# CSC535: Probabilistic Graphical Models 

Midterm Review
Prof. Jason Pacheco

## Administrative Items

- Midterm out (obviously)
- Due Friday @ 11:59pm
- 4 questions (15 points) + 1 Extra Credit (2 points)
- You may provide handwritten responses (scanned PDF)
- Make sure handwriting is clear and easy-to-read
- No office hours Friday (I will be traveling)


## Midterm

## Problem 1 (4 points)

- Provide Bayes Net and Factor graphs for a model
- Give formula for sum-product messages in model
- Show dependence / independence


## Problem 2 (3 points)

## Extra Credit (2 points)

- Derive Poisson maximum likelihood estimate
- Derive MAP estimate with Gamma prior
- Two player game, best of 7 rounds wins
- Compute probability of winning conditioned on current score


## Problem 3 (4 points)

- Show variable elimination for two different elimination orderings
- Bound on maximal clique size


## Problem 4 (4 points)

- Show variable elimination for two different elimination orderings
- Bound on maximal clique size
- Probability and Statistics
- Probabilistic Graphical Models
- Message Passing Inference
- Parameter Learning

Topics

- Probability and Statistics
- Probabilistic Graphical Models
- Message Passing Inference
- Parameter Learning


## Probability and Random Events

## Fundamental Rules of Probability

$>$ Conditional: $p(X \mid Y)=\frac{p(X, Y)}{p(Y)}=\frac{p(X, Y)}{\sum_{x} p(X=x, Y)}$
$>$ Law of total probability: $p(Y)=\sum_{x} p(Y, X=x)$
$>$ Probability chain rule: $p(X, Y)=p(Y) p(X \mid Y)$

## Independence of RVs

> Two RVs X \& Y are independent iff: $p(X \mid Y)=p(X)$
> Equivalently: $p(X, Y)=p(X) p(Y)$
$>\mathrm{X} \& \mathrm{Y}$ are conditionally independent given Z iff: $p(X \mid Y, Z)=p(X \mid Z)$
> Equivalently: $p(X, Y \mid Z)=p(X \mid Z) p(Y \mid Z)$

Tabular Method
Let $X, Y$ be binary $R V$ s with the joint probability table
$P\left(y_{1}\right)=P\left(x_{1}, y_{1}\right)+P\left(x_{2}, y_{1}\right)$
$P\left(y_{2}\right)=P\left(x_{1}, y_{2}\right)+P\left(x_{2}, y_{2}\right)$
[i.e., sum down columns]

For Binomial use K-by-K probability table.

## $Y$

Tabular Method


Tabular Method


## Bayes' Rule

Posterior represents all uncertainty after observing data...


## Bayesian Inference Example

About 29\% of American adults have high blood pressure (BP). Home test has $30 \%$ false positive rate and no false negative error.


## A recent home test states that you have high BP. Should you start medication?

An Assessment of the Accuracy of Home Blood Pressure Monitors When Used in Device Owners

Jennifer S. Ringrose, ${ }^{1}$ Gina Polley, ${ }^{1}$ Donna McLean, ${ }^{2-4}$ Ann Thompson, ${ }^{1,5}$ Fraulein Morales, ${ }^{1}$ and Raj Padwal ${ }^{1,4,6}$

## Bayesian Inference Example

About 29\% of American adults have high blood pressure (BP). Home test has $30 \%$ false positive rate and no false negative error.


- Latent quantity of interest is hypertension: $\theta \in\{$ true, false $\}$
- Measurement of hypertension: $y \in\{$ true, false $\}$
- Prior: $p(\theta=$ true $)=0.29$
- Likelihood: $p(y=$ true $\mid \theta=$ false $)=0.30$

$$
p(y=\operatorname{true} \mid \theta=\operatorname{true})=1.00
$$

## Bayesian Inference Example

About 29\% of American adults have high blood pressure (BP). Home test has $30 \%$ false positive rate and no false negative error.


Suppose we get a positive measurement, then posterior is:

$$
\begin{aligned}
p(\theta=\text { true } \mid y=\text { true }) & =\frac{p(\theta=\operatorname{true}) p(y=\text { true } \mid \theta=\text { true })}{p(y=\text { true })} \\
& =\frac{0.29 * 1.00}{0.29 * 1.00+0.71 * 0.30} \approx 0.58
\end{aligned}
$$

## Bayesian Estimation

Task: produce an estimate $\hat{\theta}$ of $\theta$ after observing data $y$
Bayes estimators minimize expected loss function:

$$
\mathbb{E}[L(\theta, \hat{\theta}) \mid y]=\int p(\theta \mid y) L(\theta, \hat{\theta}) d \theta
$$

Example: Minimum mean squared error (MMSE):

$$
\hat{\theta}^{\mathrm{MMSE}}=\arg \min \mathbb{E}\left[(\hat{\theta}-\theta)^{2} \mid y\right]=E[\theta \mid y]
$$

Posterior mean always minimizes squared error.

## - Probability and Statistics

- Probabilistic Graphical Models
- Message Passing Inference
- Parameter Learning


## Directed Graphical Models

- Distribution factorized as product of conditionals via chain rule

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

- Choose ordering where terms simplify due to conditional independence

Eg. Suppose $x_{4} \perp x_{1} \mid x_{3}$ and $x_{2} \perp x_{4} \mid x_{1}$ then:

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

- Directed graph encodes factorized distribution via conditional independence properties

- Test independence using canonical subgraphs:
- Straightforward simulation via ancestral sampling



## Bayes Ball Algorithm

To test if $X_{A} \perp X_{B} \mid X_{C}$ roll ball from every node in $X_{A} \ldots$


If any ball reaches any node in $X_{B}$ then $X_{A} \not \perp X_{B} \mid X_{C}$

Otherwise:
$X_{A} \perp X_{B} \mid X_{C}$

Tests for property of directed separation (d-separation): if $X_{C}$ separates / blocks $X_{A}$ from $X_{B}$ then $X_{A} \perp X_{B} \mid X_{C}$

## Bayes Ball Algorithm



## Undirected Graphical Models

- Joint factorization as nonnegative factors (potentials) over subsets:

$$
p(x) \propto \prod_{f \in \mathcal{F}} \psi_{f}\left(x_{f}\right)
$$

- Easier to specify models compared to Bayes nets since:
- Factors do not need to be normalized conditional probabilities
- May specify up to unknown normalization constant
- Easier to verify Markov independence via separating sets
- Factorization ambiguous in MRFs, but explicit in factor graphs (factor graphs generally preferred)
- Simulation is not easy in general. Can't do ancestral sampling.



## Conditional Independence (Undirected)

We say $x_{A}$ and $x_{C}$ are conditionally independent $x_{A} \Perp x_{C} \mid x_{B}$ given variables $x_{B}$ iff,
$p\left(x_{A}, x_{C} \mid x_{B}\right)=p\left(x_{A} \mid x_{B}\right) p\left(x_{C} \mid x_{B}\right)$

Def. We say $p(x)$ is globally Markov w.r.t. $\mathcal{G}$ if $x_{A} \Perp x_{C} \mid x_{B}$ in any separating set of $\mathcal{G}$.


Conditional independence in undirected graphical models is defined by separating sets

## Markov Random Fields (MRFs)

A factor $\psi_{c}\left(x_{c}\right)$ corresponds to a clique $c \in \mathcal{C}$ (fully connected subgraph) in the MRF

An MRF does not imply a unique factorization, for example either of the following are "valid":

$$
\begin{gathered}
\psi\left(x_{1}, x_{2}, x_{3}\right) \psi\left(x_{3}, x_{4}\right) \psi\left(x_{3}, x_{5}\right) \\
\psi\left(x_{1}, x_{2}\right) \psi\left(x_{2}, x_{3}\right) \psi\left(x_{1}, x_{3}\right) \psi\left(x_{3}, x_{4}\right) \psi\left(x_{3}, x_{5}\right)
\end{gathered}
$$

A factorization is valid if it satisfies the Global Markov property, defined by conditional independencies

## Factor Graphs

Factor graphs make factorization explicit...


Factor node for each product term in the joint factorization:

$$
p(x) \propto \prod_{f \in \mathcal{F}} \psi_{f}\left(x_{f}\right)
$$

where $x_{f}=\left\{x_{i}: i \in f\right\}$ the set of variables in factor $f$. For example:

$$
\psi\left(x_{1}\right) \psi\left(x_{2}\right) \psi\left(x_{1}, x_{2}, x_{3}\right) \psi\left(x_{3}, x_{4}\right) \psi\left(x_{3}, x_{5}\right)
$$

Factor nodes correspond to MRF cliques

- Probability and Statistics
- Probabilistic Graphical Models
- Message Passing Inference
- Parameter Learning


## Bayes Net $\rightarrow$ MRF



## Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:
$\mathcal{O}\left(K^{3}\right)$


$$
\phi(D, E, G)=\mathcal{O}\left(K^{3}\right)
$$

## Variable Elimination

Elimination order D, E, H, G, S, L

## Worst-case Complexity: $\mathcal{O}\left(K^{3}\right)$



$$
\phi(E, G, S)=\mathcal{O}\left(K^{3}\right)
$$

## Variable Elimination

Elimination order D, E, H, G, S, L

Fill-in Edge

## Worst-case Complexity: <br> $\mathcal{O}\left(K^{3}\right)$



$$
\phi(E, G, S)=\mathcal{O}\left(K^{3}\right)
$$

## Variable Elimination

Elimination order D, E, H, G, S, L

## Worst-case Complexity: <br> $\mathcal{O}\left(K^{3}\right)$



$$
\phi(H, G, J)=\mathcal{O}\left(K^{3}\right)
$$

## Variable Elimination

Elimination order D, E, H, G, S, L

Worst-case Complexity:
$\mathcal{O}\left(K^{4}\right)$


$$
\phi(G, S, L, J)=\mathcal{O}\left(K^{4}\right)
$$

## Variable Elimination

Elimination order D, E, H, G, S, L

## Worst-case Complexity: $\mathcal{O}\left(K^{4}\right)$



$$
\phi(S, L, J)=\mathcal{O}\left(K^{3}\right)
$$

## Variable Elimination

Elimination order D, E, H, G, S, L

## Worst-case

 Complexity:$\mathcal{O}\left(K^{4}\right)$


$$
\phi(L, J)=\mathcal{O}\left(K^{2}\right)
$$

## Variable Elimination

Elimination order D, E, H, G, S, L

## Worst-case

 Complexity:$\mathcal{O}\left(K^{4}\right)$

What if we choose a different elimination order?

$$
\phi(L, J)=\mathcal{O}\left(K^{2}\right)
$$

## Computational Complexity

## Add fill-in edges to connect all neighbors

Eliminate G first...


Complexity
depends on
elimination order...

## For $N$ variables

 worst case is:$$
\mathcal{O}\left(K^{N}\right)
$$

$$
\phi(G, D, E, L, H, J)=\mathcal{O}\left(K^{6}\right)
$$

## Computational Complexity



## Computational Complexity

## Clique Tree



Elimination order $\prec$ induces graph with maximal cliques $\mathcal{C}(\prec)$ and width:


$$
w(\prec)=\max _{c \in \mathcal{C}(\prec)}|c|-1
$$

$>$ Complexity of variable elimination is $\mathcal{O}\left(K^{w(\prec)+1}\right)$
$>$ Lowest complexity given by the treewidth:

$$
w^{*}=\min _{\prec} \max _{c \in \mathcal{C}(\prec)}|c|-1
$$

It is NP-hard to compute treewidth, and therefore an optimal elimination order (of course...)

## Variable Elimination Summary

$>$ Variable elimination allows computation of marginals / conditionals
$>$ Algorithm is valid for any graphical model
$>$ Suffices to show variable elimination for MRFs, since Bayes nets $\rightarrow$ MRFs by moralization
$>$ Worst-case complexity is dependent on elimination order, and is exponential in number of variables
$>$ Optimal ordering $=$ treewidth, is NP-hard to compute

## Sum-Product Belief Propagation



Pass messages from leaves-to-root, then root-to-leaves

Forward-Backward extends to any tree-structured pairwise MRF

Marginal given by incoming messages (e.g. node C):


$$
p(C) \propto \psi(C) m_{A}(C) m_{F}(C) m_{G}(C)
$$

## Pairwise MRF Sum-Product Belief Propagation

Message updates depend only on Markov blanket...


Message $m_{t s}\left(x_{s}\right)=\sum_{x_{t}} \psi_{s t}\left(x_{s}, x_{t}\right) \psi_{t}\left(x_{t} \prod_{k}\right) \Gamma(t) \backslash s m_{k t}\left(x_{t}\right)$
Marginal $p\left(x_{t}\right) \propto \psi_{t}\left(x_{t}\right) \prod_{k \in \Gamma(t)} m_{k t}\left(x_{t}\right)$

## Factor Graph Sum-Product Belief Propagation



Variable node $x_{m}$ gathers messages, $\mu_{f, \rightarrow x_{m}}$, and sends

$$
\mu_{x_{m} \rightarrow f_{s}}\left(x_{m}\right)=\prod_{l \exists f_{l} \in n\left(x_{m}\right) \backslash f_{s}} \mu_{f_{l} \rightarrow x_{m}}\left(x_{m}\right)
$$



Factor $f_{s}$ gathers messages $\mu_{x_{m} \rightarrow f_{s}}\left(x_{m}\right)$, and sends
$\mu_{f_{s} \rightarrow x}(x)=\sum_{x_{1}} \sum_{x_{2}} \cdots \sum_{x_{w}} f_{s}\left(x, x_{1}, x_{2}, \ldots, x_{M}\right) \prod_{m \in n a\left(f_{s}\right) \backslash x} \mu_{x_{m} \rightarrow f_{s}}\left(x_{m}\right)$

Marginal is product of incoming factor-to-variable messages:

$$
p\left(x_{m}\right) \propto \prod_{f_{l} \in n e\left(x_{m}\right)} \mu_{f_{l} \rightarrow x_{m}}\left(x_{m}\right)
$$

## Marginal Inference Algorithms

## One Marginal

All Marginals


## Junction Tree

Clique tree edges are separator sets in original MRF...so clique tree encodes conditional independencies

$$
X_{1} \perp X_{5} \mid\left\{X_{2}, X_{3}\right\}
$$



Theorem A clique tree resulting from variable elimination satisfies the running intersection property and is thus a junction tree

## Junction Tree

Definition (Running intersection) For any pair of clique nodes $\mathrm{V}, \mathrm{W}$ all cliques on the unique path between V and W contain shared variables

Junction Tree


Not A Junction Tree
$\left\{X_{2}, X_{3}, X_{5}\right\} \cap\left\{X_{2}, X_{5}, X_{6}\right\}=\left\{X_{2}, X_{5}\right\}$


Theorem A clique tree resulting from variable elimination satisfies the runniing intersection property and is thus a junction tree

## Junction Trees and Triangulation



- A chord is an edge connecting two non-adjacent nodes in some cycle
- A cycle is chordless if it contains no chords
- A graph is triangulated (chordal) if it contains no chordless cycles of length 4 or more

Theorem: The maximal cliques of a graph have a corresponding junction tree if and only if that undirected graph is triangulated

Lemma: For a non-complete triangulated graph with at least 3 nodes, there is a decomposition of the nodes into disjoint sets $A, B$, $S$ such that $S$ separates $A$ from $B$, and $S$ is complete.
$>$ Key induction argument in constructing junction tree from triangulation
> Implies existence of elimination ordering which introduces no new edges

## Induced Graph

Recall the induced graph is the union over intermediate graphs from running variable elimination
The induced graph is chordal thus:

- Maximal cliques of the induced graph form a junction tree
- It admits an elimination ordering that introduces no new edges

Logic of junction tree algorithm:

1. Triangulate the graph
a. Implies a junction tree
b. Induces an elimination order

2. Run sum-product BP on junction tree to compute all clique marginals

## Loopy Belief Propagation (sum-product)

## Initialize Messages

Constant: $m_{s t}^{0}\left(x_{t}\right)=$ const.
Random: $m_{s t}^{0}\left(x_{t}\right) \sim U([0,1])$

## Parallel (Synchronous) Updates

At iteration $i$ update all messages in parallel using current messages $\mathrm{m}^{\mathrm{i}-1}$ from previous iteration:

$$
m_{s t}^{i}\left(x_{t}\right)=\sum_{x_{s}} \psi_{s t}\left(x_{s}, x_{t}\right) \prod_{k \in \Gamma(s) \backslash t} m_{k s}^{i-1}\left(x_{s}\right)
$$

- Store, both, the previous messages (from iteration $i-1$ ) and current messages (from iteration $i$ )
- Many convergence results assume parallel updates



## Loopy Belief Propagation (sum-product)

## Initialize Messages

Constant: $m_{s t}^{0}\left(x_{t}\right)=$ const.
Random: $m_{s t}^{0}\left(x_{t}\right) \sim U([0,1])$

## Asynchronous (Sequential) Updates

Choose an ordering of nodes and update using the latest available messages:

$$
m_{s t}\left(x_{t}\right)=\sum_{x_{s}} \psi_{s t}\left(x_{s}, x_{t}\right) \prod_{k \in \Gamma(s) \backslash t} m_{k s}\left(x_{s}\right)
$$

- Simplifies updates since only need to keep track of one copy of messages
- Makes parallel processing trickier



## Pseudocode from Murphy's Textbook

Algorithm 22.1: Loopy belief propagation for a pairwise MRF
1 Input: node potentials $\psi_{s}\left(x_{s}\right)$, edge potentials $\psi_{s t}\left(x_{s}, x_{t}\right)$;
2 Initialize messages $m_{s \rightarrow t}\left(x_{t}\right)=1$ for all edges $s-t$;
3 Initialize beliefs $\operatorname{bel}_{s}\left(x_{s}\right)=1$ for all nodes $s$;

## 4 repeat

5 Send message on each edge

$$
m_{s \rightarrow t}\left(x_{t}\right)=\sum_{x_{s}}\left(\psi_{s}\left(x_{s}\right) \psi_{s t}\left(x_{s}, x_{t}\right) \prod_{u \in \operatorname{nbr}_{s} \backslash t} m_{u \rightarrow s}\left(x_{s}\right)\right) ;
$$

$6 \quad$ Update belief of each node $\operatorname{bel}_{s}\left(x_{s}\right) \propto \psi_{s}\left(x_{s}\right) \prod_{t \in \text { nbr }_{s}} m_{t \rightarrow s}\left(x_{s}\right)$;
7 until beliefs don't change significantly;
8 Return marginal beliefs bel ${ }_{s}\left(x_{s}\right)$;

## Loopy BP on Factor Graphs

Set of neighbors of node s: $\quad \Gamma(s)=\{f \in \mathcal{F} \mid s \in f\}$


Loopy BP:
Message updates can be iteratively computed on graphs with cycles.

## But marginals not

$x_{w}$ guaranteed correct!


$$
m_{f s}\left(x_{s}\right)=\sum_{x_{f \backslash s}} \psi_{f}\left(x_{f}\right) \prod_{t \in f \backslash s} \bar{m}_{t f}\left(x_{t}\right)
$$

Marginal Distribution of Each Variable:

$$
p_{s}\left(x_{s}\right) \propto \prod_{f \in \Gamma(s)} m_{f s}\left(x_{s}\right)
$$

Marginal Distribution of Each Factor: Clique of variables linked by factor.

$$
p_{f}\left(x_{f}\right) \propto \psi_{f}\left(x_{f}\right) \prod_{s \in f} \bar{m}_{s f}\left(x_{s}\right)
$$

## Message Passing Inference Summary

- Brute-force enumeration exponential regardless of graph
- Sum-Product BP
- Exact inference in tree-structure graphs in $\mathrm{O}\left(\mathrm{TK}^{2}\right)$ time for T nodes, each taking K states
- Reduces to Forward-Backward in HMMs
- Same for Max-Product BP (reduces to Viterbi in HMMs)
- Variable elimination
- Exact marginals in general graphs
- Worst-case complexity exponential in size of largest clique
- Need to rerun from scratch for each marginal
- Complexity dependent on elimination order (NP-hard to optimize)


## Message Passing Inference Summary

## - Junction Tree Algorithm

- Exact marginals in general graphs
- Caches messages to compute all marginals
- Worst-case complexity exponential in size of largest clique
- Optimizing Jtree is NP-hard (corresponds to finding treewidth)
- Loopy BP
- BP updates only depend on tree-structured Markov blanket
- Approximate inference in loopy graphs
- No guarantees, but works well empirically in many instances
- Some techniques to improve convergence
- Message damping
- Asynchronous message update schedules
- Probability and Statistics
- Probabilistic Graphical Models
- Message Passing Inference
- Parameter Learning


## Maximum Likelihood Estimation

$$
\theta^{\mathrm{MLE}}=\arg \max _{\theta} p(\mathcal{Y} \mid \theta)=\arg \max _{\theta} \log p(\mathcal{Y} \mid \theta)
$$

If concave then just solve for zero-gradient solution,

$$
\mathcal{L}(\theta) \equiv \log p(\mathcal{Y} \mid \theta) \quad \nabla_{\theta} \mathcal{L}\left(\theta^{\mathrm{MLE}}\right)=0
$$

Log-Likelihood Function doesn't change argmax since log is monotonic

Logarithm serves a couple of practical purposes:

1) Simplifies derivatives for conditionally independent data

$$
\nabla_{\theta} \mathcal{L}(\theta)=\sum_{i=1}^{N} \nabla_{\theta} \log p\left(y_{i} \mid \theta\right)
$$

2) Avoids numerical under/overflow

## MLE of Gaussian Mean

Assume data are i.i.d. univariate Gaussian,

$$
p(\mathcal{Y} \mid \theta)=\prod_{i=1}^{N} \mathcal{N}\left(y_{i} \mid \theta, \sigma^{2}\right)
$$

Log-likelihood function:

$$
\mathcal{L}(\theta)=\sum_{i=1}^{N} \log \left(\frac{1}{\sqrt{2 \pi \sigma^{2}}} \exp \left(-\frac{1}{2}\left(y_{i}-\theta\right)^{2} \sigma^{-2}\right)\right)
$$

Constant doesn't depend on mean

$$
=\text { const. }-\frac{1}{2} \sum_{i=1}^{N}\left(\left(y_{i}-\theta\right)^{2} \sigma^{-2}\right)
$$

MLE doesn't change when we:

1) Drop constant terms (in $\theta$ )
2) Minimize negative log-likelihood

MLE estimate is least squares estimator:

$$
\theta^{\mathrm{MLE}}=-\frac{1}{2 \sigma^{2}} \arg \max _{\theta} \sum_{i=1}^{N}\left(y_{i}-\theta\right)^{2}=\arg \min _{\theta} \sum_{i=1}^{N}\left(y_{i}-\theta\right)^{2}
$$

## Maximum A Posteriori (MAP) Estimation

Recall the MAP estimator maximizes posterior probability,

$$
\begin{array}{rlrl}
\theta^{\mathrm{MAP}} & =\arg \max _{\theta} p(\theta \mid \mathcal{Y}) \\
& =\arg \max _{\theta} p(\theta, \mathcal{Y}) & & \\
& =\arg \max _{\theta} p(\mathcal{Y} \mid \theta) p(\theta) & & \text { ( Probabes' rule ) } \\
& =\arg \max _{\theta} \log p(\mathcal{Y} \mid \theta)+\log p(\theta) & & \text { (Monotonicity Chain Rule ) }
\end{array}
$$

Prior serves as regularizer in regularized MLE:

$$
\theta^{\mathrm{MLE}}=\arg \max _{\theta} \mathcal{L}(\theta)-\lambda R(\theta)
$$

## Learning Summary

Maximum a posteriori (MAP) maximizes posterior probability,

$$
\theta^{\mathrm{MAP}}=\arg \max _{\theta} \log p(\theta \mid \mathcal{Y})=\arg \max _{\theta} \mathcal{L}(\theta)+\log p(\theta)
$$

Parameters are random quantities with prior $p(\theta)$.

Corresponds to regularized MLE for specific prior/regularizer pair,

$$
\hat{\theta}=\arg \max _{\theta} \mathcal{L}(\theta)-\lambda \mathcal{R}(\theta)
$$

Gaussian prior=L2, Laplacian prior=L1

Straightforward sequential updating, e.g. Bayesian linear regression

