

732A96 Advanced Machine Learning

Graphical Models and Hidden Markov Models

Jose M. Peña
IDA, Linköping University, Sweden

Lecture 1: Causal Models, Bayesian Networks and Markov Networks

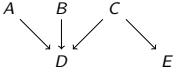
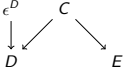

Contents

- ▶ Causal Models
- ▶ Bayesian Networks
 - ▶ Definition
 - ▶ Causal Reasoning
 - ▶ Probabilistic Reasoning
- ▶ Markov Networks
 - ▶ Definition
 - ▶ Probabilistic Reasoning

Literature

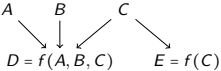
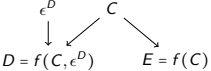
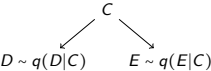
- ▶ Main source
 - ▶ Bishop, C. M. *Pattern Recognition and Machine Learning*. Springer, 2006. Chapter 8.
- ▶ Additional source
 - ▶ Koski, T. J. T. and Noble, J. M. A Review of Bayesian Networks and Structure Learning. *Mathematica Applicanda* 40, 51-103, 2012.

Causal Models: Qualitative

Microscopic DAG	Macroscopic DAG	Macroscopic Violates assumption
 <pre>graph TD; A --> D; B --> D; C --> D; C --> E;</pre>	 <pre>graph TD; epsilonD["epsilon^D"] --> D; C --> D; C --> E;</pre>	 <pre>graph TD; epsilonD["epsilon^D"] --> D; epsilonE["epsilon^E"] --> E; D -.- E;</pre>

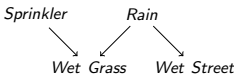
- ▶ At the **microscopic** level, every system is a causal system, **assuming** Reichenbach's principle of common cause: "No correlation without causation".
- ▶ Then, at the **microscopic** level, every system can be represented by a causal model.
- ▶ The structure of the causal model can be represented as a **directed and acyclic graph (DAG)**.
- ▶ At the **macroscopic** level, every system can be represented by a causal model **if no unmodeled variable** is cause of two or more modeled variables. The unmodeled causes of a variable X are aggregated into an error variable ϵ^X .

Causal Models: Quantitative

Microscopic DAG Functional	Macroscopic DAG Functional	Macroscopic DAG Probabilistic
 <p>$A \rightarrow D = f(A, B, C)$ $B \rightarrow D = f(A, B, C)$ $C \rightarrow D = f(A, B, C)$ $C \rightarrow E = f(C)$</p>	 <p>$\epsilon^D \rightarrow D = f(C, \epsilon^D)$ $C \rightarrow D = f(C, \epsilon^D)$ $C \rightarrow E = f(C)$</p>	 <p>$C \rightarrow D \sim q(D C)$ $C \rightarrow E \sim q(E C)$</p>

- ▶ **Assuming** Laplace's demon, every variable is a **deterministic** function of its causes at the **microscopic** level.
- ▶ Then, every variable is a **probabilistic** function of its modeled causes at the **macroscopic** level.
- ▶ Both Reichenbach's principle of common cause and Laplace's demon have been disproven. Human reasoning seem to comply with both of them, though.
- ▶ Then, probabilistic DAGs may not be ontological but epistemological models. They also help to identify key questions about reasoning.

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

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

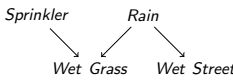

Bayesian Networks: Separation

- ▶ We now show that many of the independencies in p can be read off G without numerical calculations.
- ▶ Let ρ be a path between two 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 $U \perp_p V | Z$.
- ▶ 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 $p(X) = \prod_i q(X_i | pa_G(X_i))$ if and only if it satisfies all the independencies identified by the separation criterion.

Bayesian Networks: Separation

- ▶ **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

UG	Potentials assuming binary random variables
	$\varphi(A, B, C) = (1, 1, 1, 1, 1, 1, 1)$ $\varphi(B, C, D) = (2, 2, 2, 2, 2, 2, 2)$ $p(A, B, C, D) = \varphi(A, B, C)\varphi(B, C, D)/Z$ 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.
- ▶ 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

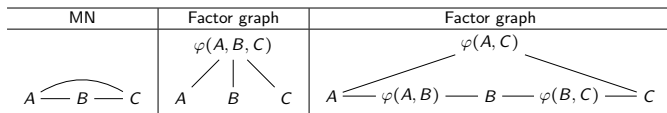
- ▶ We now show that many of the independencies in p can be read off G without numerical calculations.
- ▶ A path ρ between two nodes α and β in G is Z -open with $Z \subseteq X \setminus \{\alpha, \beta\}$ when no node in ρ is in Z .
- ▶ Let U , V and Z be three disjoint subsets of X . Then, U and V 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 $U \perp_G V|Z$ if and only if $U \perp_p V|Z$.
- ▶ 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: Factor Graphs

- ▶ What if $\varphi(C_i) = \prod_j \varphi(C_i^j)$ 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.



- ▶ 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.

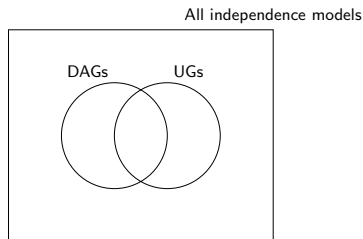
Markov Networks: Probabilistic Reasoning

- ▶ In the first example before, what is the state of a random variable A if a random variable B is **observed** to be in the state b ?

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

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

Intersection of Bayesian Networks 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 $I(G) = I(H)$ if and only if G has no unshielded colliders.
- ▶ Given an UG G , there is a DAG H such that $I(G) = I(H)$ if and only if G is triangulated.