

732A96/TDDE15 Advanced Machine Learning

Graphical Models and Hidden Markov Models

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Lecture 1: Causal Models, Bayesian Networks and Markov Networks

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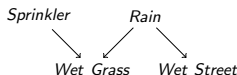
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Literature

- ▶ Main source
 - ▶ Bishop, C. M. *Pattern Recognition and Machine Learning*. Springer, 2006. Chapter 8.
- ▶ Additional source
 - ▶ Koski, T. J. T. and Noble, J. M. A Review of Bayesian Networks and Structure Learning. *Mathematica Applicanda* 40, 51-103, 2012.

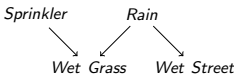
Causal Models

- ▶ Assume that we want to represent the causal relations between a set of random variables, e.g. the latter may represent the state of the components of a system.
- ▶ A natural and intuitive representation consists of a **graph** where the random variables are the nodes, and the causal relations are the edges. We call the graph a **causal model**.



- ▶ What happens if some random variables are not modeled ?
 - ▶ Nothing if they have at most one modeled effect, e.g. mediators.
 - ▶ Problems otherwise, i.e. $WG \rightarrow WS$ and $WG \leftarrow WS$ are both wrong.
- ▶ **Exercise.** Produce a causal model for the domain *Temperature*, *Ice cream sales* and *Soda sales*.
- ▶ **Exercise.** Produce a causal model for Boyle's law, which relates the pressure and volume of a gas as $Pressure \cdot Volume = constant$ if the temperature and amount of gas remain unchanged within a closed system.

Bayesian Networks: Definition

DAG	Parameter values for the conditional probability distributions
 <pre> graph TD Sprinkler --> Wet Rain --> Grass Rain --> Wet Wet --> Street </pre>	$q(S) = (0.3, 0.7)$ $q(R) = (0.5, 0.5)$ $q(WG r_0, s_0) = (0.1, 0.9)$ $q(WG r_0, s_1) = (0.7, 0.3)$ $q(WG r_1, s_0) = (0.8, 0.2)$ $q(WG r_1, s_1) = (0.9, 0.1)$ $q(WS r_0) = (0.1, 0.9)$ $q(WS r_1) = (0.7, 0.3)$ $p(S, R, WG, WS) = q(S)q(R)q(WG S, R)q(WS R)$

- ▶ A **Bayesian network (BN)** over a finite set of **discrete** random variables $X = X_{1:n} = \{X_1, \dots, X_n\}$ consists of
 - ▶ a DAG G whose nodes are the elements in X , and
 - ▶ parameter values θ_G specifying conditional probability distributions $q(X_i|pa_G(X_i))$.
- ▶ The BN represents a **causal** model of the system.
- ▶ The BN also represents a **probabilistic** model of the system, namely $p(X) = \prod_i q(X_i|pa_G(X_i))$.

Bayesian Networks: Definition

- ▶ We now show that $p(X) = \prod_i q(X_i | pa_G(X_i))$ is a probability distribution.
- ▶ Clearly, $0 \leq \prod_i q(X_i | pa_G(X_i)) \leq 1$.
- ▶ Assume without loss of generality that $pa_G(X_i) \subseteq X_{1:i-1}$ for all i . Then

$$\sum_x \prod_i q(x_i | pa_G(X_i)) = \sum_{x_1} [q(x_1) \dots \sum_{x_{n-1}} [q(x_{n-1} | pa_G(X_{n-1})) \sum_{x_n} q(x_n | pa_G(X_n))] \dots] = 1$$

- ▶ Moreover, $p(X_j | pa_G(X_j)) = q(X_j | pa_G(X_j))$. To see it, note that

$$\begin{aligned} p(X_j | pa_G(X_j)) &= \frac{p(X_j, pa_G(X_j))}{p(pa_G(X_j))} = \frac{\sum_{X \setminus \{X_j, pa_G(X_j)\}} \prod_i q(X_i | pa_G(X_i))}{\sum_{X \setminus pa_G(X_j)} \prod_i q(X_i | pa_G(X_i))} \\ &= \frac{\sum_{X_{1:j} \setminus \{X_j, pa_G(X_j)\}} \prod_{i \leq j} q(X_i | pa_G(X_i))}{\sum_{X_{1:j} \setminus pa_G(X_j)} \prod_{i \leq j} q(X_i | pa_G(X_i))} = q(X_j | pa_G(X_j)) \end{aligned}$$

Bayesian Networks: Separation

- ▶ We now show that many of the independencies in p can be read off G without numerical calculations.
- ▶ A path in G is a sequence of adjacent nodes, i.e. the direction of the edge is irrelevant. A node B is a descendant of a node A in G if there is a path $A \rightarrow \dots \rightarrow B$.
- ▶ Let ρ be a path between the nodes α and β in G .
- ▶ A node B in ρ is a **collider** when $A \rightarrow B \leftarrow C$ is a subpath of ρ .
- ▶ Moreover, ρ is Z -open with $Z \subseteq X \setminus \{\alpha, \beta\}$ when
 - ▶ no non-collider in ρ is in Z , and
 - ▶ every collider in ρ is in Z or has a descendant in Z .
- ▶ Let U , V and Z be three disjoint subsets of X . Then, U and V are **separated** given Z in G (i.e. $U \perp_G V | Z$) when there is no Z -open path in G between a node in U and a node in V .
- ▶ The separation criterion is **sound**, i.e. if $U \perp_G V | Z$ then $U \perp_p V | Z$.
- ▶ For instance, $S \perp_p R$, $S \not\perp_p R | WG$, $S \not\perp_p WS | WG$, $S \perp_p WS | WG, R$.

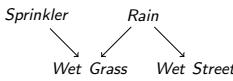



- ▶ Note that we read independencies from G , never dependencies.

Bayesian Networks: Separation

- ▶ Moreover, the separation criterion is also **complete**, i.e. p may be such that $U \perp_G V|Z$ if and only if $U \perp_p V|Z$.
- ▶ Moreover, p factorizes as $p(X) = \prod_i q(X_i | pa_G(X_i))$ if and only if it satisfies all the independencies identified by the separation criterion.
- ▶ **Exercise.** Prove that $A \perp_p B|C$ for the DAGs $A \rightarrow C \rightarrow B$, $A \leftarrow C \rightarrow B$ and $A \leftarrow C \leftarrow B$, i.e. prove that $p(A, B|C) = p(A|C)p(B|C)$.
- ▶ **Exercise.** Prove that $A \perp_p B|\emptyset$ for the DAG $A \rightarrow C \leftarrow B$, i.e. prove that $p(A, B) = p(A)p(B)$.
- ▶ **Exercise.** Find the minimal set of nodes that separates a given node from the rest. This set is called the Markov blanket of the given node.

Bayesian Networks: Causal Reasoning

Original	After $do(r_1)$
 <p> $q(S) = (0.3, 0.7)$ $q(R) = (0.5, 0.5)$ $q(WG r_0, s_0) = (0.1, 0.9)$ $q(WG r_0, s_1) = (0.7, 0.3)$ $q(WG r_1, s_0) = (0.8, 0.2)$ $q(WG r_1, s_1) = (0.9, 0.1)$ $q(WS r_0) = (0.1, 0.9)$ $q(WS r_1) = (0.7, 0.3)$ </p> <p> $p(S, R, WG, WS) = q(S)q(R)q(WG S, R)q(WS R)$ </p>	 <p> $q(S) = (0.3, 0.7)$ $q(WG s_0) = (0.8, 0.2)$ $q(WG s_1) = (0.9, 0.1)$ $q(WS) = (0.7, 0.3)$ </p> <p> $p(S, WG, WS) = q(S)q(WG S)q(WS)$ </p>

- What would be the state of the system if a random variable X_j is **forced** to take the state x_j , i.e. $p(X \setminus X_j | do(x_j))$?
 - Remove X_j and all the edges from and to X_j from G .
 - Remove $q(X_j | pa_G(X_j))$.
 - If $X_j \in pa_G(X_i)$, then replace $q(X_i | pa_G(X_i))$ with $q(X_i | pa_G(X_i) \setminus X_j, x_j)$
 - Set $p(X \setminus X_j | do(x_j)) = \prod_i q(X_i | pa_G(X_i))$.
- So, the result of $do(x)$ on a BN is a **BN**.

Bayesian Networks: Probabilistic Reasoning

- What is the state of the system if a random variable X_i is **observed** to be in the state x_i , i.e. $p(X \setminus X_i | x_i)$?

- $$p(X \setminus X_i | x_i) = \frac{p(X \setminus X_i, x_i)}{p(x_i)} = \frac{p(X \setminus X_i, x_i)}{\sum_{X \setminus X_i} p(X \setminus X_i, x_i)}$$
- $$p(R, WG, WS | s) = \frac{q(s)q(R)q(WG|s,R)q(WS|R)}{\sum_{r, wg, ws} q(s)q(r)q(wg|s,r)q(ws|r)}$$
$$= \frac{q(s)q(R)q(WG|s,R)q(WS|R)}{q(s) \sum_r [q(r) \sum_{wg} [q(wg|s,r) \sum_{ws} q(ws|r)]]}$$


- What is the state of a random variable Y if a random variable X_i is **observed** to be in the state x_i , i.e. $p(Y | x_i)$?

- $$p(Y | x_i) = \frac{p(Y, x_i)}{p(x_i)} = \frac{\sum_{X \setminus \{X_i, Y\}} p(X \setminus X_i, x_i)}{\sum_{X \setminus X_i} p(X \setminus X_i, x_i)}$$
- $$p(WS | s) = \frac{\sum_{r, wg} q(s)q(r)q(wg|s,r)q(WS|r)}{\sum_{r, wg, ws} q(s)q(r)q(wg|s,r)q(ws|r)}$$
$$= \frac{q(s) \sum_r [q(r)q(WS|r) \sum_{wg} q(wg|s,r)]}{q(s) \sum_r [q(r) \sum_{wg} [q(wg|s,r) \sum_{ws} q(ws|r)]]}$$

- What is the state of a random variable Y if a random variable X_i is **observed** to be in the state x_i , after **forcing** a random variable X_j to take the state x_j , i.e. $p(Y | x_i, do(x_j))$?
- Answering questions like the one above can be computationally hard.
- A BN is an efficient formalism to compute a posterior probability distribution from a prior probability distribution in the light of observations, hence the name.

Markov Networks: Definition

- ▶ A BN represents asymmetric (causal) relations, whereas a Markov network represents **symmetric** relations, e.g. physical laws.

UG	Potentials assuming binary random variables
 <pre> graph LR A --- B A --- C B --- D C --- D </pre>	$\varphi(A, B, C) = (1, 1, 1, 1, 2, 2, 2, 2)$ $\varphi(B, C, D) = (1, 2, 3, 4, 5, 6, 7, 8)$ $p(A, B, C, D) = \varphi(A, B, C)\varphi(B, C, D)/Z$ with $Z = \sum_{a,b,c,d} \varphi(a, b, c)\varphi(b, c, d)$

- ▶ A **Markov network (MN)** over X consists of
 - ▶ an undirected graph (UG) G whose nodes are the elements in X , and
 - ▶ a set of non-negative functions $\varphi(K)$ over the cliques $Cl(G)$ of G .
- ▶ A clique is a maximal complete set of nodes. The functions are called potentials. They represent **compatibility** relations between the random variables in the cliques.
- ▶ The MN represents a **probabilistic** model of the system, namely

$$p(X) = \frac{1}{Z} \prod_{K \in Cl(G)} \varphi(K)$$

where Z is a normalization constant, i.e.

$$Z = \sum_x \prod_{K \in Cl(G)} \varphi(k)$$

- ▶ Clearly, $p(X)$ is a probability distribution.

Markov Networks: Separation

- ▶ We now show that many of the independencies in p can be read off G without numerical calculations.
- ▶ A path ρ between two nodes α and β in G is Z -open with $Z \subseteq X \setminus \{\alpha, \beta\}$ when no node in ρ is in Z .
- ▶ Let U , V and Z be three disjoint subsets of X . Then, U and V are **separated** given Z in G (i.e. $U \perp_G V | Z$) when there is no Z -open path in G between a node in U and a node in V .
- ▶ The separation criterion is **sound**, i.e. if $U \perp_G V | Z$ then $U \perp_p V | Z$.
- ▶ Moreover, it is also **complete**, i.e. p may be such that $U \perp_p V | Z$ if and only if $U \perp_G V | Z$.
- ▶ Moreover, p factorizes as $p(X) = \frac{1}{Z} \prod_{K \in Cl(G)} \varphi(K)$ if and only if it satisfies all the independencies identified by the separation criterion.

Markov Networks: Separation

- ▶ **Exercise.** Prove that $A \perp_p B | C$ for the UG $A - C - B$, i.e. prove that $p(A, B | C) = f(A, C)g(B, C)$ for some functions f and g .
- ▶ **Exercise.** Find the minimal set of nodes that separates a given node from the rest. This set is called the Markov blanket of the given node.

Markov Networks: Probabilistic Reasoning

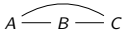
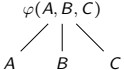
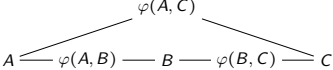
- ▶ What is the state of a random variable A if a random variable B is **observed** to be in the state b ?

$$p(A|b) = \frac{\sum_{c,d} \varphi(A, b, c) \varphi(b, c, d) / Z}{\sum_{a,c,d} \varphi(a, b, c) \varphi(b, c, d) / Z} = \frac{\sum_c [\varphi(A, b, c) \sum_d \varphi(b, c, d)]}{\sum_{a,c} [\varphi(a, b, c) \sum_d \varphi(b, c, d)]}$$

- ▶ Answering questions like the one above can be computationally hard.
- ▶ A MN is an efficient formalism to answer such questions.

Markov Networks: Factor Graphs

- What if $\varphi(A, B, C) = \varphi(A, B)\varphi(B, C)\varphi(A, C)$? I.e. $\varphi(C_i) = \prod_j \varphi(C_i^j)$ with $C_i^j \subset C_i$.
- A MN may obscure the structure of the potentials. Solution: Factor graphs.
- A **factor graph** over X consists of an UG G with two types of nodes: The elements in X and a set of potentials $\varphi(K)$ over subsets of X . All the edges in G are between a potential and the elements of X that are in the potential's domain.

MN	Factor graph	Factor graph
		

- The factor graph represents a **probabilistic** model of the system, namely

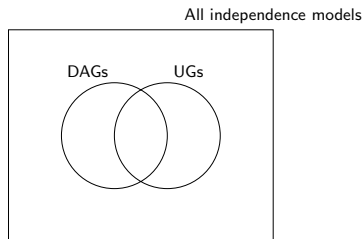
$$p(X) = \frac{1}{Z} \prod_K \varphi(K)$$

where Z is a normalization constant, i.e.

$$Z = \sum_x \prod_K \varphi(k)$$

- Factor graphs: Finer-grained parameterization of MNs.

Intersection of Bayesian and Markov Networks



- ▶ An **unshielded collider** in a DAG is a subgraph of the form $A \rightarrow C \leftarrow B$ such that A and B are not adjacent in the DAG.
- ▶ An UG is **triangulated** if every cycle in it contains a chord, i.e. an edge between two non-consecutive nodes in the cycle.
- ▶ Given a DAG G , there is an UG H such that $\perp_G \equiv \perp_H$ if and only if G has no unshielded colliders.
- ▶ Given an UG G , there is a DAG H such that $\perp_G \equiv \perp_H$ if and only if G is triangulated.

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Thank you