Probabilistic Graph Models: Factor Graphs, Belief Propagation

ECE/CS 498 DS U/G

Lecture 23: Belief Propagation, ICA 5

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Announcements

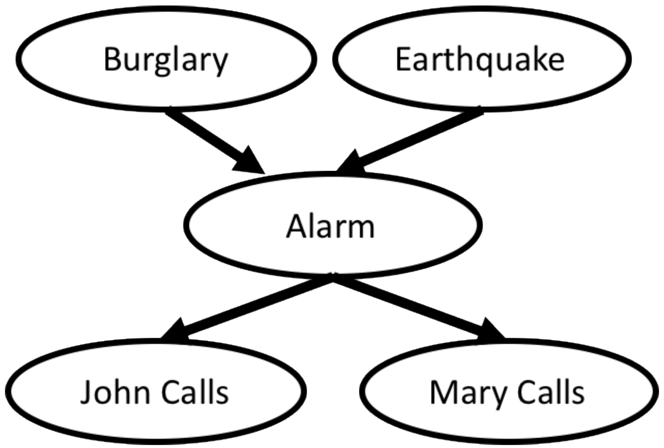
- Course Timeline:
  - Wed 4/15: Belief Propagation, ICA 5 on Factor Graphs
  - Mon 4/20: Support Vector Machines, Cross Validation
- HW 4 released today
  - Covers forward-backward algorithm, factor graphs, belief propagation
  - Due **Wed 4/22 @ 11:59 PM** on Compass 2G
- Final Project progress report 2 due **Friday April 17 @ 11:59 PM** on Compass2G
  - There should be *substantial* progress with projects by this point (i.e. meaningful results, ML/AI models)
- Discussion section on Friday 4/17
  - Practice with factor graphs and belief propagation

Belief Propagation

Inference on Graphical Models

Problems we have already looked at:

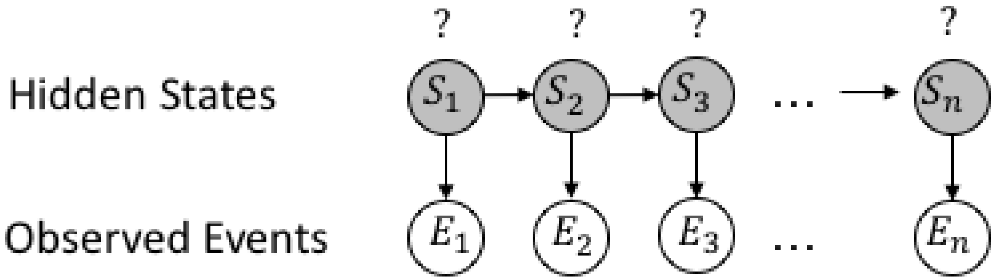
Bayes Network



Calculate the joint probability $P(B, J, A, E, M) = P(J|A)\, P(M|A) P(A|B, E) P(B) P(E)$

Calculate the state probability $P(B) = \sum_{J,A,E,M} P(B, J, A, E, M)$

Hidden Markov Model



Calculate the conditional distribution

$P(S_t|E_1, \dots, E_n)$

Factorize (Bayes Theorem)

$\propto P(S_t|E_1, \dots, E_t) * P(E_{t+1}, \dots, E_n|S_t, E_1, \dots, E_t)$

Use the Markov Property

$= P(S_t|E_1, \dots, E_t) * P(E_{t+1}, \dots, E_n|S_t)$

Forward Backward Algorithm

$= \alpha_t \odot \beta_t$

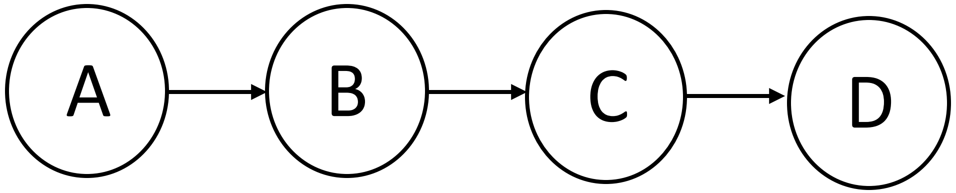
Just involves computation of joint distributions and its marginalization

Example of inference on a Bayesian Network

Consider the following Bayesian Network

- $A \in \{a^1, a^2\}, B \in \{b^1, b^2\}, C \in \{c^1, c^2\}, D \in \{d^1, d^2\}$

Inference task: Compute P(D)



$$P(D) = \sum_{A,B,C} P(A,B,C,D) = \sum_{A,B,C} P(A)P(B|A)P(C|B)P(D|C)$$

- Simple way would be to generate each possible sequence (A,B,C,D) and sum over them
  - Exponential in the number of variables

Example of inference on Bayesian Network

- Enumerating all combinations
- Each term has 3 multiplications
- 8+8 = 16 terms
- Total multiplication ops = 16x3 = 48

- 7 additions for $d^1$and 7 additions for d^2
- Total additions ops = 7+7=14

$$
\begin{array}{rllll}
 & P(a^1) & P(b^1 \mid a^1) & P(c^1 \mid b^1) & P(d^1 \mid c^1) \\
+ & P(a^2) & P(b^1 \mid a^2) & P(c^1 \mid b^1) & P(d^1 \mid c^1) \\
+ & P(a^1) & P(b^2 \mid a^1) & P(c^1 \mid b^2) & P(d^1 \mid c^1) \\
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\end{array}
$$

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\end{array}
$$

All terms involved in computation of $P(d^1)$ and $P(d^2)$ respectively.

Example of inference on Bayesian Network

Can we reduce the number of computations?

- Many terms are common; they can be computed once and reused

Consider the orange highlighted box, $P(c^1|b^1)P(d^1|c^1)$ is common.

Compute: $P(a^1)P(b^1|a^1) + P(a^2)P(b^1|a^2)$

Consider the blue highlighted box, $P(c^1|b^2)P(d^1|c^1)$ is common.

Compute: $P(a^1)P(b^2|a^1) + P(a^2)P(b^2|a^2)$

Define: $\tau_1(B) = P(a^1)P(B|a^1) + P(a^2)P(B|a^2)$

where $B \in \{b^1, b^2\}$

$$
\begin{array}{lllll}
 & P(a^1) & P(b^1 \mid a^1) & P(c^1 \mid b^1) & P(d^1 \mid c^1) \\
+ & P(a^2) & P(b^1 \mid a^2) & P(c^1 \mid b^1) & P(d^1 \mid c^1) \\
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\end{array}
$$

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\end{array}
$$

All terms involved in computation of $P(d^1)$ and $P(d^2)$ respectively.

Example of inference on Bayesian Network

Consider the orange highlighted box, $P(d^1|c^1)$ is common.

Compute: $\tau_1(b^1)P(c^1|b^1) \; + \tau_1(b^2)P(c^1|b^2)$

Consider the blue highlighted box, $P(d^1|c^2)$ is common.

Compute: $\tau_1(b^1)P(c^2|b^1) \; + \tau_1(b^2)P(c^2|b^2)$

Define: $\tau_2(C) \; = \tau_1(b^1)P(C|b^1) + \tau_1(b^2)P(C|b^2)$

where $C \in \{c^1, c^2\}$

$$\boxed{\begin{array}{llll} & \tau_1(b^1) & P(c^1 \mid b^1) & P(d^1 \mid c^1) \\ + & \tau_1(b^2) & P(c^1 \mid b^2) & P(d^1 \mid c^1) \end{array}}$$
$$\boxed{\begin{array}{llll} + & \tau_1(b^1) & P(c^2 \mid b^1) & P(d^1 \mid c^2) \\ + & \tau_1(b^2) & P(c^2 \mid b^2) & P(d^1 \mid c^2) \end{array}}$$

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All terms involved in computation of $P(d^1)$ and $P(d^2)$ respectively. The sum is simplified because of use of $\tau_1(B)$.

Example of inference on Bayesian Network

- Computation shown alongside is easy and gives $P(D)$
- Previous steps are equivalent to **pushing summation inside**

$$P(D) = \sum_C \sum_B \sum_A P(A)P(B|A)P(C|B)P(D|C)$$

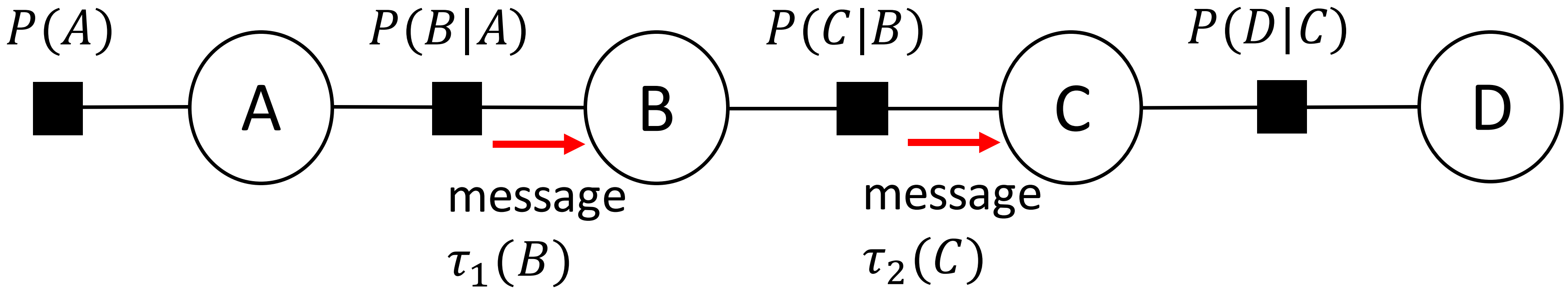
$$P(D) = \sum_C P(D|C) \overbrace{\sum_B P(C|B) \underbrace{\sum_A P(A)P(B|A)}_{\tau_1(B)}}^{\tau_2(C)}$$

$$\begin{aligned} & \tau_2(c^1) \quad P(d^1 \mid c^1) \\ + \; & \tau_2(c^2) \quad P(d^1 \mid c^2) \end{aligned}$$

$$\begin{aligned} & \tau_2(c^1) \quad P(d^2 \mid c^1) \\ + \; & \tau_2(c^2) \quad P(d^2 \mid c^2) \end{aligned}$$

Computation of $P(D)$ is simplified because of use of $\tau_1(B)$, $\tau_2(C)$.

Flow of computations (messages) in Factor Graph corresponding to the given BN



Sum-product algorithm reduces computations

- Pushing summations inside reduced the number of computations
  - Simple way: 48 multiplications + 14 additions
  - Pushing summations inside: 4x3 multiplications + 2x3 additions
  - Can be up to linear in number of variables (much better than exponential!)

- What helped in addressing the exponential blowup of marginalizing the joint distribution?
  - Graph structure – because of structure of Bayesian Network, some subexpression in the joint depend only on a small number of variables
  - Pushing summation inside – by computing these expressions once and caching the results, we can avoid generating them exponentially many times

- Referred to as **sum-product algorithm** or **Belief Propagation**

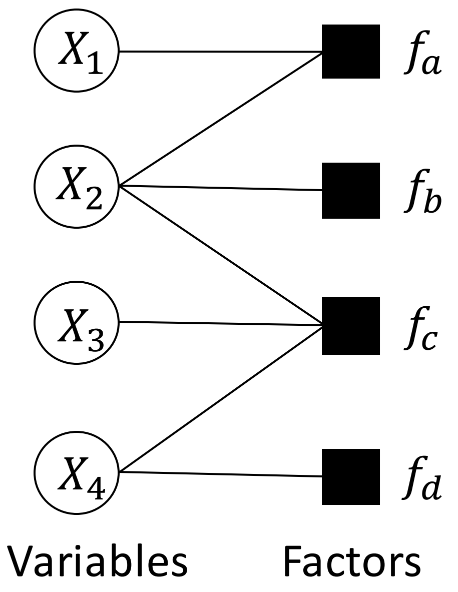
Inference problem on Factor Graphs

What is the problem we are trying to solve?

- Marginalization on Factor Graphs

Marginal probability $$P(X_i) = \sum_{\boldsymbol{X} \setminus X_i} P(\boldsymbol{X})$$

All variables except X_i



Challenge:

- Computationally expensive because the sum is calculated on all variables except one

$X_i \in \{0,1\}$ is a discrete variable e.g., a Boolean variable

Approach:

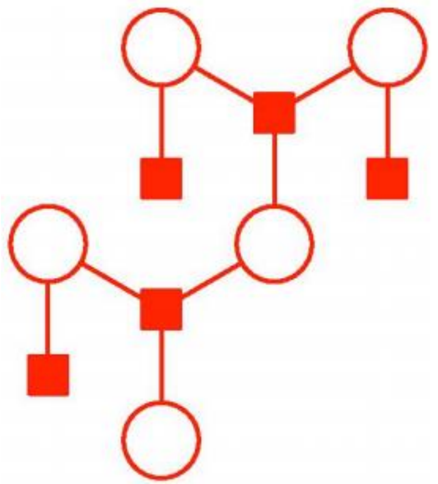
- Factorize the joint distribution according the structure
- Use belief propagation to reduce computations

$f_c(X_c)$ is a tensor on a set of variables X_c

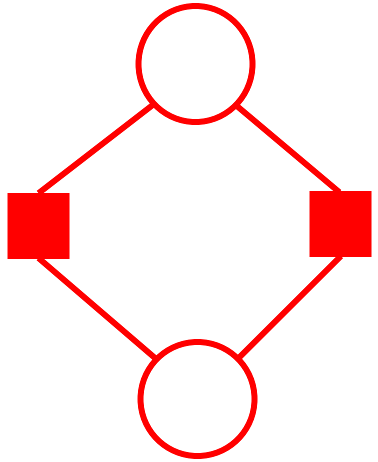
Belief propagation

- Also known as sum-product algorithm
- Computes marginal distributions by “pushing in summations”
- Exact inference for linear graphs and trees
- Approximate inference for graphs with loops; performs remarkably well

- In case of Factor Graphs, involves two types of **messages**
  - From factor to variables
  - From variables to factors



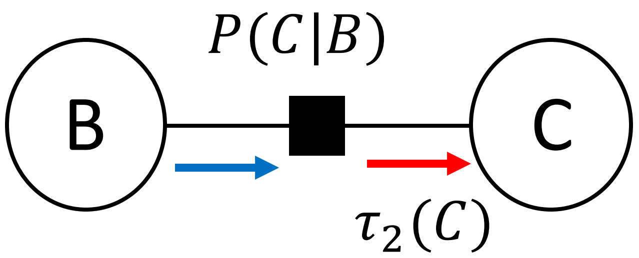
Tree Factor graph



Factor graph with loop

Belief Propagation – Message from factor to variable

Recall from previous example:

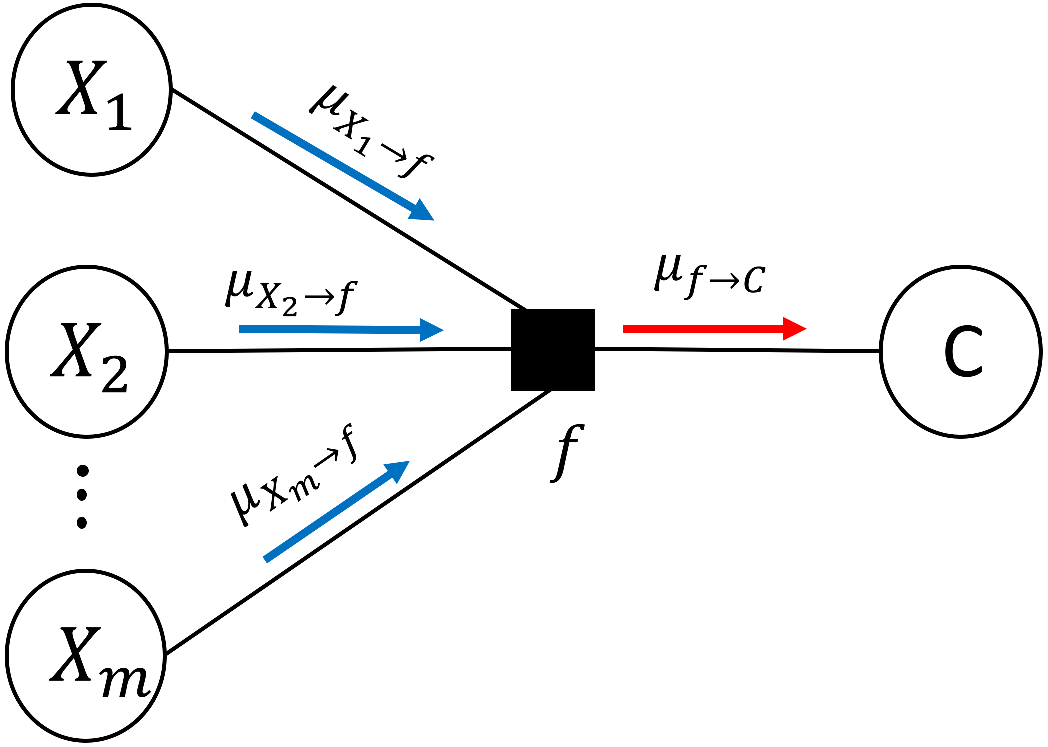


$$\tau_2(C) = \sum_B P(C|B)\tau_1(B)$$

To get the general expression, denote by:

$$f(B,C) = P(C|B)$$
$$\mu_{f\to C}(C) = \tau_2(C)$$
$$\mu_{B\to f}(B) = \tau_1(B)$$

In general:

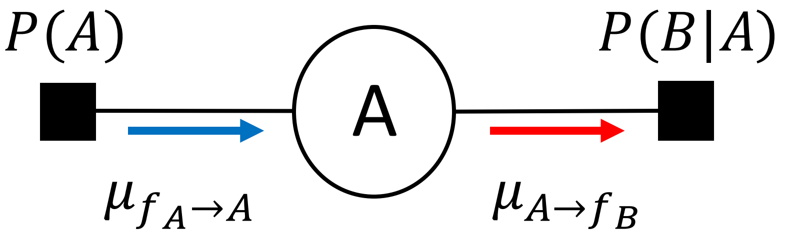


$$\mu_{f\to C}(C) = \sum_{X_1,X_2,\dots,X_m} f(C,X_1,\dots,X_m)\prod_{i=1}^{m}\mu_{X_i\to f}(X_i)$$

Message from factor to variable: Product of all incoming messages and factor, sum out previous variables

Belief Propagation – Message variable to factor

Recall from previous example:

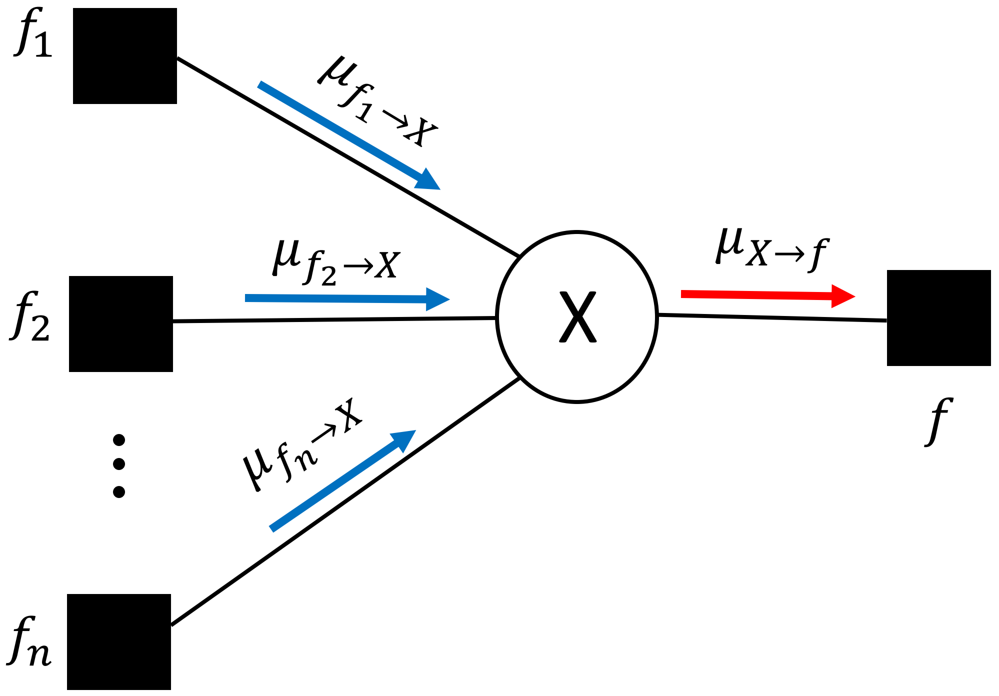


$$\mu_{A \to f_B}(A) = \mu_{f_A \to A}(A) = P(A)$$

Where,

$$f_A(A) = P(A)$$
$$f_B(A, B) = P(B|A)$$

In general:



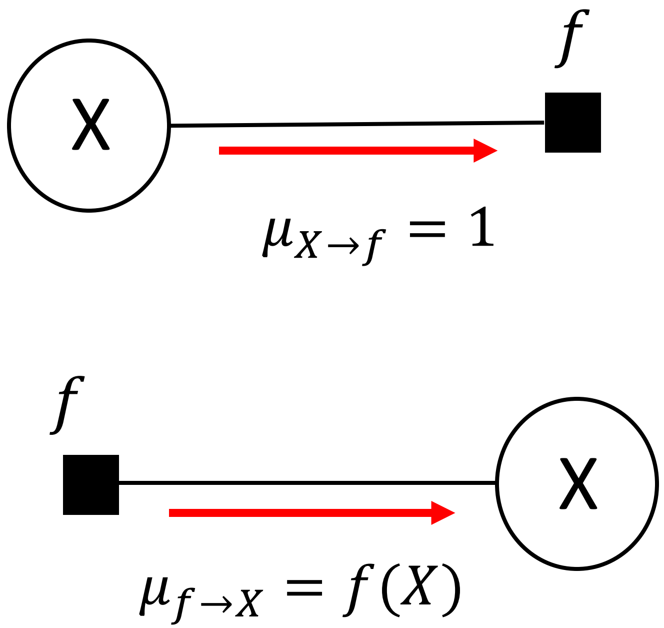
$$\mu_{X \to f}(X) = \prod_{i=1}^{n} \mu_{f_i \to X}(X)$$

Message from variable to factor: Product of all incoming messages

Belief Propagation: General Algorithm

Steps to compute marginal distribution for all variables

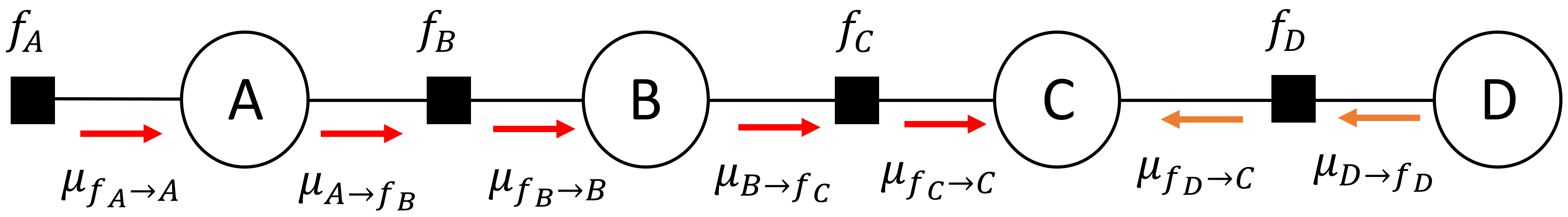
- How to start the algorithm
  - Choose a node in the factor graph as root node
  - Compute all the leaf-to-root messages
  - Compute all the root-to-leaf messages
- Initial Conditions
  - Starting from a factor leaf/root node, the initial factor-to-variable message is the factor itself
  - Starting from a variable leaf/root node, the initial variable-to-factor message is a vector of ones
- Computing marginals
  - Marginal is given by the product of all incoming messages; normalize if necessary



Initialization

Example of belief propagation

Compute $P(C)$



$$\mu_{f_A \to A}(A) = f_A(A) = P(A)$$

$$\mu_{A \to f_B}(A) = \mu_{f_A \to A}(A) = P(A)$$

$$\mu_{f_B \to B}(B) = \sum_A f_B(A, B)\, \mu_{f_A \to A}(A)$$

$$= \sum_A P(B|A)\, P(A)$$

$$\mu_{B \to f_C}(B) = \mu_{f_B \to B}(B)$$

$$= \sum_A P(B|A)\, P(A)$$

$$\mu_{f_C \to C}(C) = \sum_B f_C(B, C)\, \mu_{B \to f_B}(B)$$

$$= \sum_B P(C|B) \sum_A P(B|A) P(A)$$

$$\mu_{D \to f_D}(D) = 1$$

$$\mu_{f_D \to C}(C)$$

$$= \sum_D f_D(C, D)\, \mu_{f_D \to C}(C)$$

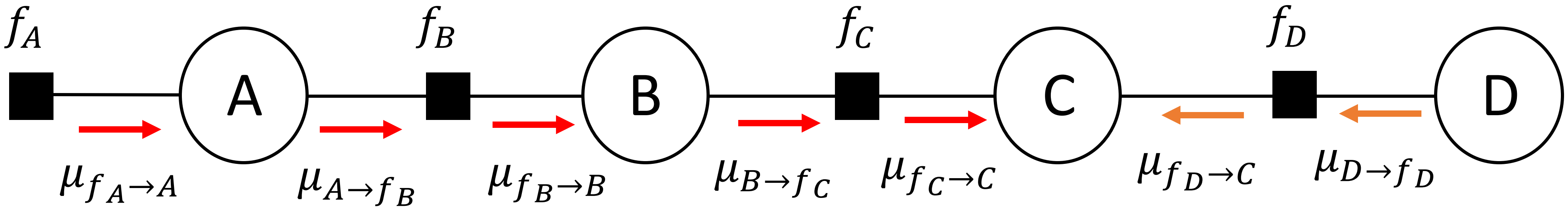
$$= \sum_D P(D|C)$$

Example of belief propagation

$$\mu_{f_D \to C}(C) = \sum_D P(D|C)$$

$$\mu_{f_C \to C}(C) = \sum_B P(C|B) \sum_A P(B|A)P(A)$$

Compute $P(C)$



$$P(C) = \mu_{f_C \to C}(C)\mu_{f_D \to C}(C)$$

Verifying that the above computation gives the marginal distribution

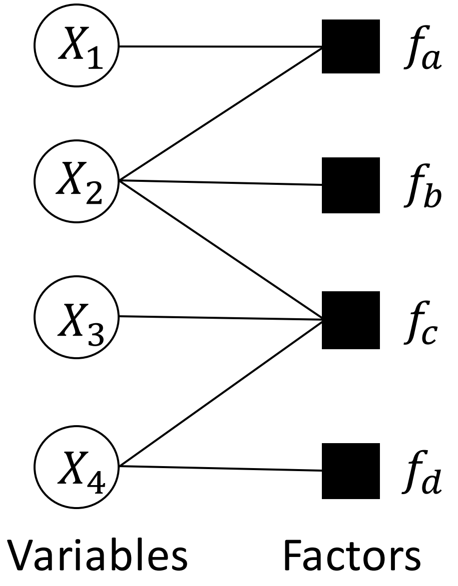
$$P(C) = \left(\sum_B P(C|B) \sum_A P(B|A)P(A)\right)\left(\sum_D P(D|C)\right) = \sum_B P(C|B) \sum_A P(B|A)P(A) \sum_D P(D|C)$$

$$= \sum_A \sum_B \sum_D P(A)P(B|A)P(C|B)P(D|C) = \sum_{A,B,D} P(A,B,C,D)$$

Marginalization on Factor Graphs

Marginal probability $$P(X_i) = \sum_{\boldsymbol{X} \backslash X_i} P(\boldsymbol{X})$$

All variables except X_i



Inference method	Description
Belief Propagation	Exact inference on non-loop FG
Sampling - Markov Chain Monte Carlo, Gibbs	Approximate inference
Variational Inference	Approximate inference

$X_i \in \{0,1\}$ is a discrete variable e.g., a Boolean variable

$f_c(X_c)$ is a tensor on a set of variables X_c

References

- Daphne Koller, Nir Friedman's textbook on Graphical Models
- https://www.doc.ic.ac.uk/~mpd37/teaching/ml_tutorials/2016-11-09-Svensson-BP.pdf

Begin ICA 5