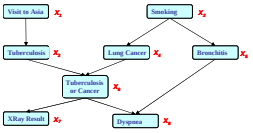
Machine Learning

10-701/15-781, Spring 2008

Graphical Models

Eric Xing



Lecture 18, March 26, 2008

Reading: Chap. 8, C.B book

What is a graphical model?

--- example from medical diagnostics

- A possible world for a patient with lung problem:

Visit to Asia X_1

Smoking X_2

Tuberculosis X_3

Lung Cancer X_4

Bronchitis X_5

Tuberculosis or Cancer X_6

XRay Result X_7

Dyspnea X_8

Recap of Basic Prob. Concepts

- Representation: what is the joint probability dist. on multiple variables?

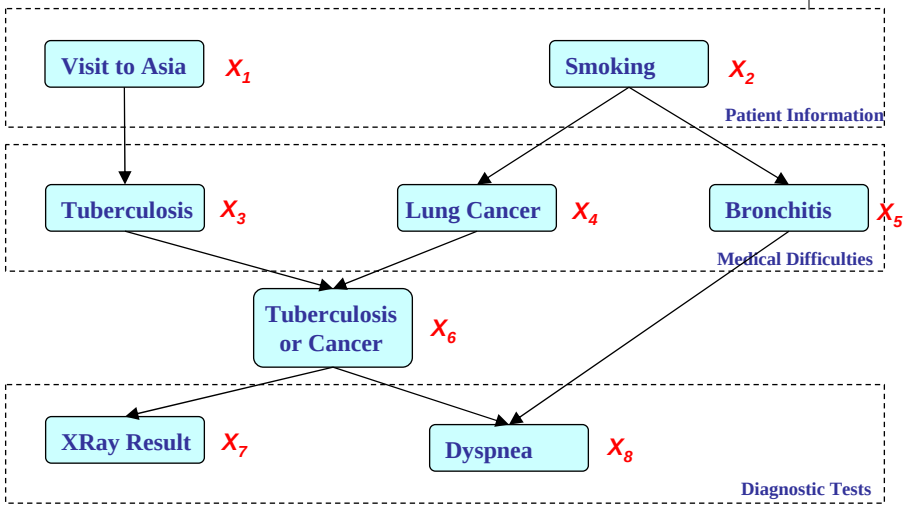
$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8,)$$

  - How many state configurations in total? --- 2^8
  - Are they all needed to be represented?
  - Do we get any scientific/medical insight?

- Learning: where do we get all this probabilities?
  - Maximal-likelihood estimation? but how many data do we need?
  - Where do we put domain knowledge in terms of plausible relationships between variables, and plausible values of the probabilities?

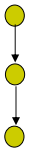
- Inference: If not all variables are observable, how to compute the conditional distribution of latent variables given evidence?

Dependencies among variables



Probabilistic Graphical Models

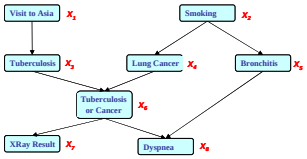
- Represent dependency structure with a graph
  - Node <-> random variable
  - Edges encode dependencies
    - Absence of edge -> conditional independence
  - Directed and undirected versions



- Why is this useful?
  - A language for communication
  - A language for computation
  - A language for development
- Origins:
  - Wright 1920's
  - Independently developed by Spiegelhalter and Lauritzen in statistics and Pearl in computer science in the late 1980's

Probabilistic Graphical Models, con'd

- If X_i's are **conditionally independent** (as described by a **PGM**), the joint can be factored to a product of simpler terms, e.g.,



$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$$
$$= P(X_1)\,P(X_2)\,P(X_3|X_1)\,P(X_4|X_2)\,P(X_5|X_2)\,P(X_6|X_3, X_4)\,P(X_7|X_6)\,P(X_8|X_5, X_6)$$

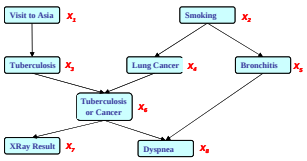
- Why we may favor a PGM?
  - Representation cost: how many probability statements are needed?

    2+2+4+4+4+8+4+8=36, an 8-fold reduction from 2^8!
  - Algorithms for systematic and efficient inference/learning computation
    - Exploring the graph structure and probabilistic (e.g., Bayesian, Markovian) semantics
  - Incorporation of domain knowledge and causal (logical) structures

Two types of GMs

- Directed edges give causality relationships (**Bayesian Network** or **Directed Graphical Model**):
- Undirected edges simply give (physical or symmetric) correlations between variables (**Markov Random Field** or **Undirected Graphical model**):

Bayesian Network: Factorization Theorem



$$P(X_1, X_2, X_3, X_4, X_5, X_6, X_7, X_8)$$
$$= P(X_1)\, P(X_2)\, P(X_3|\, X_1)\, P(X_4|\, X_2)\, P(X_5|\, X_2)$$
$$P(X_6|\, X_3, X_4)\, P(X_7|\, X_6)\, P(X_8|\, X_5, X_6)$$

- **Theorem:**

  Given a DAG, The most general form of the probability distribution that is consistent with the graph factors according to "node given its parents":

$$P(\mathbf{X}) = \prod_i P(X_i \mid \mathbf{X}_{\pi_i})$$

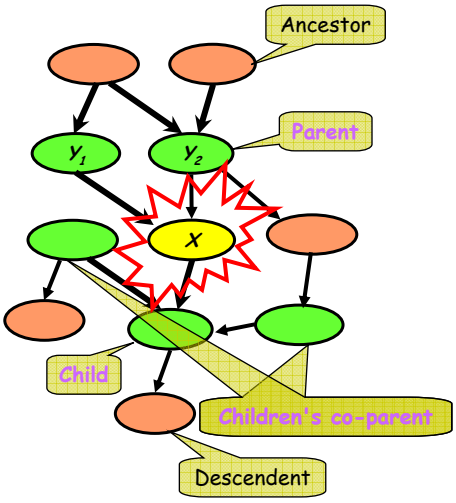
  where $\mathbf{X}_{\pi_i}$ is the set of parents of xi. d is the number of nodes (variables) in the graph.

Bayesian Network: Conditional Independence Semantics

$P(X \mid X') = P(X \mid X_{MB})$

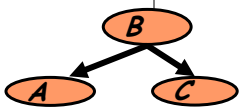
Structure: ***DAG***

- Meaning: a node is **conditionally independent** of every other node in the network outside its **Markov blanket**
- Local conditional distributions (**CPD**) and the **DAG** completely determine the **joint** dist.
- Give **causality** relationships, and facilitate a **generative** process



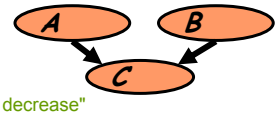
Local Structures & Independencies

- Common parent
  - Fixing B decouples A and C
    "given the level of gene B, the levels of A and C are independent"



- Cascade
  - Knowing B decouples A and C
    "given the level of gene B, the level gene A provides no extra prediction value for the level of gene C"

- V-structure
  - Knowing C couples A and B
    because A can "explain away" B w.r.t. C
    "If A correlates to C, then chance for B to also correlate to B will decrease"

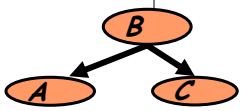


- The language is compact, the concepts are rich!

A simple justification

$P(A, C \mid B)$

$= P(A \mid B) P(C \mid B)$



$A \perp C \mid B$

$P(A, B, C) = P(B) P(A \mid B) P(C \mid B)$

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

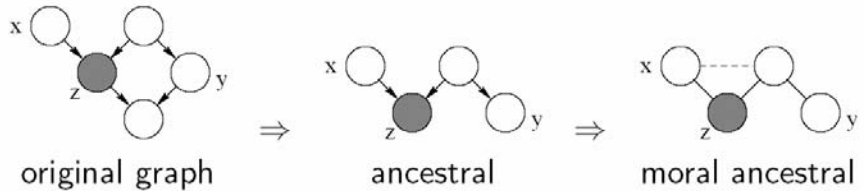
$= P(A \mid B) P(C \mid B)$

Graph separation criterion

- D-separation criterion for Bayesian networks (D for Directed edges):

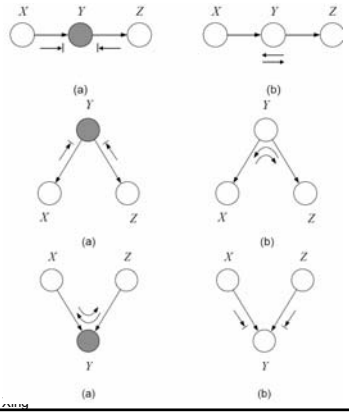
  Definition: variables x and y are *D-separated* (conditionally independent) given z if they are separated in the *moralized* ancestral graph

- Example:



Global Markov properties of DAGs

- X is **d-separated** (directed-separated) from Z given Y if we can't send a ball from any node in X to any node in Z using the "*Bayes-ball*" algorithm illustrated bellow (and plus some boundary conditions):

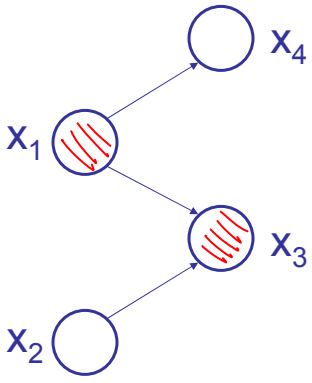


- Defn: $\mathcal{I}(\mathcal{G})$=all independence properties that correspond to d-separation:

$$\mathrm{I}(G) = \left\{X \perp Z | Y : \mathrm{dsep}_G(X; Z | Y)\right\}$$

- D-separation is sound and complete

Example:



- Complete the I(G) of this graph:

$X_2 \perp\!\!\!\perp X_1 \mid -$

$X_2 \perp\!\!\!\perp X_4$

$X_4 \perp\!\!\!\perp X_3 \mid X_1$

$X_4 \perp\!\!\!\perp X_2 \mid X_1$

$X_2 \perp\!\!\!\perp X_4 \mid X_1, X_3.$

Towards quantitative specification of probability distribution

- Separation properties in the graph imply independence properties about the associated variables
- For the graph to be useful, any conditional independence properties we can derive from the graph should hold for the probability distribution that the graph represents

$P(X_1 \cdots X_N) = \prod_i P(X_i \mid X_{\pi_i})$

$P(\cdots) = ?$

- **The Equivalence Theorem**

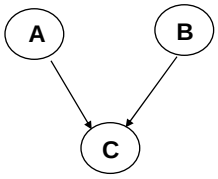
  For a graph G,

  Let $\mathcal{D}_1$ denote the family of all distributions that satisfy I(G),

  Let $\mathcal{D}_2$ denote the family of all distributions that factor according to G,

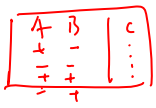
  Then $\mathcal{D}_1 \equiv \mathcal{D}_2$.

Example



$\longleftrightarrow$ $p(A,B,C) = P(C \mid A,B)P(A)P(B)$

$P(C \mid A,B)$



$P(A)$

$P(B)$

$\leftarrow \cdot \rightarrow$

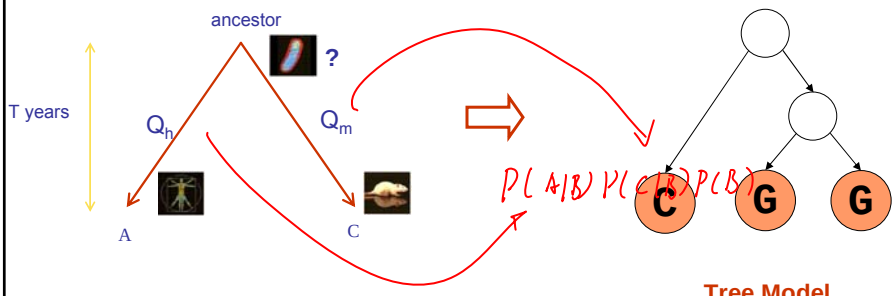
$N(\mu_C, \Sigma_C)$ $\mu_C = \mu_A + \mu_B$

$N(\mu_A, \Sigma_A)$

$N(\mu_B, \Sigma_B)$

Example, con'd

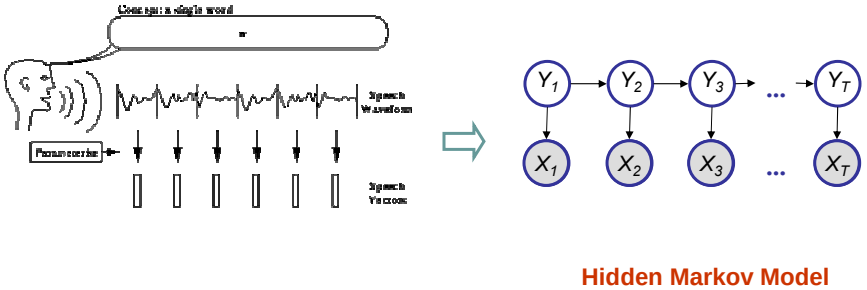
- Evolution



Tree Model

Example, con'd

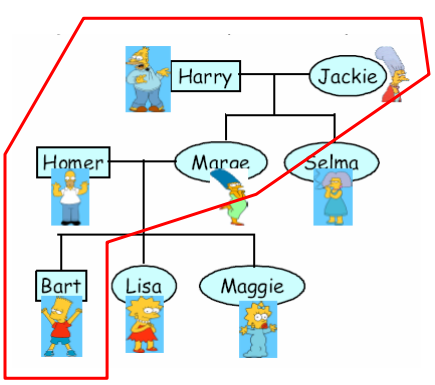
- Speech recognition

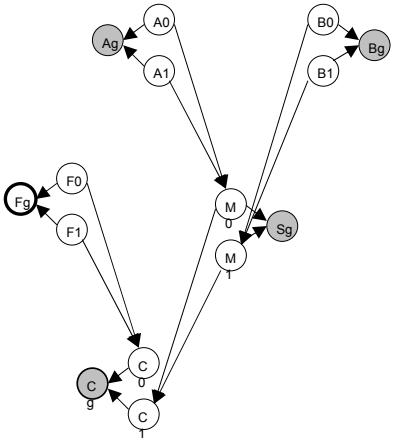


Hidden Markov Model

Example, con'd

- Genetic Pedigree



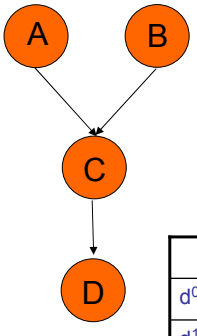


Conditional probability tables (CPTs)

a^0	0.75
a^1	0.25

b^0	0.33
b^1	0.67

P(a,b,c.d) = P(a)P(b)P(c|a,b)P(d|c)



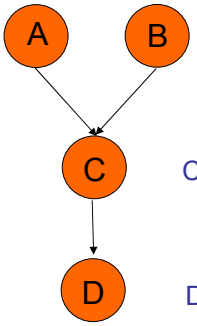
	a^0b^0	a^0b^1	a^1b^0	a^1b^1
c^0	0.45	1	0.9	0.7
c^1	0.55	0	0.1	0.3

	c^0	c^1
d^0	0.3	0.5
d^1	07	0.5

Conditional probability density func. (CPDs)

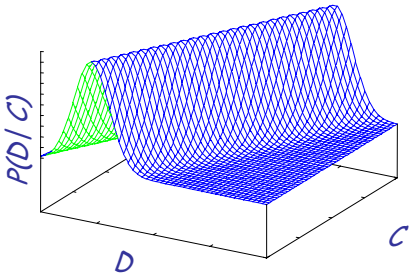
A~N(μ_a, Σ_a) B~N(μ_b, Σ_b)

P(a,b,c.d) = P(a)P(b)P(c|a,b)P(d|c)

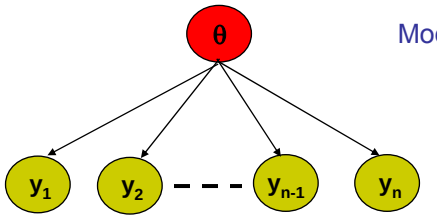


C~N(A+B, Σ_c)

D~N(μ_a+C, Σ_a)



Conditionally Independent Observations

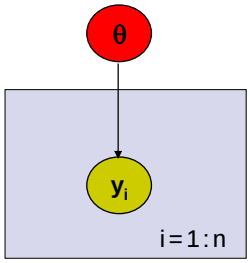


Model parameters

Data

$p(y_1, \cdots y_n, \theta) = p(\theta) \prod_i p(y_i|\theta)$

"Plate" Notation



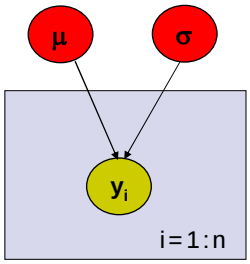
Model parameters

Data = $\{y_1,\ldots y_n\}$

Plate = rectangle in graphical model

variables within a plate are replicated
in a conditionally independent manner

Example: Gaussian Model



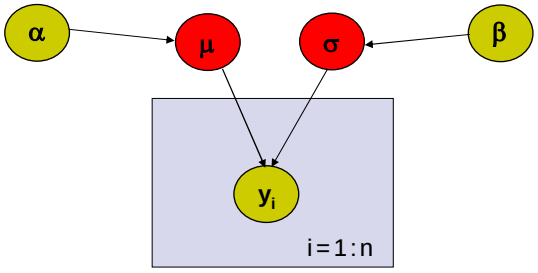
Generative model:

$p(y_1,\ldots y_n \mid \mu, \sigma) = \prod_i p(y_i \mid \mu, \sigma)$
$= p(\text{data} \mid \text{parameters})$
$= p(D \mid \theta)$

where $\theta = \{\mu, \sigma\}$

- Likelihood = p(data | parameters)
  = p(D | θ)
  = L (θ)
- Likelihood tells us how likely the observed data are conditioned on a particular setting of the parameters
  - Often easier to work with log L (θ)

Example: Bayesian Gaussian Model

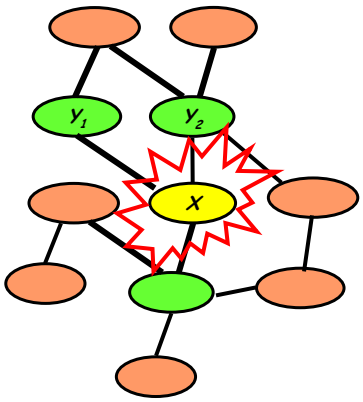


Note: priors and parameters are assumed independent here

Markov Random Fields

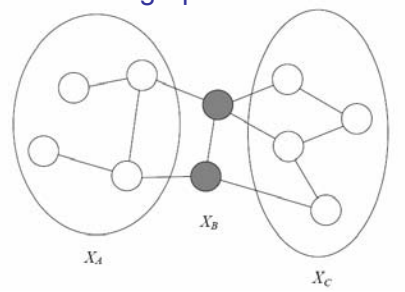
Structure: an ***undirected graph***

- Meaning: a node is **conditionally independent** of every other node in the network given its **Directed neighbors**
- Local contingency functions (**potentials**) and the **cliques** in the graph completely determine the **joint** dist.
- Give **correlations** between variables, but no explicit way to generate samples



Semantics of Undirected Graphs

- Let *H* be an undirected graph:



- *B* ***separates*** *A* and *C* if every path from a node in *A* to a node in *C* passes through a node in *B*: $\text{sep}_H(A;C|B)$
- A probability distribution satisfies the ***global Markov property*** if for any disjoint *A*, *B*, *C*, such that *B* separates *A* and *C*, *A* is independent of *C* given *B*: $\text{I}(H) = \{A \perp C|B) : \text{sep}_H(A;C|B)\}$

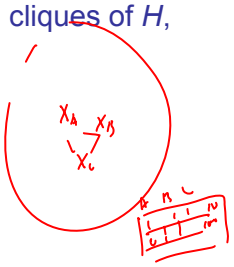
Representation

- Defn: an undirected graphical model represents a distribution $P(X_1,\ldots,X_n)$ defined by an undirected graph *H*, and a set of positive ***potential functions*** y_c associated with cliques of *H*, s.t.

$$P(x_1,\ldots,x_n) = \frac{1}{Z}\prod_{c\in C}\psi_c(\mathbf{x}_c)$$

where *Z* is known as the partition function:

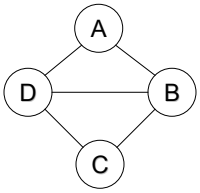
$$Z = \sum_{x_1,\ldots,x_n}\prod_{c\in C}\psi_c(\mathbf{x}_c)$$



- Also known as Markov Random Fields, Markov networks …
- The ***potential function*** can be understood as an contingency function of its arguments assigning "pre-probabilistic" score of their joint configuration.

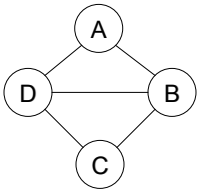
Cliques

- For $G=\{V,E\}$, a complete subgraph (clique) is a subgraph $G'=\{V'\subseteq V, E'\subseteq E\}$ such that nodes in V' are fully interconnected
- A (maximal) clique is a complete subgraph s.t. any superset $V''\supseteq V'$ is not complete.
- A sub-clique is a not-necessarily-maximal clique.



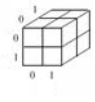
- Example:
  - max-cliques = {*A*,*B*,*D*}, {*B*,*C*,*D*},
  - sub-cliques = {*A*,*B*}, {*C*,*D*}, …→ all edges and singletons

Example UGM – using max cliques



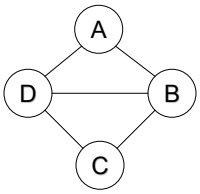
$$P(x_1,x_2,x_3,x_4)=\frac{1}{Z}\psi_c(\mathbf{x}_{124})\times\psi_c(\mathbf{x}_{234})$$

$$Z=\sum_{x_1,x_2,x_3,x_4}\psi_c(\mathbf{x}_{124})\times\psi_c(\mathbf{x}_{234})$$



- For discrete nodes, we can represent $P(X_{1:4})$ as two 3D tables instead of one 4D table

Example UGM – using subcliques



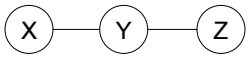
$$P(x_1, x_2, x_3, x_4) = \frac{1}{Z}\prod_{ij}\psi_{ij}(\mathbf{x}_{ij})$$

$$= \frac{1}{Z}\psi_{12}(\mathbf{x}_{12})\psi_{14}(\mathbf{x}_{14})\psi_{23}(\mathbf{x}_{23})\psi_{24}(\mathbf{x}_{24})\psi_{34}(\mathbf{x}_{34})$$

$$Z = \sum_{x_1,x_2,x_3,x_4}\prod_{ij}\psi_{ij}(\mathbf{x}_{ij})$$

- For discrete nodes, we can represent $P(X_{1:4})$ as 5 2D tables instead of one 4D table

Interpretation of Clique Potentials



- The model implies $X \perp Z | Y$. This independence statement implies (by definition) that the joint must factorize as:

$$p(x, y, z) = p(y)p(x \mid y)p(z \mid y)$$

- We can write this as: $p(x, y, z) = p(x, y)p(z \mid y)$, but $p(x, y, z) = p(x \mid y)p(z, y)$
  - **cannot** have all potentials be marginals
  - **cannot** have all potentials be conditionals
- The positive clique potentials can only be thought of as general "compatibility", "goodness" or "happiness" functions over their variables, but not as probability distributions.

Exponential Form

- Constraining clique potentials to be positive could be inconvenient (e.g., the interactions between a pair of atoms can be either attractive or repulsive). We represent a clique potential $\psi_c(\mathbf{x}_c)$ in an unconstrained form using a real-value "energy" function $\phi_c(\mathbf{x}_c)$:

$$\psi_c(\mathbf{x}_c) = \exp\{-\phi_c(\mathbf{x}_c)\}$$

For convenience, we will call $\phi_c(\mathbf{x}_c)$ a potential when no confusion arises from the context.

- This gives the joint a nice additive strcuture

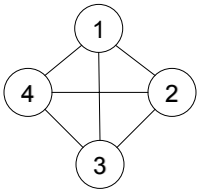
$$p(\mathbf{x}) = \frac{1}{Z}\exp\left\{-\sum_{c\in C}\phi_c(\mathbf{x}_c)\right\} = \frac{1}{Z}\exp\{-H(\mathbf{x})\}$$

where the sum in the exponent is called the "free energy":

$$H(\mathbf{x}) = \sum_{c\in C}\phi_c(\mathbf{x}_c)$$

- In physics, this is called the "Boltzmann distribution".
- In statistics, this is called a log-linear model.

Example: Boltzmann machines



- A fully connected graph with pairwise (edge) potentials on binary-valued nodes (for $x_i \in \{-1,+1\}$ or $x_i \in \{0,1\}$) is called a Boltzmann machine

$$P(x_1,x_2,x_3,x_4) = \frac{1}{Z}\exp\left\{\sum_{ij}\phi_{ij}(x_{i,}x_j)\right\}$$

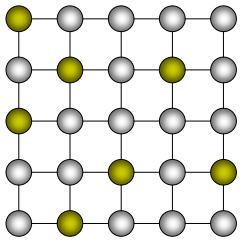
$$= \frac{1}{Z}\exp\left\{\sum_{ij}\theta_{ij}x_ix_j + \sum_i\alpha_ix_i + C\right\}$$

- Hence the overall energy function has the form:

$$H(x) = \sum_{ij}(x_i-\mu)\Theta_{ij}(x_j-\mu) = (x-\mu)^T\Theta(x-\mu)$$

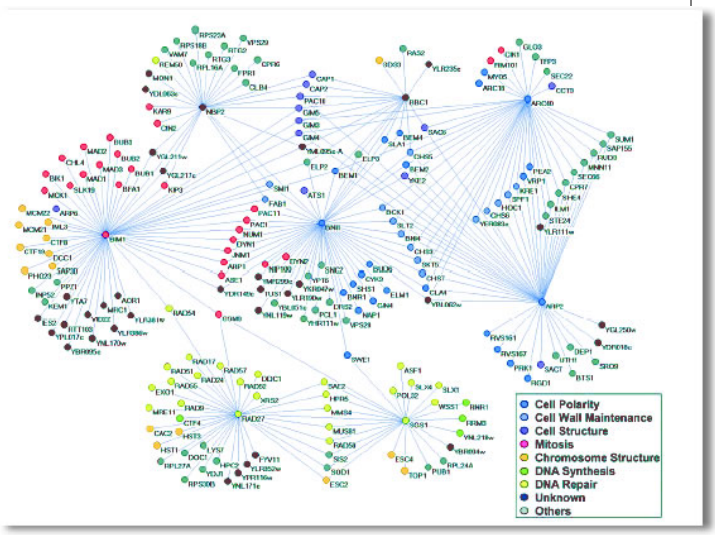
Example: Ising (spin-glass) models

- Nodes are arranged in a regular topology (often a regular packing grid) and connected only to their geometric neighbors.

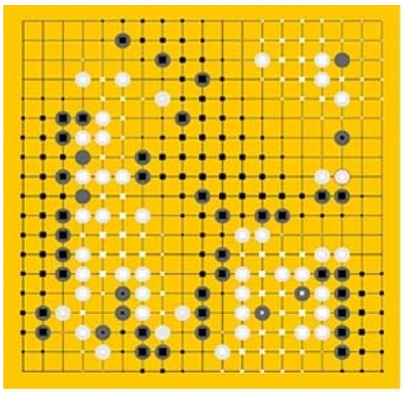


- Same as sparse Boltzmann machine, where $\theta_{ij} \neq 0$ iff i,j are neighbors.
  - e.g., nodes are pixels, potential function encourages nearby pixels to have similar intensities.
- Potts model: multi-state Ising model.

Example: Protein-Protein interaction networks



Example: Modeling Go



This is the middle position of a Go game. Overlaid is the estimate for the probability of becoming black or white for every intersection. Large squares mean the probability is higher.

GMs are your old friends

Density estimation

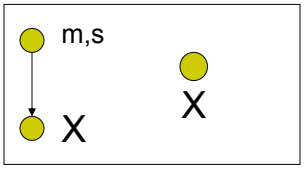
Parametric and nonparametric methods

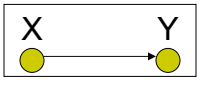
Regression

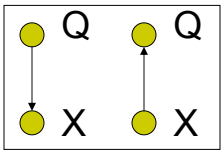
Linear, conditional mixture, nonparametric

Classification

Generative and discriminative approach



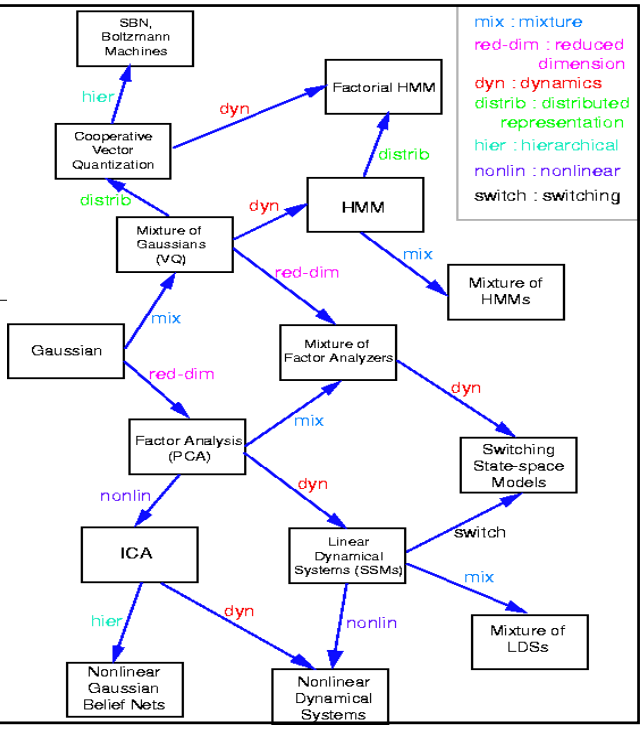




$p(\ldots) = \prod_i p(x_i \mid x_{\pi_i})$

$\log p(\ldots) = \sum_i \log p(x_i \mid x_{\pi_i})$

An (incomplete) genealogy of graphical models



(Picture by Zoubin Ghahramani and Sam Roweis)

Probabilistic Inference

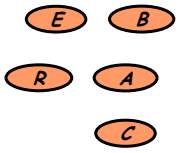
- Computing statistical queries regarding the network, e.g.:
  - Is node X independent on node Y given nodes Z,W ?
  - What is the probability of X=true if (Y=false and Z=true)? $p(X \mid Y, Z)$
  - What is the joint distribution of (X,Y) if Z=false?
  - What is the likelihood of some full assignment?
  - What is the most likely assignment of values to all or a subset the nodes of the network?

- General purpose algorithms exist to fully automate such computation
  - Computational cost depends on the topology of the network
  - Exact inference:
    - The junction tree algorithm
  - Approximate inference;
    - Loopy belief propagation, variational inference, Monte Carlo sampling

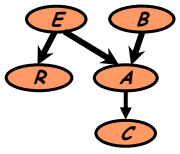
Learning Graphical Models

The goal:

Given set of independent samples (***assignments*** of random variables), find the ***best*** (the most likely?) Bayesian Network (both DAG and CPDs)



(B,E,A,C,R)=(T,F,F,T,F)
(B,E,A,C,R)=(T,F,T,T,F)
……..
(B,E,A,C,R)=(F,T,T,T,F)

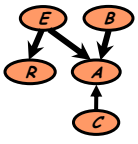


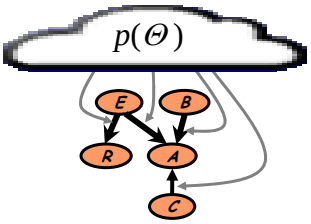
E	B	P(A | E,B)	
e	b	0.9	0.1
e	$\bar{b}$	0.2	0.8
$\bar{e}$	b	0.9	0.1
$\bar{e}$	$\bar{b}$	0.01	0.99

A Bayesian Learning Approach

For model $p(\mathbf{A}|Q)$:

- Treat parameters/model Q as unobserved random variable(s)
- probabilistic statements of Q is conditioned on the values of the observed variables **A**obs





- Bayes' rule: $p(\Theta \mid \mathbf{A}) \propto p(\mathbf{A} \mid \Theta)\, p(\Theta)$
  posterior likelihood prior
- Bayesian estimation: $\Theta_{Bayes} = \int \Theta p(\Theta \mid \mathbf{A}) d\Theta$

Why graphical models

- **Probability theory** provides the **glue** whereby the parts are combined, ensuring that the system as a whole is consistent, and providing ways to interface models to data.
- The **graph theoretic** side of graphical models provides both an intuitively appealing interface by which humans can model highly-interacting sets of variables as well as a data structure that lends itself naturally to the design of efficient general-purpose algorithms.
- **Many of the classical multivariate probabilistic systems** studied in fields such as statistics, systems engineering, information theory, pattern recognition and statistical mechanics **are special cases of the general graphical model formalism**

  -- examples include mixture models, factor analysis, hidden Markov models, Kalman filters and Ising models.
- The graphical model framework provides a way to view all of these systems as instances of a **common underlying formalism**.

--- M. Jordan