

## Lecture 13 - graphs; DGM

Tuesday, October 13, 2020 14:34

- today :
- graph theory
- DGM

### Graphical model

graph. model  $\rightsquigarrow$  prob. theory + C.S.  
 ↓  
 R.V.      graph

graph  $\rightarrow$  efficient data structure

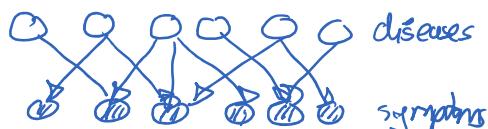
e.g.  $X_1, \dots, X_n$  R.V.s

$$X_i \in \{0, 1\}$$

$n = 100s$

$\Rightarrow 2^{100}$  #'s table  $\rightarrow$  intractable

GMR



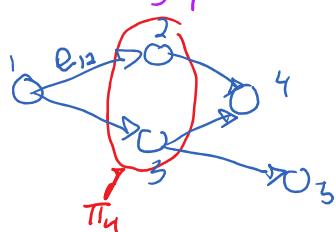
diseases  
symptoms

### Graph theory review:

directed graph  
"digraph"

$$G = (V, E)$$

$V = \{1, \dots, n\}$  "nodes/vertices"



$E \subseteq V \times V$  "directed edges"

$$e_{12} = (1, 2)$$

directed graph

$$\begin{array}{l} 1 \text{ to } 4 \\ (1, 2), (2, 4) \\ \text{or} \\ (1, 3), (3, 4) \end{array}$$

$\rightarrow$  compatible seq. of edges

$$\pi_i \triangleq \{j \in V : \exists (j, i) \in E\}$$

set of parents of  $i$

$$\text{children}(i) \triangleq \{j \in V : \exists (i, j) \in E\}$$

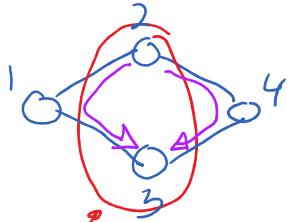
(note: no self loop in this class  
i.e.  $|E| = 2$ )

undirected graph :  $G = (V, E)$

where elements of  $E$  are 2-sets  
(set of 2 elements)

$$\text{thus we have } \{i, j\} = \{j, i\}$$

vs.  $(i, j) \neq (j, i)$  [order matters]



"neighbors" of node 4 or 1

$$N(i) \text{ for neighbors of } i = \{j \in V : \exists (i, j) \in E\}$$

undirected path  $2 \rightsquigarrow 3$

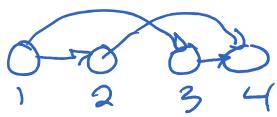
$\otimes$  neighbors → replace the parents/children terminology from a digraph

def : DAG = directed acyclic graph = digraph with no cycles

def : An ordering  $I: V \rightarrow \{1, \dots, |V|\}$  is said to be topological for G

iff nodes in  $\pi_i$  appear before  $i$  in  $I \quad \forall i$

$$(j \in \pi_i \Rightarrow I(j) < I(i))$$

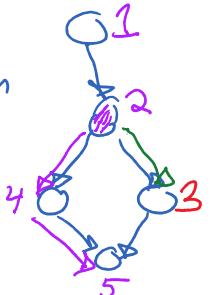


$\rightarrow$  if dep. ordering  
 $\Rightarrow$  all edges go from left to right  
 [no "back edge"]

prop: digraph  $G$  is DAG  $\Leftrightarrow \exists$  a topological ordering of  $G$

proof:  $\Leftarrow$ ) Trivial : no back edge  $\Rightarrow$  no cycle

$\Rightarrow$ ) use DFS algorithm to label nodes in decreasing order when have no children  
 to construct a top. sort  
 in  $O(|E| + |V|)$



Notation for graph models:

n discrete R.V.  $X_1, \dots, X_n$

$\hookrightarrow$  discrete R.V. for simplicity conditional dist. concept is  
 trying to formalize

$V \leftarrow$  set of vertices  
 one available per node

shorthand see Borel-kolmogorov paradox

joint  $p(x_1=x_1, \dots, x_n=x_n) \stackrel{?}{=} p(x_1, \dots, x_n) = p(x_r) \stackrel{(?)}{=} p(x)$

for any  $A \subseteq V$

$$p(x_A) = p\{X_i=x_i : i \in A\} = \sum_{x_{A^C}} p(x_A, x_{A^C})$$

subset of  
 "subspace"

$$\{x_1, x_2, x_3\} \leftrightarrow \{x_1, x_2, x_4\}$$

summing over all possible  
 values of  $x_i(x_i) \in \cup_{A \subseteq V} x_{A^C}$  can take

question : is  $p(x_1, x_2, x_4) \stackrel{?}{=} p(x_2, x_1, x_4)$  ?

yes! usually in this class, we use "typical convention"

revisit cond. indep.:

let  $A, B, C \subseteq V$

⊗  $X_A \perp\!\!\!\perp X_B \mid X_C$

$$(F) \Leftrightarrow p(x_A, x_B \mid x_C) = p(x_A \mid x_C)p(x_B \mid x_C) \quad \forall x_A, x_B, x_C \\ \text{s.t. } p(x_C) > 0$$

$$(C) \Leftrightarrow p(x_A \mid x_B, x_C) = p(x_A \mid x_C) \quad \forall x_A, x_B, x_C \\ \text{s.t. } p(x_B, x_C) > 0$$

⊗ "marginal independence":  $X_A \perp\!\!\!\perp X_B \mid \begin{matrix} \emptyset \\ \text{or} \\ X_C \end{matrix}$   
 $p(x_A, x_B) = p(x_A)p(x_B)$

2 facts about C.I.:

1) can repeat variables in statement  $X \perp\!\!\!\perp Y, Z \mid \underline{\exists}, W$  is fine to say  
(for convenience)  
does not do anything

2) decomposition:  $X \perp\!\!\!\perp (Y, Z) \mid W \Rightarrow \begin{matrix} X \perp\!\!\!\perp Y \mid W \\ X \perp\!\!\!\perp Z \mid W \end{matrix}$

⊗ pairwise indep.  $\not\Rightarrow$  mutual indep. → see lecture 3

$$Z = X \oplus Y$$
  
⊕  
xor

⊗ chain rule  $p(x_V) = \prod_{i=1}^n p(x_i \mid x_{1:n-1})$   
(always true)

assumption in DGM

last cond.  $p(x_n \mid x_{1:n-1})$  ↗ table with

$p(x_V) = \prod_{i=1}^n p(x_i \mid x_{\pi_i})$  → tables of  $2^{\max_i |\pi_i|}$  ≈  $2^n$  entries

15h38

Directed graph. model

Let  $G = (V, E)$  be a DAG

a directed graphical model (DGM) (associated with  $G$ ) (aka a Bayesian network)

is a family of distributions over  $X_V$

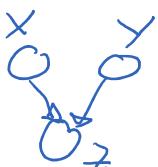
is a family of distributions over  $X_V$

$$\mathcal{F}(G) = \left\{ p \text{ is a dist. over } X_V : \exists \text{ legal factors } f_i \text{ s.t. } p(x_V) = \prod_{i=1}^n f_i(x_i | x_{\pi_i}) \right\}$$

$\hookrightarrow f_i : \Omega_{X_i} \times \Omega_{X_{\pi_i}} \rightarrow [0, 1]$   
 s.t.  $\sum_{x_i} f_i(x_i | x_{\pi_i}) = 1 \quad \forall x_{\pi_i}$   
 $\Rightarrow f_i$  is like a CPT  
 (conditional prob. table)

terminology: if we can write  $p(x_V) = \prod_i f_i(x_i | \dots)$  (this determines G)  
 then we say that " $p$  factors according to  $G$ "

one example:



$$p \in \mathcal{F}(G) \Leftrightarrow \exists f_x, f_y, f_z \text{ legal}$$

s.t.  $p(x, y, z) = f_x(x) f_y(y) f_z(z | y)$

"leaf plucking" property (fundamental property of DGM)

let  $p \in \mathcal{F}(G)$ ; let  $n$  be a leaf in  $G$  (i.e.  $n$  has no children)

a) then  $p(x_{1:n-1}) \in \mathcal{F}(G - \{n\})$

P means remove node n from G

b) moreover, if  $p(x_{1:n}) = \prod_{i=1}^n f_i(x_i | x_{\pi_i})$  then  $p(x_{1:n-1}) = \prod_{i=1}^{n-1} f_i(x_i | x_{\pi_i})$

proof:

$$p(x_n, x_{1:n-1}) = f_n(x_n | x_{\pi_n}) \prod_{j \neq n} f_j(x_j | x_{\pi_j})$$

$$p(x_{1:n-1}) = \sum_{x_n} p(x_n, x_{1:n-1}) = \left( \sum_{x_n} f_n(x_n | x_{\pi_n}) \right) \left( \prod_{j \neq n} f_j(x_j | x_{\pi_j}) \right)$$

no  $n$  in any  $x_j$   
by def

//

proposition: if  $p \in \mathcal{F}(G)$

let  $\{f_i\}$  be a factorization w.r.t.  $G$  for  $p$

$$\text{then } \text{inf}(x_{1:n-1}) = \text{C}(x_{1:n-1}) \times \text{inf}(x_n)$$

Let  $\{f_i\}$  be a factorization w.r.t to  $G$  for  $p$

$$\text{then } \forall i, p(x_i | x_{\pi_i}) = f_i(x_i | x_{\pi_i}) \quad \forall \pi_i$$

i.e. factors are correct conditionals  
(and are unique)

proof: WLOG, let  $(1, \dots, n)$  be a top sorting of  $G$  (possible since  $G$  is a DAG)

let  $i$  be fixed; we want to show that  $p(x_i | x_{\pi_i}) = f_i(x_i | x_{\pi_i})$

- $n$  is a leaf  $\rightarrow$  "pluck it" to get  $p(x_{1:n-1}) = \prod_{j=1}^{n-1} f_j(x_j | x_{\pi_j})$   
factorization for a DAG where  $x_{n-1}$  is now a leaf

- pluck  $n-1$  as well? (as leaf because of top order)

- keep doing this [in reverse order  $n-1, n-2, \dots, i+1$ ] to get

$$p(x_{1:i}) = f_i(x_i | x_{\pi_i}) \prod_{j=1}^{i-1} f_j(x_j | x_{\pi_j}) \stackrel{\text{i.e. no } x_i \text{ by top-sort property}}{\triangleq} g(x_{1:i})$$

partition  $1:i$  as  $\{i\} \cup \pi_i \cup A$  [ $A \triangleq 1:(i-1) \setminus \pi_i$ ]

$$p(x_{1:i}) = p(x_i, x_{\pi_i}, x_A)$$

$$p(x_i | x_{\pi_i}) = \sum_{x_A} p(x_i, x_{\pi_i}, x_A) = f_i(x_i | x_{\pi_i}) \left( \sum_{x_A} g(x_{1:i-1}) \right) = f_i(x_i | x_{\pi_i})$$

$$\sum_{x_i} \sum_{x_A} p(x_i, x_{\pi_i}, x_A) \left( \sum_{x_A} f_i(x_i | x_{\pi_i}) \right) \leq g(x_{1:i-1})$$

There is no  $x_i$  there //

\* (now) we can safely write

$$\mathcal{L}(G) = \{ p : p(x_v) = \prod_{i=1}^n p(x_i | x_{\pi_i}) \}$$

Properties:

adding edges  $\Rightarrow$  more distributions

i.e.  $G = (V, E)$  and  $G' = (V, E')$  with  $E' \supseteq E$

then  $\mathcal{L}(G) \subseteq \mathcal{L}(G')$

$\leftarrow \cup = V(D)$  and  $\cup - V, \subseteq$ , with  $\cup = L$

then  $\mathcal{Z}(G) \subseteq \mathcal{Z}(G')$

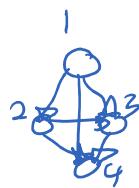
examples:

- $E = \emptyset$  (trivial graph)  $\Rightarrow \mathcal{Z}(G)$  contains only fully independent distributions

$$\text{ie. } p(x_v) = \prod_{i=1}^n p(x_i) / p(\emptyset)$$

- complete digraph (DAG)

for all  $i \neq j$  either  $(i,j) \in E$   
or  $(j,i) \in E$



get wlog

$$p(x_v) = \prod_{i=1}^n p(x_i | x_{\neq i})$$

(like chain rule)

$\Rightarrow$  all dist. one in  $\mathcal{Z}(G)$  (complete)  
on  $x_v$

~~⊗~~ removing edges impose more factorization constraints

(and thus <sup>more</sup> cond. indep. assumptions)