CSE 847: Statistical Machine Learning

Graphical Models

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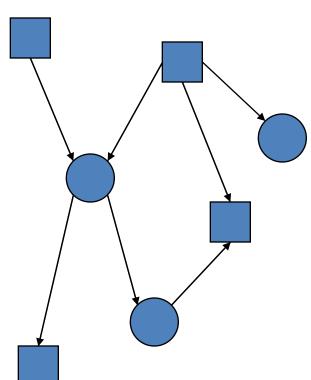
What is a graphical model?

A graphical model is a way of representing probabilistic relationships between random variables.

Conditional (in)dependencies are represented by (missing) edges:

Undirected edges simply give correlations between variables (Markov Random Field or Undirected Graphical model):

Directed edges give causality relationships (Bayesian Network or Directed Graphical Model):



"Graphical models are a marriage between probability theory and graph theory.

They provide a natural tool for dealing with two problems that occur throughout applied mathematics and engineering — uncertainty and complexity —

and in particular they are playing an increasingly important role in the design and analysis of machine learning algorithms.

Fundamental to the idea of a graphical model is the notion of modularity — a complex system is built by combining simpler parts.

The graphical model framework provides a way to view all of these systems as instances of a common underlying formalism.

This view has many advantages -- in particular, specialized techniques that have been developed in one field can be transferred between research communities and exploited more widely.

Moreover, the graphical model formalism provides a natural framework for the design of new systems."

--- Michael Jordan, 1998.

Why can we do with graphical models?

- ☐ Graphs are an intuitive way of representing and visualising the relationships between many variables. (Examples: family trees, electric circuit diagrams, neural networks)
- ☐ Graphical models allow us to define general messagepassing algorithms that implement probabilistic inference efficiently. Thus we can answer queries like "What is P(A|C = c)?" without enumerating all settings of all variables in the model.
- A graph allows us to abstract out the conditional independence relationships between the variables from the details of their parametric forms. Thus we can answer questions like: "Is A dependent on B given that we know the value of C?" just by looking at the graph.

Applications of graphical models

- ☐ Information extraction
- ☐ Speech recognition
- ☐ Computer vision
- ☐ Modeling of gene regulatory networks
- ☐ Gene finding and diagnosis of diseases
- ☐ Graphical models for protein structure

Probability Distributions

- \square Let $X_1,...,X_p$ be discrete random variables
- \square Let P be a joint distribution over $X_1,...,X_p$

 \square If the variables are binary, then we need $O(2^p)$ parameters to describe P

- ☐ Can we do better?
 - ☐ Key idea: use properties of independence

Independent Random Variables

- □Two variables X and Y are independent if
 P(X = x|Y = y) = P(X = x) for all values x, y
 That is, learning the values of Y does not change prediction of X
- ☐ If X and Y are independent then P(X,Y) = P(X|Y)P(Y) = P(X)P(Y)
- □ In general, if $X_1,...,X_p$ are independent, then $P(X_1,...,X_p) = P(X_1)...P(X_p)$

Conditional Independence

- ☐ Unfortunately, most of random variables of interest are not independent of each other
- □A more suitable notion is that of conditional independence
- ☐ Two variables X and Y are conditionally independent given Z if

P(X = x | Y = y,Z=z) = P(X = x | Z=z) for all values x,y,z

That is, learning the values of Y does not change prediction of X once we know the value of Z

notation: $X \perp Y \mid Z$

Example: Naïve Bayesian Model

- ☐A common model in early diagnosis:
 - Symptoms are conditionally independent given the disease (or fault)
- ☐Thus, if
 - X₁,...,X_p denote whether the symptoms exhibited by the patient (headache, high-fever, etc.) and
 - H denotes the hypothesis about the patients health
- then, $P(X_1,...,X_p,H) = P(H)P(X_1|H)...P(X_p|H)_{,}$
- ☐ This **naïve Bayesian** model allows compact representation
 - It does embody strong independence assumptions

Probabilistic Graphical Models I

- ☐ Probabilities play a central role in modern pattern recognition.
- ☐ The probabilistic inference and learning may be complex.
- ☐ It is advantageous to augment the analysis using diagrammatic representations of probability distributions, called probabilistic graphical models.

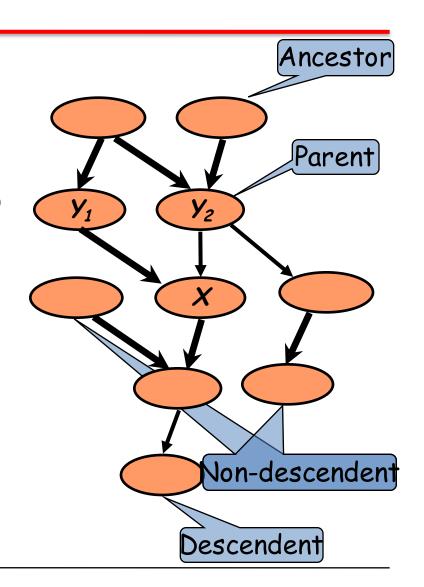
Probabilistic Graphical Models II

☐ Insights into the properties of the model, including conditional independence properties, can be obtained by inspection of the graph.

☐ Complex computations, required to perform inference and learning in sophisticated models, can be expressed in terms of graphical manipulations, in which underlying mathematical expressions are carried along implicitly.

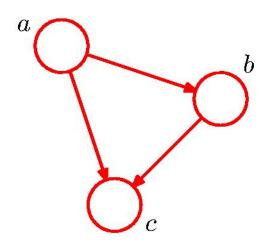
A Few Definitions

- ☐ Nodes (vertices) + links (arcs, edges)
 - ☐ Node: a random variable
 - ☐ Link: a probabilistic relationship
- ☐ Directed graphical models or Bayesian networks.
- ☐ Undirected graphical models or Markov random fields.
- ☐ Factor graphs convenient for solving inference problems



Bayesian Networks

Directed Acyclic Graph (DAG)



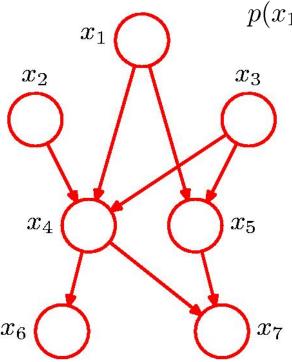
This graph is fully connected because there is a link between every pair of nodes.

$$p(a,b,c) = p(c|a,b)p(a,b) = p(c|a,b)p(b|a)p(a)$$

$$p(x_1,\ldots,x_K) = p(x_K|x_1,\ldots,x_{K-1})\ldots p(x_2|x_1)p(x_1)$$

Bayesian Networks

The absence of links conveys important information about the properties of the class of distributions that the graph represents.



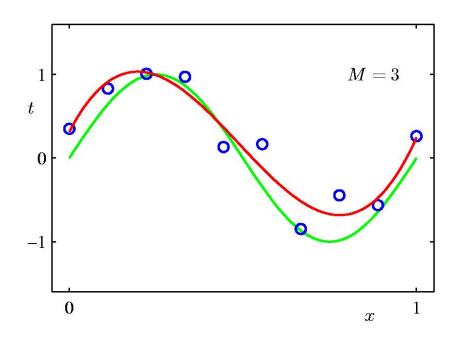
$$p(x_1, \dots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$
$$p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

General Factorization

$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k | \mathbf{pa}_k)$$

Directed acyclic graphs, or DAGs

Bayesian Curve Fitting (1)



Polynomial

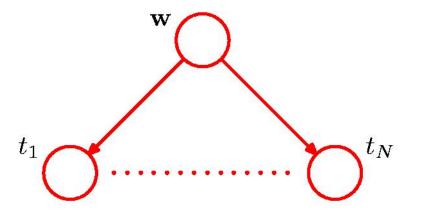
$$y(x, \mathbf{w}) = \sum_{j=0}^{M} w_j x^j$$

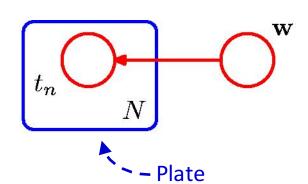
$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{w}) \prod_{n=1}^{N} p(t_n | y(\mathbf{w}, x_n))$$

Random variables: polynomial coefficients w and the observed data t.

Bayesian Curve Fitting (2)

$$p(\mathbf{t}, \mathbf{w}) = p(\mathbf{w}) \prod_{n=1}^{N} p(t_n | y(\mathbf{w}, x_n))$$

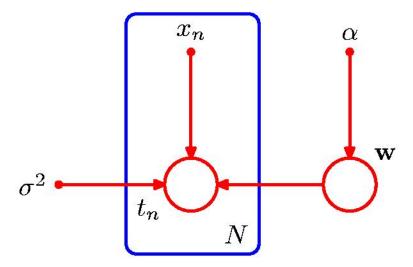




Bayesian Curve Fitting (3)

Input variables and explicit hyperparameters

$$p(\mathbf{t}, \mathbf{w} | \mathbf{x}, \alpha, \sigma^2) = p(\mathbf{w} | \alpha) \prod_{n=1}^{N} p(t_n | \mathbf{w}, x_n, \sigma^2).$$

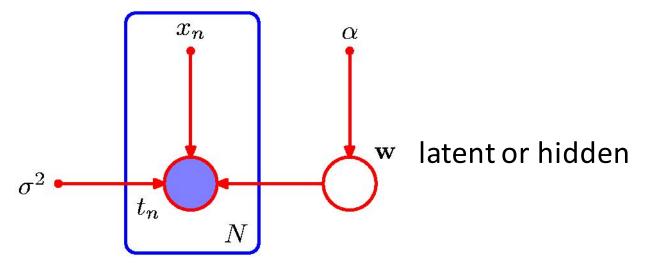


Deterministic parameters shown by small nodes

Bayesian Curve Fitting—Learning

Condition on data

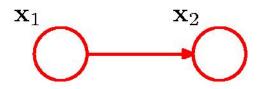
$$p(\mathbf{w}|\mathbf{t}) \propto p(\mathbf{w}) \prod_{n=1}^{N} p(t_n|\mathbf{w})$$



Shaded nodes are set to observed values

Discrete Variables (1)

General joint distribution: K^{2} { 1 parameters



$$p(\mathbf{x}_1, \mathbf{x}_2 | \boldsymbol{\mu}) = \prod_{k=1}^K \prod_{l=1}^K \mu_{kl}^{x_{1k} x_{2l}}$$

Independent joint distribution: $2(K \{ 1) \text{ parameters})$

$$\mathbf{x}_1$$

$$\sum_{i=1}^{n}$$

$$\hat{p}(\mathbf{x}_1, \mathbf{x}_2 | \boldsymbol{\mu}) = \prod_{k=1}^K \mu_{1k}^{x_{1k}} \prod_{l=1}^K \mu_{2l}^{x_{2l}}$$

Discrete Variables (2)

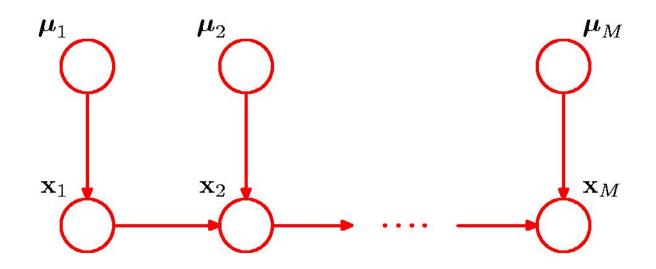
General joint distribution over M variables: $K^M \ \{ \ 1 \ parameters \ \}$

M -node Markov chain: K { 1+(M { $1)}$ K(K { $1)}$ parameters



Sparse connectivity results in fewer parameters.

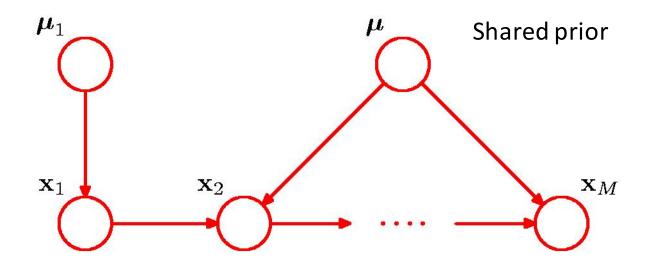
Discrete Variables: Bayesian Parameters (1)



$$p(\{\mathbf{x}_m, \boldsymbol{\mu}_m\}) = p(\mathbf{x}_1 | \boldsymbol{\mu}_1) p(\boldsymbol{\mu}_1) \prod_{m=2}^{M} p(\mathbf{x}_m | \mathbf{x}_{m-1}, \boldsymbol{\mu}_m) p(\boldsymbol{\mu}_m)$$

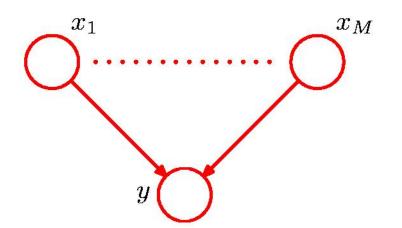
$$p(\boldsymbol{\mu}_m) = \operatorname{Dir}(\boldsymbol{\mu}_m | \boldsymbol{\alpha}_m)$$

Discrete Variables: Bayesian Parameters (2)



$$p(\{\mathbf{x}_m\}, \boldsymbol{\mu}_1, \boldsymbol{\mu}) = p(\mathbf{x}_1 | \boldsymbol{\mu}_1) p(\boldsymbol{\mu}_1) \prod_{m=2}^{M} p(\mathbf{x}_m | \mathbf{x}_{m-1}, \boldsymbol{\mu}) p(\boldsymbol{\mu})$$

Parameterized Conditional Distributions



If x_1,\ldots,x_M are discrete, K-state variables, $p(y=1|x_1,\ldots,x_M)$ in general has $O(K^M)$ parameters.

The parameterized form (more restricted form of conditional distribution)

$$p(y = 1|x_1, \dots, x_M) = \sigma\left(w_0 + \sum_{i=1}^M w_i x_i\right) = \sigma(\mathbf{w}^T \mathbf{x})$$

requires only M+1 parameters

Linear-Gaussian Models

Directed Graph

$$p(x_i|pa_i) = \mathcal{N}\left(x_i \left| \sum_{j \in pa_i} w_{ij} x_j + b_i, v_i \right)\right)$$

Each node is Gaussian, the mean is a linear function of the parents.

Vector-valued Gaussian Nodes

$$p(\mathbf{x}_i|\mathrm{pa}_i) = \mathcal{N}\left(\mathbf{x}_i\left|\sum_{j\in\mathrm{pa}_i}\mathbf{W}_{ij}\mathbf{x}_j + \mathbf{b}_i, \mathbf{\Sigma}_i
ight)$$

Conditional Independence

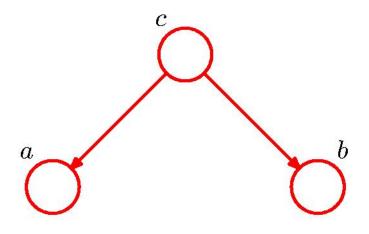
a is independent of b given c

$$p(a|b,c) = p(a|c)$$

$$p(a,b|c) = p(a|b,c)p(b|c)$$
$$= p(a|c)p(b|c)$$

Notation

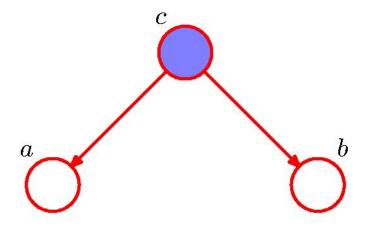
$$a \perp \!\!\!\perp b \mid c$$



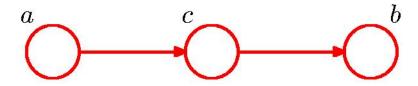
$$p(a, b, c) = p(a|c)p(b|c)p(c)$$

$$p(a,b) = \sum_{c} p(a|c)p(b|c)p(c)$$

$$a \not\perp \!\!\!\perp b \mid \emptyset$$



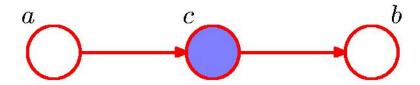
$$p(a, b|c) = \frac{p(a, b, c)}{p(c)}$$
$$= p(a|c)p(b|c)$$
$$a \perp \!\!\! \perp b \mid c$$



$$p(a, b, c) = p(a)p(c|a)p(b|c)$$

$$p(a,b) = p(a) \sum_{c} p(c|a)p(b|c) = p(a)p(b|a)$$

$$a \not\perp \!\!\!\perp b \mid \emptyset$$

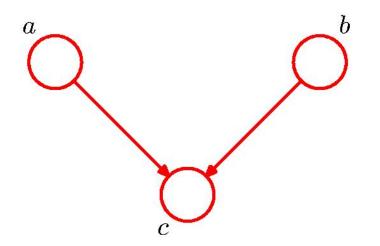


$$p(a,b|c) = \frac{p(a,b,c)}{p(c)}$$

$$= \frac{p(a)p(c|a)p(b|c)}{p(c)}$$

$$= p(a|c)p(b|c)$$

$$a \perp \!\!\!\perp b \mid c$$

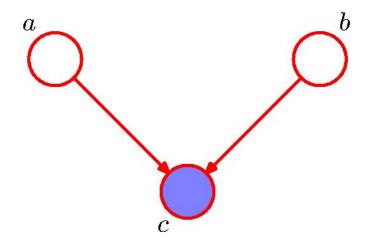


$$p(a,b,c) = p(a)p(b)p(c|a,b)$$

$$p(a,b) = p(a)p(b)$$

$$a \perp \!\!\!\perp b \mid \emptyset$$

Note: this is the opposite of Example 1, with c unobserved.



$$p(a,b|c) = \frac{p(a,b,c)}{p(c)}$$
$$= \frac{p(a)p(b)p(c|a,b)}{p(c)}$$

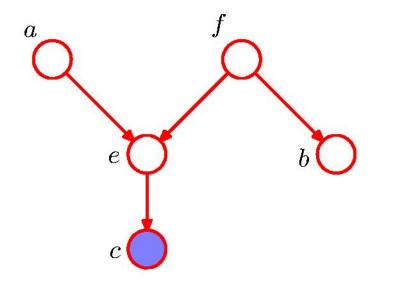
 $a \not\perp \!\!\!\perp b \mid c$

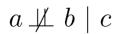
Note: this is the opposite of Example 1, with c observed.

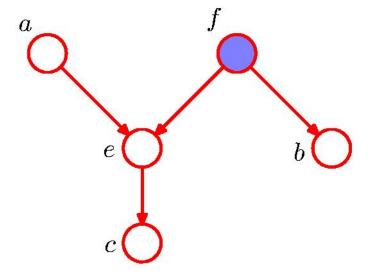
D-separation

- A, B, and C are non-intersecting subsets of nodes in a directed graph.
- A path from A to B is blocked if it contains a node such that either
 - a) the arrows on the path meet either head-to-tail or tailto-tail at the node, and the node is in the set C, or
 - b) the arrows meet head-to-head at the node, and neither the node, nor any of its descendants, are in the set C.
- If all paths from A to B are blocked, A is said to be d-separated from B by C.
- If A is d-separated from B by C, the joint distribution over all variables in the graph satisfies $A \perp \!\!\! \perp B \mid C$.

D-separation: Example

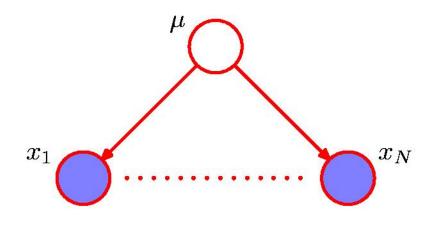






$$a \perp \!\!\! \perp b \mid f$$

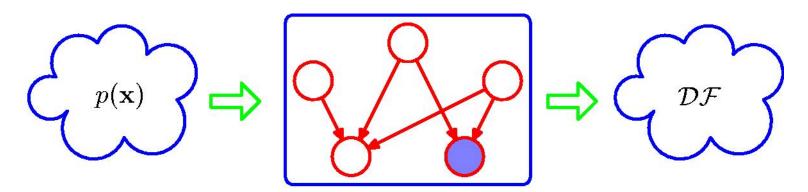
D-separation: I.I.D. Data



$$p(\mathcal{D}|\mu) = \prod_{n=1}^{N} p(x_n|\mu)$$

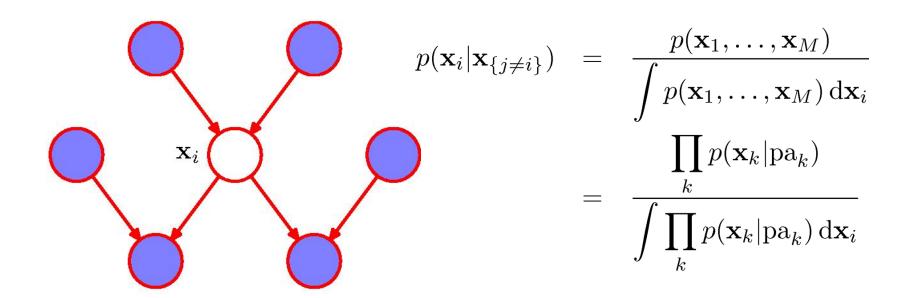
$$p(\mathcal{D}) = \int_{-\infty}^{\infty} p(\mathcal{D}|\mu) p(\mu) d\mu \neq \prod_{n=1}^{N} p(x_n)$$

Directed Graphs as Distribution Filters



- \square We can view a graphical model as a filter in which a probability distribution p(x) is allowed through the filter if, and only if, it satisfies the directed factorization property .
 - ☐ The set of all possible probability distributions p(x) that pass through the filter is denoted DF.
- ☐ We can alternatively use the graph to filter distributions according to whether they respect all of the conditional independencies implied by the d-separation properties of the graph.

The Markov Blanket

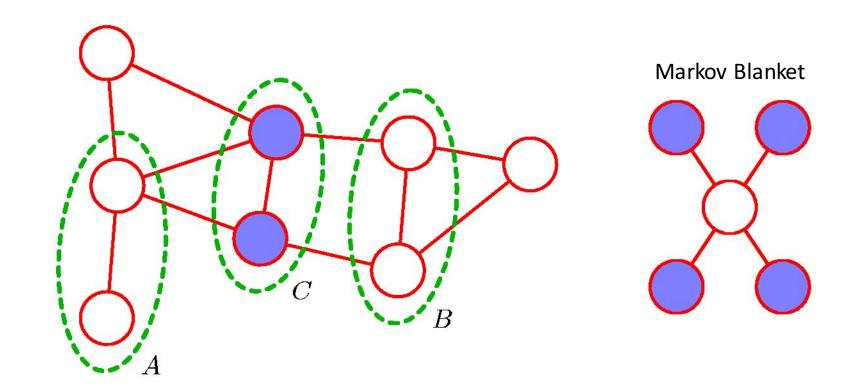


Factors independent of x_i cancel between numerator and denominator.

Conditional Independence

- ☐ Conditional independence properties simplify both the structure of a model and the computations needed to perform inference and learning under that model.
- ☐ Given an expression for the joint distribution, we can check conditional independence by repeated application of the sum and product rules of probability.
- ☐ An important and elegant feature of graphical models is that conditional independence properties of the joint distribution can be read directly from the graph.

Markov Random Fields



 $A \perp \!\!\! \perp B | C$

Markov random field, also known as Markov network or undirected graphical model

Factorization (1)

- ☐ In directed graphical models, the joint distribution can be factored as the product of conditional distributions.
- Seek a factorization rule for undirected graphs that will correspond to the above conditional independence test.
 - ☐ Express the joint distribution p(x) as a product of functions defined over sets of variables that are local to the graph.

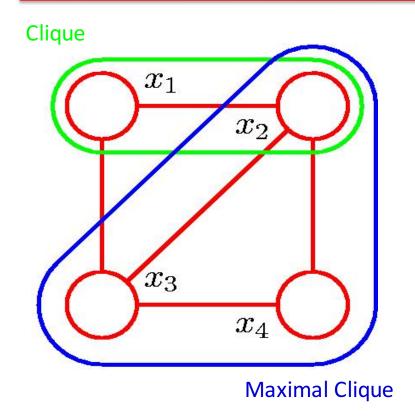
Factorization (2)

- □ Consider two nodes x_i and x_j that are not connected by a link:
 - ☐ They are conditionally independent given all other nodes in the graph.

$$p(x_i, x_j | \mathbf{x}_{\backslash \{i,j\}}) = p(x_i | \mathbf{x}_{\backslash \{i,j\}}) p(x_j | \mathbf{x}_{\backslash \{i,j\}})$$

 \square In the factorization of the joint distribution, x_i and x_j do not appear in the same factor.

Cliques and Maximal Cliques



- Olique is defined as a subset of the nodes in a graph such that there exists a link between all pairs of nodes in the subset.
- □A maximal clique is a clique such that it is not possible to include any other nodes from the graph in the set without it ceasing to be a clique.
- ☐ Define the factors in the decomposition of the joint distribution to be functions of the variables in the cliques.

Joint Distribution (1)

lacksquare Express the joint distribution as $p(\mathbf{x}) = rac{1}{Z} \prod_C \psi_C(\mathbf{x}_C)$

where $\psi_C(\mathbf{x}_C)$ is the potential over clique C and the partition function Z:

$$Z = \sum_{\mathbf{x}} \prod_{C} \psi_C(\mathbf{x}_C)$$

is the normalization coefficient.

- ☐ We do not restrict the choice of potential functions to those that have a specific probabilistic interpretation as marginal or conditional distributions.
- One consequence of the generality of the potential functions is that their product will in general not be correctly normalized.
 - \square M K-state variables \rightarrow K^M terms in Z.

Joint Distribution (2)

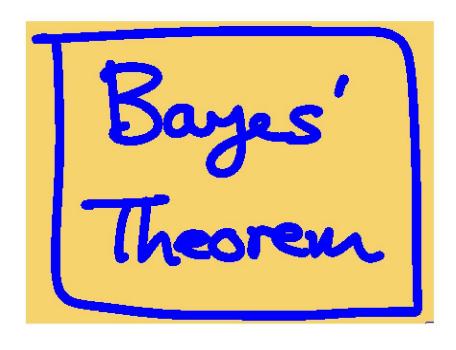
- We are restricted to potential functions which are strictly positive
- ☐ Energies and the Boltzmann distribution

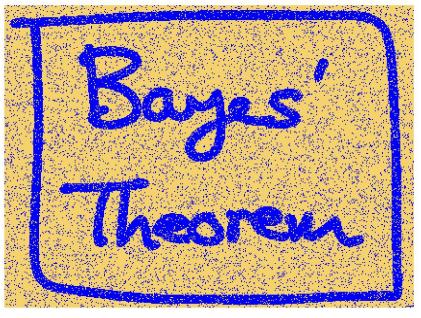
Energy function

$$\psi_C(\mathbf{x}_C) = \exp\left\{-E(\mathbf{x}_C)\right\}$$

- ☐ The potentials in an undirected graph do not have a specific probabilistic interpretation. (greater flexibility)
- ☐ How to motivate a choice of potential function for a particular application?
 - ☐ Find a good balance in satisfying the (possibly conflicting) influences of the clique potentials.

Illustration: Image De-Noising (1)



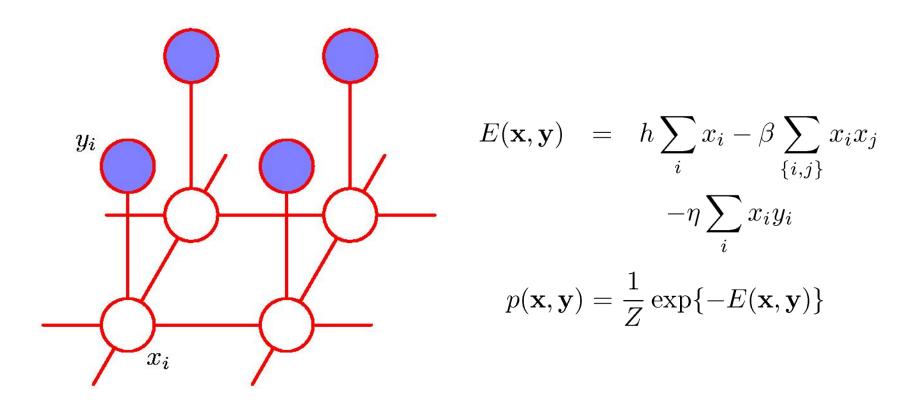


Original Image

Noisy Image

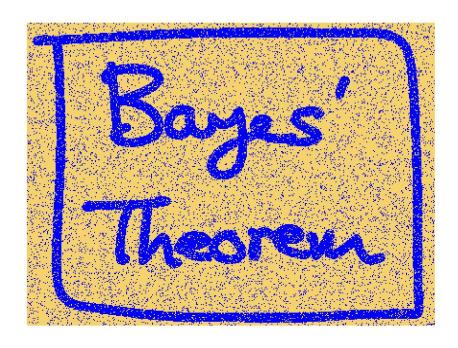
flipping the sign of the pixels with probability 10%

Illustration: Image De-Noising (2)

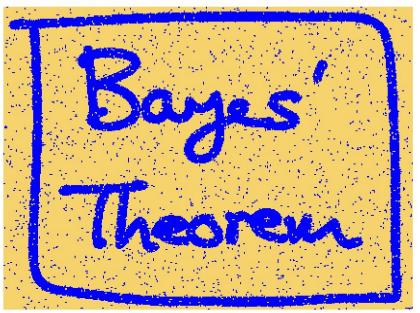


Iterated conditional modes, or ICM: coordinate-wise gradient ascent

Illustration: Image De-Noising (3)



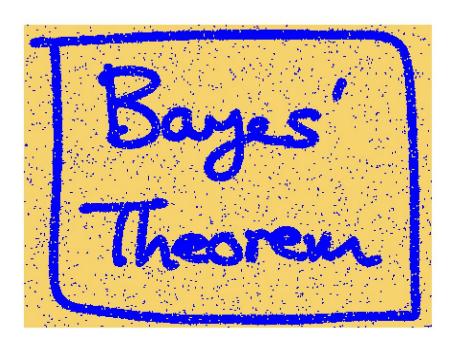
Noisy Image



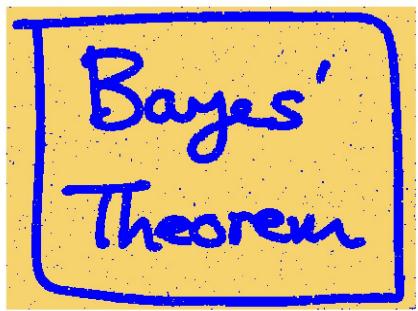
Restored Image (ICM)

$$\beta = 1.0$$
, $\eta = 2.1$, $h = 0$.

Illustration: Image De-Noising (4)

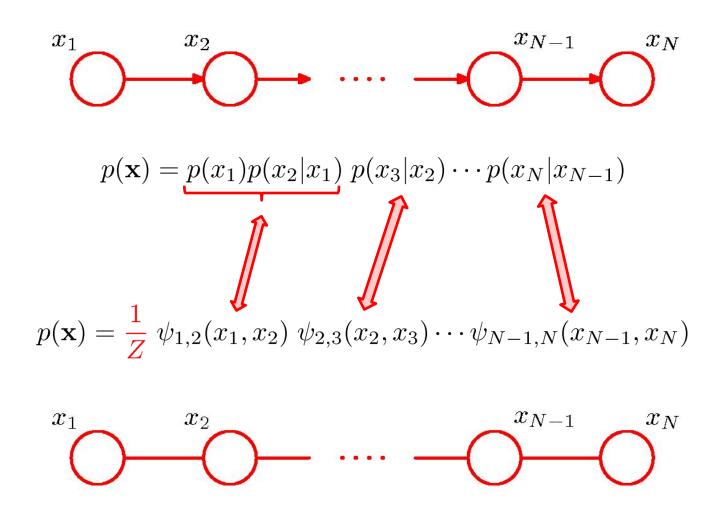


Restored Image (ICM)



Restored Image (Graph cuts)

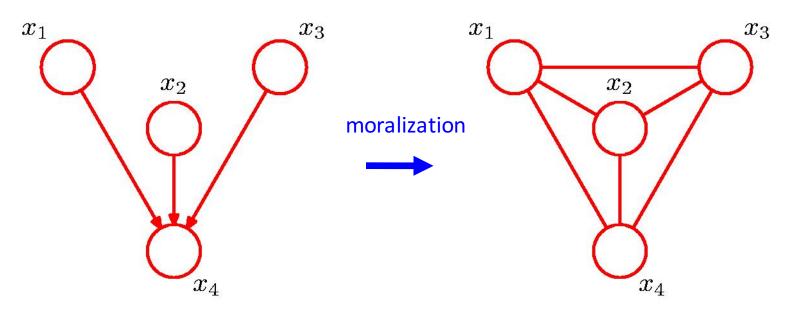
Converting Directed to Undirected Graphs (1)



Converting Directed to Undirected Graphs (2)

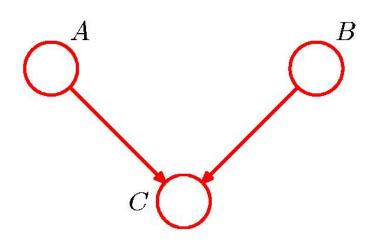
Additional links

moral graph

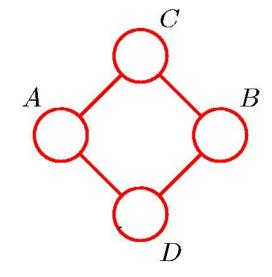


$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)$$
$$= \frac{1}{Z}\psi_A(x_1, x_2, x_3)\psi_B(x_2, x_3, x_4)\psi_C(x_1, x_2, x_4)$$

Directed vs. Undirected Graphs



$$A \perp \!\!\!\perp B \mid \emptyset$$
 $A \perp \!\!\!\!\perp B \mid C$



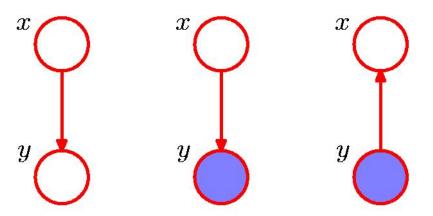
$$A \not\perp \!\!\!\perp B \mid \emptyset$$

$$A \perp \!\!\!\!\perp B \mid C \cup D$$

$$C \perp \!\!\!\!\perp D \mid A \cup B$$

Inference in Graphical Models

- ☐ Inference in graphical models
 - □Some of the nodes in a graph are clamped to observed values, and we wish to compute the posterior distributions of one or more subsets of other nodes.



$$p(y) = \sum_{x'} p(y|x')p(x') \qquad p(x|y) = \frac{p(y|x)p(x)}{p(y)}$$



$$p(\mathbf{x}) = \frac{1}{Z}\psi_{1,2}(x_1, x_2)\psi_{2,3}(x_2, x_3)\cdots\psi_{N-1,N}(x_{N-1}, x_N)$$

$$p(x_n) = \sum_{x_1} \cdots \sum_{x_{n-1}} \sum_{x_{n+1}} \cdots \sum_{x_N} p(\mathbf{x})$$

- ☐ In a naive implementation, we would first evaluate the joint distribution and then perform the summations explicitly.
 - \square N variables each with K states => there are K^N values for **x**

□Obtain a much more efficient algorithm by exploiting the conditional independence properties of the graphical model.

■ Key Idea: Rearrange the order of the summations and the multiplications to allow the required marginal to be evaluated much more efficiently.

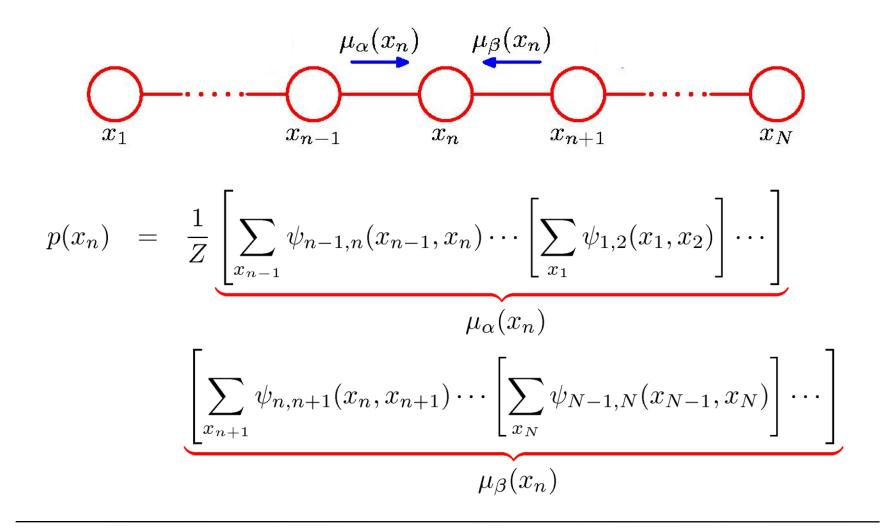
$$p(\mathbf{x}) = \frac{1}{Z} \psi_{1,2}(x_1, x_2) \psi_{2,3}(x_2, x_3) \cdots \psi_{N-1,N}(x_{N-1}, x_N)$$
$$p(x_n) = \sum_{x_1} \cdots \sum_{x_{n-1}} \sum_{x_{n+1}} \cdots \sum_{x_N} p(\mathbf{x})$$

Consider for instance the summation over x_N :

$$\mu_{\beta}(x_{N-1}) \Leftarrow \sum_{x_N} \psi_{N-1,N}(x_{N-1},x_N)$$
 Only one that depends on x_N

$$\mu_{\beta}(x_{N-2}) \Leftarrow \sum_{x_{N-1}} \psi_{N-2,N-1}(x_{N-2},x_{N-1}) \mu_{\beta}^{\bullet}(x_{N-1})$$

Each summation effectively removes a variable from the distribution. This can be viewed as the removal of a node from the graph.



$$\mu_{\alpha}(x_{n-1}) \qquad \mu_{\alpha}(x_n) \qquad \mu_{\beta}(x_n) \qquad \mu_{\beta}(x_{n+1})$$

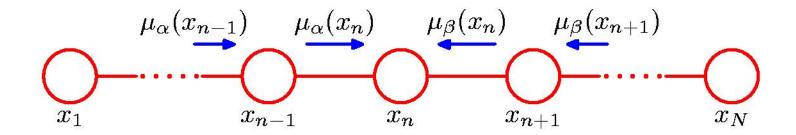
$$x_{n-1} \qquad x_n \qquad x_{n+1} \qquad x_n$$

$$\mu_{\alpha}(x_n) = \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \left[\sum_{x_{n-2}} \cdots \right]$$

$$= \sum_{x_{n-1}} \psi_{n-1,n}(x_{n-1}, x_n) \mu_{\alpha}(x_{n-1}).$$

$$\mu_{\beta}(x_n) = \sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \left[\sum_{x_{n+2}} \cdots \right]$$

$$= \sum_{x_{n+1}} \psi_{n,n+1}(x_n, x_{n+1}) \mu_{\beta}(x_{n+1}).$$



$$\mu_{\alpha}(x_2) = \sum_{x_1} \psi_{1,2}(x_1, x_2)$$

$$\mu_{\beta}(x_{N-1}) = \sum_{x_N} \psi_{N-1,N}(x_{N-1}, x_N)$$

$$Z = \sum_{x_n} \mu_{\alpha}(x_n) \mu_{\beta}(x_n)$$

Total time complexity: $O(NK^2)$. This is linear in the length of the chain, in contrast to the exponential cost of a naive approach.

We now try to understand the simple chain example using first-order principles



Using definition of probability, we have

$$P(e) = \sum_{a} \sum_{c} \sum_{b} \sum_{a} P(a,b,c,d,e)$$



By chain decomposition, we get

$$P(e) = \sum_{a} \sum_{c} \sum_{b} \sum_{a} P(a,b,c,d,e)$$

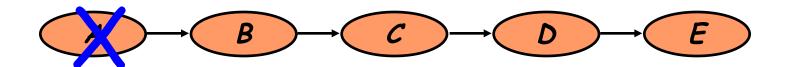
$$= \sum_{a} \sum_{c} \sum_{b} \sum_{a} P(a)P(b \mid a)P(c \mid b)P(d \mid c)P(e \mid d)$$



Rearranging terms ...

$$P(e) = \sum_{d} \sum_{c} \sum_{b} \sum_{a} P(a)P(b | a)P(c | b)P(d | c)P(e | d)$$

$$= \sum_{d} \sum_{c} \sum_{b} P(c | b)P(d | c)P(e | d) \sum_{a} P(a)P(b | a)$$

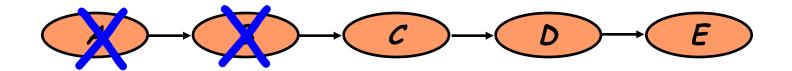


Now we can perform innermost summation

$$P(e) = \sum_{d} \sum_{c} \sum_{b} P(c \mid b) P(d \mid c) P(e \mid d) \sum_{a} P(a) P(b \mid a)$$

$$= \sum_{d} \sum_{c} \sum_{b} P(c \mid b) P(d \mid c) P(e \mid d) p(b)$$

This summation, is exactly the first step in the forward iteration we describe before



Rearranging and then summing again, we get

$$P(e) = \sum_{d} \sum_{c} \sum_{b} P(c \mid b) P(d \mid c) P(e \mid d) p(b)$$

$$= \sum_{d} \sum_{c} P(d \mid c) P(e \mid d) \sum_{b} P(c \mid b) p(b)$$

$$= \sum_{d} \sum_{c} P(d \mid c) P(e \mid d) p(c)$$

To compute local marginals:

- Compute and store all forward messages, $\mu_{\alpha}(x_n)$.
- Compute and store all backward messages, $\mu_{\beta}(x_n)$.
- Compute Z at any node x_m
- Compute

$$p(x_n) = \frac{1}{Z} \mu_{\alpha}(x_n) \mu_{\beta}(x_n)$$

for all variables required.

Inference on a Chain: Summary

- □ Exact inference on a graph comprising a chain of nodes can be performed efficiently
 - ☐ Message passing along the chain
- ☐ This can't be extended to an arbitrary graph.
- □Inference can be performed efficiently using local message passing on a broader class of graphs called trees.
 - □Sum-product algorithm