# Machine Learning (CSE 446): Probabilistic Graphical Models

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#### Notation

Let  $V = \langle V_1, V_2, \dots, V_\ell \rangle$  be a collection of random variables (not necessarily a sequence).

Val(V) will denote the values of a r.v. V.

 $oldsymbol{V}_I$  denotes a subset of the r.v.s  $oldsymbol{V}$  with indices  $i \in I.$ 

$$oldsymbol{V}_{
eg I} = oldsymbol{V} \setminus oldsymbol{V}_I$$

#### Recall:

- $ullet p(oldsymbol{V}) = \prod_{i=1}^\ell p(V_i \mid V_1, \dots, V_{i-1})$  (always true, for any ordering)
- ▶  $p(V_I, V_J \mid V_K) = p(V_I \mid V_K) \cdot p(V_J \mid V_K)$  if and only if  $V_I \perp V_J \mid V_K$  (conditional independence)
- ullet  $p(m{V}_I = m{v}_I) = \sum_{m{v}_{\lnot I} \in \mathrm{Val}(m{V}_{\lnot I})} p(m{V}_I = m{v}_I, m{V}_{\lnot I} = m{v}_{\lnot I})$  (marginalization)

### Factor Graphs

Two kinds of vertices:

- ▶ Random variables (denoted by circles, " $V_i$ ")
- ▶ Factors (denoted by squares, " $f_j$ ")

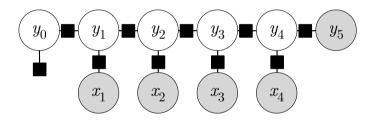
The graph is *bipartite*; every edge connects some variable to some factor. Let  $I_j \subseteq \{1, \dots, \ell\}$  be the set of variables  $f_j$  is connected to.

Factor  $f_j$  defines a map  $\operatorname{Val}(\boldsymbol{V}_{I_j}) \to \mathbb{R}_{\geq 0}$ .

The graph and factors define a probability distribution:

$$p(oldsymbol{V}=oldsymbol{v}) \propto \prod_{i} f_j(oldsymbol{v}_{I_j})$$

# Example



#### Two Kinds of Factors

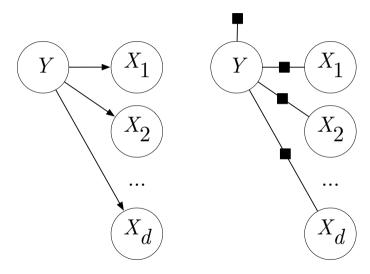
Conditional probability tables. E.g., if  $I_j = \{1, 2, 3\}$ :

$$f_j(v_1, v_2, v_3) = p(V_3 = v_3 \mid V_1 = v_1, V_2 = v_2)$$

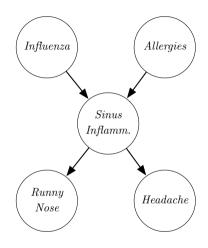
Lead to Bayesian networks (with some constraints).

Potential functions (arbitrary nonnegative values). Lead to **Markov random fields** (a.k.a. Markov networks).

# Naïve Bayes as a Bayesian Network and a Factor Graph



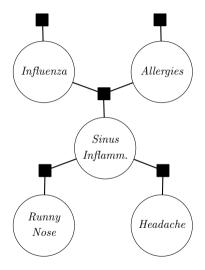
# Yucky Bayesian Network



Sinus inflammation is caused by flu, but also by allergies.

Runny nose and headache are both caused by sinus inflammation.

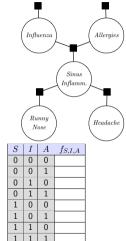
## Yucky Factor Graph



Sinus inflammation is caused by flu, but also by allergies.

Runny nose and headache are both caused by sinus inflammation.

# Yucky Factor Graph



I	$f_I$
0	
1	

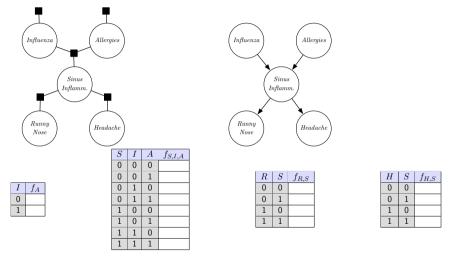
I	$f_A$
0	
1	

S	$f_{R,S}$	H	S
0		0	0
1		0	1
0		1	0
1		1	1

< ←	<b>&gt;</b>	4	3	Þ	4	$\equiv$	<b>.</b>	 na	0

 $f_{H,S}$ 

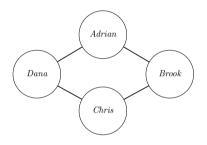
# Yucky Factor Graph



$$\begin{aligned} p(i,a,s,r,h) &= f_I(i) \cdot f_A(a) \cdot f_{S,I,A}(s,i,a) \cdot f_{R,S}(r,s) \cdot f_{H,S}(h,s) \\ &= p(i) \cdot p(a) \cdot p(s \mid i,a) \cdot p(r \mid s) \cdot p(h \mid s) \end{aligned}$$

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## Contagious Markov Random Field



Independencies:  $A \perp C \mid B, D$ ;

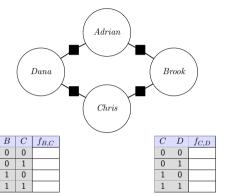
 $B \perp D \mid A, C$ ;

 $\neg A \bot C$ ;

 $\neg B \bot D$ 

# Contagious Factor Graph

 $f_{A,B}$ 



$$p(a, b, c, d) = \frac{f_{A,B}(a, b) \cdot f_{B,C}(b, c) \cdot f_{C,D}(c, d) \cdot f_{D,A}(d, a)}{\sum_{a' \in D} \sum_{b' \in D} \sum_{c' \in D} \int_{d' \in D} f_{A,B}(a', b') \cdot f_{B,C}(b', c') \cdot f_{C,D}(c', d') \cdot f_{D,A}(d', a')}$$

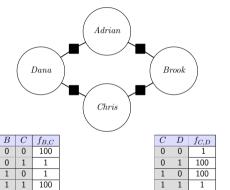
 $f_{D,A}$ 

 $f_{A,B}$ 

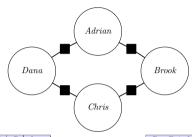
30

10

0







A	B	$f_{A,B}$
0	0	30
0	1	5
1	0	1
1	1	10

B	C	$f_{B,C}$
0	0	100
0	1	1
1	0	1
1	1	100

C	D	$f_{C,D}$
0	0	1
0	1	100
1	0	100
1	1	1

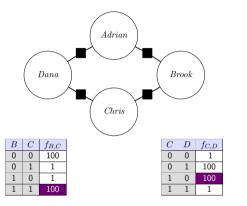
D	A	$f_{D,A}$
0	0	100
0	1	1
1	0	1
1	1	100

$$\sum_{\substack{a' \in \text{Val}(A) \text{Val}(B) \text{Val}(C) \text{Val}(D) \\ = 7,201,840}} \sum_{\substack{c' \in \text{Val}(C) \text{Val}(D) \\ = 1,201,840}} f_{A,B}(a',b') \cdot f_{B,C}(b',c') \cdot f_{C,D}(c',d') \cdot f_{D,A}(d',a')$$

 $f_{A,B}$ 

30

10

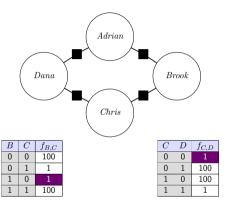


D	A	$f_{D,A}$
0	0	100
0	1	1
1	0	1
1	1	100

$$p(A = 0, B = 1, C = 1, D = 0) = \frac{5,000,000}{7,201,840} \approx 0.69$$

 $f_{A.B}$ 

30



D	A	$f_{D,A}$
0	0	100
0	1	1
1	0	1
1	1	100

$$p(A = 1, B = 1, C = 0, D = 0) = \frac{10}{7,201,840} \approx 0.0000014$$

### Structure and Independence

#### Bayesian networks:

► A variable is conditionally independent of its non-descendants given its parents.

#### Markov networks:

► Conditional independence derived from "Markov blanket" and separation properties.

Local configurations can be used to check *all* conditional independence questions; almost no need to look at the values in the factors!

## Independence "Spectrum"

$$\prod_{i=1}^{\ell} f_{V_i}(V_i)$$
  $f_{oldsymbol{V}}(oldsymbol{V})$ 

everything is independent

minimal expressive power

fewer parameters

everything can be interdependent

arbitrary expressive power

more parameters

Nothing past this point will be on the exam.

## Operations on Factors: Multiplication

Given two factors  $f_U$  and  $f_V$ , we can create a new "product" factor such that:

$$f_{U \cup V}(u \cup v) = f_{U}(u) \cdot f_{V}(v)$$

for all  $u \in \mathrm{Val}(U)$  and all  $v \in \mathrm{Val}(V)$ .

A	В	$f_{A,B}$
0	0	30
0	1	5
1	0	1
1	1	10

B	C	$f_{B,C}$
0	0	100
0	1	1
1	0	1
1	1	100

A	B	C	$f_{A,B,C}$
0	0	0	3,000
0	0	1	30
0	1	0	5
0	1	1	500
1	0	0	100
1	0	1	1
1	1	0	10
1	1	1	1,000

## Operations on Factors: Multiplication

Given two factors  $f_{m{U}}$  and  $f_{m{V}}$ , we can create a new "product" factor such that:

$$f_{U \cup V}(u \cup v) = f_{U}(u) \cdot f_{V}(v)$$

for all  $u \in Val(U)$  and all  $v \in Val(V)$ .

A	B	$f_{A,B}$
0	0	30
0	1	5
1	0	1
1	1	10

$f_{A,B}$		B	C	$f_{B,C}$	
30		0	0	100	
5	•	0	1	1	
1		1	0	1	
10		1	1	100	

A	B	C	$f_{A,B,C}$
0	0	0	3,000
0	0	1	30
0	1	0	5
0	1	1	500
1	0	0	100
1	0	1	1
1	1	0	10
1	1	1	1,000

This might remind you of a **join** operation on a database.

## Operations on Factors: Multiplication

Given two factors  $f_{m{U}}$  and  $f_{m{V}}$ , we can create a new "product" factor such that:

$$f_{U \cup V}(u \cup v) = f_{U}(u) \cdot f_{V}(v)$$

for all  $u \in Val(U)$  and all  $v \in Val(V)$ .

A	B	$f_{A,B}$
0	0	30
0	1	5
1	0	1
1	1	10

B	C	$f_{B,C}$
0	0	100
0	1	1
1	0	1
1	1	100

A	B	C	$f_{A,B,C}$
0	0	0	3,000
0	0	1	30
0	1	0	5
0	1	1	500
1	0	0	100
1	0	1	1
1	1	0	10
1	1	1	1,000

What happens if you multiply out all the factors in a factor graph?

## Operations on Factors: Maximization

Given a factor  $f_U$  and a variable  $V \not\in U$ , we can transform  $f_{U,V}$  into  $f_U$  by:

$$f_{\boldsymbol{U}}(\boldsymbol{u}) = \max_{v \in \operatorname{Val}(V)} f_{\boldsymbol{U},V}(\boldsymbol{u},v)$$

max

for all  $u \in Val(U)$ .

A	C	$f_{A,C}$	
0	0	<i>f</i> <sub>A,C</sub> 3,000	١
0	1	500	
1	0	100	
1	1	1,000	

A	B	C	$f_{A,B,C}$
0	0	0	3,000
0	0	1	30
0	1	0	5
0	1	1	500
1	0	0	100
1	0	1	1
1	1	0	10
1	1	1	1,000

## Operations on Factors: Marginalization

Given a factor  $f_U$  and a variable  $V \not\in U$ , we can transform  $f_{U,V}$  into  $f_U$  by:

$$f_{\boldsymbol{U}}(\boldsymbol{u}) = \sum_{v \in Val(V)} f_{\boldsymbol{U},V}(\boldsymbol{u},v)$$

for all  $u \in Val(U)$ .

A	C	$f_{A,C}$
0	0	3,000 + 5
0	1	30 + 500
1	0	100 + 10
1	1	1 + 1,000

$$\sum_{i}$$

B	C	$f_{A,B,C}$
0	0	3,000
0	1	30
1	0	5
1	1	500
0	0	100
0	1	1
1	0	10
1	1	1,000
	0 0 1 1 0	0 0 0 1 1 0 1 1 0 0 0 1

## Operations on Factors: Marginalization

Given a factor  $f_U$  and a variable  $V \not\in U$ , we can transform  $f_{U,V}$  into  $f_U$  by:

$$f_{\boldsymbol{U}}(\boldsymbol{u}) = \sum_{v \in Val(V)} f_{\boldsymbol{U},V}(\boldsymbol{u},v)$$

for all  $u \in Val(U)$ .

$A \mid C \mid f_{A,C}$
0 0 3,000 + 5
0 1 30 + 500
1 0 100 + 10
1 1 1 + 1,000

A	B	C	$f_{A,B,C}$
0	0	0	3,000
0	0	1	30
0	1	0	5
0	1	1	500
1	0	0	100
1	0	1	1
1	1	0	10
1	1	1	1,000

If you multiply out all the factors in a factor graph, then sum out each variable, one by one, until none are left, what do you get?

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- ▶ Products are associative:  $(f_1 \cdot f_2) \cdot f_3 = f_1 \cdot (f_2 \cdot f_3)$
- ▶ Sums are commutative:  $\sum_{X} \sum_{Y} f = \sum_{Y} \sum_{X} f$
- $\blacktriangleright$  Maximizations are commutative:  $\max_X \max_Y f = \max_X \max_X f$
- ► Multiplication distributes over marginalization and maximization:

$$\sum_{X} (f_1 \cdot f_2) = f_1 \cdot \sum_{X} f_2$$
$$\max_{X} (f_1 \cdot f_2) = f_1 \cdot \max_{X} f_2$$

(assuming X is not in the scope of  $f_1$ ).

Most general definition: "reason about some variables, optionally given values of some others." Let O be the observed variables and U be the unobserved ones;  $V = O \cup U$ .

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Three inference problems, all given  $O = o \dots$ 

▶ Marginal inference: what is the marginal distribution over  $Q \subset U$ ?  $(p(Q \mid o),$ marginalizing out the rest.)

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  - Related: draw samples from that distribution.

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- ▶ Most probable explanation (MPE): what is the most probable assignment to U? ( $\operatorname{argmax}_{\boldsymbol{u}} p(\boldsymbol{u} \mid \boldsymbol{o})$ )

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- ▶ Maximum a posteriori (MAP): what is the most probable assignment to  $Q \subset U$ ? ( $\operatorname{argmax}_{q} p(q \mid o)$ )

#### Inference

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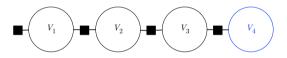
Three inference problems, all given  $O = o \dots$ 

- ▶ Marginal inference: what is the marginal distribution over  $Q \subset U$ ?  $(p(Q \mid o),$  marginalizing out the rest.)
  - Related: draw samples from that distribution.
- ▶ Most probable explanation (MPE): what is the most probable assignment to U? ( $\operatorname{argmax}_{\boldsymbol{u}} p(\boldsymbol{u} \mid \boldsymbol{o})$ )
  - ▶ Related: what is the most *dangerous* assignment to *U*?
- ▶ Maximum a posteriori (MAP): what is the most probable assignment to  $Q \subset U$ ? (argmax<sub>q</sub>  $p(q \mid o)$ )
  - Related: what values of Q have the lowest expected cost?

Lecture ended here; keep reading if you're interested!

Given a factor graph with variables V, find the marginal distribution over some  $V_i \in V$ ,  $p(V_i)$ .

Simple chain example, focusing on i = 4:



$V_1$	$f_{V_1}$
0	
1	

$V_1$	$V_2$	$f_{V_1,V_2}$
0	0	
0	1	
1	0	
1	1	

	$V_2$	$V_3$	$f_{V_2,V_3}$	
	0	0		
	0	1		
	1	0		
ĺ	1	1		

$V_3$	$V_4$	$f_{V_3,V_4}$
0	0	
0	1	
1	0	
1	1	

▶ If we had a single  $f_{V_4}$ , we could easily renormalize it to get  $p(V_4)$ .

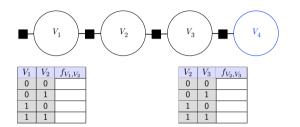
- ▶ If we had a single  $f_{V_4}$ , we could easily renormalize it to get  $p(V_4)$ .
- ▶ Correct:  $f_{V_4} = \sum_{V_1} \sum_{V_2} \sum_{V_3} f_{V_1} \cdot f_{V_1,V_2} \cdot f_{V_2,V_3} \cdot f_{V_3,V_4}$

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- ▶ Correct:  $f_{V_4} = \sum_{V_1} \sum_{V_2} \sum_{V_3} f_{V_1} \cdot f_{V_1,V_2} \cdot f_{V_2,V_3} \cdot f_{V_3,V_4}$ 
  - lacksquare But that multiplied-out factor would have  $\prod_i |\mathrm{Val}(V_i)|$  values!

- ▶ If we had a single  $f_{V_4}$ , we could easily renormalize it to get  $p(V_4)$ .
- ► Correct:  $f_{V_4} = \sum_{V_2} \sum_{V_2} \sum_{V_2} f_{V_1} \cdot f_{V_1, V_2} \cdot f_{V_2, V_3} \cdot f_{V_3, V_4}$ 
  - lacktriangle But that multiplied-out factor would have  $\prod_i |\mathrm{Val}(V_i)|$  values!
- ► Reorganize calculations:

$$\sum_{V_1} \sum_{V_2} \sum_{V_3} f_{V_1} \cdot f_{V_1, V_2} \cdot f_{V_2, V_3} \cdot f_{V_3, V_4}$$

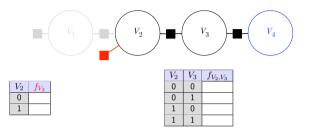
$$= \sum_{V_3} f_{V_3, V_4} \cdot \left( \sum_{V_2} f_{V_2, V_3} \cdot \left( \sum_{V_1} f_{V_1, V_2} \cdot f_{V_1} \right) \right)$$



$V_3$	$V_4$	$f_{V_3,V_4}$
0	0	0 13,14
0	1	
1	0	
1	1	

$$\sum_{V_1} \sum_{V_2} \sum_{V_3} f_{V_1} \cdot f_{V_1, V_2} \cdot f_{V_2, V_3} \cdot f_{V_3, V_4}$$

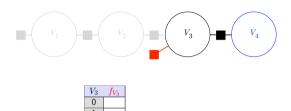
$$= \sum_{V_3} f_{V_3, V_4} \cdot \left( \sum_{V_2} f_{V_2, V_3} \cdot \left( \sum_{V_1} f_{V_1, V_2} \cdot f_{V_1} \right) \right)$$



$V_3$	$V_4$	$f_{V_3,V_4}$
0	0	
0	1	
1	0	
1	1	

$$\sum_{V_1} \sum_{V_2} \sum_{V_3} f_{V_1} \cdot f_{V_1, V_2} \cdot f_{V_2, V_3} \cdot f_{V_3, V_4}$$

$$= \sum_{V_3} f_{V_3, V_4} \cdot \left(\sum_{V_2} f_{V_2, V_3} \cdot f_{V_2}\right)$$



$V_3$	$V_4$	$f_{V_3,V_4}$
0	0	
0	1	
1	0	
1	1	

$$\sum_{V_1} \sum_{V_2} \sum_{V_3} f_{V_1} \cdot f_{V_1, V_2} \cdot f_{V_2, V_3} \cdot f_{V_3, V_4}$$

$$= \sum_{V_3} f_{V_3, V_4} \cdot f_{V_3}$$



$V_4$	$f_{V_4}$
0	
1	

$$\sum_{V_1} \sum_{V_2} \sum_{V_3} f_{V_1} \cdot f_{V_1, V_2} \cdot f_{V_2, V_3} \cdot f_{V_3, V_4}$$

$$= f_{V_4}$$

#### Variable Elimination

Given a factor graph with factors f, eliminate variable V.

- 1. Let  $f_{elim} \subset f$  be the factors connected to V
- 2. Let  $oldsymbol{f}_{keep} = oldsymbol{f} \setminus oldsymbol{f}_{elim}$  be the rest
- 3. Let  $f_{new} = \sum_{V} \prod_{f \in \boldsymbol{f}_{elim}} f$
- 4. Return  $\boldsymbol{f}_{keep} \cup \{f_{new}\}$

Uses the graph structure to avoid exponential blowup; this is an example of dynamic programming.

# Marginal Inference by Variable Elimination (No Evidence)

Given a factor graph with variables V and factors f, find the marginal distribution over some  $V_{keep} \subset V$ .

- 1. Order the variables in  $oldsymbol{V} \setminus oldsymbol{V}_{keep}.$
- 2. For each  $V \in \mathbf{V} \setminus \mathbf{V}_{keep}$ :
  - lacktriangle Eliminate V; i.e., remove factors connected to V and replace with the derived  $f_{new}$ .

The resulting factor graph is proportional to  $p(V_{keep})$ .

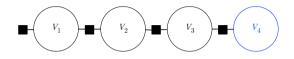
# Marginal Inference by Variable Elimination (No Evidence)

Given a factor graph with variables V and factors f, find the marginal distribution over some  $V_{keep} \subset V$ .

- 1. Order the variables in  $V \setminus V_{keep}$ . The ordering can make a huge difference!
- 2. For each  $V \in \mathbf{V} \setminus \mathbf{V}_{keep}$ :
  - lacktriangle Eliminate V; i.e., remove factors connected to V and replace with the derived  $f_{new}$ .

The resulting factor graph is proportional to  $p(V_{keep})$ .

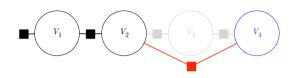
# A Less Good Ordering



$$\sum_{V_1} \sum_{V_2} \sum_{V_3} f_{V_1} \cdot f_{V_1, V_2} \cdot f_{V_2, V_3} \cdot f_{V_3, V_4}$$

$$= \sum_{V_1} f_{V_1} \cdot \left( \sum_{V_2} f_{V_1, V_2} \cdot \left( \sum_{V_3} f_{V_2, V_3} \cdot f_{V_3, V_4} \right) \right)$$

# A Less Good Ordering



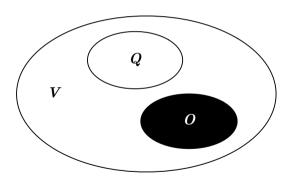
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### What About Evidence?

Original problem: given O = o, what is the marginal distribution over  $Q \subset U$ ? (I.e.,  $p(Q \mid O = o)$ .)



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This adds a step at the beginning: reduce factors to "respect the evidence."

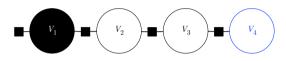
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This will remind you of a **select ... where** operation in a database.

#### Suppose $V_1$ is observed to take value 1.



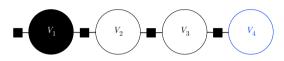
$V_1$	$f_{V_1}$
0	
1	

$V_1$	$V_2$	$f_{V_1,V_2}$
0	0	
0	1	
1	0	
1	1	

$V_2$	$V_3$	$f_{V_2,V_3}$
0	0	
0	1	
1	0	
1	1	

$V_3$	$V_4$	$f_{V_3,V_4}$
0	0	
0	1	
1	0	
1	1	

#### Suppose $V_1$ is observed to take value 1.



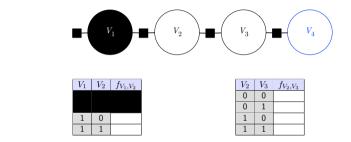


$V_1$	$V_2$	$f_{V_1,V_2}$
1	0	
1	1	

$V_2$	$V_3$	$f_{V_2,V_3}$
0	0	
0	1	
1	0	
1	1	

$V_3$	$V_4$	$f_{V_3,V_4}$
0	0	
0	1	
1	0	
1	1	

Suppose  $V_1$  is observed to take value 1.



•	
n imnovo it	
n ignore it.	

 $f_{V_3,V_4}$ 

Note that  $f_{V_1}$  is now a constant; since we renormalize at the end, we can ignore it. Observed nodes may create a "separation" between variables of interest and some factors.

### Marginal Inference by Variable Elimination with Evidence

Given a factor graph with variables V and factors f, and given O = o (where  $O \subset V$ ), find the marginal distribution over  $Q \subseteq U = V \setminus O$ .

- 1. Reduce factors connected to *O* to respect the evidence.
- 2. Order the variables in  $U \setminus Q$ .
- 3. For each  $V \in \boldsymbol{U} \setminus \boldsymbol{Q}$ :
  - lacktriangle Eliminate V; i.e., remove factors connected to V and replace with the derived  $f_{new}$ .

The resulting factor graph is proportional to  $p(Q \mid O = o)$ .

### Remarks on Computational Complexity

In general, denser graphs are more expensive.

Runtime and space depend on the size of the original and intermediate factors. (This is why ordering matters so much.)

Finding the best ordering is NP-hard.

Certain graphical structures allow inference in linear time with respect to the size of the *original* factors.

- ▶ Bayesian networks: polytrees
- Markov networks: chordal graphs

### MPE Inference

$$\mathop{\mathrm{argmax}}_{\boldsymbol{u} \in \mathrm{Val}(\boldsymbol{U})} p(\boldsymbol{U} = \boldsymbol{u} \mid \boldsymbol{O} = \boldsymbol{o})$$

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Variable elimination and exact inference are identical to the marginal case!

#### MPE Inference

$$\operatorname*{argmax}_{\boldsymbol{u} \in \mathrm{Val}(\boldsymbol{U})} p(\boldsymbol{U} = \boldsymbol{u} \mid \boldsymbol{O} = \boldsymbol{o})$$

Variable elimination and exact inference are identical to the marginal case!

Just replace each sum operation with a max operation, and add bookkeeping to recover the most probable assignment.

### Rocket Science: True MAP

Given a factor graph with variables V and factors f, and given O = o (where  $O \subset V$ ), find the most probable assignment of  $Q \subset U = V \setminus O$ .

Let  $oldsymbol{R} = oldsymbol{U} \setminus oldsymbol{Q}$ .

$$\begin{aligned} & \operatorname*{argmax}_{\boldsymbol{q} \in \operatorname{Val}(\boldsymbol{Q})} p(\boldsymbol{Q} = \boldsymbol{q} \mid \boldsymbol{O} = \boldsymbol{o}) \\ & = \operatorname*{argmax}_{\boldsymbol{q} \in \operatorname{Val}(\boldsymbol{Q})} \sum_{\boldsymbol{r} \in \operatorname{Val}(\boldsymbol{R})} p(\boldsymbol{Q} = \boldsymbol{q}, \boldsymbol{R} = \boldsymbol{r} \mid \boldsymbol{O} = \boldsymbol{o}) \end{aligned}$$

Solution: first use marginal inference to eliminate R, then use max inference to solve for Q.

#### Alternative Inference Methods

Huge range of techniques!

#### Exact:

► Integer linear programming

#### Inexact:

- ► randomized (e.g., Gibbs sampling, importance sampling, simulated annealing)
- deterministic (e.g., mean field variational, loopy belief propagation, linear programming relaxations, dual decomposition, beam search)

#### References I

Daphne Koller, Nir Friedman, Lise Getoor, and Ben Taskar. Graphical models in a nutshell, 2007. URL https://ai.stanford.edu/~koller/Papers/Koller+al:SRL07.pdf.