732A96/TDDE15 Advanced Machine Learning

Graphical Models

Jose M. Peña
IDA, Linköping University, Sweden

Lecture 1: Bayesian and Markov Networks

Contents

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.

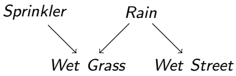
Causal Structures

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

$$\begin{tikzcd} \mathit{Sprinkler} \arrow[dr] & & \mathit{Rain} \arrow[dl] \arrow[dr] & \\ & \mathit{Wet\ Grass} & & \mathit{Wet\ Street} \end{tikzcd}$$

- **Exercise**. Produce a causal structure for the domain *Temperature*, *Ice cream sales* and *Soda sales*.
- **Exercise**. Produce a causal structure for Boyle's law, which relates the pressure and volume of a gas as $\mathit{Pressure} \cdot \mathit{Volume} = \mathit{constant}$ if the temperature and amount of gas remain unchanged within a closed system.

Bayesian Networks: Definition

DAG	Parameter values for the conditional probability distributions
	$q(s) = (0.3, 0.7) = (\theta_{s_0}, \theta_{s_1})$ $q(r) = (0.5, 0.5) = (\theta_{r_0}, \theta_{r_1})$ $q(wg \mid r_0, s_0) = (0.1, 0.9) = (\theta_{wg_0 \mid r_0, s_0}, \theta_{wg_1 \mid r_0, s_0})$ $q(wg \mid r_0, s_1) = (0.7, 0.3) = (\theta_{wg_0 \mid r_0, s_1}, \theta_{wg_1 \mid r_0, s_1})$ $q(wg \mid r_1, s_0) = (0.8, 0.2) = (\theta_{wg_0 \mid r_1, s_0}, \theta_{wg_1 \mid r_1, s_0})$ $q(wg \mid r_1, s_1) = (0.9, 0.1) = (\theta_{wg_0 \mid r_1, s_1}, \theta_{wg_1 \mid r_1, s_1})$ $q(ws \mid r_0) = (0.1, 0.9) = (\theta_{ws_0 \mid r_0}, \theta_{ws_1 \mid r_0})$ $q(ws \mid r_1) = (0.7, 0.3) = (\theta_{ws_0 \mid r_1}, \theta_{ws_1 \mid r_1})$ $p(s, r, wg, ws) = q(s)q(r)q(wg \mid s, r)q(ws \mid r)$

- A **Bayesian network (BN)** over a finite set of **discrete** random variables $X = X_{1:n} = \{X_1, \dots, X_n\}$ consists of
  - a directed acyclic graph (DAG) G whose nodes are the elements in X, and
  - parameter values θ specifying probability distributions $q(x_i \mid pa_i)$, where Pa_i are the parents of X_i in G, i.e. the nodes with an edge into X_i.
- The BN represents a causal model of the system.
- And also a probabilistic model of the system as $p(x) = \prod_i q(x_i \mid pa_i)$.

Bayesian Networks: Definition

- We now show that $p(x) = \prod_i q(x_i|pa_i)$ is a probability distribution.
- Clearly, $0 \leq \prod_i q(x_i|pa_i) \leq 1$.
- Assume without loss of generality that $Pa_i \subseteq X_{1:i-1}$ for all i. Then
$$\sum_x \prod_i q(x_i|pa_i) = \sum_{x_1}[q(x_1) \ldots \sum_{x_{n-1}}[q(x_{n-1}|pa_{n-1}) \sum_{x_n} q(x_n|pa_n)] \ldots] = 1$$
- Moreover, $p(x_j|pa_j) = q(x_j|pa_j)$. To see it, note that

$$\begin{aligned} p(x_j|pa_j) = \frac{p(x_j, pa_j)}{p(pa_j)} &= \frac{\sum_{x \setminus \{x_j, pa_j\}} \prod_i q(x_i|pa_i)}{\sum_{x \setminus pa_j} \prod_i q(x_i|pa_i)} \\ &= \frac{\sum_{x_{1:j} \setminus \{x_j, pa_j\}} \prod_{i \leq j} q(x_i|pa_i)}{\sum_{x_{1:j} \setminus pa_j} \prod_{i \leq j} q(x_i|pa_i)} = q(x_j|pa_j) \end{aligned}$$

Bayesian Networks: Separation

- We now show that many of the independencies in p can be read off G without numerical calculations. Consider the following DAG.

$$\begin{tikzcd}
Age \arrow[rr] & & Battery \arrow[dl] \arrow[dr] & & Bulb \arrow[dl] \\
& Radio & & Lights &
\end{tikzcd}$$

- **Chain**: $Age \rightarrow Battery \rightarrow Radio$
  - $Age \not\perp Radio | \varnothing$ not sperated
  - $Age \perp Radio | Battery$ sperated
- **Fork**: $Radio \leftarrow Battery \rightarrow Lights$
  - $Radio \not\perp Lights | \varnothing$
  - $Radio \perp Lights | Battery$
- **Collider**: $Battery \rightarrow Lights \leftarrow Bulb$
  - $Battery \perp Bulb | \varnothing$
  - $Battery \not\perp Bulb | Lights$
- **Chain + collider**: $Age \rightarrow Battery \rightarrow Lights \leftarrow Bulb$
  - $Age \perp Bulb | \varnothing$
  - $Age \not\perp Bulb | Lights$
  - $Age \perp Bulb | Lights, Battery$

Bayesian Networks: Separation

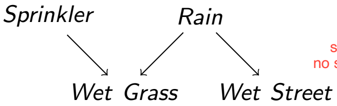
$$\begin{tikzcd} \mathit{Age} \arrow[rr] & & \mathit{Battery} \arrow[dl] \arrow[dr] & & \mathit{Bulb} \arrow[dl] \\ & \mathit{Radio} & & \mathit{Lights} & \end{tikzcd}$$

- A path in G is a sequence of distinct and 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 $A \to \ldots \to B$. child
  - E.g., $\mathit{Age} \to \mathit{Battery} \to \mathit{Lights} \leftarrow \mathit{Bulb}$ is a path.
  - E.g., Lights is a descendant of Age.
- Let ρ be a path in G between the nodes α and β.
- A node B in ρ is a **collider** when $A \to B \leftarrow C$ is a subpath of ρ.
  - E.g., Lights is a collider in the path $\mathit{Age} \to \mathit{Battery} \to \mathit{Lights} \leftarrow \mathit{Bulb}$.
- 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.
  - E.g., the path $\mathit{Age} \to \mathit{Battery} \to \mathit{Lights} \leftarrow \mathit{Bulb}$ is Z-open with $Z = \{\mathit{Lights}\}$.
- 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.
  - E.g., $\mathit{Age}, \mathit{Battery} \perp_G \mathit{Bulb} | \varnothing$.

Bayesian Networks: Separation

separate means independence

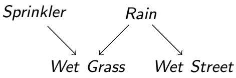
- The separation criterion is **sound**, i.e. if $U \perp_G V | Z$ then $U \perp_p V | Z$.
- For instance, $S \perp_p R$ and $S \perp_p WS | WG, R$ follow from the DAG



sep -> independent
no sep not-> dependent

- Note that we read independencies from G, never dependencies. That is, $S \not\perp_G R | WG$ and $S \not\perp_G WS | WG$ follow from the DAG, but not $S \not\perp_p R | WG$ or $S \not\perp_p WS | WG$.
- **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 $A \perp_p B | \varnothing$ 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.
- **Exercise**. How many free parameters do we have in the wet grass BN ? How many do we have if we specify the distribution without the assistance of a BN, i.e. as a table ?

Bayesian Networks: Causal Inference

Original	After $do(r_1)$
 $q(s) = (0.3, 0.7)$ $q(r) = (0.5, 0.5)$ $q(wg \mid r_0, s_0) = (0.1, 0.9)$ $q(wg \mid r_0, s_1) = (0.7, 0.3)$ $q(wg \mid r_1, s_0) = (0.8, 0.2)$ $q(wg \mid r_1, s_1) = (0.9, 0.1)$ $q(ws \mid r_0) = (0.1, 0.9)$ $q(ws \mid r_1) = (0.7, 0.3)$ $p(s, r, wg, ws) = q(s)q(r)q(wg \mid s, r)q(ws \mid r)$	 $q(s) = (0.3, 0.7)$ $q(wg \mid s_0) = (0.8, 0.2)$ $q(wg \mid s_1) = (0.9, 0.1)$ $q(ws) = (0.7, 0.3)$ $p(s, wg, ws) = q(s)q(wg \mid s)q(ws)$

- What would be the state of the system if a random variable X_j is forced to take the state x_j ?
  - Remove X_j and all the edges from and to X_j from G.
  - Remove $q(x_j|pa_j)$.
  - If $X_j \in Pa_i$, then replace $q(x_i|pa_i)$ with $q(x_i|pa_i \setminus x_j, x_j)$
  - Set $p(x \setminus x_j|do(x_j)) = \prod_i q(x_i|pa_i)$.
- So, the result of $do(x)$ on a BN **is a BN**. No more on causality in this course.

Bayesian Networks: Probabilistic Inference

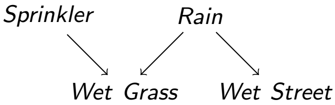
- What is the state of a random variable X_k if a random variable X_i is observed to be in the state x_i ?

$$p(x_k|x_i) = \frac{p(x_k, x_i)}{p(x_i)} = \frac{\sum_{x \setminus \{x_i, x_k\}} p(x)}{\sum_{x \setminus x_i} p(x)}$$

- For instance,

$$p(ws|s) = \frac{\sum_{r,wg} p(r, wg, ws, s)}{\sum_{r,wg,ws} p(r, wg, ws, s)} = \frac{\sum_{r,wg} q(s)q(r)q(wg|s,r)q(ws|r)}{\sum_{r,wg,ws} q(s)q(r)q(wg|s,r)q(ws|r)}$$

for the DAG

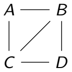


- Answering questions like the one above can be computationally hard.
- A BN is an efficient (because it uses the independences encoded) formalism to compute a posterior probability distribution from a prior probability distribution in the light of observations, hence the name. More on probabilistic inference in Lecture 2.

Markov Networks: Definition

in MN, we still can use parameter number reduction techniques

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

UG	Potentials assuming binary random variables
	2^3 = 8 non-neg number, it is not prob, it is a combination number $\varphi(a,b,c) = (0,0,0,0,1,1,1,1)$ we need normalise them $\varphi(b,c,d) = (1,2,3,4,5,6,7,8)$ $p(a,b,c,d) = \varphi(a,b,c)\varphi(b,c,d)/Z$ with $Z = \sum_{a,b,c,d} \varphi(a,b,c)\varphi(b,c,d)$

- A **Markov network (MN)** over X consists of A-B is a clique, when no super set(full connected)
  - 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, i.e. the maximal complete sets of nodes in G. 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 in G between two nodes α and β 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 $U \perp_p V|Z$.

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.
- **Exercise**. How many free parameters do we have in the ABCD MN ? How many do we have if we specify the distribution without the assistance of a MN ? How many if the variables have three states ?

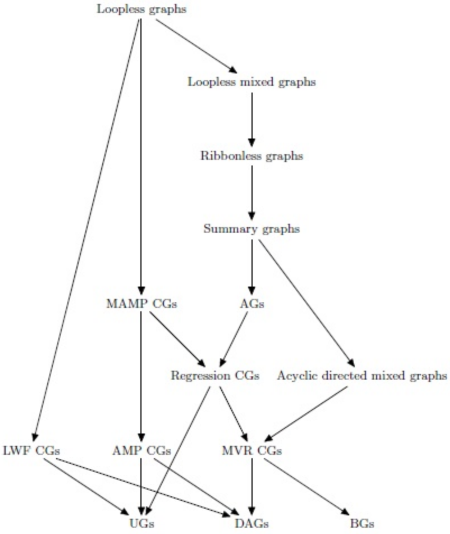
Markov Networks: Probabilistic Inference

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

$$p(a|b) = \frac{\sum_{c,d} \varphi(a,b,c)\varphi(b,c,d)/Z}{\sum_{a,c,d} \varphi(a,b,c)\varphi(b,c,d)/Z}$$

- Answering questions like the one above can be computationally hard.
- A MN is an efficient (because it uses the independences encoded) formalism to answer such questions. More on probabilistic inference in Lecture 2.

Families of Graphical Models



Contents

Thank you