Advanced Probabilistic Machine Learning
SSY316

Graphical Models (1)

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Graphical models

A powerful framework to represent and learn structured probabilistic models

Capture way in which a joint distribution can be factorized into product of factors, each depending only on a subset of variables

Useful for

- Visualize the structure of a probabilistic model
- Encode structural information (dependencies) about involved RVs
- Structure computations: provide graph-based algorithms for computation, inference, and forecasting

Graphical models

- Image Processing
- Speech Processing
- Natural Language Processing
- Document Processing
- Pattern Recognition
- Bioinformatics
- Computer Vision
- Economics
- Physics
- Social Sciences
- ...

Graphical models

Three types of graphical models:

- Bayesian networks (directed acyclic graphs): Represent a set of RVs and their conditional dependence structure
- Markov random fields (undirected graphs): Represent a set of RVs and their Markov structure
- Factor graphs: More convenient for the purposes of inference and learning

Bayesian networks (Bayes nets)

Bayesian networks: encode a factorization of a joint distribution.

Two types of elements:

- Nodes: represent RVs
  - Empty nodes: unobserved RVs
  - Shaded nodes: observed RVs
- Edges: represent relationships between RVs

Bayesian networks

Bayesian networks: encode a factorization of a joint distribution.

K RVs $\{\mathsf{x}_1, \ldots, \mathsf{x}_K\}$ with joint probability distribution $p(x_1, \ldots, x_K)$

Chain rule:

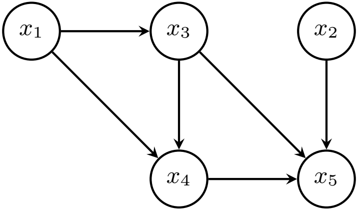
$$\begin{aligned} p(x_1, \ldots, x_K) &= p(x_1)p(x_2|x_1) \cdots p(x_K|x_1, \ldots, x_{K-1}) \\ &= \prod_{k=1}^{K} p(x_k|x_1, \ldots, x_{k-1}) \end{aligned}$$

To build BN:

1. Introduce a node for each x; associate node with $p(x|\cdot)$
2. For each $p(x|\cdot)$ draw a directed edge to node x from nodes corresponding to RVs on which the distribution is conditioned
3. Edge from node x to node $\tilde{x}$: x parent of $\tilde{x}$, $\tilde{x}$ child of x

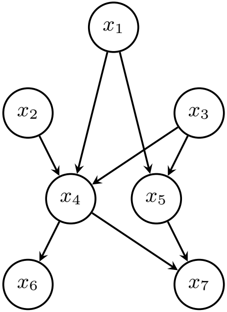
Bayesian networks
(from joint distribution to BN)

$$p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_2)p(x_3|x_1)p(x_4|x_1, x_3)p(x_5|x_2, x_3, x_4)$$



1. Introduce a node for each x; associate node with $p(x|\cdot)$
2. For each $p(x|\cdot)$ draw a directed edge to node x from nodes corresponding to RVs on which distribution is conditioned

Bayesian networks (from BN to joint distribution)



$$p(x_1, \ldots, x_7) = p(x_1)p(x_2)p(x_3)p(x_4|x_1, x_2, x_3)p(x_5|x_1, x_3)p(x_6|x_4)p(x_7|x_4, x_5)$$

Factorization into conditional distributions given by structure of BN.

Bayesian networks

Bayesian network: A directed acyclic graph (DAG) whose nodes represent RVs $\{\mathsf{x}_1, \ldots, \mathsf{x}_K\}$ with an associated joint distribution that factorizes as

$$p(x_1, \ldots, x_K) = \prod_{k=1}^{K} p(x_k | x_{\mathcal{P}(x_k)})$$

$\mathcal{P}(x_k)$: set of indices of parents of node x_k in the DAG.

- $\mathsf{x}_{\mathcal{P}(\mathsf{x}_k)}$: Account for statistical dependence of x_k with all the preceding variables $\mathsf{x}_1, \ldots, \mathsf{x}_{k-1}$ according to selected order
- BN encodes

$$\mathsf{x}_k \perp \{\mathsf{x}_1, \ldots, \mathsf{x}_{k-1}\} \backslash \mathcal{P}(\mathsf{x}_k)$$

Example: Bayesian polynomial regression

Goal: Make predictions for target variable t given some new value x.

- Training data set $\mathcal{D} = (x_{\mathcal{D}}, t_D) = \{(x_1, t_1), \ldots, (x_N, t_N)\}$

Model:

For $\boldsymbol{\phi}(x) = (1, x^2, \ldots, x^M)^\mathsf{T}$,

$$\begin{aligned} t &= \boldsymbol{w}^\mathsf{T}\boldsymbol{\phi}(x) + \varepsilon, \qquad \varepsilon \sim \mathcal{N}(0, \beta^{-1}) \\ \boldsymbol{w} &\sim p(\boldsymbol{w}) \end{aligned}$$

Equivalently,

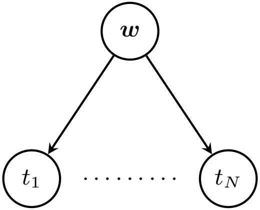
$$p(t|x, \boldsymbol{w}, \beta) = \mathcal{N}(t|\mu(x, \boldsymbol{w}), \beta^{-1})$$

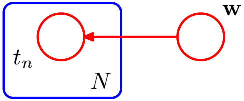
RVs: $\boldsymbol{w}$ and $t_{\mathcal{D}}$
Parameters: $(x_1, \ldots, x_N)$, σ^2, α

Example: Polynomial regression

Joint distribution $p(t_{\mathcal{D}}, \boldsymbol{w})$:

$$p(\boldsymbol{t}_{\mathcal{D}}, \boldsymbol{w}) = p(\boldsymbol{t}_{\mathcal{D}}|\boldsymbol{w})p(\boldsymbol{w}) = p(\boldsymbol{w}) \prod_{i=1}^{N} p(t_i|\boldsymbol{w})$$

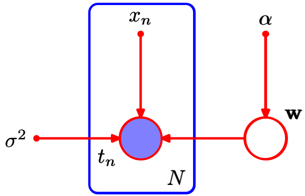




Example: Polynomial regression

- Joint distribution conditioned on input data and model parameters,

$$p(t_{\mathcal{D}}, \boldsymbol{w} | x_{\mathcal{D}}, \alpha, \sigma^2) = p(\boldsymbol{w}|\alpha) \prod_{i=1}^{N} p(t_i | \boldsymbol{w}, x_i, \sigma^2)$$



- Deterministic parameters represented by smaller solid circles
- Some RVs are observed $\longrightarrow$ shaded nodes
- Unobserved RVs: latent or hidden RVs (e.g., $\boldsymbol{w}$)

Bayesian networks

When are they useful?

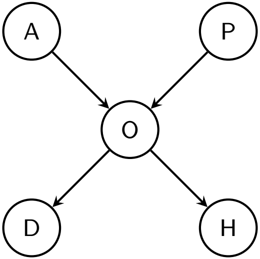
- When can identify causality relationships among RVs $\longrightarrow$ a natural order on variables; RVs that appear later caused by subset of preceding variables

Causing RVs for RV x_k included in $\mathcal{P}(x_k)$ $\longrightarrow$ when conditioning on $\mathsf{x}_{\mathcal{P}(\mathsf{x}_k)}$, x_k independent on all other preceding RVs.

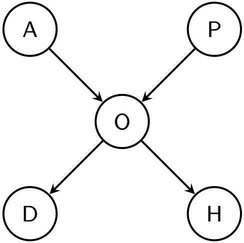
Bayesian networks: Example

- Lack of physical activity (A) and bad dietary patterns (P) cause obesity (O)
- Obesity causes diabetes (D) and heart disease (H)

Bayesian network:



Bayesian networks: Example



Joint distribution:

$$p(\mathsf{A},\mathsf{P},\mathsf{O},\mathsf{D},\mathsf{H}) = p(\mathsf{A})p(\mathsf{P})p(\mathsf{O}|\mathsf{A},\mathsf{P})p(\mathsf{D}|\mathsf{O})p(\mathsf{H}|\mathsf{O})$$

Marginal distribution:

$$p(\mathsf{H}) = \int p(\mathsf{A},\mathsf{P},\mathsf{O},\mathsf{D},\mathsf{H})\mathsf{d}a\,\mathsf{d}p\,\mathsf{d}o\,\mathsf{d}d$$

Ancestral sampling

Problem: Obtaining marginals is not easy

Idea: Draw samples from a given probability distribution.

- Easy to draw samples from a BN! $\longrightarrow$ Ancestral sampling

Ancestral sampling

Assume:

$$p(x_1, \ldots, x_K) = \prod_{k=1}^{K} p(x_k | x_{\mathcal{P}(x_k)})$$

(ordered variables $\{\mathrm{x}_1, \ldots, \mathrm{x}_K\}$, with no arrow from any node to any lower numbered node)

Goal: Draw samples from $p(x_1, \ldots, x_K)$

Ancestral sampling:

1. Draw sample for $\mathrm{x}_1 \sim p(x_1)$
2. Draw sample for $\mathrm{x}_2 \sim p(x_2 | x_{\mathcal{P}(2)})$
3. ...
4. Draw sample for $\mathrm{x}_K \sim p(x_K | x_{\mathcal{P}(K)})$

We have obtained a sample from the joint distribution.

Ancestral sampling

Sample from a marginal distribution:

- Take sampled values for required nodes and ignore those for remaining ones
- $p(x_2, x_4)$: sample from $p(x_1, \ldots, x_K)$, retain $\hat{x}_2, \hat{x}_4$ and discard $\{\hat{x}_{j \neq 2,4}\}$

Conditional independence

- Two RVs a and b are conditionally independent given c if

$$p(a, b|c) = p(a|c)p(b|c)$$

We write $a \perp b|c$

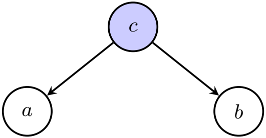
- Can also be written as

$$p(a|b, c) = \frac{p(a, b|c)}{p(b|c)} = \frac{p(a|c)p(b|c)}{p(b|c)} = p(a|c)$$

Graphical models: Conditional independence properties can be read directly from graph (d-separation).

Conditional independence

Tail-to-tail nodes:

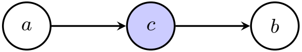


$$p(a, b|c) = \frac{p(a, b, c)}{p(c)} = \frac{p(a|c)p(b|c)p(c)}{p(c)} = p(a|c)p(b|c) \implies \mathsf{a} \perp \mathsf{b}|\mathsf{c}$$

a and b independent if node in between is observed

Conditional independence

Head-to-tail nodes:

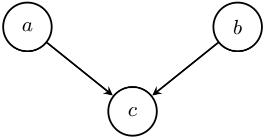


$$p(a,b|c) = \frac{p(a,b,c)}{p(c)} = \frac{p(a)p(c|a)p(b|c)}{p(c)} = p(a|c)p(b|c) \implies \mathsf{a} \perp \mathsf{b}|\mathsf{c}$$

a and b independent if node in between is observed

Conditional independence

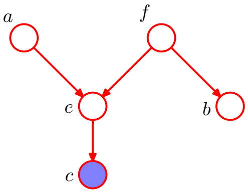
Head-to-head nodes:



$$p(a,b) = \int p(a,b,c)dc = \int p(c|a,b)p(a)p(b)dc = p(a)p(b) \quad \Longrightarrow \quad \mathsf{a} \perp \mathsf{b}|\emptyset$$

a and b independent if node in between and any of its descendants are not observed

d-separation



- Are a and b conditionally independent given c?
- More in general: Is a given subset of variables $\mathcal{A}$ independent of another set $\mathcal{B}$ conditioned on a third subset $\mathcal{C}$? ($\mathsf{x}_{\mathcal{A}} \perp \mathsf{x}_{\mathcal{B}} | \mathsf{x}_{\mathcal{C}}$)

Goal: Determine independencies directly from the directed acyclic graph.

d-separation: If all paths from from any node in $\mathcal{A}$ to any node in $\mathcal{B}$ given the nodes in $\mathcal{C}$ are blocked, then $\mathcal{A} \perp \mathcal{B} | \mathcal{C}$

d-separation

Previous examples giving blocked paths:

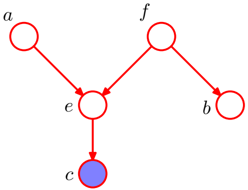
- observed tail-to-tail nodes
- observed head-to-tail nodes
- unobserved head-to-head nodes (with unobserved descendants)

d-separation: Let G be a directed graph and $\mathcal{A}$, $\mathcal{B}$, and $\mathcal{C}$ disjoint sets of nodes (RVs). Then, if all paths from any node in $\mathcal{A}$ to any node in $\mathcal{B}$ given the nodes in $\mathcal{C}$ are blocked, $\mathcal{A}$ and $\mathcal{B}$ are said to be d-separated by $\mathcal{C}$ and $\mathcal{A} \perp \mathcal{B} | \mathcal{C}$.

A path between $\mathcal{A}$ and $\mathcal{B}$ is blocked if the path includes either:

- A head-to-tail or tail-to-tail node which is in $\mathcal{C}$; or
- A head-to-head node, and neither the node nor any of its descendants in $\mathcal{C}$

d-separation

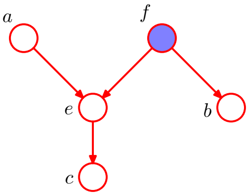


Are a and b conditionally independent given c?

- Path from a to b not blocked by f, since a tail-to-tail node and f unobserved
- Path not blocked by e, as a head-to-head node with an observed descendant

Hence, $a \perp b | c$ does not follow from the DAG

d-separation

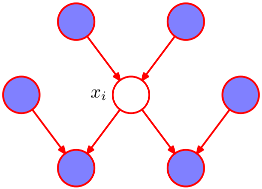


Are a and b conditionally independent given f?

- Path from a to b blocked by f, since a tail-to-tail node and observed
- Path blocked by e, as a head-to-head node and neither it its descendants are observed

Hence, $a \perp b|c$ follows from the DAG

Markov blanket



In a directed graphical model: A node is conditionally independent of all other nodes given its parents, children, and co-parents.

Markov blanket of node x_i: The minimal set of nodes that isolates x_i from the rest of the graph.

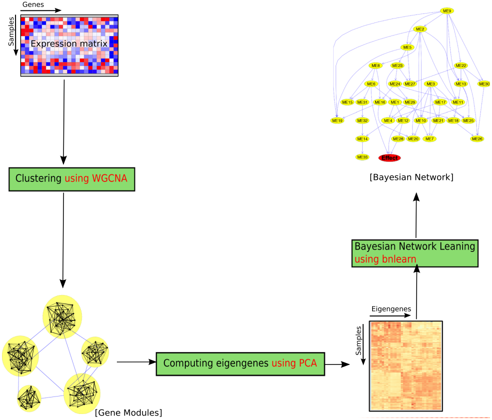
Structure Learning

What if the Bayesian network is not known?

Bayesian networks can be learned from data without a pre-specified structure:

- Different algorithms can be employed to learn network structure by analyzing the data and inferring most likely graph structure that best fits observed dependencies.
- Once structure and parameters are learned, Bayesian networks can be used for prediction

Predicting blood disease from gene expression profile



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Bayesian networks: Examples

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F. B. Hatipoglu, U. Uyar, “Examining the dynamics of macroeconomic indicators and banking stock returns with bayesian networks, *Business and Economics Research Journal*, 2019.

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Reading

"Pattern recognition and machine learning,"

Chapter 8 (Intro, 8.1 (until 8.1.2), 8.2)