## Probabilistic Graphical Models

## Lecture 2: Graphical Models. Belief Propagation

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## Outline

(1) Graphical Models

(2) Belief Propagation

## Literature

Excellent book about graphical models and belief propagation, written by one of the pioneers in these topics:

- Pearl, J.

Probabilistic Reasoning in Intelligent Systems (1990)

## The Need to Factorize

Variables $x_{1}, x_{2}, \ldots, x_{n}$

$$
P\left(x_{1}\right)=\sum_{x_{2}} \cdots \sum_{x_{n}} P\left(x_{1}, x_{2}, \ldots, x_{n}\right)
$$

Marginalization: Exponential time
Storage: $\quad$ Exponential space $\Rightarrow$ Need factorization

- Independence?

But probabilistic modelling is about dependencies!

## The Need to Factorize

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But probabilistic modelling is about dependencies!

- Conditional independence

Dependencies may have simple structure

## Towards Bayesian Networks

Tracking a fly

- Path pretty random


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## Remember

$$
\begin{aligned}
P\left(x_{1}, \ldots, x_{n}\right)= & P\left(x_{1}\right) P\left(x_{2} \mid x_{1}\right) \ldots \\
& P\left(x_{n} \mid x_{n-1}, \ldots, x_{1}\right) ?
\end{aligned}
$$



Here: $P\left(x_{n} \mid x_{n-1}, \ldots, x_{1}\right)=P\left(x_{n} \mid x_{n-1}\right) \Rightarrow$ Linear storage Causal factorization $\Rightarrow$ Bayesian networks

## Bayesian Networks (Directed Graphical Models)

Causal factorization:

$$
P\left(x_{1}, \ldots, x_{n}\right)=\prod_{i=1}^{n} P\left(x_{i} \mid \boldsymbol{x}_{\pi_{i}}\right)
$$

## Bayesian network

 (aka directed graphical model, aka causal network):- Graphical representation of ancestry [DAG]
- $P\left(x_{i} \mid \boldsymbol{x}_{\pi_{i}}\right)$ : Conditional probability table (CPT)



## Conditional Independence

$$
\mathcal{A} \perp \mathcal{B} \mid \mathcal{C} \Leftrightarrow P(\mathcal{A}, \mathcal{B} \mid \mathcal{C})=P(\mathcal{A} \mid \mathcal{C}) P(\mathcal{B} \mid \mathcal{C}) \Leftrightarrow P(\mathcal{A} \mid \mathcal{C}, \mathcal{B})=P(\mathcal{A} \mid \mathcal{C})
$$

## Did It Rain Tonight?

$$
P(R=y)=0.2 \quad P(S=y)=0.1
$$



| $R$ | $P(W=y \mid R)$ |
| :---: | :---: |
| y | 1 |
| n | 0.2 |


| $R$ | $S$ | $P(H=y \mid R, S)$ |
| :---: | :---: | :---: |
| y | y | 1 |
| y | n | 1 |
| n | y | 0.9 |
| n | n | 0.01 |

## Monty Hall Problem



- Let's make a deal!
- Door with car (hidden)
- First choice of yours (remains closed)
- Host opens door with goat, $H \neq F, D$
- Do you switch?


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- Do you switch?
- "Intuition": Fifty-fifty.
$F, H$ give no information. He would be stupid, wouldn't he?


## Winning with Bayes (I)



- Intuition "H does not tell anything" correct in principle. But about what?
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Will use Bayes to see that.


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- OK, but $P($ Switch wins $)=P(I=0 \mid F, H)=P(I=0)=2 / 3$ !
- Bayes makes you switch and double your chance of winning!



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If $F=D$, host picks random goat

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## Working with Graphical Models

- Intermediate between lots of headscratching and doing all sums
- Powerful division of inference in manageable, local steps


## Why Graphical Models?

(1) Easy way of communicating ideas about dependencies, models
(2) Precise semantics: Conditional independence constraints on distributions. Efficient algorithms for testing these
(3) Lead to large savings in computations (belief propagation)

## Graphical Models in Practice

Dependency structures, and efficient ways to propagate information or constraints, are fundamental.
Coding / Information Theory

- LDPC codes and BP decoding revolutionized this field (resurrection of Gallager codes)
- Used from deep space
 communication (Mars rovers) over satellite transmission to CD players / hard drives


Courtesy MacKay: Information Theory
(2003)

## Graphical Models in Practice

Dependency structures, and efficient ways to propagate information or constraints, are fundamental.
Expert systems done right

- QMR-DT: Invert causal network for helping medical diagnoses
- Hugin: Advanced decision support (Lauritzen)
http://www.hugin.com/


4000

- Promedas: Medical diagnostic advisory system (SNN Nimegen)


## Graphical Models in Practice

Dependency structures, and efficient ways to propagate information or constraints, are fundamental.
Computer Vision:
Markov Random Fields

- Denoising, super-resolution, restoration (early work by Besag)
- Depth / reconstruction from stereo, matching, correspondences
- Segmentation, matting,
 blending, stitching, impainting,

Courtesy MSR

## Conditional Independence Semantics

- Graphical model formally equivalent to long (finite) list of conditional independence constraints:
$\boldsymbol{x}_{A_{1}} \perp \boldsymbol{x}_{B_{1}}\left|\boldsymbol{x}_{C_{1}}, \boldsymbol{x}_{A_{2}} \perp \boldsymbol{x}_{B_{2}}\right| \boldsymbol{x}_{C_{2}}, \ldots$ Which do you prefer?


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- Distribution consistent with graph iff all Cl constraints are met. $P\left(x_{1}\right) P\left(x_{2}\right) \ldots P\left(x_{n}\right)$ : Consistent with all graphs


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- How do I see whether $\boldsymbol{x}_{A} \perp \boldsymbol{x}_{B} \mid \boldsymbol{x}_{C}$ from the graph? Graph separation: If paths $A \leftrightarrow B$ blocked by $C$
- For Bayesian networks (directed graphical models): d-separation. $\Rightarrow$ You'll find out in the exercises!


## Undirected Graphical Models (Markov Random Fields)

- Bayesian Networks: Describe Cls with directed graphs (DAGs) Markov Random Fields: Describe Cls with undirected graphs


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- Bayesian Networks:

Describe Cls with directed graphs (DAGs) Markov Random Fields: Describe Cls with undirected graphs

- Cl semantics of undirected models: Really just graph separation



## Undirected Graphical Models (II)

- Why two frameworks?
- Each can capture setups the other cannot
- More important: In practice, some problems are much easier to parameterize (therefore: to learn) as MRFs, others much easier as Bayes nets


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- Why two frameworks?
- Each can capture setups the other cannot
- More important: In practice, some problems are much easier to parameterize (therefore: to learn) as MRFs, others much easier as Bayes nets
- How do distributions $P$ for MRF graph $\mathcal{G}$ look like? Hammersley / Clifford:
- Maximal cliques (completely connected parts) $C_{j}$ of $\mathcal{G}$
- $P(\boldsymbol{x})$ consistent with MRF $G \Leftrightarrow$

$$
P(\boldsymbol{x})=Z^{-1} \prod_{j} \Phi_{j}\left(\boldsymbol{x}_{C_{j}}\right), \quad Z:=\sum_{\boldsymbol{x}} \prod_{j} \Phi_{j}\left(\boldsymbol{x}_{C_{j}}\right)
$$

with potentials $\Phi_{j}\left(\boldsymbol{x}_{C_{j}}\right) \geq 0$. $Z$ : Partition function.

- Potentials need not normalize to 1


## Undirected Graphical Models (III)



$$
\begin{gathered}
P(\mathbf{x})=Z^{-1} \phi_{1}\left(\mathbf{x}_{123}\right) \phi_{2}\left(\mathbf{x}_{145}\right) \phi_{3}\left(\mathbf{x}_{156}\right) \\
\phi_{4}\left(\mathbf{x}_{4578}\right) \phi_{5}\left(x_{9}\right)
\end{gathered}
$$

## Directed vs. Undirected

- Sampling $\boldsymbol{x} \sim P(\boldsymbol{x})$ :

Always simple from Bayes net. Can be very hard for an MRF

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- Implicit, symmetrical knowledge? Little idea about causal links (pixels of image, correspondences)? MRFs more useful then
- Bottomline: Usually, one or the other is much more suitable. Better know well about both!


## Towards Efficient Marginalization

- With sufficient Markovian Cl constraints (directed or undirected):

$$
P\left(x_{1}, \ldots, x_{n}\right) \propto \prod_{j} \Phi_{j}\left(\boldsymbol{x}_{N_{j}}\right), \quad\left|N_{j}\right| \ll n
$$

Can store that. But what about computation?

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Can store that. But what about computation?

- Short answer: It depends on global graph structure properties, beyond local factorization

Storage: $\quad$ Linear in $n$
Computation: Exponential in $n^{1 / 2}[\mathrm{P} \neq \mathrm{NP}]$


## Node Elimination



Chain:

$$
P\left(x_{1}, \ldots, x_{7}\right)=\Phi_{1}\left(x_{1}, x_{2}\right) \Phi_{2}\left(x_{2}, x_{3}\right) \ldots \Phi_{6}\left(x_{6}, x_{7}\right)
$$

## Node Elimination

## (1)-(2)-(5)-(5)

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\sum_{x_{4}} P\left(x_{1}, \ldots, x_{4}, \ldots, x_{7}\right)
\end{gathered}
$$

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$$

$$
\begin{aligned}
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= & \Phi_{1}\left(x_{1}, x_{2}\right) \Phi_{2}\left(x_{2}, x_{3}\right)\left(\sum_{x_{4}} \Phi_{3}\left(x_{3}, x_{4}\right) \Phi_{4}\left(x_{4}, x_{5}\right)\right) \Phi_{5}\left(x_{5}, x_{6}\right) \Phi_{6}\left(x_{6}, x_{7}\right)
\end{aligned}
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## (1)-(2)-5 5

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= & \Phi_{1}\left(x_{1}, x_{2}\right) \Phi_{2}\left(x_{2}, x_{3}\right) M_{35}\left(x_{3}, x_{5}\right) \Phi_{5}\left(x_{5}, x_{6}\right) \Phi_{6}\left(x_{6}, x_{7}\right)
\end{aligned}
$$

Belief Propagation
Tree Graphs


## Factor Graphs

Factor graphs: Yet another type of graphical model

- Bipartite graph: variable / factor nodes
- No probability semantics
- Just for deriving Markovian propagation algorithms
- Factor graph = tree $\Rightarrow$ Fast computation



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Undirected GM $\rightarrow$ Factor graph: Immediate
Directed GM $\rightarrow$ Factor graph: Easy exercise

## Towards Belief Propagation



## What is a Message?



## What is a Message?

- Formally: Directed potential over one variable
- Intuition: Message $T_{2} \rightarrow a$ : What $T_{2}$ thinks $x_{a}$ should be
- Naive "definition":
- Product: All $T_{2}$, and edge $\rightarrow a$
- Sum: All except $x_{a}$

$\Rightarrow$ Real definition recursive ( $\mathcal{G}$ tree!)


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- Strictly speaking: Two types of messages: $\bigcirc \rightarrow \square, \square \rightarrow \bigcirc$ $\Rightarrow$ Understand idea, behind formalities


## Message Passing: The Recipe

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(2) Product: Gather potentials

- $\Phi_{j}\left(x_{a}, x_{b_{1}}, x_{b_{2}}\right)$
- All $\mu_{? \rightarrow b_{1}}\left(x_{b_{1}}\right)$, except $b_{1} \leftarrow \Phi_{j}$
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(3) Sum: Over $x_{b_{1}}, x_{b_{2}}$

$\mu_{T \rightarrow a}\left(x_{a}\right) \propto \sum_{x_{b_{1}, x_{b_{2}}}} \Phi_{j}\left(\boldsymbol{x}_{a b_{1} b_{2}}\right)\left(\prod_{\tilde{\tau}: T_{1} \backslash b_{1}} \mu_{\tilde{T} \rightarrow b_{1}}\left(x_{b_{1}}\right)\right)\left(\prod_{\tilde{\tilde{T}}: T_{2} \backslash b_{2}} \mu_{\tilde{T} \rightarrow b_{2}}\left(x_{b_{2}}\right)\right)$


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- Marginal distributions (our goal!) are obtained by combining messages $\leftrightarrow$ combining information from all parts
- MP works on trees, because information cannot go around in cycles


## Belief Propagation: More than Node Elimination

- Marginalization by message passing:

$$
P\left(x_{a}\right)=\sum_{\boldsymbol{x} \backslash x_{a}} P(\boldsymbol{x}) \propto \Phi_{a}\left(x_{a}\right) \prod_{j \in \mathcal{N}_{a}} \mu_{T_{j} \rightarrow a}\left(x_{a}\right)
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$\mathcal{N}_{a}$ : Factor nodes neighbouring $a \leftrightarrow$ factors $\Phi_{j}\left(x_{a}, \ldots\right)$
$\Phi_{a}:$ Can $b e \equiv 1$

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- All marginals $P\left(x_{1}\right), P\left(x_{2}\right), \ldots$ ? Do this $n$ times. Right?
$\Rightarrow$ NO! Do this twice only!
$\Rightarrow$ If you understand that, you've understood belief propagation


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## Belief Propagation on Trees

- Message uniquely defined, independent of use, order of computation
- Message can be computed once all inputs received. Once computed, it does not change anymore
- Compute all messages (2 per edge) $\Rightarrow$ All marginals, $\mathrm{O}(1)$ each


## Implementation of Belief Propagation

## Belief Propagation (Sum-Product) on Trees

(1) Designate node (any will do!) as root
(2) Inward pass: Compute messages leaves $\rightarrow$ root
(3) Outward pass: Compute messages root $\rightarrow$ leaves

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Messages can be normalized at will:

$$
\mu_{T \rightarrow a}\left(x_{a}\right)=\sum_{\boldsymbol{x}_{C_{j} \backslash a}} \Phi_{j}\left(\boldsymbol{x}_{C_{j}}\right) \prod C \mu_{\tilde{T} \rightarrow b_{1}}\left(x_{b_{1}}\right) \ldots
$$

## Implementation of Belief Propagation

## Belief Propagation (Sum-Product) on Trees

(1) Designate node (any will do!) as root
(2) Inward pass: Compute messages leaves $\rightarrow$ root
(3) Outward pass: Compute messages root $\rightarrow$ leaves

Messages can be normalized at will:

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Avoiding underflow / overflow (yes, it does matter):

- Renormalize each message to sum to 1
- Better: Work in log domain (log-messages, log-potentials):
$\prod \rightarrow+$
$\sum \rightarrow$ logsumexp [careful with zeros!]
$\operatorname{logsumexp}(\boldsymbol{v}):=\log \sum_{i=1}^{k} e^{v_{i}}=\underbrace{M+\log \sum_{i=1}^{k} e^{v_{i}-M}}_{\text {numerically stable }}, \quad M=\max _{i} v_{i}$


## Searching for the Mode: Max-Product

Decoding:

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\boldsymbol{x}_{*} \in \underset{\boldsymbol{x}}{\operatorname{argmax}} P(\boldsymbol{x})
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- Back-pointer tables:

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## Wrap-Up

- Belief propagation (sum-product) on trees: All marginals in linear time, by local information propagation
- Max-product, max-sum, logsumexp-sum, ... : What matters is the graph!


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What matters is the graph!

- What about general graphs?
- Decomposable graphs. Treewidth of a graph
- Junction tree algorithm

Interested?

- PMR Edinburgh slides:
http://www.inf.ed.ac.uk/teaching/courses/pmr/slides/jta-2x2.pdf
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- Beware (not surprising): Inference on general graphs is NP hard. In general, approximations are a must

