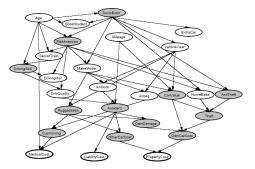
Topic 9: MESSAGE PASSING ALGORITHMS

STAT 37710/CAAM 37710/CMSC 35400 Machine Learning

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Directed graphical models

Also called Bayes nets or Belief Networks. Each vertex $v \in V$ corresponds to a random variable. Graph must be acyclic but not necessarily a tree.



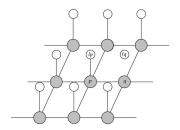
The general form of the joint distribution of all the variables is

$$p(\mathbf{x}) = \prod_{v \in V} p(x_v | \mathbf{x}_{\mathsf{pa}(v)}),$$

where pa(v) are all the parents of v in the graph.

Undirected graphical models

Also called Markov Random Fields. Graph can be any undirected graph. Common example used for image segmentation:



The general form of the joint distribution over all the variables is

$$p(\mathbf{x}) = \frac{1}{Z} \prod_{c \in \mathsf{Cliques}(\mathcal{G})} \phi_c(\mathbf{x}_c)$$

where each ϕ_c is a potentially different clique potential (just a positive function) and Z is the normalizing factor $Z = \sum_{\mathbf{x}} \prod_{c \in \text{Cliques}(\mathcal{G})} \phi_c(\mathbf{x}_c)$.

Tasks for graphical models

- Model selection (i.e., learn the graph itself from data)
- Learn the parameters of the model from data (i.e., the individual conditionals or clique potentials)
- Deduce conditional independence relations
- Infer marginals and conditional distributions

Inference

Partition V, the set of nodes, into three sets:

- 1. the set O of observed nodes
- 2. the set Q of query nodes
- 3. the set L of latent nodes

$$\text{Interested in} \quad p(\mathbf{x}_Q | \mathbf{x}_O) = \frac{\sum_{\mathbf{x}_L} p(\mathbf{x}_Q, \mathbf{x}_L, \mathbf{x}_O)}{\sum_{\mathbf{x}_L, \mathbf{x}_Q} p(\mathbf{x}_Q, \mathbf{x}_L, \mathbf{x}_O)}$$

Essential for both

- Training, when we are trying to learn the distribution of some of the nodes from data.
- Prediction, when we are trying to predict the values of some nodes (the output) given the values of some other nodes (the input)

Question: How can we do this in less than $m^{|Q|+|L|}$ time?

Inference

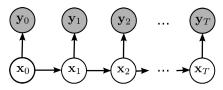
There are two approaches to inference:

- Exact inference
 - Variable elimination
 - Message passing algorithms
- Approximate inference
 - Sampling methods
 - Variational inference

In this course we focus on exact inference, specifically message passing.

Example: Hidden Markov Models

Hidden Markov Models (HMM)

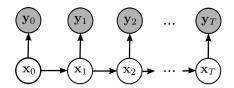


Recall that in an HMM, y_1, y_2, \dots, y_t are observed and x_1, x_2, \dots, x_T are hidden (latent). Applications:

- speech recognition (which phoneme/word/etc.)
- part of speech tagging (is it a NP, VP, etc.)?
- biological sequence analysis (intron or extron)?
- time series analysis (finance, climate, etc.)
- robotics (what is the actual location of the robot)?
- tracking

Parametrizing HMMs: stationary

case

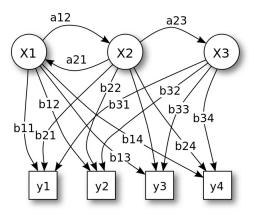


- Starting probabilities: $p(x_0 = i) = \pi_i$
- Emission probabilities: $p(y_t = j \mid x_t = i) = \omega_{i,j}$
- Transition probabilities: $p(x_{t+1} = j \mid x_t = i) = \theta_{i,j}$

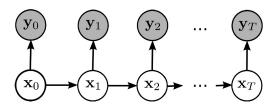
$$p(x_0, \dots, x_T, y_0, \dots, y_T) = p(x_0) \left(\prod_{t=1}^T p(x_t | x_{t-1}) \right) \left(\prod_{t=0}^T p(y_t | x_t) \right)$$

$$= \pi_{x_0} \left(\prod_{t=1}^T \theta_{x_{t-1}, x_t} \right) \left(\prod_{t=0}^T \omega_{x_t, y_t} \right)$$

Analogy with probabilistic finite state machines



HMM tasks



- 1. **Filtering:** compute $p(x_t|y_0,\ldots,y_t) \rightarrow$ forward algorithm
- 2. Smoothing: compute $p(x_t|y_0,\ldots,y_t,\ldots,y_T) \to \text{forward-backward}$ alg
- 3. Most likely explanation: compute $\arg\max_{x_0...x_T} p(x_0...x_T|y_0...y_T) \rightarrow \text{Viterbi algorithm}$
- 4. **Parameter learning:** estimate $\pi, \theta, \omega \rightarrow \text{Baum-Welch algorithm (EM)}$

1. Filtering

The "forward" algorithm

Exploiting indepence

Goal: compute the conditional of a given hidden state x_t given all past observations:

$$p(x_t|y_0,\ldots,y_t) = \frac{p(x_t,y_0,\ldots,y_t)}{\sum_{x'_t} p(x'_t,y_0,\ldots,y_t)}.$$

Naive approach:

$$p(x_t|y_0,\ldots,y_t) = \frac{\sum_{x_0,\ldots,x_{t-1}} p(x_0,\ldots,x_t,y_0,\ldots,y_t)}{\sum_{x_0,\ldots,x_{t-1},x_t'} p(x_0,\ldots,x_t',y_0,\ldots,y_t)}$$

- \rightarrow assuming $x_0,\ldots,x_t\in\{1,\ldots,k\}$, this takes $O(k^{t+1})$ time.
- Instead, exploit the independence $\{X_t,Y_t\} \perp \!\!\! \perp \{Y_0,\ldots,Y_{t-1}\} \|X_{t-1}$.

Exploiting indepence

Using $\{X_t, Y_t\} \perp \!\!\! \perp \{Y_0, \dots, Y_{t-1}\} || X_{t-1}$:

$$p(x_t, x_{t-1}, y_0, \dots, y_t) = p(x_t, y_t | x_{t-1}, y_0, \dots, y_{t-1}) p(x_{t-1}, y_0, \dots, y_{t-1})$$

$$= p(x_t, y_t | x_{t-1}) p(x_{t-1}, y_0, \dots, y_{t-1})$$

$$= p(y_t | x_t) p(x_t, x_{t-1}) p(x_{t-1}, y_0, \dots, y_{t-1}).$$

Therefore,

$$p(x_t, y_0, \dots, y_t) = \sum_{x_{t-1}} p(y_t|x_t) p(x_t|x_{t-1}) p(x_{t-1}, y_0, \dots, y_{t-1}).$$

Natural iterative algorithm: use this recursion to first compute $\ p(x_0,y_0)$, then $\ p(x_1,y_0,y_1)$, then $\ p(x_2,y_0,y_1,y_2)$, etc..

The "forward" algorithm

Define
$$\alpha_t(x_t) = p(x_t, y_0, \dots, y_t)$$
.

- 1. Seed: $\alpha_0(x_0) = p(y_0|x_0) \, \pi_{x_0}$
- 2. Iterate: $\alpha_t(x_t) = p(y_t|x_t) \sum_{x_{t-1}} p(x_t|x_{t-1}) \alpha_{t-1}(x_{t-1})$

$$p(x_t|y_0,...,y_t) = \frac{p(x_t, y_0,...,y_t)}{\sum_{x_t'} p(x_t', y_0,...,y_t)} = \frac{\alpha_t(x_t)}{\sum_{x_t'} \alpha_t(x_t')}$$

 \rightarrow Reduces the complexity from $O(k^{t+1})$ to $O(tk^2)$!!!

2. Smoothing

The "forward-backward" algorithm

Exploiting indepence

Goal: compute the conditional of a hidden state $\,x_t\,$ given all observations:

$$p(x_t|y_0,\ldots,y_T) = \frac{p(x_t,y_0,\ldots,y_T)}{\sum_{x_t'} p(x_t',y_0,\ldots,y_T)}.$$

Naive approach:

$$p(x_t|y_0,\ldots,y_{t-1}) = \frac{\sum_{x_0,\ldots,x_{t-1},x_{t+1},x_T} p(x_0,\ldots,x_T,y_0,\ldots,y_T)}{\sum_{x_0,\ldots,x_{t-1},x_t',x_{t+1},x_T} p(x_0,\ldots,x_T',y_0,\ldots,y_T)}$$

 \rightarrow assuming $x_0, \dots, x_T \in \{1, \dots, k\}$, this takes $O(k^{T+1})$ time.

• Instead, exploit the independences

$$\{X_t, Y_t\} \perp \!\!\!\perp \{Y_0, \dots, Y_{t-1}\} || X_{t-1}$$

 $\{Y_{t+1}, \dots, Y_T\} \perp \!\!\!\perp \{X_0, \dots, X_{t-1}, Y_0, Y_t\} || X_t$

•

Exploiting indepence

Using
$$\{X_t, Y_t\} \perp \!\!\! \perp \{Y_0, \dots, Y_{t-1}, Y_{t+1}, \dots, Y_T\} \| \{X_{t-1}, X_{t+1}\} :$$

$$p(x_t, y_0, \dots, y_T) = p(y_{t+1}, \dots, y_T | x_t) \underbrace{p(x_t, y_0, \dots, y_t)}_{\text{from forward alg}}.$$

Moreover,

$$p(y_{t+1},\ldots,y_T|x_t) = \sum_{x_{t+1}} p(y_{t+2},\ldots,y_T|x_{t+1}) p(y_{t+1}|x_{t+1}) p(x_{t+1}|x_t).$$

Natural iterative algorithm: use this recursion to first compute $\ p(y_T|x_{T-1})$, then $\ p(y_{T-1},y_T|x_{T-2})$, then $\ p(y_{T-2},y_{T-1},y_T|x_{T-3})$, etc..

The "forward-backward" algorithm

Define
$$\beta_t(x_t) = p(y_{t+1}, \dots, y_T | x_t)$$
.

- 1. Seed: $\beta_T(x_T) = 1$
- 2. Iterate: $\beta_t(x_t) = \sum_{x_{t+1}} p(x_{t+1}|x_t) p(y_{t+1}|x_{t+1}) \beta_{t+1}(x_{t+1})$

$$p(x_t|y_0, \dots, y_T) = \frac{p(x_t, y_0, \dots, y_T)}{\sum_{x_t'} p(x_t', y_0, \dots, y_T)} = \frac{\alpha_t(x_t)\beta_t(x_t)}{\sum_{x_t'} \alpha_t(x_t')\beta_t(x_t')}$$

ightarrow Reduces the complexity from $O(k^{T+1})$ to $O(Tk^2)$!!!

The Viterbi algorithm

3. Finding the most likely hidden sequence

Exploiting independence

Goal: find the most likely sequence of hidden variables

$$(\widehat{x}_0, \dots, \widehat{x}_T) = \underset{(x_0, \dots, x_T)}{\operatorname{argmax}} p(x_0, \dots, x_T, y_0, \dots, y_T).$$

Naively, this requires $O(Tk^T)$ time.

To exploit independence, define

$$V_t(x_t) = \max_{x_0...x_{t-1}} p(x_0, ..., x_t, y_0, ..., y_t),$$

i.e., the probability of the most likely way of ending up at x_t given the observations y_0, \ldots, y_t . Similar to the marginal $p(x_t, y_0, \ldots, y_t)$.

Exploiting independence: forward

Since

$$p(x_0 \dots x_t, y_0 \dots y_t) = p(y_t|x_t) p(x_t|x_{t-1}) p(x_0 \dots x_{t-1}, y_0 \dots y_{t-1}),$$

$$\max_{x_0 \dots x_{t-1}} p(x_0, \dots, x_t, y_0, \dots, y_t)
= \max_{x_0 \dots x_{t-1}} \left[p(y_t | x_t) p(x_t | x_{t-1}) p(x_0 \dots x_{t-1}, y_0 \dots y_{t-1}) \right]
= p(y_t | x_t) \max_{x_{t-1}} \left[p(x_t | x_{t-1}) \max_{x_0 \dots x_{t-2}} p(x_0 \dots x_{t-1}, y_0 \dots y_{t-1}) \right].$$

So

$$V_t(x_t) = p(y_t|x_t) \max_{x_{t-1}} \left[p(x_t|x_{t-1}) V_{t-1}(x_{t-1}) \right]$$

This is the forward pass (same as in smoothing, except \sum replaced by \max .

Exploiting independence: backward

The last element of the most likely sequence is $\widehat{x}_T = \operatorname{argmax}_{x_T} V_t(x_T)$. Furthermore,

$$\widehat{x}_{t-1}|(\widehat{x}_t,\ldots,\widehat{x}_T) = \underset{x_{t-1}}{\operatorname{argmax}} [p(\widehat{x}_t|x_{t-1})V_{t-1}(x_{t-1})].$$

So starting with \widehat{x}_T , we can recover $\widehat{x}_{T-1}, \widehat{x}_{T-2}, \ldots$ by the reursion

$$\widehat{x}_{t-1} = \arg \max_{x_{t-1}} (p(\widehat{x}_t | x_{t-1}) V_{t-1}(x_{t-1})).$$

The Viterbi algorithm (1967)

Forward sweep:

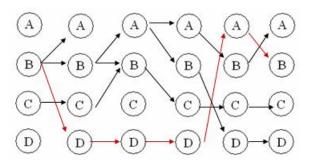
- 1. Seed: $V_0(x_0) = p(y_0|x_0) \, \pi_{x_0}$
- 2. Iterate: $V_t(x_t) = p(y_t|x_t) \max_{x_{t-1}} (p(x_t|x_{t-1}) V_{t-1}(x_{t-1}))$

Backward sweep:

- 1. Seed: $\widehat{x}_T = \arg \max V_T(x_T)$
- 2. Iterate: $\widehat{x}_{t-1} = \arg \max_{x_{t-1}} (p(\widehat{x}_t|x_{t-1}) V_{t-1}(x_{t-1}))$

Once again, the overal complexity is linear in $O(Tk^2)$.

The Viterbi algorithm



When computing each $V_t(x_t)$ if we store a pointer to $\max_{x_{t-1}} \left(p(x_t|x_{t-1}) \, V_{t-1}(x_{t-1}) \right)$, this is literally just retracing the pointers.

4. Learning the parameters

The Baum-Welch algorithm

The Baum–Welch algorithm

Need to jointly compute the distr. over the x_t 's and the setting of the parameters $\Theta=(\pi,\omega,\theta)$ that maximizes the log likelihood $\ell(\pi,\omega,\theta|x_{0:T},y_{0:T})$.

The expectation maximization (EM) approach is to iterate

1. **E-step:** compute the expectation of ℓ w.r.t. $x_{0:T}$:

$$\overline{\ell}_{\widehat{\Theta}_{\mathrm{old}}}(\Theta) = \mathbb{E}(\ell_{\widehat{\Theta}_{\mathrm{old}}}(\Theta)) = \sum_{x_{0:T}} p(x_{0:T}, y_{0:T} | \widehat{\Theta}_{\mathrm{old}}) \, \ell(\Theta | x_{0:T}, y_{0:T})$$

2. M-step:

$$\widehat{\Theta} = \operatorname*{argmax}_{\Theta} \overline{\ell}_{\widehat{\Theta}_{\mathrm{old}}}(\Theta)$$

until convergence (similar to k-means).

The Baum-Welch algorithm

Recall

$$p(x_t|y_0,\ldots,y_T) = \frac{\alpha_t(x_t)\,\beta_t(x_t)}{\sum_{x'}\alpha_t(x_t')\,\beta_t(x_t')} =: \gamma_t(x_t)$$

Also define

$$p(x_t, x_{t+1}|y_0, \dots, y_T) = \frac{1}{Z} \alpha_t(x_t) p(x_{t+1}|x_t) p(y_{t+1}|x_{t+1}) \beta_{t+1}(x_{t+1}) = \frac{\gamma_t(x_t)}{\beta_t(x_t)} p(x_{t+1}|x_t) p(y_{t+1}|x_{t+1}) \beta_{t+1}(x_{t+1}) =: \xi_t(x_t, x_{t+1})$$

The Baum–Welch algorithm

Doing the math, (in the stationary case) the EM approach boils down to

$$\pi_i^{(i+1)} = \gamma_0(i)$$

$$\omega_{i,j}^{(i+1)} = \frac{\sum_{t:y_t=j} \gamma_t(i)}{\sum_{t=0}^T \gamma_t(i)}$$

$$\theta_{i,j}^{(i+1)} = \frac{\sum_{t=0}^{T-1} \xi_t(i,j)}{\sum_{t=0}^{T-1} \gamma_t(i)},$$

which are effectively the "observed freuquencies" of transitions and emissions. Local minima a possibility, so initialization is important. Of course can use a Dirichlet prior or pseudocounts if necessary.

Numbers in logarithmic form

For any reasonable length chain, the $\alpha_t(x_t)$ and $\beta_t(x_t)$ numbers get too small for machine precision. The solution is to instead store their logarithms. We need two operations:

Multiplication:

$$\log(xy) = \log x + \log y$$

• Addition: if $\log y \le \log x$ use

$$\log(x+y) = \log(x(1+y/x)) = \log x + \log(1 + e^{\log y - \log x}).$$

If $\log x < \log y$ use

$$\log(x+y) = \log(y(1+x/y)) = \log y + \log(1 + e^{\log x - \log y}).$$

You can write your own class "logdouble" for this.

Extensions of HMMs

- Hierarchical HMMs
- Auto-regressive HMMs
- Input-output HMMs
- Factorial HMMs
- Variable number of states
- State space models (continuous hidden states) → "Kalman filter"

MESSAGE PASSING IN UNDIRECTED TREES

Factorizing sums

Inference in graphical models involves computing huge sums of products like

$$p(x_1|x_6) = \sum_{x_2} \sum_{x_3} \sum_{x_4} \sum_{x_5} p(x_1) p(x_2|x_1) p(x_3|x_1) p(x_4|x_2) p(x_5|x_3) p(x_6|x_5|x_5) p(x_5|x_5) p(x_5|x_$$

Factorizing such sums is a general problem in math. First we will find a solution for sums arising from undirected tree-shaped models.

The marginal of x_r (regarded as the root) in a tree structured undirected model is

$$p(x_r) = \frac{1}{Z} \sum_{\mathbf{x}_{V \setminus \{r\}}} \prod_{(i,j) \in \mathsf{Cliques}(\mathcal{G})} \phi_{i,j}(x_i, x_j)$$

Now factor it according to the children of the root:

$$p(x_r) = \frac{1}{Z} \prod_{u \in \mathsf{chi}(r)} \left[\underbrace{\sum_{\mathbf{x}_{V_u}} \, \phi_{r,u}(x_r, x_u) \prod_{(i,j) \in E_u} \phi_{i,j}(x_i, x_j)}_{m_{u \to r}(x_r)} \right]$$

where ${\rm chi}(r)$ is the set of children of the root, and V_u and E_u are the vertices and edges of the subtree rooted at u, respectively.

Marginal:

$$p(x_r) = \frac{1}{Z} \prod_{r \in P(r)} m_{u \to r}(x_r)$$

Messages to the root:

$$m_{u \to r}(x_r) = \sum_{x_u} \phi_{r,u}(x_r, x_u) \sum_{\mathbf{x}_{V_u \setminus \{u\}}} \prod_{(i,j) \in E_u} \phi_{i,j}(x_i, x_j)$$

$$m_{u \to r}(x_r) = \sum_{x_u} \phi_{r,u}(x_r, x_u) \underbrace{\sum_{\mathbf{x}_{V_u \setminus \{u\}}} \prod_{(i,j) \in E_u} \phi_{i,j}(x_i, x_j)}_{\text{Factorizes further!}}$$

$$\prod_{v \in \mathsf{chi}(u)} \left[\ \sum_{x_v} \phi_{u,v}(x_u, x_v) \underbrace{\sum_{\mathbf{x}_{V_v \setminus \{v\}}} \prod_{(i,j) \in E_v} \phi_{i,j}(x_i, x_j)}_{\mathsf{Factorizes further!}} \ \right]$$

and so on...

Overall we have the following recursive process:

ullet If v is a leaf (note: observed notes automatically become leaves), set

$$m_{v \to u}(x_u) = \sum_{x_v} \phi_{v,u}(x_v, x_u)$$

else set

$$m_{v \to u}(x_u) = \sum_{x_v} \ \phi_{v,u}(x_v,x_u) \prod_{w \in \mathrm{chi(v)}} m_{w \to v}(x_v).$$

· Read off result

$$p(x_r) = \frac{1}{Z} \prod_{u \in \mathsf{chi}(r)} m_{u \to r}(x_r).$$

What if we want to compute marginals for several nodes? No problem! Just keep passing messages.

trees

Summary:

1. Collect phase (leaves to root)

$$m_{v\to u}(x_u)=\sum_{x_v}\,\phi_{v,u}(x_v,x_u)\qquad\text{or}$$

$$m_{v\to u}(x_w)=\sum_{x_v}\,\phi_{v,u}(x_v,x_u)\prod_{w\in\text{chi(v)}}m_{w\to v}(x_v)$$

2. Distribute phase

$$m_{u \rightarrow v}(x_v) = \sum_{x_u} \phi_{u,v}(x_u, x_v) \prod_{z \in \mathrm{chi}(u) \cup \mathrm{pa}(u) \backslash \{v\}} m_{z \rightarrow u}(x_u)$$

3. Read off marginals

$$p(x_v) = \frac{1}{Z} \prod_{u \in \operatorname{chi}(u) \mid \operatorname{log}(u)} m_{u \to v}(x_v)$$

Semirings

A set R with two binary operations $+: R \times R \to R$ and $\cdot: R \times R \to \mathbb{R}$ is a **semiring** if it satisfies the following axioms:

- a + (b + c) = (a + b) + c
- $\exists 0 \in R$ such that 0 + a = a + 0 = a
- a + b = b + a
- $a \cdot (b \cdot c) = (a \cdot b) \cdot c$
- $\exists 1 \in R$ such that $1 \cdot a = a \cdot 1 = a$
- $a \cdot (b+c) = a \cdot b + a \cdot c$
- $(b+c) \cdot a = b \cdot a + c \cdot a$
- $\bullet \quad 0 \cdot a = a \cdot 0 = 0$

Since the only thing that message passing uses is distributivity, we can use it on any semiring \rightarrow sum-product algorithm.

Semirings

Examples of semirings:

- Any ring, e.g., $(\mathbb{R},+,\cdot)$, $(\mathbb{Q},+,\cdot)$
- $(\mathbb{R}^+, +, \cdot), (\mathbb{N}^+, +, \cdot)$
- $(\mathbb{R}^{+n\times n},+,\cdot)$
- Booelan semiring: $(\{T, F\}, \vee, \wedge)$
- Log-semiring: $(\mathbb{R} \cup \{\pm \infty\}, \oplus, +)$ where $x \oplus y = -\log(e^{-x} + e^{-y})$
- Tropical semiring: $(\mathbb{R} \cup \{-\infty\}, \max, +)$
- $(\mathbb{R}^+ \cup \{0\}, \max, \cdot)$

Using the sum-product algorithm on $(\mathbb{R}^+ \cup \{0\}, \max, \cdot) \to MAP$ (maximum a posteriori) inference.

The above is a special case of a general procedure called the **sum-product algorithm**.

Hinges only on the fact that multiplication distributes over addition.

Therefore, has analogs for max-product and min-sum.

MESSAGE PASSING IN OTHER MODELS

Message passing in non-trees

Can we generalize message passing to graphs with cycles?

- Why not just run the same algorithm? Iterate the same scheme and see if
 it converges to something reasonable

 Loopy belief propagation.

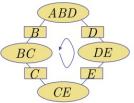
 (approximate algorithm with no theoretical guarantees but often works

 suprisingly well)
- Convert graph into a tree by identifying its multiply connected parts and treating them as single nodes
 — Junction tree algorithm. (exact algorithm, but often unfeasible)

Message passing in non-trees

IDEA: Unify the cliques into single vertices and treat them as single variables. If some original variable is present in multiple cliques, use the conditionals to tie them together.

Question: Can a spanning tree of the resulting graph enforce all the ties? (running intersection property)

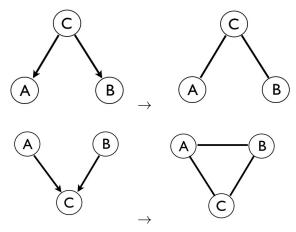


Yes, if the graph is a **junction tree**. Sufficient condition for this is that the original graph must be triangulated (no cycles of length 4 with no subcycles).

Junction tree algorithm: 1. Triangulate 2. Form junction tree from cliques 3. Run message passing.

Message passing for directed models

IDEA: Convert directed model to undirected one!



Marry the parents!!! (moralize)

Message passing for directed models

Summary:

- 1. Moralize (marry the parents)
- 2. Drop arrows
- 3. Triangulate
- 4. Form junction tree
- 5. Run message passing

FURTHER READING

- David Barber: Bayesian Reasoning and Machine Learning (online)
- Daphne Koller and Nir Friedman: Probabilistic Graphical Models
- Tutorial by Sam Roweis: http://videolectures.net/mlss06tw roweis mlpgm/
- Coursera course "Probabilistic Graphical Models" by Daphne Koller