Probabilistic Graphical models

Machine Learning (MIIS 2021-2022)

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Outline

1. Introduction to probabilistic Graphical Models
   - Bayesian networks
   - Markov Random Fields
   - Factor graphs
   - Inference and message passing algorithms
   - Learning Graphical Models

Most of the material of these slides has been taken from :

- Chapter 8 of C. Bishop's book
- D. Mackay's book
- Tutorial on Graphical Models of Z. Ghahramani (MLSS 2012)

- Unifying language to express many existing problems
- Intersection of many different scientific areas
  - probability theory
  - computer science
  - decision theory
  - optimization
  - ...
- Examples of applications: medical and fault diagnosis, image understanding, reconstruction of biological networks, speech recognition, natural language processing, decoding of messages sent over a noisy communication channel, robot navigation, and many more

- Defines a family of joint probability distributions in terms of a graph
  - directed : Bayesian Network (AI community)
  - undirected : Markov Random Field (stat.physics, computer vision)
  - bipartite factor graph (general class, coding theory)
- Joint probability factorizes as a product of potential functions defined on *small* subsets of variables (nodes in the graph)
- Independencies encoded in the structure of the graph

Computational tasks

- **Inference**: estimate probabilities for a given fixed joint distribution
  - Posterior marginals or belief $p(\mathbf{x}|\mathbf{e})$ over latent variables
  - Probability of evidence $p(\mathbf{e})$
  - Maximum a Posteriori hypothesis (map) $p(\mathbf{z}|\mathbf{e})$
- **Learning**: find best graphical model that explains given data
  - Learning parameters
  - Structure learning

Introduction: Quick recap on probability theory

Definitions:

- X is a **random variable**, takes values $x \in \mathcal{A}_X = \{a_1, a_2, \ldots, a_i, \ldots, a_I\}$ with probabilities $\mathcal{P}_X = \{p_1, p_2, \ldots, p_i, \ldots, p_I\}$
  - $p(x = a_i) = p_i, p_i \geq 0$
  - $\sum_{a_i \in \mathcal{A}_X} P(x = a_i) = 1$
- Probability of a **subset**: if T is a subset of $\mathcal{A}_X$ then: $P(T) = P(x \in T) = \sum_{a_i \in T} P(x = a_i)$
- if XY is an ordered pair of variables where then $P(x, y)$ is the **joint probability** of x and y
- **Marginal** probability: $P(x = a_i) = \sum_{y \in \mathcal{A}_y} P(x = a_i, y)$
- **Conditional** probability:

$$P(x = a_i | y = b_j) = \frac{P(x = a_i, y = b_j)}{P(y = b_j)}, \text{if } P(y = b_j) \neq 0$$

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Rules of probability:

- Product rule $P(x, y|\mathcal{H}) = P(x|y, \mathcal{H})P(y|\mathcal{H}) = P(y|x, \mathcal{H})P(x|\mathcal{H})$
- Sum rule $P(x|\mathcal{H}) = \sum_y P(x, y|\mathcal{H}) = \sum_y P(x|y, \mathcal{H})P(y|\mathcal{H})$
- Bayes theorem

$$P(y|x, \mathcal{H}) = \frac{p(x|y, \mathcal{H})P(y|\mathcal{H})}{P(x|\mathcal{H})} = \frac{p(x|y, \mathcal{H})P(y|\mathcal{H})}{\sum_{y'} p(x|y', \mathcal{H})P(y'|\mathcal{H})}$$

- Marginal independence: X and Y are independent $X \perp\!\!\!\perp Y|\emptyset$ if and only if

$$P(x, y) = P(x)P(y)$$

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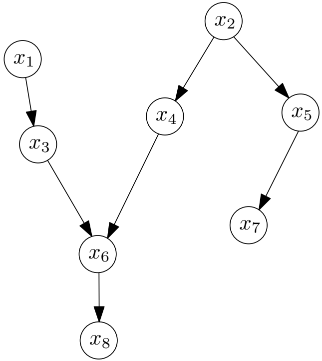
Asia network

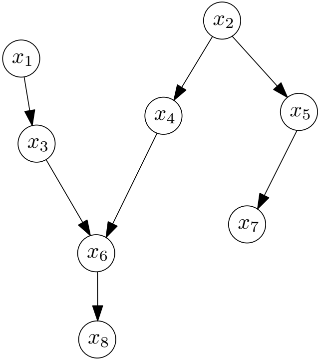


- x_1 : Visit to Asia
- x_2 : Smoker
- x_3 : Has Tuberculosis
- x_4 : Has Lung Cancer
- x_5 : Has Bronquitis
- x_6 : Tuberculosis or Cancer
- x_7 : X-Ray result
- x_8 : Dyspnea

Naive factorization: $p(\mathbf{x}) = p(x_1|x_2,\ldots,x_8)p(x_2|x_3,\ldots,x_8)\ldots p(x_8)$

Requires table with $\mathbf{2^8}$ elements!

Asia network



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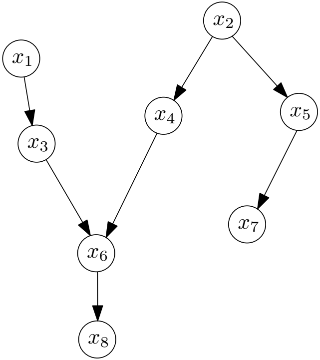
$$p(\mathbf{x}) = p(x_3|x_1)p(x_1)p(x_4|x_2)p(x_5|x_2)p(x_2)p(x_6|x_3, x_4)p(x_7|x_5)p(x_8|x_6)$$

Requires table with $\mathbf{2^3}$ elements!

Asia network



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In general $p(\mathbf{x}) = \prod_i p(x_i | \text{parents}_i)$

a	b	c	$p(a,b,c)$
0	0	0	0.192
0	0	1	0.144
0	1	0	0.048
0	1	1	0.216
1	0	0	0.192
1	0	1	0.064
1	1	0	0.048
1	1	1	0.096

Exercise (8.3 Bishop)

- Binary variables a, b, c with joint probability as above. Show that:
  - they are not marginally independent, i.e., $p(a,b) \neq p(a)p(b)$
  - they become independent when conditioned on c, i.e., $p(a,b|c) = p(a|c)p(b|c)$

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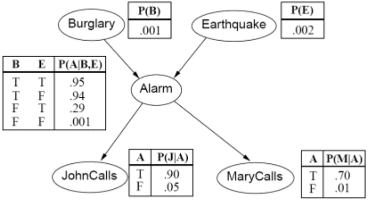
Exercise (8.4 Bishop)

- Binary variables a, b, c with joint probability as above.
  - Evaluate the distributions $p(a), p(b|c)$ and $p(c|a)$ and show that $p(a,b,c) = p(a)p(b|c)p(c|a)$
  - Draw the corresponding directed graph

- Let $\texttt{NonDescendants}_{X_i}$ denote the variables that are non descendants of X_i in the graph
- For each variable X_i we have that

$$\{X_i \perp\!\!\!\perp \texttt{NonDescendants}_{X_i} | \text{parents}_i\}$$

- Example

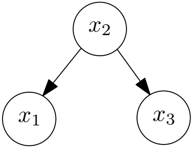


$$\{B \perp\!\!\!\perp E|\emptyset, \quad J \perp\!\!\!\perp M|A, \quad \ldots\}$$

Bayesian networks

Conditional independence: D-Separation

- Given:
  - A directed graphical model
  - Evidence set C
  - Two sets of variables A and B
- Automated way to check independence of A and B given C?
- D-Separation, [Pearl, 1988]
- Based on the three canonical models



$$p(x_1, x_2, x_3) = p(x_1|x_2)p(x_3|x_2)p(x_2)$$
$$p(x_1, x_3) = \sum_{x_2} p(x_1|x_2)p(x_3|x_2)p(x_2)$$

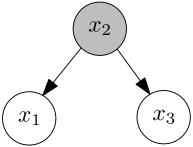
In general

$$p(x_1, x_3) \neq p(x_1)p(x_3)$$
$$x_1 \not\perp x_3 | \emptyset$$

tail-to-tail node

Common parent. Example:

- x_1 : Shoe size, x_2 : Age, x_3 : Amount of gray hair



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$$p(x_1, x_3|x_2) = p(x_1|x_2)p(x_3|x_2)$$

Therefore

$$x_1 \perp\!\!\!\perp x_3 | x_2$$

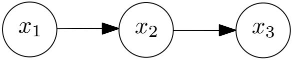
tail-to-tail node

Common parent. Example:

- x_1 : Shoe size, x_2 : Age, x_3 : Amount of gray hair
- Hidden variable explains the observed dependence between x_1 and x_3

Bayesian networks

Conditional independence: canonical models (2/3)



$$p(x_1, x_2, x_3) = p(x_1)p(x_2|x_1)p(x_3|x_2)$$

$$\begin{aligned} p(x_1, x_3) &= p(x_1) \sum_{x_2} p(x_3|x_2)p(x_2|x_1) \\ &= p(x_1) \sum_{x_2} p(x_3|x_2, x_1)p(x_2|x_1) \\ &= p(x_1)p(x_3|x_1) \end{aligned}$$

In general: $p(x_1, x_3) \neq p(x_1)p(x_3)$

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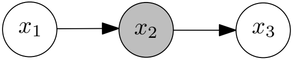
head-to-tail node

Markov chain. Example:

- x_1 : Past, x_2 : Present, x_3 : Future



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Therefore

$$x_1 \perp\!\!\!\perp x_3|x_2$$

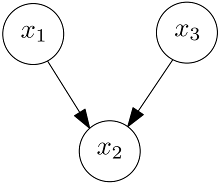
head-to-tail node

Markov chain. Example:

- x_1 : Past, x_2 : Present, x_3 : Future
- Given the present, past is independent of future

Bayesian networks

Conditional independence: canonical models (3/3)



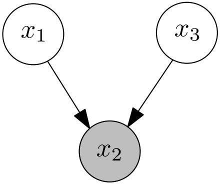
$$p(x_1, x_2, x_3) = p(x_1)p(x_3)p(x_2|x_1, x_3)$$
$$\sum_{x_2} p(x_1, x_2, x_3) = \sum_{x_2} p(x_1)p(x_3)p(x_2|x_1, x_3)$$
$$p(x_1, x_3) = p(x_1)p(x_3) \sum_{x_2} p(x_2|x_1, x_3)$$
$$p(x_1, x_3) = p(x_1)p(x_3)$$

Therefore $x_1 \perp\!\!\!\perp x_3 | \emptyset$

head-to-head node

Multiple parents. "Explaining away" phenomenon:

- x_1 : Easy exam, x_2 : Excellent grade, x_3 : Being Too Smart
- Easy exam and Being Too Smart are marginally unrelated



$$\frac{p(x_1, x_2, x_3)}{p(x_2)} = \frac{p(x_1)p(x_3)p(x_2|x_1, x_3)}{p(x_2)}$$
$$p(x_1, x_3|x_2) \neq p(x_1|x_2)p(x_3|x_2)$$

Therefore $\quad x_3 \not\perp\!\!\!\perp x_1 | x_2$

head-to-head node

Multiple parents. "Explaining away" phenomenon:

- x_1 : Easy exam, x_2 : Excellent grade, x_3 : Being Too Smart
- Easy exam and being too smart become related once we observe Excellent grade

D-Separation

1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
   - It is a head-to-tail or tail-to-tail node and the node is in C
   - It is a head-to-head node and neither the node, **nor any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B|C$

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   - It is a head-to-tail or tail-to-tail node and the node is in C
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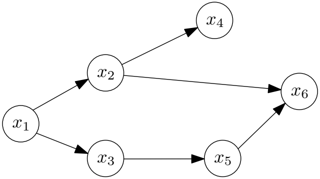
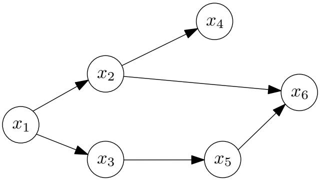
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B|C$



$$x_2 \perp\!\!\!\perp x_3|\emptyset??$$

D-Separation

1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
    - It is a head-to-tail or tail-to-tail node and the node is in C
    - It is a head-to-head node and neither the node, **not any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B | C$

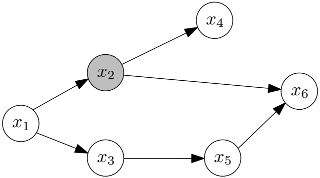


$$x_2 \perp\!\!\!\perp x_3 | \emptyset ??$$

NO!! path through x_1 is not blocked

D-Separation

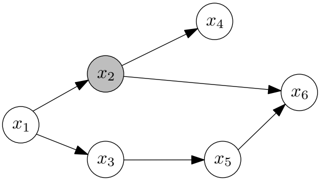
1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
   - It is a head-to-tail or tail-to-tail node and the node is in C
   - It is a head-to-head node and neither the node, **not any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B|C$



$$x_4 \perp\!\!\!\perp \{x_1, x_3\}|x_2??$$

D-Separation

1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
   - It is a head-to-tail or tail-to-tail node and the node is in C
   - It is a head-to-head node and neither the node, **not any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B|C$

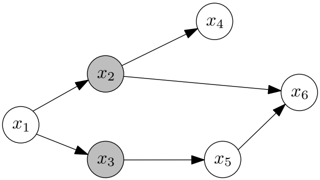


$$x_4 \perp\!\!\!\perp \{x_1, x_3\}|x_2??$$

YES!! paths through x_2 are blocked

D-Separation

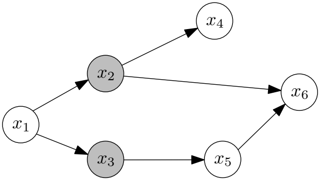
1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
   - It is a head-to-tail or tail-to-tail node and the node is in C
   - It is a head-to-head node and neither the node, **not any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B | C$



$$x_1 \perp\!\!\!\perp x_6 | \{x_2, x_3\}??$$

D-Separation

1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
   - It is a head-to-tail or tail-to-tail node and the node is in C
   - It is a head-to-head node and neither the node, **not any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B|C$

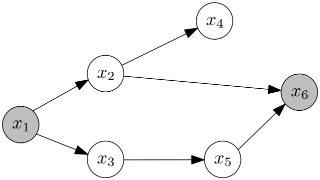


$$x_1 \perp\!\!\!\perp x_6|\{x_2, x_3\}??$$

YES!! all two paths are blocked

D-Separation

1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
   - It is a head-to-tail or tail-to-tail node and the node is in C
   - It is a head-to-head node and neither the node, **not any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B|C$



$$x_2 \perp\!\!\!\perp x_3|\{x_1, x_6\}??$$

D-Separation

1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
   - It is a head-to-tail or tail-to-tail node and the node is in C
   - It is a head-to-head node and neither the node, **not any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
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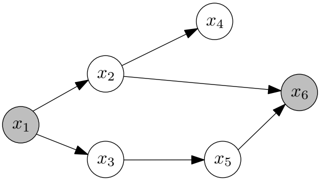


$$x_2 \perp\!\!\!\perp x_3|\{x_1, x_6\}??$$

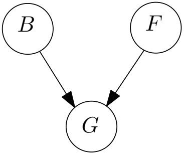
NO!! path through x_6 is opened!

D-Separation

1. A, B and C non-intersecting subsets of nodes
2. An (undirected) path from A to B is blocked if it contains a node s.t.
   - It is a head-to-tail or tail-to-tail node and the node is in C
   - It is a head-to-head node and neither the node, **not any of its descendants** are in C
3. If all paths from A and B are blocked, A is d-separated from B by C
4. Then $A \perp\!\!\!\perp B|C$

- Try yourself! : `http://aispace.org/bayes/`
- Load an existing model : `File->Load Sample Problem`
- Make three queries : Click on `Independence Quiz`
- Reason about them

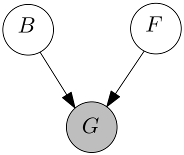
Example: B battery, F fuel tank and G fuel electric sensor



$$P(G=1|B=1,F=1)=0.8$$
$$P(G=1|B=1,F=0)=0.2$$
$$P(G=1|B=0,F=1)=0.2$$
$$P(G=1|B=0,F=0)=0.1$$
$$P(B=1)=0.9$$
$$P(F=1)=0.9$$

Without evidence, the prior probability of the tank being empty is $P(F=0)=0.1$

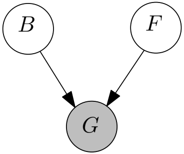
Example: B battery, F fuel tank and G fuel electric sensor



$$P(G = 1|B = 1, F = 1) = 0.8$$
$$P(G = 1|B = 1, F = 0) = 0.2$$
$$P(G = 1|B = 0, F = 1) = 0.2$$
$$P(G = 1|B = 0, F = 0) = 0.1$$
$$P(B = 1) = 0.9$$
$$P(F = 1) = 0.9$$

Observe sensor $G = 0$. What is the probability of the tank being empty?

Example: B battery, F fuel tank and G fuel electric sensor

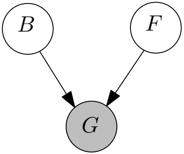


$$P(G=1|B=1,F=1)=0.8$$
$$P(G=1|B=1,F=0)=0.2$$
$$P(G=1|B=0,F=1)=0.2$$
$$P(G=1|B=0,F=0)=0.1$$
$$P(B=1)=0.9$$
$$P(F=1)=0.9$$

$$P(G=0)=\sum_{B=\{0,1\}}\sum_{F=\{0,1\}}p(G=0|B,F)p(B)p(F)=0.315$$

$$P(G=0|F=0)=\sum_{B=\{0,1\}}p(G=0|B,F=0)p(B)=0.81$$

Example: B battery, F fuel tank and G fuel electric sensor

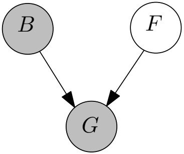


$$P(G=1|B=1,F=1)=0.8$$
$$P(G=1|B=1,F=0)=0.2$$
$$P(G=1|B=0,F=1)=0.2$$
$$P(G=1|B=0,F=0)=0.1$$
$$P(B=1)=0.9$$
$$P(F=1)=0.9$$

$$P(F=0|G=0)=\frac{P(G=0|F=0)P(F=0)}{P(G=0)}\approx 0.257$$

$$P(F=0|G=0)>P(F=0)$$

Example: B battery, F fuel tank and G fuel electric sensor

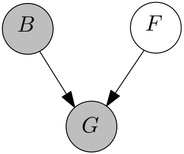


$$P(G = 1|B = 1, F = 1) = 0.8$$
$$P(G = 1|B = 1, F = 0) = 0.2$$
$$P(G = 1|B = 0, F = 1) = 0.2$$
$$P(G = 1|B = 0, F = 0) = 0.1$$
$$P(B = 1) = 0.9$$
$$P(F = 1) = 0.9$$

Suppose that we check the battery and it is flat $B = 0$. What is the new probability of the fuel being empty?

$$P(F = 0|G = 0, B = 0) = ?$$

Example: B battery, F fuel tank and G fuel electric sensor

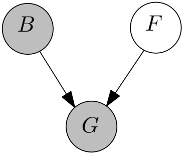


$$P(G=1|B=1,F=1)=0.8$$
$$P(G=1|B=1,F=0)=0.2$$
$$P(G=1|B=0,F=1)=0.2$$
$$P(G=1|B=0,F=0)=0.1$$
$$P(B=1)=0.9$$
$$P(F=1)=0.9$$

Suppose that we check the battery and it is flat $B=0$. What is the new probability of the fuel being empty?

$$P(F=0|G=0,B=0)=\frac{P(G=0|B=0,F=0)P(F=0)}{\sum_{F=\{0,1\}}P(G=0|B=0,F)P(F)}\approx 0.111$$

Example: B battery, F fuel tank and G fuel electric sensor

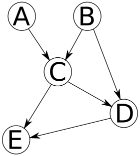


$$
\begin{aligned}
P(G=1|B=1,F=1) &= 0.8\\
P(G=1|B=1,F=0) &= 0.2\\
P(G=1|B=0,F=1) &= 0.2\\
P(G=1|B=0,F=0) &= 0.1\\
P(B=1) &= 0.9\\
P(F=1) &= 0.9
\end{aligned}
$$

Suppose that we check the battery and it is flat $B=0$. What is the new probability of the fuel being empty?

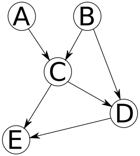
$$P(F=0|G=0,B=0) = \frac{P(G=0|B=0,F=0)P(F=0)}{\sum_{F=\{0,1\}} P(G=0|B=0,F)P(F)} \approx 0.111$$

$$P(F=0|G=0,B=0) < P(F=0|G=0) \qquad \mathbf{F} \not\perp \mathbf{B}|\mathbf{G}$$



$$p(A, B, C, D, E) = p(A)p(B)p(C|A, B)p(D|B, C)p(E|C, D)$$

Inference: Evaluate the probability distribution over some set of variables, given values of another set of variables Ex: $p(A|C = c)$? (binary variables)



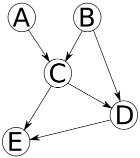
$$p(A,B,C,D,E) = p(A)p(B)p(C|A,B)p(D|B,C)p(E|C,D)$$

Inference: Evaluate the probability distribution over some set of variables, given values of another set of variables Ex: $p(A|C=c)$? (binary variables)
Naive:

$$p(A, C=c) = \sum_{B,D,E} p(A,B,C=c,D,E) \qquad \text{[16 terms]}$$

$$p(C=c) = \sum_{A} p(A, C=c) \qquad \text{[2 terms]}$$

$$p(A|C=c) = \frac{p(A,C=c)}{p(C=c)} \qquad \text{[2 terms]} \qquad \rightarrow \text{total terms: } 20$$



$$p(A,B,C,D,E) = p(A)p(B)p(C|A,B)p(D|B,C)p(E|C,D)$$

Inference: Evaluate the probability distribution over some set of variables, given values of another set of variables Ex: $p(A|C=c)$? (binary variables)

More efficiently:

$$\begin{aligned} p(A, C=c) &= \sum_{B,D,E} p(A)p(B)p(C=c|A,B)p(D|B,C=c)p(E|C=c,D) \\ &= \sum_{B} p(A)p(B)p(C=c|A,B) \sum_{D} p(D|B,C=c) \sum_{E} p(E|C=c \\ &= \sum_{B} p(A)p(B)p(C=c|A,B) \qquad [4 \text{ terms}] \end{aligned}$$

Outline

1. Introduction to probabilistic Graphical Models
   - Bayesian networks
   - Markov Random Fields
   - Factor graphs
   - Inference and message passing algorithms
   - Learning Graphical Models

Factorization : over maximal cliques (fully connected subgraphs)

$$p(\mathbf{x}) = \frac{1}{Z} \prod_C \psi_C(\mathbf{x}_C) \qquad\qquad Z = \sum_{\mathbf{x}} \prod_C \psi_C(\mathbf{x}_C)$$

where $\psi_C(\mathbf{x}_C)$ is the potential over clique C and Z is the partition function

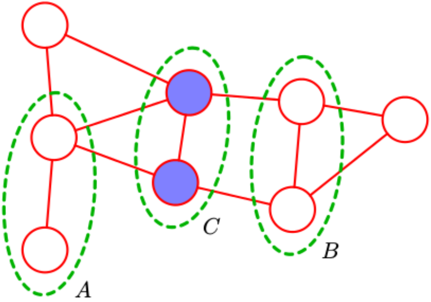
Energy models : $\psi_C(\mathbf{x}_C) = \exp(-E(\mathbf{x}_C))$
Lower energy $E \rightarrow$ Higher probability p
Higher energy $E \rightarrow$ Lower probability p

Markov Random Fields

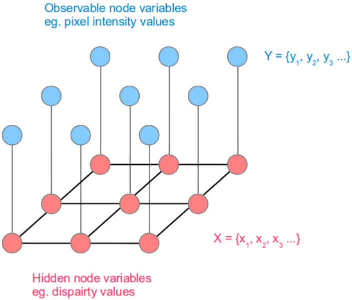
Undirected graphical models

Conditional Independences Easier! If A and B become disconnected after removing C

$$A \perp\!\!\!\perp B | C$$



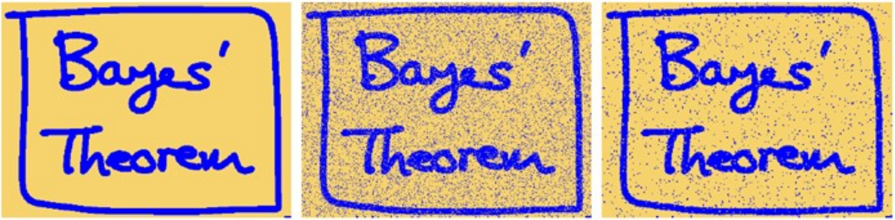
Example: image denoising as an inference task $(x_i \in \{\pm 1\}, y_i \in \{\pm 1\})$



$$E(\mathbf{x}, \mathbf{y}) = h \sum_i x_i - \beta \sum_{i,j} x_i x_j - \eta \sum_i x_i y_i$$

$$p(\mathbf{x}, \mathbf{y}) = \frac{1}{Z} \exp\{-E(\mathbf{x}, \mathbf{y})\}$$

Example: image denoising as an inference task



Left : original image

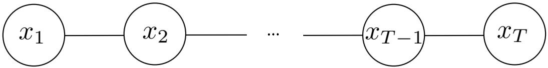
Middle : corrupted image (with $p = 0.1$ changes pixel)

Right : one local minima found over the energy landscape

Markov Random Fields

Inference on a chain

A chain of T variables, each having K possible values



Joint probability distribution :

$$p(\mathbf{x}) = \frac{1}{Z}\psi_{1,2}(x_1, x_2)\psi_{2,3}(x_2, x_3)\ldots\psi_{T-1,T}(x_{T-1}, x_T)$$

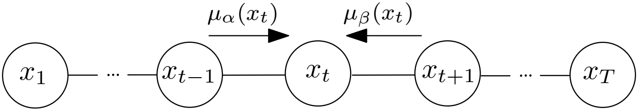
Estimate single-node marginal $p(x_t)$:

$$p(x_t) = \sum_{x_1}\ldots\sum_{x_{t-1}}\sum_{x_{t+1}}\ldots\sum_{x_T} p(\mathbf{x})$$

Naive summation has complexity $\mathcal{O}(K^T)$

Markov Random Fields

Inference on a chain

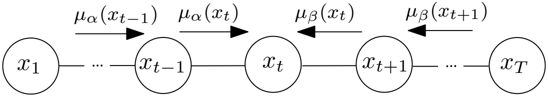


$$p(x_t) = \frac{1}{Z} \underbrace{\left[\sum_{x_{t-1}} \psi_{t-1,t}(x_{t-1}, x_t) \dots \left[\sum_{x_1} \psi_{1,2}(x_1, x_2)\right] \dots\right]}_{\mu_\alpha(x_t)} \cdot$$

$$\underbrace{\left[\sum_{x_{t+1}} \psi_{t,t+1}(x_t, x_{t+1}) \dots \left[\sum_{x_T} \psi_{T-1,T}(x_{T-1}, x_T)\right] \dots\right]}_{\mu_\beta(x_t)}$$

Markov Random Fields

Inference on a chain

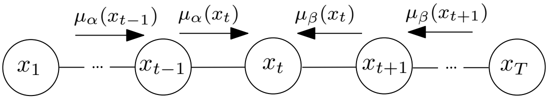


$$\mu_\alpha(x_t) = \sum_{x_{t-1}} \psi_{t-1,t}(x_{t-1}, x_t) \left[\sum_{x_{t-2}} \dots \right]$$
$$= \sum_{x_{t-1}} \psi_{t-1,t}(x_{t-1}, x_t) \mu_\alpha(x_{t-1})$$

$$\mu_\beta(x_t) = \sum_{x_{t+1}} \psi_{t,t+1}(x_t, x_{t+1}) \left[\sum_{x_{t+2}} \dots \right]$$
$$= \sum_{x_{t+1}} \psi_{t,t+1}(x_t, x_{t+1}) \mu_\beta(x_{t+1})$$

Markov Random Fields

Inference on a chain



$$\mu_\alpha(x_2) = \sum_{x_1} \psi_{1,2}(x_1, x_2) \qquad \mu_\alpha(x_{T-1}) = \sum_{x_T} \psi_{T-1,T}(x_{T-1}, x_T)$$

$$Z_{x_t} = \sum_{x_t} \mu_\alpha(x_t)\mu_\beta(x_t)$$

Computing local marginals in a chain

1. Compute forward messages $\mu_\alpha(x_t)$
2. Compute backward messages $\mu_\beta(x_t)$
3. Compute $p(x_t) = \frac{1}{Z_{x_t}}\mu_\alpha(x_t)\mu_\beta(x_t)$, Z_{x_t} sum over all x_t values
4. Complexity $\mathcal{O}(K^T) \rightarrow \mathcal{O}(TK^2)$

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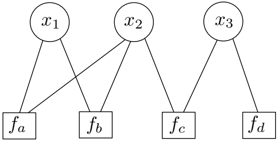
Bipartite Factor Graphs

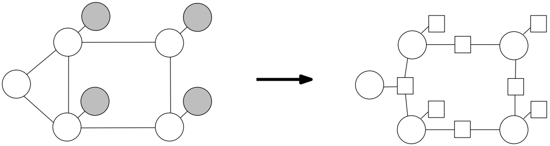
General class of graphical models

Factor graphs subsume both Bayesian networks and MRFs



Factorization: $p(\mathbf{x}) = \frac{1}{Z} f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$

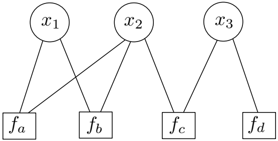
- MRF: factors correspond to maximal cliques potentials $\mathbf{x}_s$



Bipartite Factor Graphs

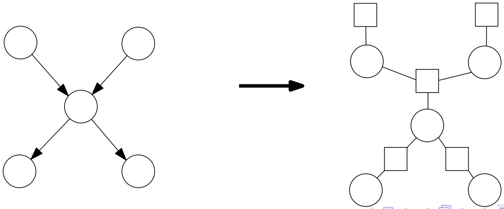
General class of graphical models

Factor graphs subsume both Bayesian networks and MRFs



Factorization: $p(\mathbf{x}) = \frac{1}{Z} f_a(x_1, x_2) f_b(x_1, x_2) f_c(x_2, x_3) f_d(x_3)$

- BN: factors correspond to conditional probability tables



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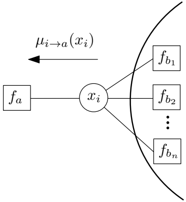
Sum-Product (belief propagation) algorithm

- Generic algorithm to compute local marginals in a factor graph
- Rediscovered several times: Gallager, J. Pearl, Kalman, ...

Iterates the following messages:

variable to factor :

$$\mu_{i\to a}(x_i) = \prod_{b\in\mathcal{N}(i)\setminus a} \mu_{b\to i}(x_i)$$



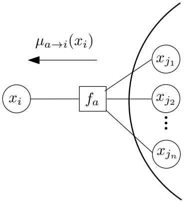
Sum-Product (belief propagation) algorithm

- Generic algorithm to compute local marginals in a factor graph
- Rediscovered several times: Gallager, J. Pearl, Kalman, ...

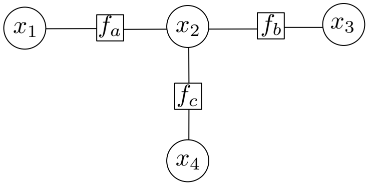
Iterates the following messages:

factor to variable

$$\mu_{a\to i}(x_i) = \sum_{\mathbf{x}_a \setminus \{i\}} f_a(\mathbf{x}_a) \prod_{j \in \mathcal{N}(a)\setminus i} \mu_{j\to a}(x_j)$$



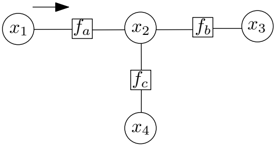
Example of inference using Belief Propagation (root node is x_3)



$$p(\mathbf{x}) \propto f_a(x_1, x_2) f_b(x_2, x_3) f_c(x_2, x_4)$$

Bipartite factor graphs

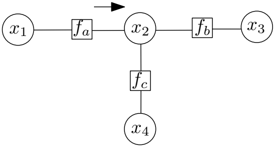
Example of inference using Belief Propagation (from leaves to root)



$$\mu_{x_1 \to f_a}(x_1) = \texttt{ones}$$

Bipartite factor graphs

Example of inference using Belief Propagation (from leaves to root)



$$\mu_{x_1 \to f_a}(x_1) = \texttt{ones}$$
$$\mu_{f_a \to x_2}(x_2) = \sum_{x_1} f_a(x_1, x_2) \mu_{x_1 \to f_a}(x_1)$$

Bipartite factor graphs

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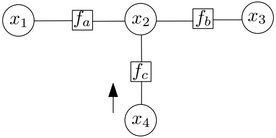

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Bipartite factor graphs

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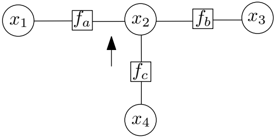

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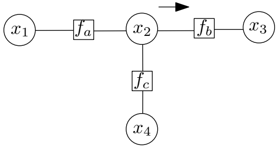

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Bipartite factor graphs

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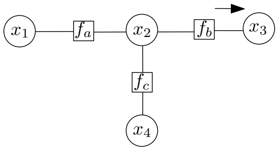

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Bipartite factor graphs

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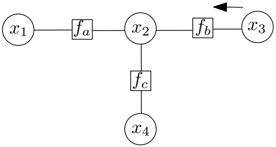

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Bipartite factor graphs

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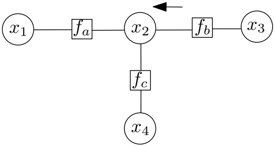

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Bipartite factor graphs

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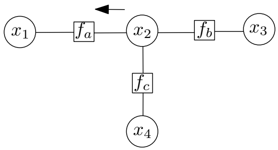

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Bipartite factor graphs

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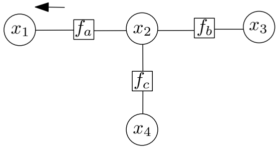

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Bipartite factor graphs

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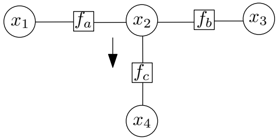

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Bipartite factor graphs

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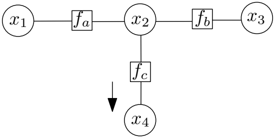

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Bipartite factor graphs

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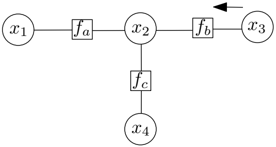

After the two passes, any single variable marginal can be computed taking the product of incoming messages and normalizing

$$Z_{x_2} = \sum_{x_2} \mu_{f_a \to x_2}(x_2)\mu_{f_b \to x_2}(x_2)\mu_{f_c \to x_2}(x_2)$$

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Bipartite factor graphs

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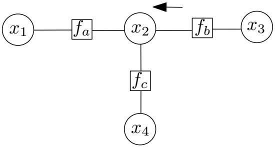

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Bipartite factor graphs

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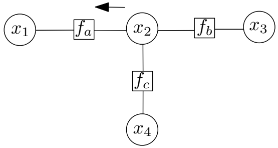

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Bipartite factor graphs

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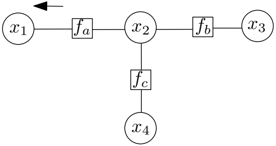

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Bipartite factor graphs

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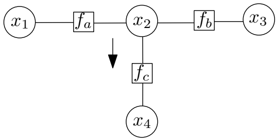

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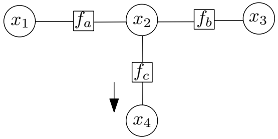

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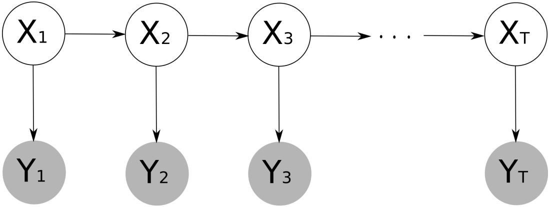
Probabilistic Inference

Hidden Markov models and Linear Gaussian state-space models



$$p(X_{1,\dots,T}, Y_{1,\dots,T}) = p(X_1)p(Y_1|X_1)\prod_{t=2}^{T} p(X_t|X_{t-1})p(Y_t|X_t)$$

- In HMMs, the states X_t are discrete
- In linear Gaussian SSMs, the states are real Gaussian vectors
- Both HMMs and SSMs can be represented as singly connected DAGs
- The **forward-backward algorithm** in HMMs and the **Kalman smoothing algorithm** in SSMs are both instances of belief propagation / factor graph representation

Sum-Product algorithm

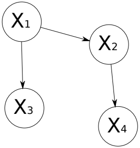
- Generic algorithm to compute local marginals in a factor graph
- Sum-Product is exact on tree graphs
- Can be an approximate algorithm on loopy graphs (LBP)
- Convergence is not guaranteed
- Variational interpretation: fixed points of LBP are stationary points of a free energy function
- Exact inference in loopy graphs
  - Compile the graph into a tree (cluster graph)
  - Run message passing on it
  - Complexity exponential in maximum clique size

Outline

1. Introduction to probabilistic Graphical Models
   - Bayesian networks
   - Markov Random Fields
   - Factor graphs
   - Inference and message passing algorithms
   - Learning Graphical Models

Learning graphical Models

Given the graph, learn the parameters



$$p(X_1)p(X_2|X_1)p(X_3|X_1)p(X_4|X_3)$$

θ_2	X_2		
X_1	0.2	0.3	0.5
	0.1	0.6	0.3

- Assume each variable X_i is discrete and can take on K_i values
- The parameters can be represented as 4 tables: θ_1 has K_1, θ_2 has entries $K_1 \times K_2$, etc...
- **Conditional Probability Tables** (CPTs) with the following semantics:

$$p(x_1 = k) = \theta_{1,k}, \qquad p(x_2 = k'|x_1 = k) = \theta_{2,k,k'}$$

- If node i has M parents, θ_i: $M+1$ dimensional table or 2-dimensional table with $(\prod_{j \in \mathrm{pa}(i)} K_j \times K_i)$ entries by collapsing all the states of the parents of node i. Note that $\sum_{k'} \theta_{i,k,k'} = 1$
- Assume a data set $\mathcal{D} = \{\mathbf{x}^n\}_{n=1}^N$

Learning graphical Models

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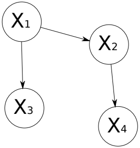

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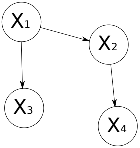

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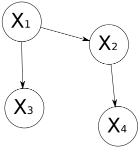

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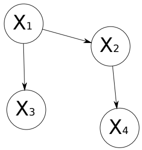

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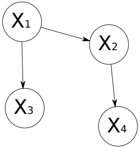
How do we learn θ from $\mathcal{D}$?



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Learning graphical Models

Given the graph, learn the parameters

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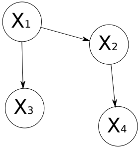

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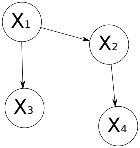

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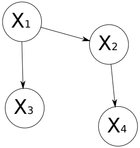

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$$\theta_{i,k,k'} = \frac{n_{i,k,k'}}{\sum_{k''} n_{i,k,k''}}$$

$n_{i,k,k''}$ is # times in $\mathcal{D}$ where $x_i = k'$ and $x_{\text{pa(i)}} = k$ (k joint configuration of the parents)

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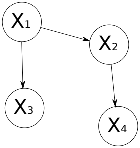

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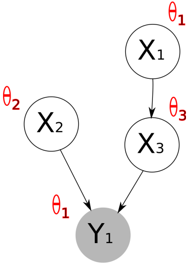
ML solution: Simply calculate frequencies!

Goal : Maximize parameter log-likelihood given observables

$$\mathcal{L}(\theta) = \log p(Y|\theta) = \log \sum_X p(Y, X|\theta)$$



The Expectation - Maximization (EM) algorithm (intuition)

Iterate between applying the following two steps:

- **The E-Step**: fill-in the hidden/missing variables
- **The M-Step**: apply complete data learning to filled-in data. Previous slide formula