EE512A – Advanced Inference in Graphical Models
— Fall Quarter, Lecture 10 —
http://j.ee.washington.edu/~bilmes/classes/ee512a_fall_2014/

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Announcements

- Read chapters 1, 2, and 3 in this book!
- Read first two chapters in above text.
Class Road Map - EE512a

- L1 (9/29): Introduction, Families, Semantics
- L2 (10/1): MRFs, elimination, Inference on Trees
- L3 (10/6): Tree inference, message passing, more general queries, non-tree
- L4 (10/8): Non-trees, perfect elimination, triangulated graphs
- L5 (10/13): triangulated graphs, $k$-trees, the triangulation process/heuristics
- L6 (10/15): multiple queries, decomposable models, junction trees
- L7 (10/20): junction trees, begin intersection graphs
- L8 (10/22): intersection graphs, inference on junction trees
- L9 (10/27): inference on junction trees, semirings,
- L10 (10/29): conditioning, hardness, LBP

- L11 (11/3):
- L12 (11/5):
- L13 (11/10):
- L14 (11/12):
- L15 (11/17):
- L16 (11/19):
- L17 (11/24):
- L18 (11/26):
- L19 (12/1):
- L20 (12/3):

Final Presentations: (12/10):

Finals Week: Dec 8th-12th, 2014.
Recap

- Message passing on junction tree nodes, definition of messages, divide out old, multiply in new.
- Messages in both directions.
- For general tree, we have MPP like in 1-tree case.
- Suff condition: locally consistent.
- Thm: MPP renders cliques locally consistent between pairs.
- In JT (r.i.p.) locally consistent ensures globally consistent.
- In JT (r.i.p.), running MPP gives marginals.
- Commutative semiring - other algebraic objects can be used.
- Time and memory complexity is $O(N^{\omega+1})$ where $\omega$ is the tree-width.
Summarizing, forward and backwards messages proceed as follows:

Recall: \( S = U \cap W \), and we initialize \( \psi_U \) and \( \psi_W \) with factors that are contained in \( U \) or \( W \).
Time-Space Tradeoffs

- Achievable region
- Unachievable region
- Approximate inference
- No need to find algorithms here
- Basic recursive conditioning
- Partial caching
- JT/elimination
- Recursive Cond. w. caching
- Other possible algorithms

Mathematical expressions:
- \( r^N \)
- \( r^{(w+1) \log N} \)
- \( N r^w \)
- \( N \)
- \( r^N \)
Recursive Conditioning, three cluster version

Example: 3-cluster version

1. $\alpha_1 \leftarrow 0$
2. for $x_{C_1} \in D_{X_{C_1}}$ do
   3. $\alpha_{2|1} \leftarrow 0$; $\alpha_{3|1} \leftarrow 0$
   4. for $x_{C_2 \setminus C_1} \in D_{X_{C_2 \setminus C_1}}$ do
      5. $\alpha_{2|1} += p(x_{C_1 \cup C_2})$
   6. for $x_{C_3 \setminus C_1} \in D_{X_{C_3 \setminus C_1}}$ do
      7. $\alpha_{3|1} += p(x_{C_1 \cup C_3})$
   8. $\alpha_1 += \alpha_{2|1} \alpha_{3|1}$

- Outer loop costs $O(|D_{X_{C_1}}|)$. Inner loops each cost $O(|D_{X_{C_2 \setminus C_1}}|)$ (assuming $C_3$ and $C_2$ are same size).
- Total cost is $O(|D_{X_{C_1 \cup C_2}}|)$, better than $O(|D_{X_{C_1 \cup C_2 \cup C_3}}|) = O(r^N)$.
- Memory: still linear.
Recursive Conditioning with good order

- We can order the cliques in a different way though. Note that this is not necessarily a junction tree, although it might be. Rather, this is more akin to a decomposition trees we saw earlier in the course, but it is not that either. Instead, it is more of a “conditioning tree”

- Depth of tree is $d = O(\log N)$
Recursive Conditioning with good order

All $\alpha$’s initialized to 0 before ‘for’ loop where they are accumulated.

for $\mathbf{x} \in \mathcal{D}_{\mathbf{x}}$ do
  for $\mathbf{y} \in \mathcal{D}_{\mathbf{y}}$ do
    $\alpha_{\mathbf{y} | \mathbf{x}} += p(\mathbf{y} | \mathbf{x})$

for $\mathbf{z} \in \mathcal{D}_{\mathbf{z}}$ do
  $\alpha_{\mathbf{z} | \mathbf{x}} = \alpha_{\mathbf{y} | \mathbf{x}}$

Lines 12-22, include at line 10 above

for $\mathbf{w} \in \mathcal{D}_{\mathbf{w}}$ do
  $\alpha_{\mathbf{w} | \mathbf{x}} = \alpha_{\mathbf{z} | \mathbf{x}}$

Include lines 12-22 here

$\alpha_1 += \alpha_2 \alpha_3 \alpha_4$
Recursive Conditioning with good order

- When we’re all done, $\alpha_1 = p(\overline{x}_E)$ (again, assuming evidence is treated as multiplies by $\delta(x, \overline{x})$).

- How much space is needed? $O(N)$ still since in worst case, depth of the tree is number of maxcliques (which is $O(N)$).

- How much time? Depends on number of $\alpha$-accumulates, or number of leaf-nodes in the tree. Depth is $d = \log N$. Each clique gets run about $r^{w+1}$ times, and runs the nodes below it about that many times.

- We get a time complexity of:

$$r^{w+1} \cdot r^{w+1} \cdot \ldots \cdot r^{w+1} \quad \text{d times} \quad \Rightarrow \quad r^{(w+1) \log N} \quad (10.21)$$
Time-Space Tradeoffs

Space complexity

\[ r \cdot N \]

\[ r^{(w+1) \log N} \]

\[ N \cdot r^w \]

\[ N \]

\[ N \cdot r^w \]

\[ r^N \]

Achievable region

No need to find algorithms here

Basic recursive conditioning

Partial caching

JT/elimination

Recursive Cond. w. caching

Other possible algorithms

Unachievable region

Approximate inference

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Recursive Conditioning with good order

- How to get other points on frontier?
- Note that in previous algorithm, for each set of variable values in intersection set (square boxes), we were solving the same sub-problem multiple times.
- We can cache the solutions for each value, at the cost of more memory. If everything is cached, space complexity will increase to $O(Nr^w)$ and time complexity will decrease to $O(Nr^w)$ (like the JT case).
Many algorithms use value specific caching. I.e., depending on the values of some variables currently conditioned on, we might actually get an entirely different set of maxcliques (or set of sets of maxcliques) below. Each should ideally be treated differently.

We can construct and memoize the dependency sets, the set of variables and their values that induce particular sub-computations. Each sub-computation might be a computation of a sum, or it might even be a computation of zero (called a no-good, or a conflict). Each of these can be memoized and re-used whenever the dependency set becomes active again.

the order of the cliques and the order of the variables in the cliques might dynamically change depending on previously instantiated values. We might not even use cliques at all, and do this at the granularity of variables and their values.
Value-Elimination

- This is the basis of the **value elimination algorithm** (Bacchus-2003), a general procedure for probabilistic inference. It gets much of its inspiration from the techniques used to produce fast SAT and constraint satisfaction problem (CSP) engines.

- This is especially useful if we have many zeros (sparsity) in the distribution and/or if there is much value specific independence.
Even with conditioning, search, etc. Complexity of exact inference is always exponential in at least the tree-width of any covering graph if we do it as we’ve been describing.
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Unfortunately, finding the best exponent (i.e., finding the best covering triangulated graph (with minimal tree-width)) is, as we saw in earlier lectures, an NP-complete optimization problem.
Even with conditioning, search, etc. Complexity of exact inference is always exponential in at least the tree-width of any covering graph if we do it as we’ve been describing.

Unfortunately, finding the best exponent (i.e., finding the best covering triangulated graph (with minimal tree-width)) is, as we saw in earlier lectures, an NP-complete optimization problem.

Even worse, inference itself is NP-complete. There are some graphs that can’t be solved in polynomial time unless P=NP (so it seems exponential cost is probably inevitable).
Hardness of Inference

- Consider the 3-SAT problem (which is a canonical NP-complete problem). Given a list of $N$ variables, and a collection of $M$ clauses (constraints), where each clause is a disjunction ("or") of 3 literals (a variable or its negation). Clauses are organized in a conjunction ("and").
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- Question: is there a satisfying truth assignment of the variables (assignment of variable values that makes the conjunction of disjunctions true).
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*Question:* is there a satisfying truth assignment of the variables (assignment of variable values that makes the conjunction of disjunctions true).

**Two examples:**

\[
\begin{align*}
(x_1 \lor x_4 \lor \bar{x}_5) \land (\bar{x}_2 \lor \bar{x}_3 \lor x_4) \land (\bar{x}_1 \lor \bar{x}_4 \lor x_3) \land (\bar{x}_3 \lor \bar{x}_4 \lor \bar{x}_5) \\
\land (\bar{x}_1 \lor x_4 \lor x_2) \land (\bar{x}_1 \lor \bar{x}_2 \lor x_3)
\end{align*}
\]

(10.1) and also

\[
\begin{align*}
(x_1 \lor \bar{x}_2 \lor x_3) \land (\bar{x}_3 \lor \bar{x}_4 \lor x_5) \land (x_5 \lor \bar{x}_6 \lor \bar{x}_7) \land (x_7 \lor x_8 \lor x_9) \\
\land (\bar{x}_9 \lor x_{10} \lor x_{11}) \land (\bar{x}_{11} \lor \bar{x}_{12} \lor \bar{x}_3)
\end{align*}
\]

(10.2)
In the general case, we have \( N \) variables and \( M \) clauses, either of which might be very large. If we can solve this problem in polynomial time in \( N \), then all NP-complete problems can be solved in polynomial time.
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To show that inference in Bayesian networks is NP-complete, all we need to do is find a BN or MRF that encodes this problem using the appropriate commutative semiring (which in our case, we’ll take to be the max-product semiring).
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Let $\{x_i\}_{i=1}^N$ be the set of variables, and let $C_j$ be the index set of the variables for clause $0 \leq j \leq M$. 

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To show that inference in Bayesian networks is NP-complete, all we need to do is find a BN or MRF that encodes this problem using the appropriate commutative semiring (which in our case, we’ll take to be the max-product semiring).

Let $\{x_i\}_{i=1}^N$ be the set of variables, and let $C_j$ be the index set of the variables for clause $0 \leq j \leq M$.

Define binary-valued functions $f_j(x_{C_j})$ such that $f_j = 1$ iff the clause is satisfied by the current values of the variables $x_{C_j}$, otherwise $f_j = 0$. 

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With this formulation, we get factorization as follows

$$p(x) \propto \prod_j f_j(x_{C_j})$$

(10.3)

which is possible to evaluate to unity iff the logic formula is satisfiable.

Next, consider BN with $N$ binary variables $\{x_i\}_{i=1}^N$ and $M$ additional variables $\{y_j\}_{j=1}^M$ with $M$ CPTs of the form:

$$p(y_j = 1|x_{C_j}) = \begin{cases} 1 & \text{if } f_j(x_{C_j}) = 1 \\ 0 & \text{else} \end{cases}$$

(10.4)

and for $x_i$ $p(x_i = 1) = 0.5$

This gives joint distribution that factorizes

$$p(x_1:N, y_1:M) = \prod_i p(x_i) \prod_j p(y_j|x_{C_j})$$
Hardness of Inference

- Create following BN, as evidence set use $y_j = 1$ for all $j \in 1 \ldots M$
- Use max-sum semi-ring, so goal is to find the assignment to the $x$ variables that maximize the joint probability.
- Resulting max evaluation is 1 iff original 3-SAT formula is satisfiable.
Hardness of Inference

- Example: $N = 5$, $M = 6$ in following 3-SAT formula and BN

\[(x_1 \lor x_4 \lor \overline{x_5}) \land (\overline{x_2} \lor \overline{x_3} \lor x_4) \land (\overline{x_1} \lor \overline{x_4} \lor x_3) \land (\overline{x_3} \lor \overline{x_4} \lor \overline{x_5}) \land (\overline{x_1} \lor x_4 \lor \overline{x_2}) \land (\overline{x_1} \lor \overline{x_2} \lor x_3)\]
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MPE/Viterbi assignment to \( x_{1:5} \) has non-zero probability iff original formula is SAT, BN inference (in general) NP-complete.
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- MPE/Viterbi assignment to $x_{1:5}$ has non-zero probability iff original formula is SAT, BN inference (in general) NP-complete.
- Doesn’t mean exact inference is always intractable, rather can’t hope for a polynomial solution in all cases unless $P = NP$.
- Moreover, even low tree-width graphs can be computationally challenging (i.e., large state space or random variable domain size).
Recap

- Time and memory complexity is $O(N^{r\omega+1})$ where $\omega$ is the tree-width.
Recap

- Time and memory complexity is $O(Nr^{\omega+1})$ where $\omega$ is the tree-width.
- We can use conditioning (e.g., cutset conditioning) to get other points. E.g., condition on a set that renders the remainder of the set a tree. Same computation less memory.
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- Recursive conditioning (and similar such algorithms) allows is to get linear memory but a time complexity of $O(τ^{(w+1)\log N})$.
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- Recursive conditioning (and similar such algorithms) allows is to get linear memory but a time complexity of $O(r^{(w+1) \log N})$.
- In general, many time-space tradeoffs for exact inference. Many algorithms along the achievable/unachievable frontier are SAT/CSP based, and use conditioning combined with various caching, and clause learning/deduction (e.g., nogood learning).
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To get a better time/space profile, need to do approximation.

For any given degree of distortion, there is a time/space tradeoff profile.
Time-Space Tradeoffs

- Conditioning
- Hardness
- Approximation
- LBP
- Next phase of class
- Refs

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Approximation: Two general approaches

- exact solution to approximate problem - approximate problem
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1. **exact solution to approximate problem** - approximate problem
   - learning with or using a model with a structural restriction, structure learning, using a $k$-tree for a lower $k$ than one knows is true. Make sure $k$ is small enough so that exact inference can be performed, and make sure that, in that low tree-width model, one has best possible graph
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- Both methods only guaranteed approximate quality solutions.
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Both methods only guaranteed approximate quality solutions.

No longer in the achievable region in time-space tradoff graph, new set of time/space tradeoffs to achieve a particular accuracy.
Belief Propagation

**Generic message definition**

\[
\mu_{i \rightarrow j}(x_j) = \sum_{x_i} \psi_{i,j}(x_i, x_j) \prod_{k \in \delta(i) \setminus \{j\}} \mu_{k \rightarrow i}(x_i)
\]  \hspace{1cm} (10.5)

- If graph is a tree, and if we obey MPP order, then we will reach a point where we've got marginals. I.e.,

\[
p(x_i) \propto \prod_{j \in \delta(i)} \mu_{j \rightarrow i}(x_i)
\]  \hspace{1cm} (10.6)

and

\[
p(x_i, x_j) \propto \psi_{i,j}(x_i, x_j) \prod_{k \in \delta(i) \setminus \{j\}} \mu_{k \rightarrow i}(x_i) \prod_{\ell \in \delta(j) \setminus \{i\}} \mu_{\ell \rightarrow j}(x_j) M
\]  \hspace{1cm} (10.7)
Often, we see that nodes have potential functions as well. I.e., we have edge potentials $\psi_{i,j}(x_i, x_j)$ for $(i, j) \in E(G)$ and $\psi_i(x_i)$ for $i \in V(G)$. Also we might normalize each step (for numerical reasons). We get:

$$
\mu_{i \rightarrow j}(x_j) \propto \sum_{x_i} \psi_{i,j}(x_i, x_j) \psi_i(x_i) \prod_{k \in \delta(i) \setminus \{j\}} \mu_{k \rightarrow i}(x_i)
$$

such that $\mu_{i \rightarrow j}(x_j)$ sums to 1. If $G$ is a tree, and we obey MPP, we get

$$
p(x_i) \propto \psi_i(x_i) \prod_{j \in \delta(i)} \mu_{j \rightarrow i}(x_i)
$$

and

$$
p(x_i, x_j) \propto \psi_{i,j}(x_i, x_j) \prod_{k \in \delta(i) \setminus \{j\}} \mu_{k \rightarrow i}(x_i) \prod_{\ell \in \delta(j) \setminus \{i\}} \mu_{\ell \rightarrow j}(x_j)
$$
\[ \psi_t(x_t, y_t) \equiv \psi_t(x_t) \]
Belief Propagation: Generality

- So far, the “belief propagation” (BP) messages are done along edges, pairwise interaction, factors of the form $\psi_{ij}(x_i, x_j)$. What about higher order interaction $\psi_C(x_C)$ where $|C| > 2$?
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- Recall a factor graph, where the factors themselves are represented on the right hand side of a bipartite graph.

$$p(x_1, x_2, x_3) = f_1(x_1, x_2)f_2(x_2, x_3)f_3(x_1, x_3)f_4(x_3)$$
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- It is common to define a form of BP on a factor graph, going back and forth, between left and right nodes.
So far, the “belief propagation” (BP) messages are done along edges, pairwise interaction, factors of the form $\psi_{ij}(x_i, x_j)$. What about higher order interaction $\psi_C(x_C)$ where $|C| > 2$?

Recall a factor graph, where the factors themselves are represented on the right hand side of a bipartite graph.

$$p(x_1, x_2, x_3) = f_1(x_1, x_2) f_2(x_2, x_3) f_3(x_1, x_3) f_4(x_3)$$

It is common to define a form of BP on a factor graph, going back and forth, between left and right nodes.

Recall, an MRF doesn’t distinguish between multiple pairwise interactions vs. one higher-order interaction.
Consider the following three graphical models, the first two factor graphs and the third a MRF.
Generality and Specificity

- Consider the following three graphical models, the first two factor graphs and the third a MRF.

\[ G_1 \quad G_2 \quad G_3 \]

- Left: any distribution that can be written as

\[
p_1(x_1, x_2, x_3) = f_1(x_1, x_2)f_2(x_2, x_3)f_3(x_3, x_1)
\]  

(10.11)
Generality and Specificity

- Consider the following three graphical models, the first two factor graphs and the third a MRF.

\[ G_1 \quad G_2 \quad G_3 \]

- **Left:** any distribution that can be written as
  \[
  p_1(x_1, x_2, x_3) = f_1(x_1, x_2)f_2(x_2, x_3)f_3(x_3, x_1)
  \] (10.11)

- **Center:** any distribution that can be written as
  \[
  p_2(x_1, x_2, x_3) = f_1(x_1, x_2)f_2(x_2, x_3)f_3(x_3, x_1)f_4(x_1, x_2, x_3)
  \] (10.12)
Generality and Specificity

- Consider the following three graphical models, the first two factor graphs and the third a MRF.

\[ p_1(x_1, x_2, x_3) = f_1(x_1, x_2)f_2(x_2, x_3)f_3(x_3, x_1) \]  
\[ p_2(x_1, x_2, x_3) = f_1(x_1, x_2)f_2(x_2, x_3)f_3(x_3, x_1)f_4(x_1, x_2, x_3) \]

- Left: any distribution that can be written as

\[ \log p(x_1, x_2, x_3) = c + c_{12}x_1x_2 + c_{23}x_2x_3 + c_{13}x_1x_3 + c_{123}x_1x_2x_3 \]
Right figure: all distributions that can be written:

\[ p_3(x_1, x_2, x_3) = \psi(x_1, x_2, x_3) \] (10.14)
Generality and Specificity

Right figure: all distributions that can be written:

\[ p_3(x_1, x_2, x_3) = \psi(x_1, x_2, x_3) \]  \hspace{1cm} (10.14)

We have \( p_1, p_2, p_3 \in \mathcal{F}(G_2, \mathcal{M}(fg)) \) and that \( p_1 \in \mathcal{F}(G_1, \mathcal{M}(fg)) \) but that \( p_2, p_3 \notin \mathcal{F}(G_1, \mathcal{M}(fg)) \). Moreover, it is clear that \( p_1, p_2, p_3 \in \mathcal{F}(G_3, \mathcal{M}(f)) \).
Generality and Specificity

Right figure: all distributions that can be written:

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Can we stay with an MRF with this limitation (i.e., MRF’s inability to discern order of interaction amongst variables in a clique)?
We can transform an MRF with higher order potentials to an MRF with only pairwise potentials, but with more variables.
Pairwise MRF representing higher order MRF

- We can transform an MRF with higher order potentials to an MRF with only pairwise potentials, but with more variables.

- Suppose we have $\psi_C(x_C)$ where $|C| > 2$. Define a new (single, scalar) variable $z_C$ where $z_C \in D_{Z_C}$ and where $|D_{Z_C}| = |D_{X_C}|$. 

\[ \psi_{Z}(z_C) = \prod_{i \in C} \psi_{z_C, x_i}(z_C, x_i) \]
Pairwise MRF representing higher order MRF

- We can transform an MRF with higher order potentials to an MRF with only pairwise potentials, but with more variables.
- Suppose we have \( \psi_C(\mathbf{x}_C) \) where \(|C| > 2\). Define a new (single, scalar) variable \( z_C \) where \( z_C \in D_{Z_C} \) and where \(|D_{Z_C}| = |D_{X_C}|\).
- Each scalar value \( z_C \in D_{Z_C} \) represents a vector of values \( \mathbf{x}_C \in D_{X_C} \), and let \( x_i(z_C) \) represent the value of \( x_i \) associated with \( z_C \), and let \( z_C(\mathbf{x}_C) \) represent the value of \( z_C \) corresponding to vector \( \mathbf{x}_C \).
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- Remove all edges between variables in $x_C$ and add pairwise factors (and edges) of the form $\psi_{z_C, x_i}(z_C, x_i)$ for $i \in C$ where $\psi_{z_C, x_i}(z_C, x_i) = 1\{x_i = x_i(z_C)\}$.
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- Create new unary factor $\psi_Z(z_C) = \psi(x_1(z_C), x_2(z_C), \ldots)$. 

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EE512a/Fall 2014/Graphical Models - Lecture 10 - Nov 3rd, 2014  
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Pairwise MRF representing higher order MRF

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- Each scalar value $z_C \in D_{Z_C}$ represents a vector of values $x_C \in D_{X_C}$, and let $x_i(z_C)$ represent the value of $x_i$ associated with $z_C$, and let $z_C(x_C)$ represent the value of $z_C$ corresponding to vector $x_C$.
- Remove all edges between variables in $x_C$ and add pairwise factors (and edges) of the form $\psi_{z_C, x_i}(z_C, x_i)$ for $i \in C$ where $\psi_{z_C, x_i}(z_C, x_i) = 1 \{x_i = x_i(z_C)\}$.
- Create new unary factor $\psi_{Z}(z_C) = \psi(x_1(z_C), x_2(z_C), \ldots)$.
- Then model of the form $\psi_C(x_C)$ has same function as a model of the form $\psi_{Z}(z_C) \prod_{i \in C} \psi_{z_C, x_i}(z_C, x_i)$ but uses only pairwise factors.
Higher order MRF choices

So, to deal with MRFs with higher order factors, we can:

- transform MRF to have only pairwise interactions, we can keep using BP on MRF edges (as done above), makes the math a bit easier, does not change the computation.
Higher order MRF choices

So, to deal with MRFs with higher order factors, we can:

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- Alternatively, we can define BP on factor graphs.
Higher order MRF choices

So, to deal with MRFs with higher order factors, we can:

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- Alternatively, could define BP directly on the maxcliques of the MRF (but maxcliques are not easy to get in a MRF when not triangulated).
Higher order MRF choices

So, to deal with MRFs with higher order factors, we can:

- transform MRF to have only pairwise interactions, we can keep using BP on MRF edges (as done above), makes the math a bit easier, does not change the computation.
- Alternatively, we can define BP on factor graphs.
- Alternatively, could define BP directly on the maxcliques of the MRF (but maxcliques are not easy to get in a MRF when not triangulated).
- For any given $p$, we know the interaction terms. If it has higher order factors, for the remainder of this term, we’ll assume we’ve done the pair-wise transformation.
We start with a general $p \in \mathcal{F}(G, M^{(f)})$ in terms of factors that might not alone have any inherent meaning or normalization.

Goal: We reparameterize $p$ so that the factor decomposition is the same but the factors are now marginals – marginal reparameterization.

Tree graph is such that we can reparameterize so that the edges and nodes are true marginals. e.g., $\phi_i(x_i) = \sum_{x_V \setminus \{i\}} p(x)$.

Can we always do this? Only when graph is triangulated and we do it in terms of cliques and separators. When graph is not triangulated, not possible in general to do this. Eg., 4-cycle.
In a tree, we achieve true marginal reparameterization by sending messages according to MPP until all messages are sent in both directions.

Alternatively, we could, say, initialize all messages to unity $\mu_{i\rightarrow j}(x_j) = 1$ or some other set of values, and sending all messages in parallel. Each parallel send of all message is considered one step.

Let $D$ be the diameter of the tree (length of longest path).

Once we have done $D$ steps, we will have “converged.” Any additional messages will not change the state.

If we have a tree, we have achieved marginal reparameterization.
State representation

Consider the set of messages \( \{ \mu_{i \rightarrow j}(x_j) \}_{i,j} \) as a large state vector \( \mu^t \) with \( 2|E(G)|r \) scalar elements.

Each sent message moves the state vector from \( \mu^t \) at time \( t \) to \( \mu^{t+1} \) at next time step.

A parallel message (sending multiple messages at the same time) moves the state vector as well.

Convergence means that any set or subset of messages sent in parallel is such that \( \mu^{t+1} = \mu^t \).
Messages as matrix multiply

\[
\mu_{i \rightarrow j}(x_j) \propto \sum_{x_i} \psi_{i, j}(x_i, x_j) \psi_i(x_i) \prod_{k \in \delta(i) \setminus \{j\}} \mu_{k \rightarrow i}(x_i) \tag{10.15}
\]

\[
= \sum_{x_i} \psi'_{i, j}(x_i, x_j) \mu_{j \rightarrow i}(x_i) \tag{10.16}
\]

\[
= (\psi'_{i, j})^T \mu_{j \rightarrow i} \tag{10.17}
\]

- Here, \(\psi'_{i, j}\) is a matrix and \(\mu_{j \rightarrow i}\) is a column vector.
- Going from state \(\mu^t\) to \(\mu^{t+1}\) is like matrix-vector multiply — group messages from \(\mu^t\) together into one vector representing \(\mu_{j \rightarrow i}\) for each \((i, j) \in E\), do the matrix-vector update, and store result in new state vector \(\mu^{t+1}\).
- If \(G\) is tree, \(\mu^t\) will converged after \(D\) steps.
Belief Propagation and Cycles

What if graph has cycles?

- MPP causes deadlock since there is no way to start sending messages.
- Like before, we can assume that messages have an initial state, e.g.,\( \mu_{i \rightarrow j}(x_j) = 1 \) for all \((i, j) \in E(G)\) - note this is bi-directional. This breaks deadlock.
- We can then start sending messages. Will we converge after \(D\) steps? What does \(D\) even mean here?
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- Like before, we can assume that messages have an initial state, e.g., $\mu_{i \to j}(x_j) = 1$ for all $(i, j) \in E(G)$ - note this is bi-directional. This breaks deadlock.
- We can then start sending messages. Will we converge after $D$ steps? What does $D$ even mean here?
- No, in fact we could oscillate forever.
Belief Propagation, Cycles, and Oscillation

- Consider odd length cycle (e.g., $C_3$, $C_5$, etc.), $C_3$ is sufficient
  \[ i \rightarrow j \rightarrow k \rightarrow i \]
Belief Propagation, Cycles, and Oscillation

- Consider odd length cycle (e.g., $C_3$, $C_5$, etc.), $C_3$ is sufficient
  
  $i \rightarrow j \rightarrow k \rightarrow i$

- Assume all messages start out at state $\mu_{i \rightarrow j} = [1, 0]^T$. 

\[
\psi_{ij}(x_i, x_j) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} (10.18)
\]

Then we have

\[
\mu_{j \rightarrow k}(x_j) = \sum x_j \psi_{jk}(x_j, x_k) \mu_{i \rightarrow j}(x_j)
\]

or in matrix form

\[
\mu_{j \rightarrow k} = (\psi_{jk})^T \mu_{i \rightarrow j}
\]

(10.20)
Belief Propagation, Cycles, and Oscillation

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  \[ i \rightarrow j \rightarrow k \rightarrow i \]
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- Consider (pairwise) edge functions, for each $i, j$

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  $$\psi_{ij}(x_i, x_j) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$  \hspace{1cm} (10.18)

- then we have

  $$\mu_{j\rightarrow k}(x_k) = \sum_{x_j} \psi_{j,k}(x_j, x_k) \mu_{i\rightarrow j}(x_j)$$  \hspace{1cm} (10.19)
Belief Propagation, Cycles, and Oscillation

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- or in matrix form
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  \mu_{j \rightarrow k} = (\psi_{j,k})^T \mu_{i \rightarrow j}
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Belief Propagation, Cycles, and Oscillation

- Let $\mu_{i \rightarrow j}^t$ be the $t^{th}$ formed message, with $\mu_{i \rightarrow j}^0$ being the starting state at $[1, 0]^T$. 
Belief Propagation, Cycles, and Oscillation

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- Then $\mu_{i \rightarrow j}^1 = [0, 1]^T$, $\mu_{i \rightarrow j}^2 = [1, 0]^T$, $\mu_{i \rightarrow j}^3 = [0, 1]^T$, and so on, never converging. In fact,
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Belief Propagation, Cycles, and Oscillation

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Belief Propagation, Cycles, and Oscillation

- Let $\mu_{i \rightarrow j}^t$ be the $t^{th}$ formed message, with $\mu_{i \rightarrow j}^0$ being the starting state at $[1, 0]^T$.
- Then $\mu_{i \rightarrow j}^1 = [0, 1]^T$, $\mu_{i \rightarrow j}^2 = [1, 0]^T$, $\mu_{i \rightarrow j}^3 = [0, 1]^T$, and so on, never converging. In fact,

$$
\mu_{i \rightarrow j}^{t+1} = (\psi_{i,j})^T \mu_{k \rightarrow i}^t
$$

(10.21)

$$
= (\psi_{i,j})^T (\psi_{k,i})^T \mu_{j \rightarrow k}^t
$$

(10.22)

$$
= (\psi_{i,j})^T (\psi_{k,i})^T (\psi_{j,k})^T \mu_{i \rightarrow j}^t
$$

(10.23)

$$
= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}^3 \mu_{i \rightarrow j}^t
$$

(10.24)

$$
= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \mu_{i \rightarrow j}^t
$$

(10.25)
Belief Propagation, Cycles, and Oscillation

- Thus, each time we go around the loop in the cycle, the message configuration for each \((i, j)\) will flip, thereby never converging.
Thus, each time we go around the loop in the cycle, the message configuration for each \((i, j)\) will flip, thereby never converging.

Damping the messages? I.e., Let \(0 \leq \gamma < 1\) and treat messages as

\[
\mu_{i \rightarrow j}^t \leftarrow \gamma \mu_{i \rightarrow j}^t + (1 - \gamma) \mu_{i \rightarrow j}^{t-1}
\]  

(10.26)
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(10.26)

Empirical Folklore - if we converge quickly without damping, the quality of the resulting marginals might be good. If we don’t converge quickly, w/o damping, might indicate some problem.
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Empirical Folklore - if we converge quickly without damping, the quality of the resulting marginals might be good. If we don’t converge quickly, w/o damping, might indicate some problem.

Ways out of this problem: Other message schedules, other forms of the interaction matrices, and other initializations.
Belief Propagation, Cycles, and Oscillation

- If we initialize messages differently, things will turn out better.
- If $\mu_{i\rightarrow j}^0 = [0.5, 0.5]^T$ then $\mu_{i\rightarrow j}^{t+1} = \mu_{i\rightarrow j}^t$.
- Damping the messages appropriately will also end up at this configuration.
- Is there a better way to characterize this?
Consider a graph with a single cycle $C_\ell$.

It could be a cycle with trees hanging off of each node. We send messages from the leaves of those dangling trees to the cycle (root) nodes, leaving only a cycle remaining.

Consider what happens to $\mu_{i \rightarrow j}^t$ as $t$ increases. w.l.o.g. consider $\mu_{\ell \rightarrow 1}^t$

Let the cycle be nodes $(1, 2, 3, \ldots, \ell, 1)$

$$\mu_{\ell \rightarrow 1}^{t+1} = \left( \prod_{i=1}^{\ell-1} (\psi_{i,i+1})^T \right) \mu_{\ell \rightarrow 1}^t$$

$$= M \mu_{\ell \rightarrow 1}^t$$

(10.27)

(10.28)

Will this converge to anything?
Belief Propagation, Single Cycle

Theorem 10.6.1 (Power method lemma)

Let $A$ be a matrix with eigenvalues $\lambda_1, \ldots, \lambda_n$ (sorted in decreasing order) and corresponding eigenvectors $x_1, x_2, \ldots, x_n$. If $|\lambda_1| > |\lambda_2|$ (strict), then the update $x^{t+1} = \alpha Ax^t$ converges to a multiple of $x_1$ starting from any initial vector $x^0 = \sum_i \beta_i x_i$ provided that $\beta_1 \neq 0$. The convergence rate factor is given by $|\lambda_2/\lambda_1|$.
From this, we the following theorem follows almost immediately.

**Theorem 10.6.2**

1. \( \mu_\ell \rightarrow 1 \) converges to the principle eigenvector of \( M \).
2. \( \mu_2 \rightarrow 1 \) converges to the principle eigenvector of \( M^T \).
3. The convergence rate is determined by the ratio of the largest and second largest eigenvalue of \( M \).
4. The diagonal elements of \( M \) correspond to correct marginal \( p(x_1) \)
5. The steady state “pseudo-marginal” \( b(x_1) \) is related to the true marginal by \( b(x_1) = \beta p(x_1) + (1 - \beta)q(x_1) \) where \( \beta \) is the ratio of the largest eigenvalue of \( M \) to the sum of all eigenvalues, and \( q(x_1) \) depends on the eigenvectors of \( M \).

**Proof.**

See Weiss2000.
What’s going on with our oscillating example?

- We had $M = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ which has row-eigenvector matrix 
  \[
  \begin{bmatrix}
  -1/\sqrt{2} & 1/\sqrt{2} \\
  1/\sqrt{2} & 1/\sqrt{2}
  \end{bmatrix}
  \]
  with corresponding eigenvalues $-1$ and $1$.

- Note that any uniform vector will be “converged”, i.e., any vector of the form $[aa]$.

- However, we don’t have the guaranteed property of convergence since we don’t have that $|\lambda_1| > |\lambda_2|$.
Belief Propagation, arbitrary graph

- This works for a graph with a single cycle, or a graph that contains a single cycle.
- It still does not tell us that we end up with correct marginals, rather we get “pseudo-marginals”, which are locally normalized, but might not be the correct marginals.
- Moreover, they might not be the correct marginals for any probability distribution.
- Also, we’d like a characterization of LBP’s convergence (if it happens) for more general graphs, with an arbitrary number of loops.

We will start on chapter 3 (we assume you will read chapters 1 and 2 on your own).

We’ll follow the Wainwright and Jordan notation, will point out where it conflicts a bit with the current notation we’ve been using.
Most of this material comes from a variety of sources. Best place to look is in our standard reading material.