# Probabilistic Graphical Models 

CMSC 478
UMBC

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A graph G that represents a probability distribution over random variables $X_{1}, \ldots, X_{N}$

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Graph $\mathrm{G}=($ vertices V , edges E )
Distribution $p\left(X_{1}, \ldots, X_{N}\right)$

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Vertices $\leftrightarrow$ random variables
Edges show dependencies among random variables

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> Graph $\mathrm{G}=($ vertices V , edges E$)$ Distribution $p\left(X_{1}, \ldots, X_{N}\right)$

Vertices $\leftrightarrow$ random variables
Edges show dependencies among random variables

Two main flavors: directed graphical models and undirected graphical models

## Outline

Directed Graphical Models Naïve Bayes

Undirected Graphical Models

> Factor Graphs
> Ising Model

Message Passing: Graphical Model Inference

## Directed Graphical Models

A directed (acyclic) graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents a probability distribution over random variables

$$
X_{1}, \ldots, X_{N}
$$

Joint probability factorizes into factors of $X_{i}$ conditioned on the parents of $X_{i}$

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Joint probability factorizes into factors of $X_{i}$ conditioned on the parents of $X_{i}$

Benefit: read the independence properties are transparent

## Directed Graphical Models

A directed (acyclic) graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents a probability distribution over random variables

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X_{1}, \ldots, X_{N}
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Joint probability factorizes into factors of $X_{i}$ conditioned on the parents of $X_{i}$

A graph/joint distribution that follows this is a Bayesian network

## Bayesian Networks: Directed Acyclic Graphs



$$
p\left(x_{1}, x_{2}, x_{\left.3, \ldots, x_{N}\right)=\prod_{i} p\left(x_{i} \mid \pi\left(x_{i}\right)\right),}^{\substack{\text { "parents of" } \\ \text { topological } \\ \text { sort }}} \mid\right.
$$

## Bayesian Networks: <br> Directed Acyclic Graphs



$$
\begin{aligned}
& p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\prod_{i} p\left(x_{i} \mid \pi\left(x_{i}\right)\right) \\
& p\left(x_{1}, x_{2}, x_{3}, x_{4}, x_{5}\right)=? ? ?
\end{aligned}
$$

## Bayesian Networks: <br> Directed Acyclic Graphs


$p\left(x_{1}, x_{2}, x_{3}, x_{4}, x_{5}\right)=$
$p\left(x_{1}\right) p\left(x_{3}\right) p\left(x_{2} \mid x_{1}, x_{3}\right) p\left(x_{4} \mid x_{2}, x_{3}\right) p\left(x_{5} \mid x_{2}, x_{4}\right)$

## Bayesian Networks: <br> Directed Acyclic Graphs



$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\prod_{i} p\left(x_{i} \mid \pi\left(x_{i}\right)\right)
$$

exact inference in general DAGs is NP-hard inference in trees can be exact

A smell of sulphur (S) can be caused either by rotten eggs (E) or as a sign of the doom brought by the Mayan Apocalypse (M). The Mayan Apocalypse also causes the oceans to boil (B). The Bayesian network and corresponding conditional probability tables for this situation are shown below. The notation $+x$ means that $x$ is true, and $-x$ means that $x$ is false. For each part, you should give either a numerical answer (e.g., 0.81 ) or an arithmetic expression in terms of numbers from the tables below (e.g., $0.9{ }^{*} 0.9$ ). Note that the latter is easier and perfectly OK.

| $P(E)$ |  |
| :---: | :---: |
| $+e$ | 0.4 |
| $-e$ | 0.6 |


| $P(S \mid E, M)$ |  |  |  |
| :---: | :---: | :---: | :---: |
| $+e$ | $+m$ | $+s$ | 1.0 |
| $+e$ | $+m$ | $-s$ | 0.0 |
| $+e$ | $-m$ | $+s$ | 0.8 |
| $+e$ | $-m$ | $-s$ | 0.2 |
| $-e$ | $+m$ | $+s$ | 0.3 |
| $-e$ | $+m$ | $-s$ | 0.7 |
| $-e$ | $-m$ | $+s$ | 0.1 |
| $-e$ | $-m$ | $-s$ | 0.9 |



| $P(M)$ |  |
| :---: | :---: |
| $+m$ | 0.1 |
| $-m$ | 0.9 |


| $P(B \mid M)$ |  |  |
| :---: | :---: | :---: |
| $+m$ | $+b$ | 1.0 |
| $+m$ | $-b$ | 0.0 |
| $-m$ | $+b$ | 0.1 |
| $-m$ | $-b$ | 0.9 |

(A) (X points) Compute the following entry from the joint distribution: $P(-e,-s,-m,-b)$
(B) (X points) What is the probability that the oceans boil?

## Directed Graphical Model Notation



## D-Separation: Testing for Conditional Independence

## d-separation

$X \& Y$ are d-separated if for all paths $P$, one of the following is true:

Variables X \& Y are conditionally
independent given $Z$ if all (undirected) paths from (any variable in) $X$ to (any variable in) $Y$ are d-separated by Z
$P$ has a chain with an observed middle node


P has a fork with an observed parent node

$P$ includes a " $v$-structure" or "collider" with all unobserved descendants


## D-Separation: Testing for Conditional Independence

Variables $X \& Y$ are conditionally independent given $Z$ if all (undirected) paths from (any variable in) $X$ to (any variable in) $Y$ are d-separated by $Z$
observing Z blocks the path from $X$ to $Y$
observing Z blocks the path from $X$ to $Y$
not observing $Z$ blocks the path from $X$ to $Y$

## d-separation

$X \& Y$ are d-separated if for all paths $P$, one of the following is true:
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## d-separation

$X \& Y$ are d-separated if for all paths $P$, one of the following is true:
$P$ has a chain with an observed middle node
 the path from $X$ to $Y$
observing Z blocks
the path from $X$ to $Y$
P has a fork with an observed parent node


P includes a " v -structure" or "collider" with all unobserved descendants

> not observing $Z$ blocks the path from $X$ to $Y$ $p(x, y, z)=p(x) p(y) p(z \mid x, y)$ $p(x, y)=\sum_{Z} p(x) p(y) p(z \mid x, y)=p(x) p(y)$


## Outline

Directed Graphical Models
Naïve Bayes

Undirected Graphical Models

> Factor Graphs
> Ising Model

Message Passing: Graphical Model Inference

## Naïve Bayes

## $\operatorname{argmax}_{Y} p(Y \mid X)$

Apply Bayes rule and take logs

## $\operatorname{argmax}_{Y} \log p(X \mid Y)+\log p(Y)$

likelihood
prior

## Naïve Bayes

## $\operatorname{argmax}_{Y} p(Y \mid X)$



Apply Bayes rule and take logs
$\operatorname{argmax}_{Y} \log p(X \mid Y)+\log p(Y)$

Represent $X$ is a D-dimensional vector (of features):
$X=\left(X_{1}, X_{2}, X_{3}, \ldots, X_{D}\right)$

## Naïve Bayes

## $\operatorname{argmax}_{Y} p(Y \mid X)$



Apply Bayes rule and take logs
$\operatorname{argmax}_{Y} \log p(X \mid Y)+\log p(Y)$


Naively generate each "feature" of $X$, conditioned on $Y$
D
$\operatorname{argmax}_{Y}$

$$
\log p\left(X_{j} \mid Y\right)+\log p(Y)
$$

$$
\overline{j=1}
$$

## The Bag of Words Representation

I love this movie! It's sweet, but with satirical humor. The dialogue is great and the adventure scenes are fun... It manages to be whimsical and romantic while laughing at the conventions of the fairy tale genre. I would recommend it to just about anyone. I've seen it several times, and I'm always happy to see it again whenever I have a friend who hasn't seen it yet!

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| , | 6 |
| :---: | :---: |
| 1 | 5 |
| the | 4 |
| to | 3 |
| and | 3 |
| seen | 2 |
| yet |  |
| would | 1 |
| whimsical |  |
| times |  |
| sweet |  |
| satirical |  |
| adventure |  |
| genre |  |
| fairy |  |
| humor |  |
| have | 1 |
| great | 1 |

## Bag of Words Representation



## Naïve Bayes: A Generative Story

Generative Story
$\phi=$ distribution over $K$ labels for label $k=1$ to $K$ :
$p(y=k)$
$\theta_{k}=$ generate parameters
$p\left(x_{i j} \mid y=k\right)$
global
parameters

$$
\sum_{j=1}^{D} \log p\left(X_{i j} \mid Y_{i}\right)+\log p\left(Y_{i}\right)
$$

## Naïve Bayes: A Generative Story

## Generative Story

$\phi=$ distribution over $K$ labels
for label $k=1$ to $K$ :

$$
\theta_{k}=\text { generate parameters }
$$

for item $i=1$ to $N$ :

$$
y_{i} \sim \operatorname{Cat}(\phi)
$$

## Naïve Bayes: A Generative Story

Generative Story
$\phi=$ distribution over $K$ labels for label $k=1$ to $K$ :
$\theta_{k}=$ generate parameters
for item $i=1$ to $N$ :

$$
y_{i} \sim \operatorname{Cat}(\phi)
$$


local
variables for each feature $j$

$$
x_{i j} \sim \mathrm{~F}_{j}\left(\theta_{y_{i}}\right)
$$

Generate each feature based on the label

$$
\sum_{j=1}^{D} \log p\left(X_{i j} \mid Y_{i}\right)+\log p\left(Y_{i}\right)
$$

## Naïve Bayes: A Generative Story

Generative Story
$\phi=$ distribution over $K$ labels for label $k=1$ to $K$ :
$\theta_{k}=$ generate parameters
for item $i=1$ to $N$ :
$y_{i} \sim \operatorname{Cat}(\phi)$
for each feature $j$

$$
x_{i j} \sim \mathrm{~F}_{j}\left(\theta_{y_{i}}\right)
$$


each $x_{i j}$ is conditionally
independent of one
another (given the label)

$$
\sum_{j=1}^{D} \log p\left(X_{i j} \mid Y_{i}\right)+\log p\left(Y_{i}\right)
$$

## Naïve Bayes: A Generative Story

Generative Story
$\phi=$ distribution over $K$ labels for label $k=1$ to $K$ :
$\theta_{k}=$ generate parameters
for item $i=1$ to $N$ :
$y_{i} \sim \operatorname{Cat}(\phi)$
for each feature $j$

$$
x_{i j} \sim \mathrm{~F}_{j}\left(\theta_{y_{i}}\right)
$$

Maximize Log-likelihood

$$
\begin{gathered}
\mathcal{L}(\theta)=\sum_{i} \sum_{j} \log F_{y_{i}}\left(x_{i j} ; \theta_{y_{i}}\right)+\sum_{i} \log \phi_{y_{i}} \text { s. t. } \\
\sum_{k} \phi_{k}=1 \quad \phi_{k} \geq 0
\end{gathered} \quad \theta_{k} \text { is valid for } F_{j} .
$$

## Multinomial Naïve Bayes: A Generative Story

Generative Story
$\phi=$ distribution over $K$ labels
for label $k=1$ to $K$ :
$\theta_{k}=$ distribution over J feature values
for item $i=1$ to $N$ :
$y_{i} \sim \operatorname{Cat}(\phi)$
for each feature $j$

$$
x_{i j} \sim \operatorname{Cat}\left(\theta_{y_{i}}\right)
$$

Maximize Log-likelihood

$$
\begin{aligned}
\mathcal{L}(\theta)= & \sum_{i} \sum_{j} \log \theta_{y_{i}, x_{i, j}}+\sum_{i} \log \phi_{y_{i}} \text { s.t. } \\
& \sum_{k} \phi_{k}=1 \quad \phi_{k} \geq 0 \quad \sum_{j} \theta_{k j}=1 \forall k \quad \theta_{k j} \geq 0,
\end{aligned}
$$

## Multinomial Naïve Bayes: A Generative Story

Generative Story
$\phi=$ distribution over $K$ labels
for label $k=1$ to $K$ :
$\theta_{k}=$ distribution over J feature values
for item $i=1$ to $N$ :
$y_{i} \sim \operatorname{Cat}(\phi)$
for each feature $j$

$$
x_{i j} \sim \operatorname{Cat}\left(\theta_{y_{i}, j}\right)
$$

Maximize Log-likelihood via Lagrange Multipliers ( $\geq \mathbf{0}$ constraints not shown)
$=\sum_{i} \sum_{j} \log \theta_{y_{i}, x_{i, j}}+\sum_{i} \log \phi_{y_{i}}-\mu\left(\sum_{k} \phi_{k}-1\right)-\sum_{k} \lambda_{k}\left(\sum_{j} \theta_{k j}-1\right)$

## Multinomial Naïve Bayes: Learning

Calculate class priors
For each $k$ :
items ${ }_{k}=$ all items with class $=k$

Calculate feature generation terms For each $k$ :
obs $_{k}=$ single object containing all items labeled as $k$

For each feature $j$

$$
n_{k j}=\# \text { of occurrences of } j \text { in obs } k
$$

$$
p(k)=\frac{\mid \text { items }_{k} \mid}{\# \text { items }}
$$

Brill and Banko (2001)
With enough data, the classifier may not matter


## Summary: Naïve Bayes is Not So Naïve, but not without issue

## Pro

Very Fast, low storage requirements

Robust to Irrelevant Features

Very good in domains with many equally important features

Optimal if the independence assumptions hold

Dependable baseline for text classification (but often not the best)

## Con

Model the posterior in one go? (e.g., use conditional maxent)

Are the features really uncorrelated?

Are plain counts always appropriate?

Are there "better" ways of handling missing/noisy data?
(automated, more principled)

## Outline

Directed Graphical Models Naïve Bayes

Undirected Graphical Models

$$
\begin{aligned}
& \text { Factor Graphs } \\
& \text { Ising Model }
\end{aligned}
$$

Message Passing: Graphical Model Inference

## Undirected Graphical Models

An undirected graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents a probability distribution over random variables

$$
X_{1}, \ldots, X_{N}
$$

Joint probability factorizes based on cliques in the graph

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An undirected graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents a probability distribution over random variables

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Joint probability factorizes based on cliques in the graph

Common name: Markov Random Fields

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An undirected graph $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents a probability distribution over random variables

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X_{1}, \ldots, X_{N}
$$

Joint probability factorizes based on cliques in the graph

## Common name: Markov Random Fields

Undirected graphs can have an alternative formulation as Factor Graphs

## Markov Random Fields: Undirected Graphs



$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)
$$

## Markov Random Fields: Undirected Graphs

clique: subset of nodes, where nodes are pairwise connected
maximal clique: a clique that cannot add a node and remain a clique


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## Markov Random Fields: Undirected Graphs

clique: subset of nodes, where nodes are pairwise connected
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$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{7} \prod_{\substack{\text { global } \\ \text { normalization }}}^{\substack{\text { maximal } \\ \text { cliques }}} \psi_{\substack{\text { potential function (not } \\ \text { necessarily a probability!) }}}^{\text {variables part }} \text { of the clique } \mathrm{c}
$$

## Markov Random Fields: Undirected Graphs

clique: subset of nodes, where nodes are pairwise connected
maximal clique: a clique that cannot add a node and remain a clique


$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{Z} \prod_{\substack{\text { global } \\ \text { normalization }}} \psi_{C}\left(x_{C}\right) \underbrace{}_{\substack{\text { maximal } \\ \text { variables part } \\ \text { of the clique } \mathrm{C}}}
$$

## Markov Random Fields: Undirected Graphs

clique: subset of nodes, where nodes are pairwise connected
maximal clique: a clique that cannot add a node and remain a clique


$$
\begin{aligned}
& p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{Z} \prod_{C} \psi_{C}\left(x_{c}\right) \\
& \text { ons should we } \\
& \text { tentials } \psi_{c} \text { ? }
\end{aligned}
$$

variables part
Q: What restrictions should we place on the potentials $\psi_{C}$ ?
maximal cliques
potential function (not necessarily a probability!)

## Markov Random Fields: Undirected Graphs

clique: subset of nodes, where nodes are pairwise connected
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& \text { ons should we }
\end{aligned}
$$

variables part

Q: What restrictions should we place on the potentials $\psi_{C}$ ?

A: $\psi_{C} \geq 0\left(\right.$ or $\left.\psi_{C}>0\right)$
normalization
maximal potential function (not cliques necessarily a probability!)

## Terminology: Potential Functions

$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{Z} \prod_{C} \psi_{C}\left(x_{C}\right)
$$

energy function (for clique C)
(get the total energy of a configuration by summing the
individual energy functions)

$$
\psi_{C}\left(x_{c}\right)=\underbrace{\exp -E\left(x_{C}\right)}_{\text {Boltzmann distribution }}
$$

## Ambiguity in Undirected Model Notation



$$
\begin{aligned}
& p(x, y, z) \propto \psi(x, y, z) \\
& \text { ーーーーーーーーーーーーーーーー } \\
& p(x, y, z) \propto \psi_{1(x, y)} \psi_{2(y, z)} \psi_{3(x, z)}
\end{aligned}
$$

## Outline

Directed Graphical Models
Naïve Bayes

Undirected Graphical Models
Factor Graphs
Ising Model

Message Passing: Graphical Model Inference

## MRFs as Factor Graphs

Undirected graphs: $\mathrm{G}=(\mathrm{V}, \mathrm{E})$ that represents $p\left(X_{1}, \ldots, X_{N}\right)$

Factor graph of $p$ : Bipartite graph of evidence nodes $X$, factor nodes $F$, and edges $T$

Evidence nodes $X$ are the random variables

Factor nodes F take values associated with the potential functions

Edges show what variables are used in which factors

## MRFs as Factor Graphs

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Evidence nodes $X$ are the random variables

Factor nodes F take values associated with the potential functions

Edges show what variables are
 used in which factors

## Different Factor Graph Notation for the Same Graph



## Example: Linear Chain

Directed (e.g., hidden Markov model [HMM]; generative)

## Example: Linear Chain

Directed (e.g., hidden Markov model [HMM]; generative)

Directed (e.g.., maximum entropy Markov model
[MEMM]; conditional)


## Example: Linear Chain

Directed (e.g., hidden Markov model [HMM]; generative)

Directed (e.g.., maximum entropy Markov model [MEMM]; conditional)

Undirected
(e.g., conditional random field [CRF])


## Example: Linear Chain

Directed (e.g., hidden Markov model [HMM]; generative)

Directed (e.g.., maximum entropy Markov model [MEMM]; conditional)

## Undirected as

 factor graph (e.g., conditional random field [CRF])

## Example: Linear Chain Conditional Random Field



Widely used in applications like part-of-speech tagging

Noun-Mod Noun Verb Noun
President Obama told Congress ...

## Example: Linear Chain Conditional Random Field



Widely used in applications like part-of-speech tagging

Noun-Mod Noun Nerb Noun
President Obama told Congress ... and named entity recognition Person Person Other Org.
President Obama told Congress ...

## Linear Chain CRFs for Part of Speech Tagging

A linear chain CRF is a conditional probabilistic model of the sequence of tags $z_{1}, z_{2}, \ldots, z_{N}$ conditioned on the entire input sequence $x_{1: N}$

## Linear Chain CRFs for Part of Speech Tagging

$$
p( \rangle)
$$

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## Linear Chain CRFs for Part of Speech Tagging

$$
p\left(z_{1}, z_{2}, \ldots, z_{N} \mid \diamond\right)
$$

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## Linear Chain CRFs for Part of Speech Tagging

$$
p\left(z_{1}, z_{2}, \ldots, z_{N} \mid x_{1: N}\right)
$$

A linear chain CRF is a conditional probabilistic model of the sequence of tags $z_{1}, z_{2}, \ldots, z_{N}$ conditioned on the entire input sequence $x_{1: N}$

## Linear Chain CRFs for Part of Speech Tagging

$$
p\left(z_{1}, z_{2}, \ldots, z_{N} \mid x_{1: N}\right)
$$



## Linear Chain CRFs for Part of Speech Tagging



$$
\begin{aligned}
& p\left(z_{1}, z_{2}, \ldots, z_{N} \mid x_{1: N}\right) \propto \\
& \prod_{i=1}^{\mathrm{N}} \exp \left(\left\langle\theta^{(f)}, f_{i}\left(z_{i}\right)\right\rangle+\left\langle\theta^{(g)}, g_{i}\left(z_{i}, z_{i+1}\right)\right\rangle\right)
\end{aligned}
$$

## Linear Chain CRFs for Part of Speech Tagging

$g_{j}$ : inter-tag features

(can depend on
any/all input words

$$
\left.x_{1: N}\right)
$$



## Linear Chain CRFs for Part of Speech Tagging



## Linear Chain CRFs for Part of Speech Tagging

$g_{j}$ : inter-tag features<br>(can depend on<br>any/all input words<br>$$
\left.x_{1: N}\right)
$$<br>$f_{i}$ : solo tag features<br>(can depend on<br>any/all input words<br>$\left.x_{1: N}\right)$

## Feature design, just like in maxent models!

## Linear Chain CRFs for Part of Speech Tagging

$g_{j}$ : inter-tag features
(can depend on
any/all input words

$$
\left.x_{1: N}\right)
$$

$f_{i}$ : solo tag features
(can depend on
any/all input words

$$
\left.x_{1: N}\right)
$$

Example:

$$
g_{j, N \rightarrow V}\left(\mathrm{z}_{\mathrm{j}}, \mathrm{z}_{\mathrm{j}+1}\right)=1\left(\text { if } \mathrm{z}_{\mathrm{j}}==\mathrm{N} \& \mathrm{z}_{\mathrm{j}+1}=\mathrm{V}\right) \text { else } 0
$$

$g_{j, \text { told }, N \rightarrow V}\left(\mathrm{z}_{\mathrm{j}}, \mathrm{z}_{\mathrm{j}+1}\right)=1\left(\right.$ if $\mathrm{z}_{\mathrm{j}}==\mathrm{N} \& \mathrm{z}_{\mathrm{j}+1}==\mathrm{V} \& \mathrm{x}_{\mathrm{j}}==$ told) else 0


## Outline

Directed Graphical Models
Naïve Bayes

Undirected Graphical Models

Factor Graphs<br>Ising Model

Message Passing: Graphical Model Inference

## Example: Ising Model

Image denoising (Bishop, 2006; Fig 8.30)


X


Y


Example: Ising Model


Example: Using Model

Image denoising (Bishop, 2006; Fig 8.30)


## Example: Ising Model

Image denoising (Bishop, 2006; Fig 8.30)



neighboring pixels
should be similar

$$
\begin{aligned}
& E(x, y)=h \sum_{i} x_{i}-\beta \sum_{i j} x_{i} x_{j}-\eta \sum_{i} x_{i} y_{i} \\
& \text { allow for a bias } \\
& x_{i} \text { and } y_{i} \text { should } \\
& \text { be correlated }
\end{aligned}
$$

## Example: Ising Model

Image denoising (Bishop, 2006; Fig 8.30)


observed (noisy) pixel/state
x : original pixel/state

$$
\begin{aligned}
& E(x, y)=h \sum_{i} x_{i}-\beta \sum_{i j} x_{i} x_{j}-\eta \sum_{i} x_{i} y_{i} \\
& \text { allow for a bias } \\
& x_{i} \text { and } y_{i} \text { should } \\
& \text { be correlated }
\end{aligned}
$$

## Example: Ising Model

Image denoising (Bishop, 2006; Fig 8.30)


Q: Why subtract $\beta$ and $\eta$ ?

$$
\begin{array}{r}
E(x, y)=h \sum_{i} x_{i}-\beta \sum_{i j} x_{i} x_{j}-\eta \sum_{i} x_{i} y_{i} \\
\text { allow for a bias }
\end{array} \begin{array}{r}
x_{i} \text { and } y_{i} \text { should } \\
\text { be correlated }
\end{array}
$$

neighboring pixels

## Example: Ising Model

Image denoising (Bishop, 2006; Fig 8.30)


Q: Why subtract $\beta$ and $\eta$ ?
neighboring pixels

| A: Better states $\rightarrow$ lower <br> energy (higher potential) <br> $\psi_{C}\left(x_{c}\right)=\exp -E\left(x_{C}\right)$ | allow for a bias |
| :--- | :--- |

## Markov Random Fields with Factor Graph Notation


factor graphs are bipartite

## Outline

Directed Graphical Models Naïve Bayes

Undirected Graphical Models

$$
\begin{aligned}
& \text { Factor Graphs } \\
& \text { Ising Model }
\end{aligned}
$$

Message Passing: Graphical Model Inference

## Two Problems for Undirected Models

$$
p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{Z} \prod_{c} \psi_{c}\left(x_{c}\right)
$$

Finding the normalizer
Computing the marginals

## Two Problems for Undirected Models

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p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{Z} \prod_{C} \psi_{C}\left(x_{c}\right)
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Finding the normalizer
Computing the marginals

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Z=\sum_{x} \prod_{c} \psi_{c}\left(x_{c}\right)
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p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{Z} \prod_{C} \psi_{C}\left(x_{c}\right)
$$

Finding the normalizer
Computing the marginals

## Sum over all variable combinations, with the $x_{n}$ coordinate fixed

$$
Z=\sum_{x} \prod_{c} \psi_{c}\left(x_{c}\right)
$$


$Z_{2}(v)=\sum_{x_{1}} \sum_{x_{3}} \prod_{c} \psi_{c}\left(x=\left(x_{1}, v, x_{3}\right)\right)$

## Two Problems for Undirected Models

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Finding the normalizer
Computing the marginals

## Sum over all variable combinations, with the $x_{n}$ coordinate fixed

$$
Z=\sum_{x} \prod_{c} \psi_{c}\left(x_{c}\right)
$$

Q: Why are these difficult?

Example: 3
variables, fix the
$2^{\text {nd }}$ dimension

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Z_{2}(v)=\sum_{x_{1}} \sum_{x_{3}} \prod_{c} \psi_{c}\left(x=\left(x_{1}, v, x_{3}\right)\right)
$$

## Two Problems for Undirected Models

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p\left(x_{1}, x_{2}, x_{3}, \ldots, x_{N}\right)=\frac{1}{Z} \prod_{C} \psi_{c}\left(x_{c}\right)
$$

Finding the normalizer
Computing the marginals

## Sum over all variable combinations, with the $x_{n}$ coordinate fixed

$$
Z=\sum_{x} \prod_{c} \psi_{c}\left(x_{c}\right)
$$

Q: Why are these difficult?
A: Many different combinations
$Z_{n}(v)=\sum_{x: x_{n}=v} \prod_{c} \psi_{c}\left(x_{c}\right)$
Example: 3
variables, fix the
$2^{\text {nd }}$ dimension

$$
Z_{2}(v)=\sum_{x_{1}} \sum_{x_{3}} \prod_{c} \psi_{c}\left(x=\left(x_{1}, v, x_{3}\right)\right)
$$

## Message Passing: Count the Soldiers

If you are the front soldier in the line, say the number 'one' to the soldier behind you.

If you are the rearmost soldier in the line, say the number 'one' to the soldier in front of you.

If a soldier ahead of or behind you says a number to you, add one to it, and say the new
number to the soldier on the other side

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## Sum-Product Algorithm

Main idea: message passing

An exact inference algorithm for tree-like graphs

## Belief propagation (forward-backward for HMMs) is a special case

## Sum-Product

definition of

$$
p\left(x_{i}=v\right)=\prod_{x: x_{i}=v} p\left(x_{1}, x_{2}, \ldots, x_{i}, \ldots, x_{N}\right)
$$



## Sum-Product

$$
\begin{gathered}
\begin{array}{c}
\text { definition of } \\
\text { marginal }
\end{array}
\end{gathered} p\left(x_{i}=v\right)=\prod_{x: x_{i}=v} p\left(x_{1}, x_{2}, \ldots, x_{i}, \ldots, x_{N}\right)
$$

main idea: use bipartite nature of graph to efficiently compute the marginals

The factor nodes can act as filters

## Sum-Product

$\begin{gathered}\text { definition of } \\ \text { marginal }\end{gathered} \quad p\left(x_{i}=v\right)=\prod_{x: x_{i}=v} p\left(x_{1}, x_{2}, \ldots, x_{i}, \ldots, x_{N}\right)$


## Sum-Product

alternative marginal computation

$$
p\left(x_{i}=v\right)=\prod_{f} r_{f \rightarrow x_{i}}\left(x_{i}\right)
$$

main idea: use bipartite nature of graph to


## Sum-Product

From variables to factors


## Sum-Product

From variables to factors

set of factors in which variable n participates

From factors to variables

$$
r_{m \rightarrow n}\left(x_{n}\right)
$$

$$
=\sum_{w_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n \prime}\right)
$$


sum over configuration of
variables for the $m^{\text {th }}$ factor, with variable $n$ fixed
set of variables that the $m^{\text {th }}$ factor depends on

## Example



Q: What are the variables?

## Example



## Example



## Example



## Example



## Example



1. Select the root, or pick one if a tree $\left(x_{3}\right)$
2. Send messages from leaves to root

$$
\begin{aligned}
& q_{x_{1} \rightarrow f_{a}}\left(x_{1}\right)=1 \\
& q_{x_{4} \rightarrow f_{c}}\left(x_{4}\right)=1
\end{aligned}
$$

$$
q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right) \quad r_{m \rightarrow n}\left(x_{n}\right)=\sum_{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n^{\prime}}\right)
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& r_{f_{a} \rightarrow x_{2}}\left(x_{2}\right)=? ? ?
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r_{m \rightarrow n}\left(x_{n}\right)=\sum_{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n \prime}\right)
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\end{aligned}
$$

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q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right)
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## Example

1. Select the root, or pick one if a tree $\left(x_{3}\right)$
2. Send messages from leaves to root
3. Send messages from root to leaves


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q_{x_{3} \rightarrow f_{b}}\left(x_{3}\right)=1
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$q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right)$
$r_{m \rightarrow n}\left(x_{n}\right)=\sum_{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n^{\prime}}\right)$

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& r_{f_{c} \rightarrow x_{4}}\left(x_{4}\right)=\sum_{k} f_{c}\left(x_{2}=k, x_{4}\right) \\
& r_{f_{a} \rightarrow x_{1}}\left(x_{1}\right)=\sum_{k} f_{a}\left(x_{1}, x_{2}=k\right)
\end{aligned}
$$

$$
q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right)
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## Example



1. Select the root, or pick one if a tree $\left(x_{3}\right)$
2. Send messages from leaves to root
3. Send messages from root to leaves
4. Use messages to compute marginal probabilities

$$
p\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right)
$$

$$
q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right)
$$

$$
r_{m \rightarrow n}\left(x_{n}\right)=\sum_{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n \prime}\right)
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& p\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right) \\
& p\left(x_{1}\right)=r_{f_{a} \rightarrow x_{1}}\left(x_{1}\right)
\end{aligned}
$$

$$
q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right) \quad r_{m \rightarrow n}\left(x_{n}\right)=\sum_{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n^{\prime}}\right)
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& p\left(x_{1}\right)=r_{f_{a} \rightarrow x_{1}}\left(x_{1}\right) \\
& p\left(x_{2}\right) \\
& =r_{f_{a} \rightarrow x_{2}}\left(x_{2}\right) r_{f_{b} \rightarrow x_{2}}\left(x_{2}\right) r_{f_{c} \rightarrow x_{2}}\left(x_{2}\right)
\end{aligned}
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$$

## Example



1. Select the root, or pick one if a tree $\left(x_{3}\right)$
2. Send messages from leaves to root
3. Send messages from root to leaves
4. Use messages to compute marginal probabilities

$$
\begin{aligned}
& p\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right) \\
& p\left(x_{1}\right)=r_{f_{a} \rightarrow x_{1}}\left(x_{1}\right) \\
& p\left(x_{2}\right) \\
& =r_{f_{a} \rightarrow x_{2}}\left(x_{2}\right) r_{f_{b} \rightarrow x_{2}}\left(x_{2}\right) r_{f_{c} \rightarrow x_{2}}\left(x_{2}\right) \\
& p\left(x_{3}\right)=r_{f_{b} \rightarrow x_{3}}\left(x_{3}\right) \\
& p\left(x_{4}\right)=r_{f_{c} \rightarrow x_{4}}\left(x_{4}\right)
\end{aligned}
$$

$$
q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right)
$$

$$
r_{m \rightarrow n}\left(x_{n}\right)=\sum_{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n^{\prime}}\right)
$$

## Example



1. Select the root, or pick one if a tree $\left(x_{3}\right)$
2. Send messages from leaves to root
3. Send messages from root to leaves
4. Use messages to compute marginal probabilities
5. Are we done?
6. If a tree structure, we've converged 2.

$$
q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right)
$$

$$
r_{m \rightarrow n}\left(x_{n}\right)=\sum_{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n^{\prime}}\right)
$$

## Example



1. Select the root, or pick one if a tree $\left(x_{3}\right)$
2. Send messages from leaves to root
3. Send messages from root to leaves
4. Use messages to compute marginal probabilities
5. Are we done?
6. If a tree structure, we've converged
7. If not:
8. Either accept the partially converged result, or...
9. 

$$
q_{n \rightarrow m}\left(x_{n}\right)=\prod_{m^{\prime} \in M(n) \backslash m} r_{m^{\prime} \rightarrow n}\left(x_{n}\right) \quad r_{m \rightarrow n}\left(x_{n}\right)=\sum_{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n^{\prime}}\right)
$$

## Example



## Max-Product (Max-Sum)

Problem: how to find the most likely (best) setting of latent variables

Replace sum (+) with max in factor $\rightarrow$ variable computations

$$
r_{m \rightarrow n}\left(x_{n}\right)=\max _{\boldsymbol{w}_{m} \backslash n} f_{m}\left(\boldsymbol{w}_{m}\right) \prod_{n^{\prime} \in N(m) \backslash n} q_{n^{\prime} \rightarrow m}\left(x_{n \prime}\right)
$$

(why max-sum? computationally,
implement with logs)

## Loopy Belief Propagation

Sum-product algorithm is not exact for general graphs

Loopy Belief Propagation (Loopy BP): run sumproduct algorithm anyway and hope for the best

Requires a message passing schedule

## Outline

Directed Graphical Models
Naïve Bayes

Undirected Graphical Models

## Factor Graphs <br> Ising Model

Message Passing: Graphical Model Inference

