_i^1|pa_i^j}, \dots, \theta_{x_i^{q_i}|pa_i^j} \mid \mathbf{m_{complete}}) = \mathrm{Dir}(\alpha_{ij1}, \dots, \alpha_{ijr_i})$ 

$$\alpha_{ijk} = \alpha \cdot p(x_i = k \mid pa_i = j)$$

So far...

parameter independence equivalence property

hyper distribution



(conjugate)  $p(\theta|\mathbf{m})$  for all complete  $\mathbf{m}$ 

Fifth assumption: Parameter modularity Heckerman, Geiger, and Chickering 1995

If a variable X<sub>i</sub> in two DAG models have the same parents, then

$$p(\theta_i \mid \mathbf{m}_1) = p(\theta_i \mid \mathbf{m}_2)$$

**Parameter Modularity: Example** 

 $p(\theta_1 \mid \mathbf{m}_1) = p(\theta_1 \mid \mathbf{m}_2)$ 

The whole story

parameter independence equivalence property

hyper distribution



(conjugate)  $p(\theta|\boldsymbol{m})$  for all complete  $\boldsymbol{m}$ 

parameter independence parameter modularity

(conjugate)  $p(\theta|\mathbf{m})$  for all  $\mathbf{m}$ 

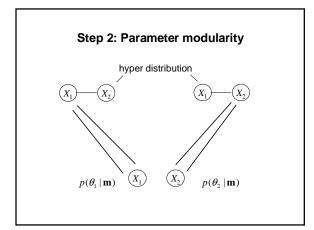
**Example: Empty graph for two variables** 

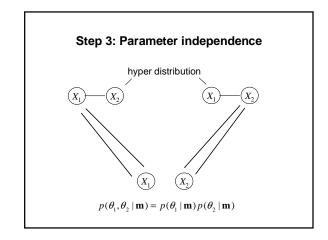
Given a hyper distribution for  $(X_1, X_2)$ , compute parameter prior for

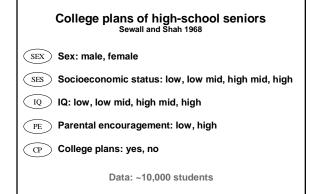
 $\mathbf{1}$ :  $(X_1)$  (

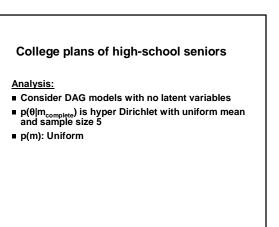
Step 1: Change of variable

hyper distribution  $\overbrace{x_1} \quad \overbrace{x_2}$ 









# Results $p(\mathbf{m} \mid \mathbf{d}) = 1.000000$

# DAG search for large domains

- Finding the DAG model with the highest marginal likelihood among those structures with at most *k* parents is NP hard for *k*>1. Chickering 1996
- Monte-Carlo methods
- Greedy/local search Heckerman et al. 1995



# DAG model selection given incomplete data

- Large sample approximations
  - BIC (Friedman 1997)
  - Laplace (Thiesson, Meek, Chickering, & Heckerman 1998) Caveat: DAG models (discrete) with latent variables are Stratified Exponential Family (Geiger, Heckerman, King, & Meek 2001)
- MCMC methods (e.g., DiCiccio et al. 1995)
- Variational methods (e.g., Attias 2000)

# Variational methods for model selection e.g. Attias 2000, Ghahramani & Beal 2000

Example: Factor analysis



$$\ln p(\mathbf{y} \mid \mathbf{m}) = \ln \int d\mathbf{x} \ d\theta \ p(\mathbf{y}, \mathbf{x}, \theta \mid \mathbf{m})$$
$$= \ln \int d\mathbf{x} \ d\theta \ q(\mathbf{x}, \theta) \frac{p(\mathbf{y}, \mathbf{x}, \theta)}{q(\mathbf{x}, \theta)}$$

$$\geq \int dx \ d\theta \ q(\mathbf{x}, \theta) \ln \frac{p(\mathbf{y}, \mathbf{x}, \theta)}{q(\mathbf{x}, \theta)}$$
 (Jensen ineq.)

Using a simple, factorized  $q(x,\theta)=q_x(x)q_{\theta}(\theta)$ :

$$\ln p(\mathbf{y} \mid \mathbf{m}) \ge \int dx \ d\theta \ q_x(\mathbf{x}) \ q_{\theta}(\theta) \ln \frac{p(\mathbf{y}, \mathbf{x}, \theta)}{q_x(\mathbf{x}) \ q_{\theta}(\theta)}$$

# Variational versus Laplace methods

- Laplace: Approximates p(θ|d) around one mode; full dependence
- Variational: p(θ|d) can be any convenient (possibly multi-model) distribution; convenience usually demands independence assumptions

# Averaging/selecting among UG models

- Decomposable: special case of DAGs; e.g., Dawid and Lauritzen 1993
- Non-decomposable
  - No closed-form marginal likelihood; MCMC used (e.g. Dellaportas & Foster 1999)

  - BIC via IPS + EM (e.g., Lauritzen 1996)
  - Heuristic method

# Heuristic method

$$X_1$$
  $X_2$   $X_3$   $p(x_1|x_2)$   $p(x_2|x_1,x_3)$   $p(x_1|x_2)$ 

Each local distribution

$$p(x_i | \text{neighbors}_i) = p(x_i | x \setminus x_i)$$

learned separately

Each local distribution can be learned efficiently (e.g., decision tree learned with Bayesian model selection)

Resulting conditionals are inconsistent, although "almost consistent"

# Microsoft applications of "Dependency Networks"

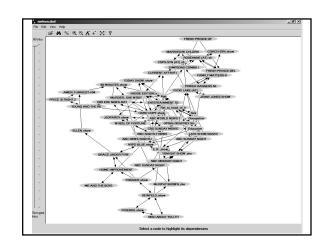
- Collaborative filtering (Commerce Server 2002)
- Exploratory data analysis (SQL Server 2000)

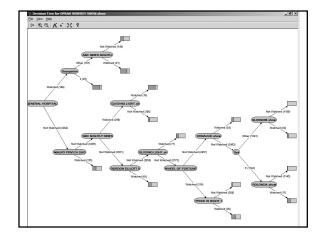
# **Exploratory data analysis**

# Example: Nielsen data, 2/6/95-2/19/95

	Age	Show1	Show2	Show3	
viewer 1	73	у	n	n	
viewer 2		n	у	У	
viewer 3	35	n	n	n	
		e	tc.		

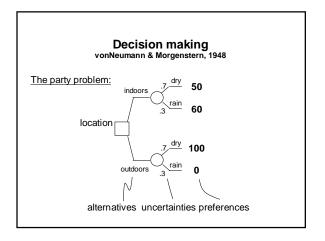
~400 shows, ~3000 viewers

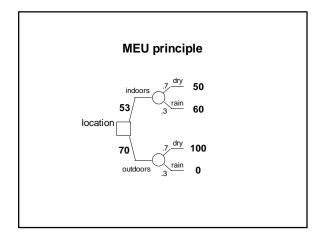


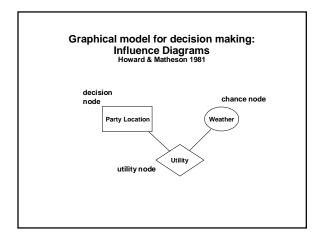


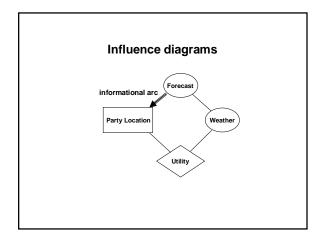
# Software

- Dependency networks, DAGs: http://research.microsoft.com/~dmax/WinMine/ Tooldoc.htm
- Many others: http://www.cs.berkeley.edu/~murphyk/Bayes/b nsoft.html



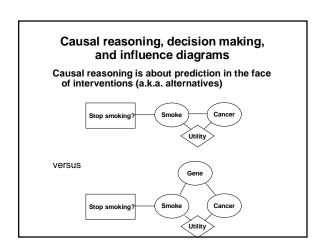






# Solving influence diagrams

- Concert to decision tree and then solve (Howard & Matheson 1981); computation grows exponentially with number of nodes
- Solve using influence diagram as data structure (Shachter 1986)



# Causal reasoning and influence diagrams

Alternative formulations of causal reasoning

- Rubin (e.g., 1978)
- Pearl (e.g. 2000)
- Spirtes, Glymous, & Scheines (e.g. 2001) involve couterfactuals

Dawid 2000: Don't need couterfactuals

Heckerman & Shacther 1995: If you want couterfactuals, they are consistent with decision theory and can be encoded with influence diagrams

### For more information...

### Tutorials:

- W. Buntine. Operations for learning with graphical models. Journal of Artificial Intelligence Research, 2, 159-225 (1994).
- D. Heckerman (1999). A tutorial on learning with Bayesian networks. In Learning in Graphical Models (Ed. M. Jordan). MIT Press.
- R. Cowell, A. P. Dawid, S. Lauritzen, and D. Spiegelhalter. Probabilistic Networks and Expert Systems. Springer-Verlag. 1999.
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http://www.cs.berkeley.edu/~murphyk/Bayes/bayes.html

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