Inference with Graphical Models – Propagation Algorithms (2)

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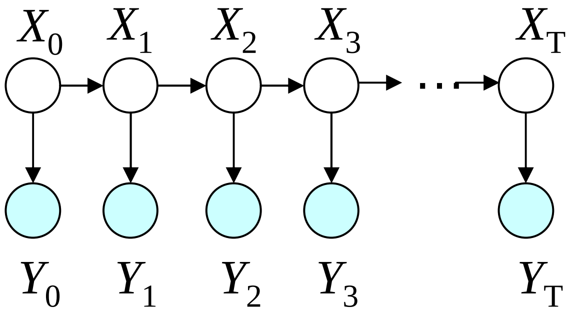
Computational Methodology in Statistical Inference II

Inference on Hidden Markov Model

Inference on Hidden Markov Model

- Review: HMM model

$$p(X,Y) = p(X_0)p(Y_0 \mid X_0)\prod_{t=1}^{T} p(X_t \mid X_{t-1})p(Y_t \mid X_t)$$



X_t: hidden state, finite

- Inference
  - Compute

$$p(X_t \mid Y_1,\ldots,Y_T) \qquad \text{for any } t$$

Naïve computation requires $O(K^T)$ operations, exponential on the sequence length.

K: number of hidden states

Belief Propagation on HMM

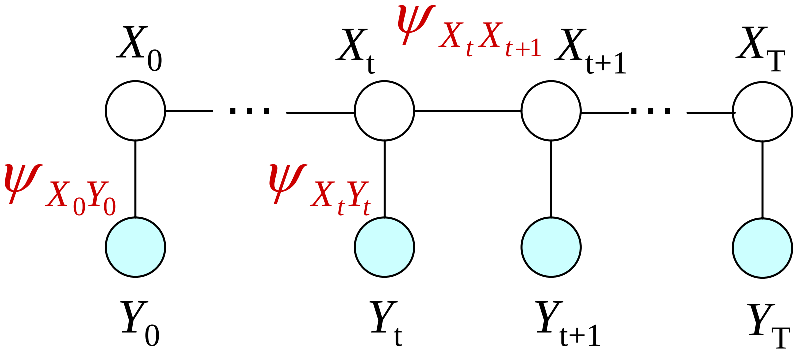
- BP for undirected tree representation
  - Clique potentials

$$\psi_{X_0Y_0}(X_0,Y_0) = p(X_0)p(Y_0 \mid X_0) = p(X_0,Y_0)$$

$$\psi_{X_tY_t}(X_t,Y_t) = p(Y_t \mid X_t) \qquad (1 \le t \le T)$$

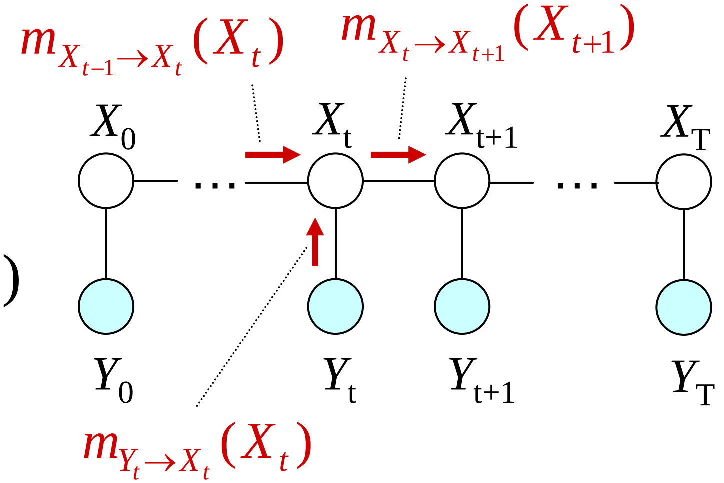
$$\psi_{X_{t-1}X_t}(X_{t-1},X_t) = p(X_t \mid X_{t-1}) \qquad (1 \le t \le T)$$

$$p(X,Y) = \psi_{X_0Y_0}(X_0,Y_0)\prod_{t=1}^{T}\psi_{X_{t-1}X_t}(X_{t-1},X_t)\psi_{X_tY_t}(X_t,Y_t)$$



Belief Propagation on HMM

- Upward message passing



$$m_{X_t\to X_{t+1}}(X_{t+1}) = \sum_{X_t} \psi_{X_t X_{t+1}}(X_t, X_{t+1}) \times m_{X_{t-1}\to X_t}(X_t) m_{Y_t\to X_t}(X_t)$$

$$m_{Y_t\to X_t}(X_t) = p(Y_t \mid X_t) \quad (Y_t \text{ is given.})$$

$$m_{X_t\to X_{t+1}}(X_{t+1}) = \sum_{X_t} p(X_{t+1} \mid X_t) m_{X_{t-1}\to X_t}(X_t) p(Y_t \mid X_t)$$

$$= \sum_{X_t} A_{X_t, X_{t+1}} \underbrace{m_{X_{t-1}\to X_t}(X_t) p(Y_t \mid X_t)}_{\alpha(X_t)}$$

(A: transition matrix)

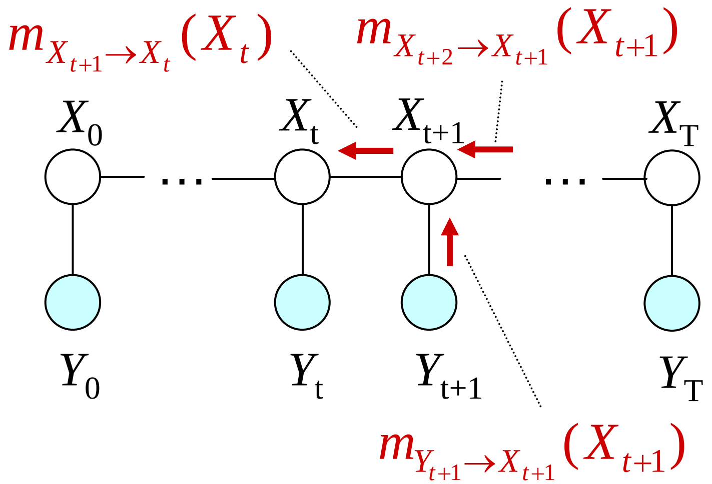
$$\alpha(X_{t+1}) = \sum_{X_t} A_{X_t, X_{t+1}} \alpha(X_t) p(Y_{t+1} \mid X_{t+1})$$

update rule

Belief Propagation on HMM

- Downward message passing

$$m_{X_{t+1}\to X_t}(X_t)=\sum_{X_{t+1}}\psi_{X_tX_{t+1}}(X_t,X_{t+1})$$
$$\times m_{X_{t+2}\to X_{t+1}}(X_{t+1})m_{Y_{t+1}\to X_{t+1}}(X_{t+1})$$



⇒

$$m_{X_{t+1}\to X_t}(X_t)=\sum_{X_{t+1}}p(X_{t+1}\mid X_t)m_{X_{t+2}\to X_{t+1}}(X_{t+1})p(Y_{t+1}\mid X_{t+1})$$
$$=\sum_{X_{t+1}}A_{X_t,X_{t+1}}m_{X_{t+2}\to X_{t+1}}(X_{t+1})p(Y_{t+1}\mid X_{t+1})$$

$$\beta(X_t)\equiv m_{X_{t+1}\to X_t}(X_t)$$

⇒

$$\beta(X_t)=\sum_{X_{t+1}}A_{X_t,X_{t+1}}\beta(X_{t+1})p(Y_{t+1}\mid X_{t+1})$$ update rule

Belief Propagation on HMM

- Marginals

$$p(X_t, Y_0, \cdots, Y_T) = m_{Y_t \to X_t}(X_t) m_{X_{t-1} \to X_t}(X_t) m_{X_{t+1} \to X_t}(X_t)$$

$$= \underbrace{p(Y_t \mid X_t) m_{X_{t-1} \to X_t}(X_t)}_{\alpha(X_t)} \underbrace{m_{X_{t+1} \to X_t}(X_t)}_{\beta(X_t)}$$

$\Rightarrow$

$$p(X_t, Y_0, \cdots, Y_T) = \alpha(X_t)\beta(X_t)$$

(Y_t's are given.)

Hence,

$$p(Y_0, \cdots, Y_T) = \sum_{X_t} \alpha(X_t)\beta(X_t)$$

and

$$p(X_t \mid Y_0, \cdots, Y_T) = \frac{\alpha(X_t)\beta(X_t)}{\sum_{X_t} \alpha(X_t)\beta(X_t)}$$

Forward-Backward Algorithm

- Summary
  - Forward-backward algorithm (α–β algorithm)

$$\alpha(X_{t+1}) = \sum_{X_t} A_{X_t,X_{t+1}} \alpha(X_t) p(Y_{t+1} \mid X_{t+1})$$

$$\beta(X_t) = \sum_{X_{t+1}} A_{X_t,X_{t+1}} \beta(X_{t+1}) p(Y_{t+1} \mid X_{t+1})$$

$$\alpha(X_0) = p(X_0, Y_0), \quad \beta(X_T) = 1$$

  - Marginals

$$p(X_t, Y_0, \cdots, Y_T) = \alpha(X_t)\beta(X_t)$$

$$p(Y_0, \cdots, Y_T) = \sum_{X_t} \alpha(X_t)\beta(X_t)$$ – likelihood of Y (any t)

$$p(X_t \mid Y_0, \cdots, Y_T) = \frac{\alpha(X_t)\beta(X_t)}{\sum_{X_t} \alpha(X_t)\beta(X_t)}$$ – smoothing

Forward-Backward Algorithm

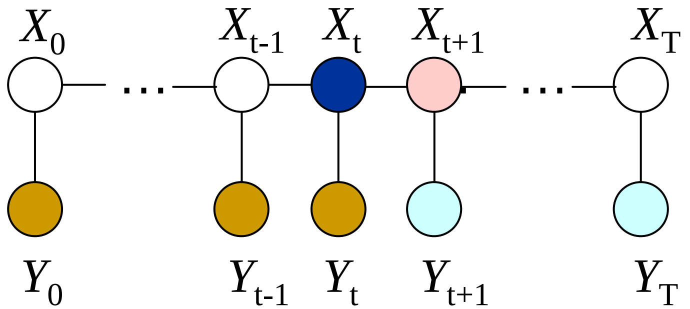
- Meaning of α and β

$$\alpha(X_t) = p(Y_0, \cdots, Y_t, X_t) \qquad (0 \le t \le T)$$

$$\beta(X_t) = p(Y_{t+1}, \cdots, Y_T \mid X_t) \qquad (0 \le t \le T-1)$$

Proof: Forward-Backward Algorithm

- Proof by induction



$\alpha(X_0) = p(X_0, Y_0)$ by definition.

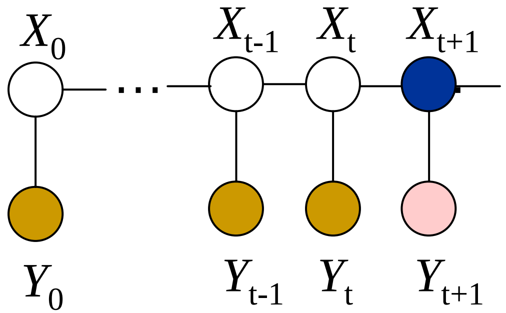
Suppose $\alpha(X_t) = p(Y_0, \cdots, Y_t, X_t)$,

(a) $\alpha(X_{t+1}) = \sum_{X_t} p(X_{t+1} \mid X_t)\alpha(X_t) p(Y_{t+1} \mid X_{t+1})$

$= \sum_{X_t} \underline{p(X_{t+1} \mid X_t) p(Y_0, \cdots, Y_t \mid X_t)} p(X_t) p(Y_{t+1} \mid X_{t+1})$

(Markov)

$= \sum_{X_t} \underline{p(Y_0, \cdots, Y_t, X_{t+1} \mid X_t)} p(X_t) p(Y_{t+1} \mid X_{t+1})$



$= p(Y_0, \cdots, Y_t, X_{t+1}) p(Y_{t+1} \mid X_{t+1})$

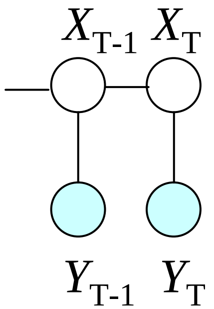
$= \underline{p(Y_0, \cdots, Y_t \mid X_{t+1}) p(Y_{t+1} \mid X_{t+1})} p(X_{t+1})$

(Markov)

$= \underline{p(Y_0, \cdots, Y_t, Y_{t+1} \mid X_{t+1})} p(X_{t+1}) \quad = p(Y_0, \cdots, Y_t, Y_{t+1}, X_{t+1})$

Proof: Forward-Backward Algorithm

$$\beta(X_{T-1}) = \sum_{X_T} p(X_T \mid X_{T-1}) \underbrace{\beta(X_T)}_{=1} p(Y_T \mid X_T) = p(Y_T \mid X_{T-1})$$



For $t \le T-2$,

If $\beta(X_{t+1}) = p(Y_{t+2}, \cdots, Y_T \mid X_{t+1})$,

(b) $$\beta(X_t) = \sum_{X_{t+1}} p(X_{t+1} \mid X_t) \beta(X_{t+1}) p(Y_{t+1} \mid X_{t+1})$$

$$= \sum_{X_{t+1}} p(X_{t+1} \mid X_t) p(Y_{t+2}, \cdots, Y_T \mid X_{t+1}) p(Y_{t+1} \mid X_{t+1})$$

(Markov)

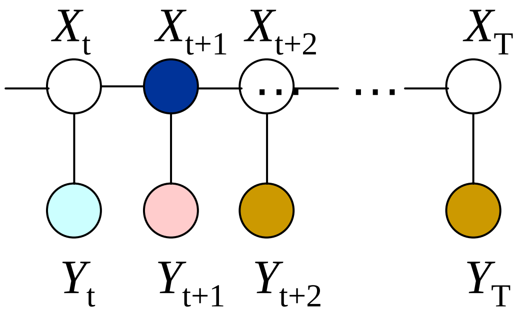
$$= \sum_{X_{t+1}} p(X_{t+1} \mid X_t) p(Y_{t+1}, Y_{t+2}, \cdots, Y_T \mid X_{t+1})$$

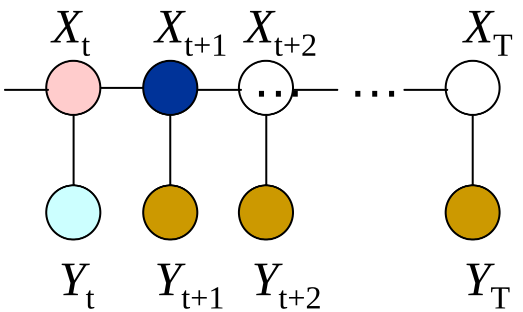
(Markov)

$$= \sum_{X_{t+1}} p(Y_{t+1}, Y_{t+2}, \cdots, Y_T, X_{t+1} \mid X_t)$$

$$= p(Y_{t+1}, Y_{t+2}, \cdots, Y_T \mid X_t)$$

Q.E.D.





Forward-Backward Algorithm

- The ordinary derivation of $\alpha\!-\!\beta$ algorithm uses

$$\alpha(X_t) = p(Y_0, \cdots, Y_t, X_t), \qquad \beta(X_t) = p(Y_{t+1}, \cdots, Y_T \mid X_t)$$

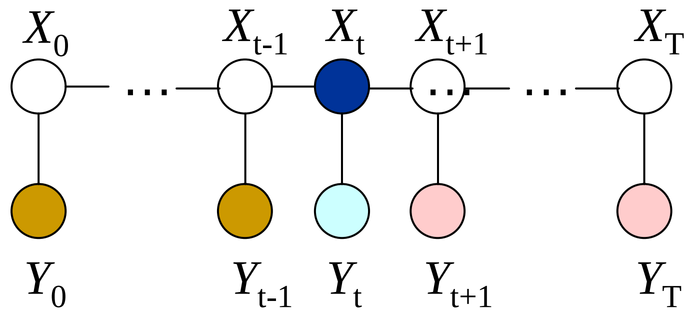
as definitions, and derives the update rules by tracing back (a) and (b).

- Confirm again

$$p(X_t, Y_0, \cdots, Y_T) = \alpha(X_t)\beta(X_t)$$

by

$$p(X_t, Y_0, \cdots, Y_T)$$
$$= p(X_t)\,p(Y_1, \cdots, Y_T \mid X_t)$$
$$= \underbrace{p(X_t)\,p(Y_1, \cdots, Y_t \mid X_t)}_{\alpha(X_t)}\,\underbrace{p(Y_{t+1}, \cdots, Y_T \mid X_t)}_{\beta(X_t)}$$



Forward-Backward Algorithm

- Computational cost of the forward-backward algorithm cost is O(K^2T), which is linear to the sequence length.
- Smoothing, filtering, and prediction are done by the algorithm;
  - smoothing:

$$p(X_t \mid Y_0, \cdots, Y_T) = \frac{\alpha(X_t)\beta(X_t)}{\sum_{X_t} \alpha(X_t)\beta(X_t)}$$

  - filtering:

$$\alpha(X_t) = p(Y_0, \cdots, Y_t, X_t),$$

$$\Rightarrow \quad p(X_t \mid Y_0, \cdots, Y_t) = \frac{p(Y_0, \cdots, Y_t, X_t)}{p(Y_0, \cdots, Y_t)} = \frac{\alpha(X_t)}{\sum_{X_t} \alpha(X_t)}$$

  - prediction:

$$p(X_{t+1} \mid Y_0, \cdots, Y_t) = \sum_{X_t} p(X_{t+1} \mid X_t) p(X_t \mid Y_0, \cdots, Y_t) = \frac{\sum_{X_t} A_{X_t, X_{t+1}} \alpha(X_t)}{\sum_{X_t} \alpha(X_t)}$$

Forward-Backward Algorithm

- Prediction and filtering are computed sequentially.

  For each time step, the update of $\alpha(X_t)$ with the new observation Y_t is sufficient.

  We do not need to access the older variables of Y_s.

Mini-Summary

- Belief propagation is applicable to the inference of HMM
  - HMM is a tree → BP is applicable.
  - BP for smoothing derives the forward-backward algorithm.
    - Smoothing for all the hidden variables is done by the computation of the cost linear in the length.
  - BP for prediction and filtering derive sequential (forward) algorithm.

Inference on Non-Tree Graphs

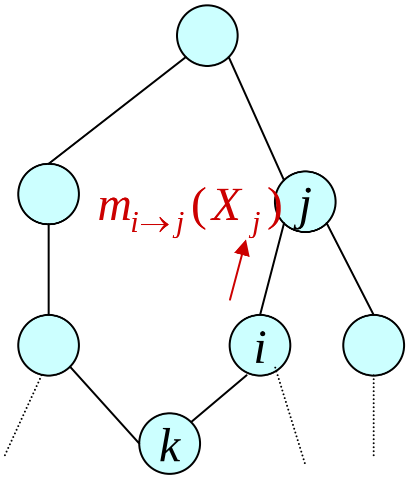
Methods for Non-tree Graphs

- Loopy Belief Propagation
  - Application of BP updates to general graphs, though they have loops.
  - An approximation algorithm.
  - There is no theoretical guarantee for convergence or correctness.

- Junction Tree Algorithm
  - Propagation algorithm on the “clique tree”.
  - Exactness of the resulting marginals are guaranteed, while the marginals are obtained only for the cliques.
  - Efficiency of the algorithm depends on the clique tree derived from the original graph.

Loopy Belief Propagation

(Murphy, K., Weiss, Y., and Jordan, M. 1999).



ALGORITHM

- The update rule is the same as the BP for trees.

$$m_{i\to j}(X_j) = \sum_{X_i} \psi_{ji}(X_j, X_i) \prod_{k\in ne(i)\setminus\{j\}} m_{k\to i}(X_i)$$

  - The order of updates is arbitrary:
    an arbitrary ordering, simultaneous updates, etc.

- Repeat the updates until some convergence criterion is satisfied.

- Compute all the (approximated) marginals by

$$p(X_i) = \frac{b(X_i)}{\sum_{X_i} b(X_i)}, \qquad b(X_i) = \prod_{j\in ne(i)} m_{j\to i}(X_i)$$

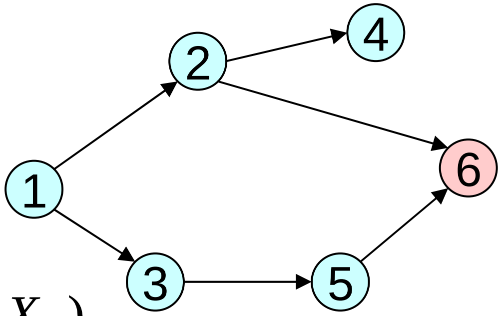
Loopy Belief Propagation

- There are no theoretical guarantees for convergence or correctness.

  → Current research issue.

- In many practical examples, loopy BP shows fast convergence and high accuracy.
  - Decoding method of error correcting codes (turbo-code)

Junction Tree Algorithm



- Basic idea: marginalization by elimination

Example

$$p(X_1, X_6 = e) = \sum_{X_2, X_3, X_4, X_5, X_6} p(X_1) p(X_2 | X_1) p(X_3 | X_1) p(X_4 | X_2) \times p(X_5 | X_3) p(X_6 = e | X_2, X_5)$$

$$= \sum_{X_2, X_3, X_5} p(X_1) p(X_2 | X_1) p(X_3 | X_1) p(X_5 | X_3) \sum_{X_6} p(X_6 = e | X_2, X_5) \sum_{X_4} p(X_4 | X_2)$$

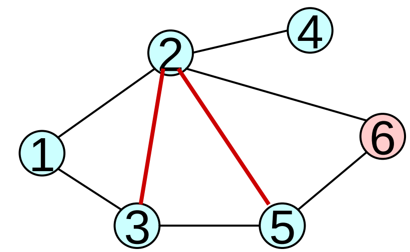
$$= \sum_{X_2, X_3} p(X_1) p(X_2 | X_1) p(X_3 | X_1) \sum_{X_5} p(X_5 | X_3) m_6(X_2, X_5)$$

$$= \sum_{X_2, X_3} p(X_1) p(X_2 | X_1) p(X_3 | X_1) m_5(X_2, X_3)$$

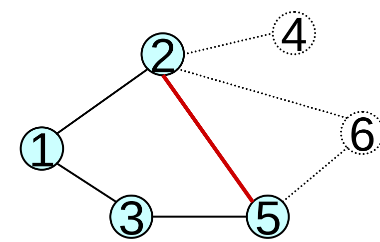
$$= \sum_{X_2, X_3} \psi(X_{1,} X_2, X_3)$$ ← marginalization is easy

Junction Tree Algorithm

New cliques appears in the process of successive eliminating variables.



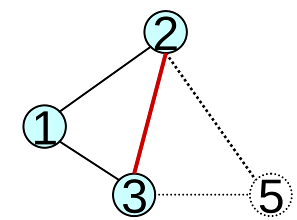
$$p(X_1, X_6 = e) = \sum_{X_2, X_3, X_4, X_5, X_6} p(X_1) p(X_2 \mid X_1) p(X_3 \mid X_1) p(X_4 \mid X_2) \times p(X_5 \mid X_3) p(X_6 = e \mid X_2, X_5)$$



$$= \sum_{X_2, X_3, X_5} p(X_1) p(X_2 \mid X_1) p(X_3 \mid X_1) p(X_5 \mid X_3) \sum_{X_6} p(X_6 = e \mid X_2, X_5) \sum_{X_4} p(X_4 \mid X_2)$$

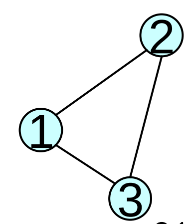
marginalizing out 6 connects 2 and 5

$$= \sum_{X_2, X_3} p(X_1) p(X_2 \mid X_1) p(X_3 \mid X_1) \sum_{X_5} p(X_5 \mid X_3) \underline{m_6(X_2, X_5)}$$



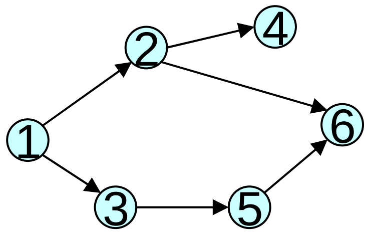
marginalizing out 5 connects 2 and 3

$$= \sum_{X_2, X_3} p(X_1) p(X_2 \mid X_1) p(X_3 \mid X_1) \underline{m_5(X_2, X_3)} = \sum_{X_2, X_3} \psi(X_1, X_2, X_3)$$

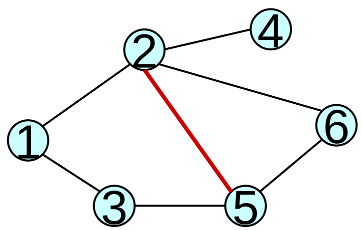


Junction Tree Algorithm

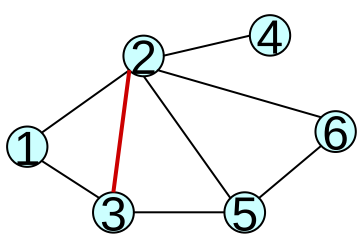
- Sketch of JT algorithm



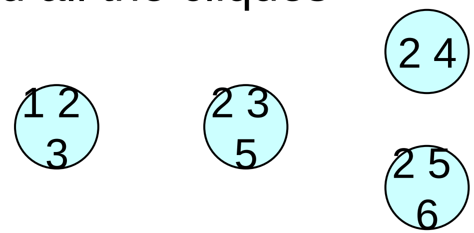
1. Moralization



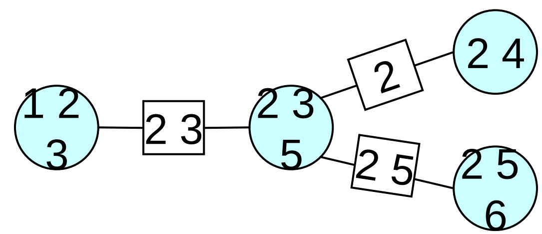
2. Triangulation.



3. Find all the cliques

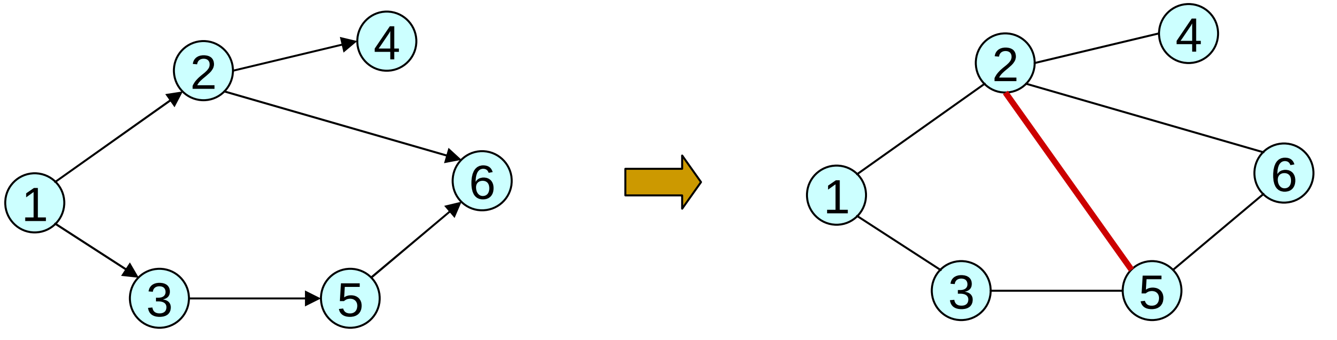


4. Make a junction tree.



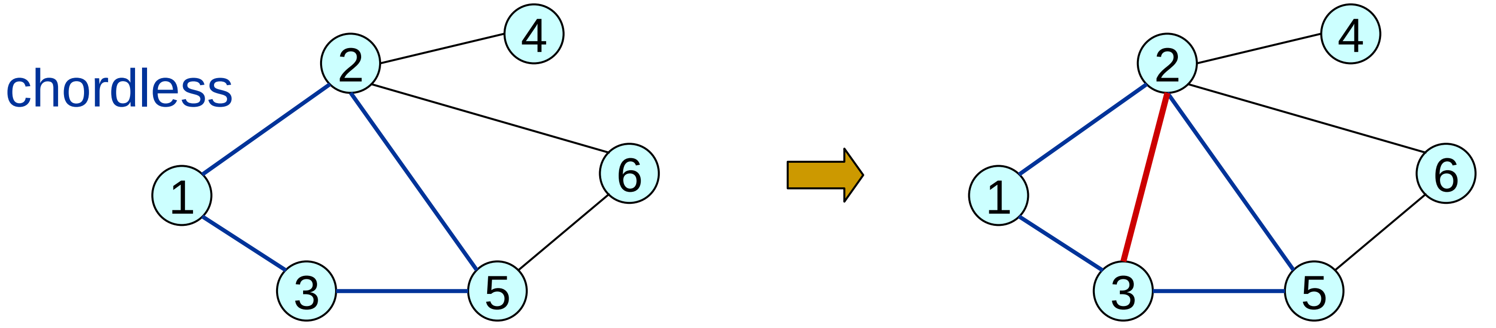
5. Propagate messages → Marginal probabilities of all the cliques.

Moralization



- Moralization: connect parents for each node.
- Make an undirected graph by removing the directions.
- No additional conditional independence relations are suggested by moralization.

Triangulation

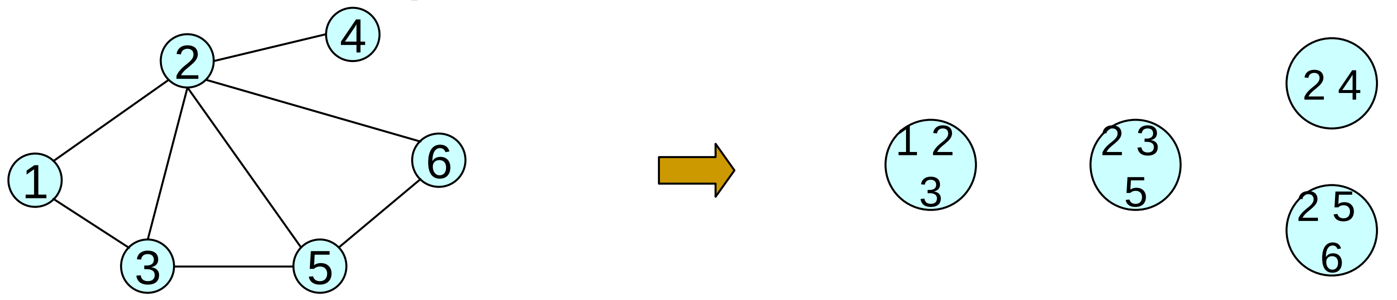


- Triangulation: make a graph such that there are no loops of length larger than 3 without chord.
  - A chord is an edge that connects non-consecutive two nodes in a loop.

- Triangulation guarantees the running intersection property of the junction tree.

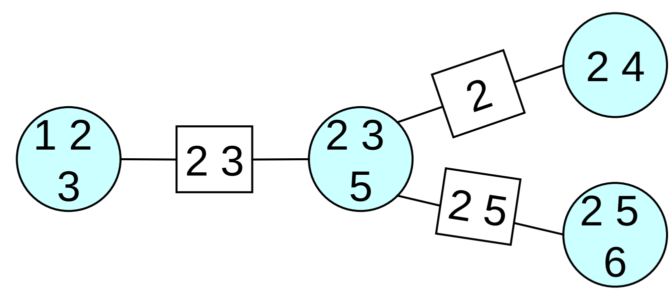
Junction Tree

- Find all the cliques



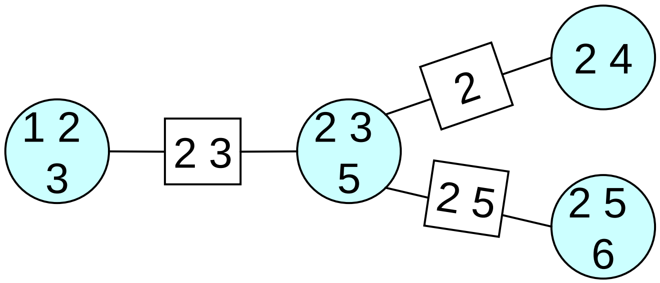
- Make a junction tree
  - Junction tree
    - Tree of the cliques
    - Each edge has a separator (intersection of connected nodes)
  - Running intersection property:

    if a variable appears in multiple nodes, it must appears in all intermediate nodes in the tree.



Junction Tree Propagation

$$p(X) = \prod_{C:\text{clique}} \psi_C(X_C)$$

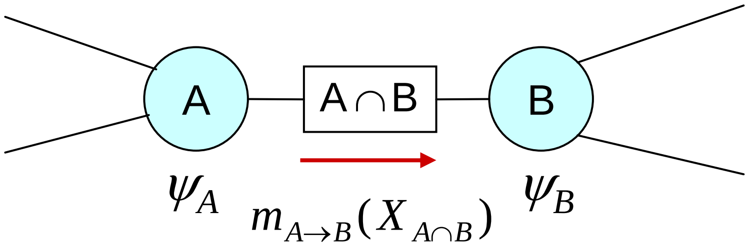


- Initial potentials

  $\psi_C(X_C)$ given by the product of potentials in C

- Run belief propagation on the junction tree

$$m_{A\to B}(X_{A\cap B}) = \sum_{X_{A\setminus B}} \psi_A(X_A) \prod_{C\in N(A)} m_{C\to A}(X_{C\cap A})$$



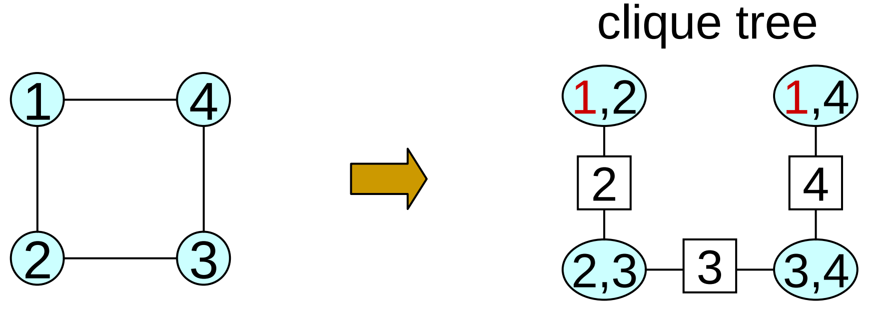
- After the upward and downward updates, the marginals are given by

$$p(X_C) = \psi_C(X_C), \quad p(X_S) = \phi_S(X_S).$$

Junction Tree Propagation

Remarks:

- The running intersection property of the junction tree ensures that the propagation procedure gives marginal-out.



Not triangulated

Running intersection does not hold.

- The computational cost of JT depends on the size of cliques.

  If the original graph is complete, there is no gain.

General Propagation Algorithm

General Propagation Algorithm

- Distribution law
  - Belief propagation = successive marginalization on a tree.

$$\sum_{X_2,X_3,X_4} p(X) = \sum_{X_2,X_3,X_4} f(X_1,X_2)g(X_2,X_3)h(X_3,X_4)$$

$$= \sum_{X_2} f(X_1,X_2)\sum_{X_3} g(X_2,X_3)\underline{\sum_{X_4} h(X_3,X_4)}$$

  - The mathematical source of efficiency is simply the distribution law of sum and product.

$$\sum_{\ell=1}^{K} a_{ijk} h_{k\ell} = a_{ijk} \sum_{\ell=1}^{K} h_{k\ell},$$

$$h_{k\ell} := h(X_3 = k, X_4 = \ell)$$
$$a_{ijk} := fg(X_1 = i, X_2 = j, X_3 = k)$$

Essentially,

$$ab + ac = a(b+c) \qquad \text{distribution law}$$

$$\sum_{i=1}^{K} ab_i = a\left(\sum_{i=1}^{K} b_i\right)$$

$2K$ operations $\qquad$ $K+1$ operations

General Propagation Algorithm

- Operations that satisfy distribution law

  In general, for two operations $\circ$ and $*$, the distribution law is

$$(a*b)\circ(a*c)=a*(b\circ c)$$

  - Sum-product $ab+ac=a(b+c)$ $(\circ=+,\ *=\times)$

  - Max-product (for non-negative values)

$$\max\{ab,ac\}=a\max\{b,c\} \qquad (\circ=\max,\ *=\times)$$

  - Max-sum

$$\max\{a+b,a+c\}=a+\max\{b,c\} \qquad (\circ=\max,\ *=+)$$

- For each pair of operations, BP-type algorithms are derived.
- BP for max-product is applicable for combinatorial maximization problems.

Mini-Summary

- Propagation algorithms for non-tree graphs
  - Loopy BP: approximation algorithm

    Direct application of the BP update rule for general graphs.
  - Junction tree algorithm: exact marginalization for cliques.
- Extension of propagation algorithm
  - BP-type algorithms are obtained if the two operations satisfy the distribution law.

    e.g. max-product, max-sum