School of Computer Science
Carnegie Mellon

10-708 Probabilistic Graphical Models

Exact Inference

Readings:

Jordan Chap. 3

Jordan Chap. 4

Matt Gormley

Lecture 7

February 3, 2016

Some slides and figures from Gormley & Eisner (2014, 2015) "Structured BP for NLP" tutorial

Housekeeping

- **Office Hours**

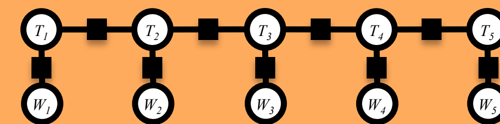
Exact Inference

1. Data

$$\mathcal{D} = \{\boldsymbol{x}^{(n)}\}_{n=1}^{N}$$

2. Model

$$p(\boldsymbol{x} \mid \boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C)$$



3. Objective

$$\ell(\theta; \mathcal{D}) = \sum_{n=1}^{N} \log p(\boldsymbol{x}^{(n)} \mid \boldsymbol{\theta})$$

5. Inference

1. Marginal Inference

$$p(\boldsymbol{x}_C) = \sum_{\boldsymbol{x}' : \boldsymbol{x}'_C = \boldsymbol{x}_C} p(\boldsymbol{x}' \mid \boldsymbol{\theta})$$

2. Partition Function

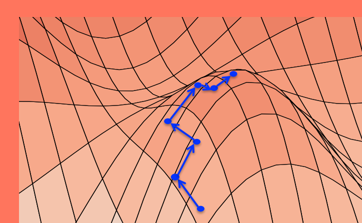
$$Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C)$$

3. MAP Inference

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{argmax}}\ p(\boldsymbol{x} \mid \boldsymbol{\theta})$$

4. Learning

$$\boldsymbol{\theta}^* = \underset{\boldsymbol{\theta}}{\operatorname{argmax}}\, \ell(\boldsymbol{\theta}; \mathcal{D})$$



Goals for Today's Lecture

1. Unify MRFs and Bayes Nets with a new representation: **factor graphs**
2. Perform exact inference on factor graphs with two algorithms: **Elimination** and **Sum-Product Belief Propagation**

1. Data

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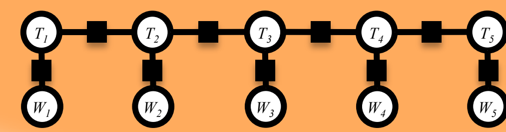

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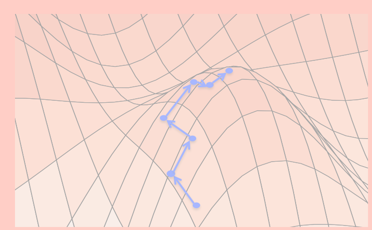
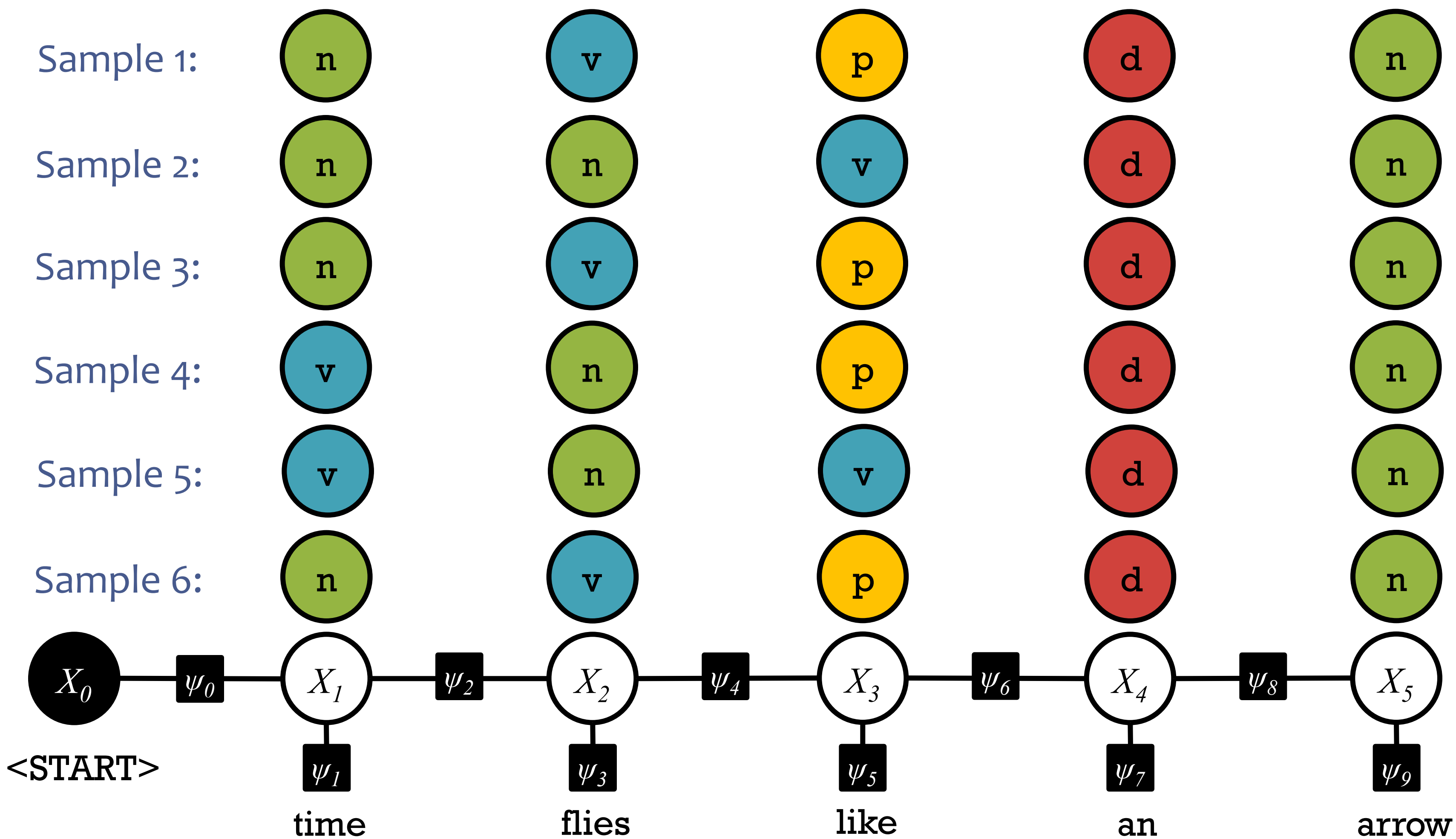


Representation of both directed and undirected graphical models

FACTOR GRAPHS

Sampling from a Joint Distribution

A **joint distribution** defines a probability $p(\boldsymbol{x})$ for each assignment of values $\boldsymbol{x}$ to variables $\boldsymbol{X}$. This gives the **proportion** of samples that will equal $\boldsymbol{x}$.



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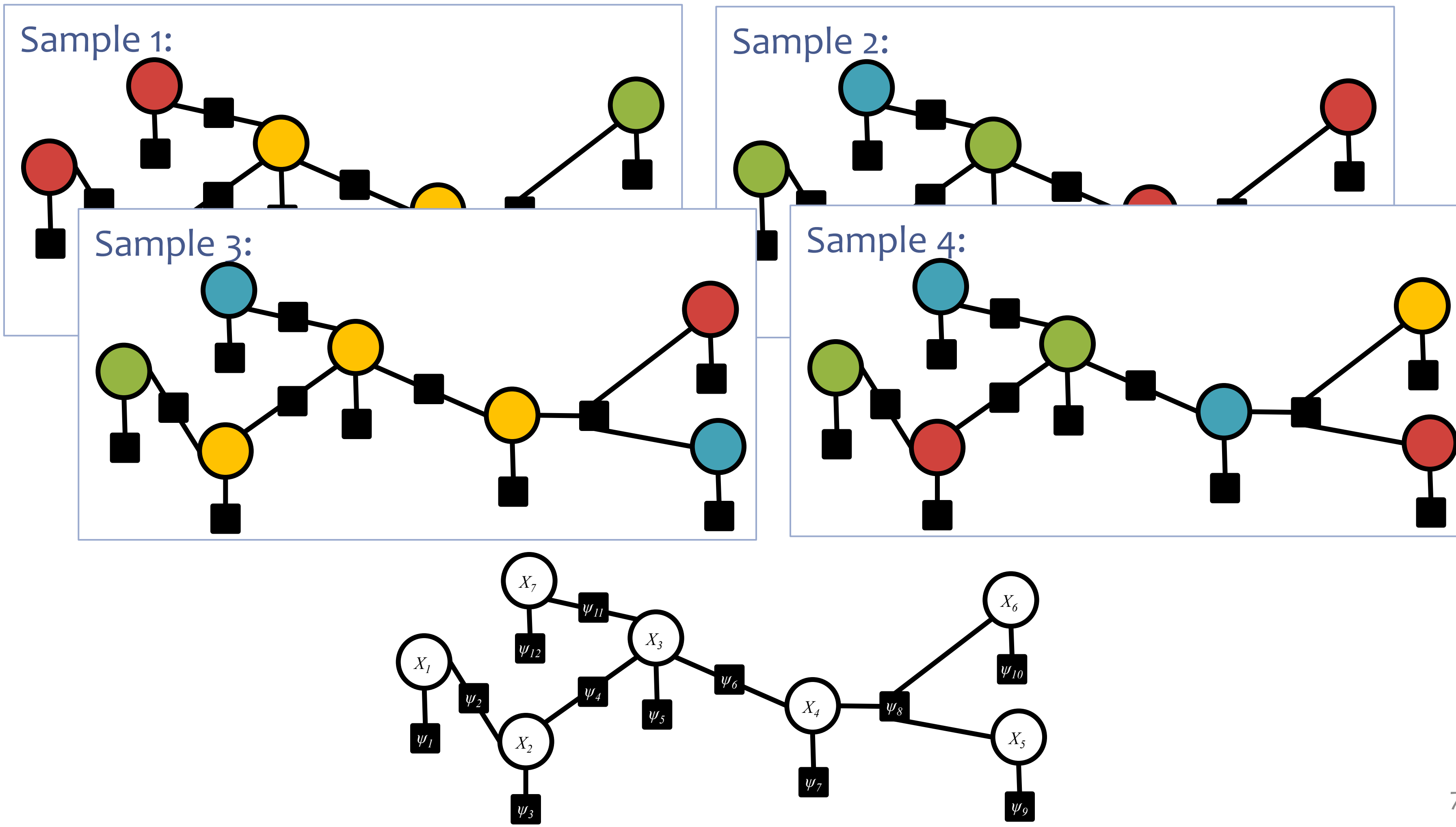

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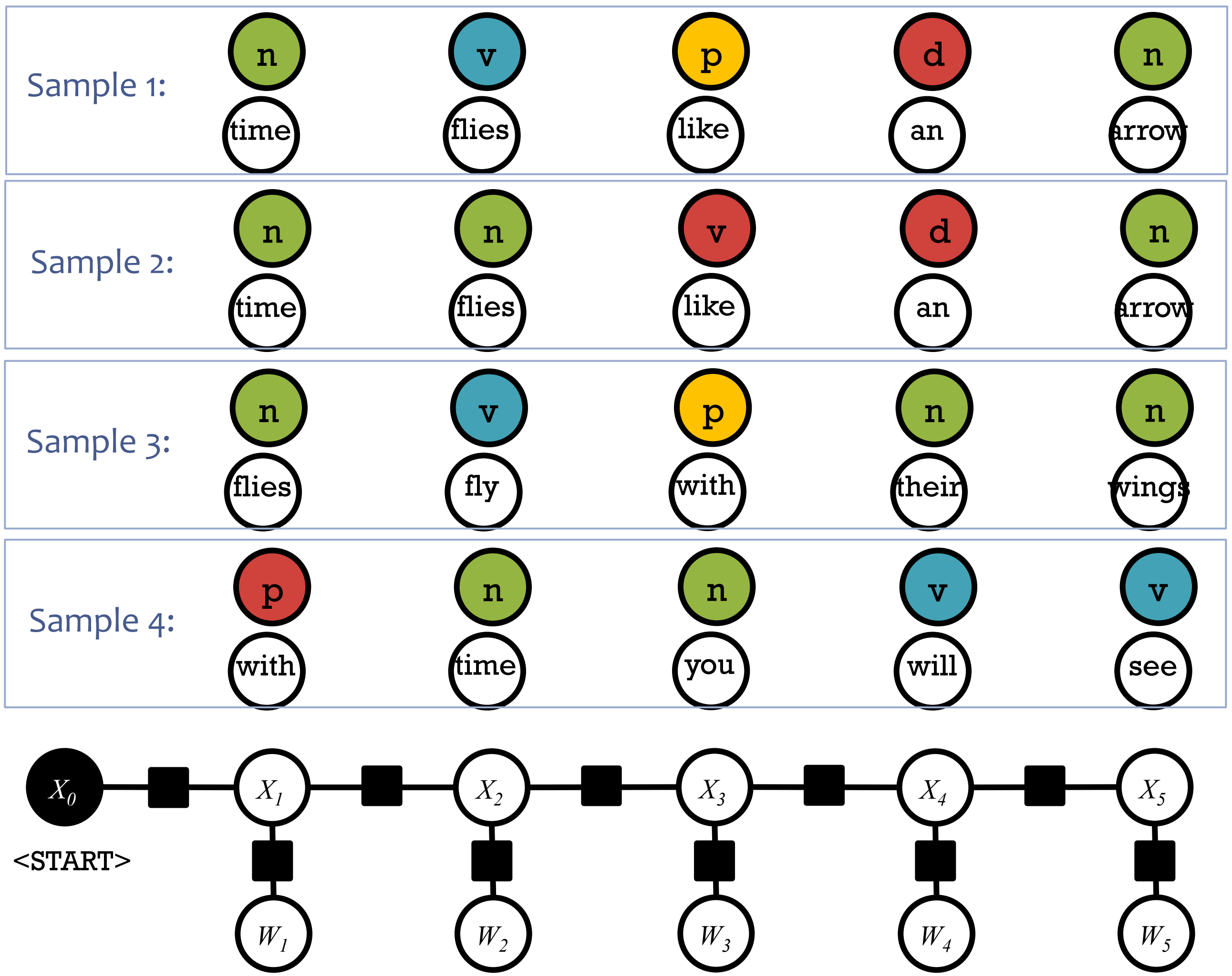

Factors have local opinions (≥ 0)

Each black box looks at *some* of the tags X_i and words W_i

Note: We chose to reuse the same factors at different positions in the sentence.

	v	n	p	d
v	1	6	3	4
n	8	4	2	0.1
p	1	3	1	3
d	0.1	8	0	0

	v	n	p	d
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n	8	4	2	0.1
p	1	3	1	3
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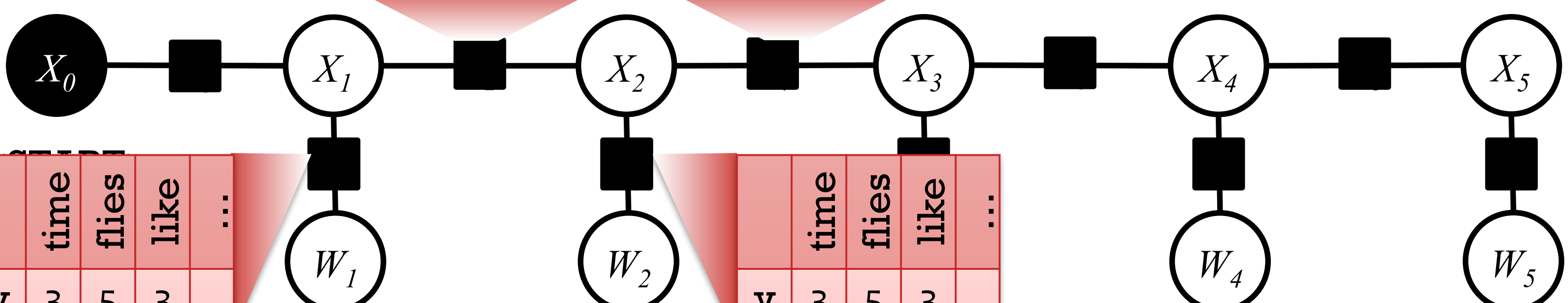

	time	flies	like	…
v	3	5	3	
n	4	5	2	
p	0.1	0.1	3	
d	0.1	0.2	0.1	

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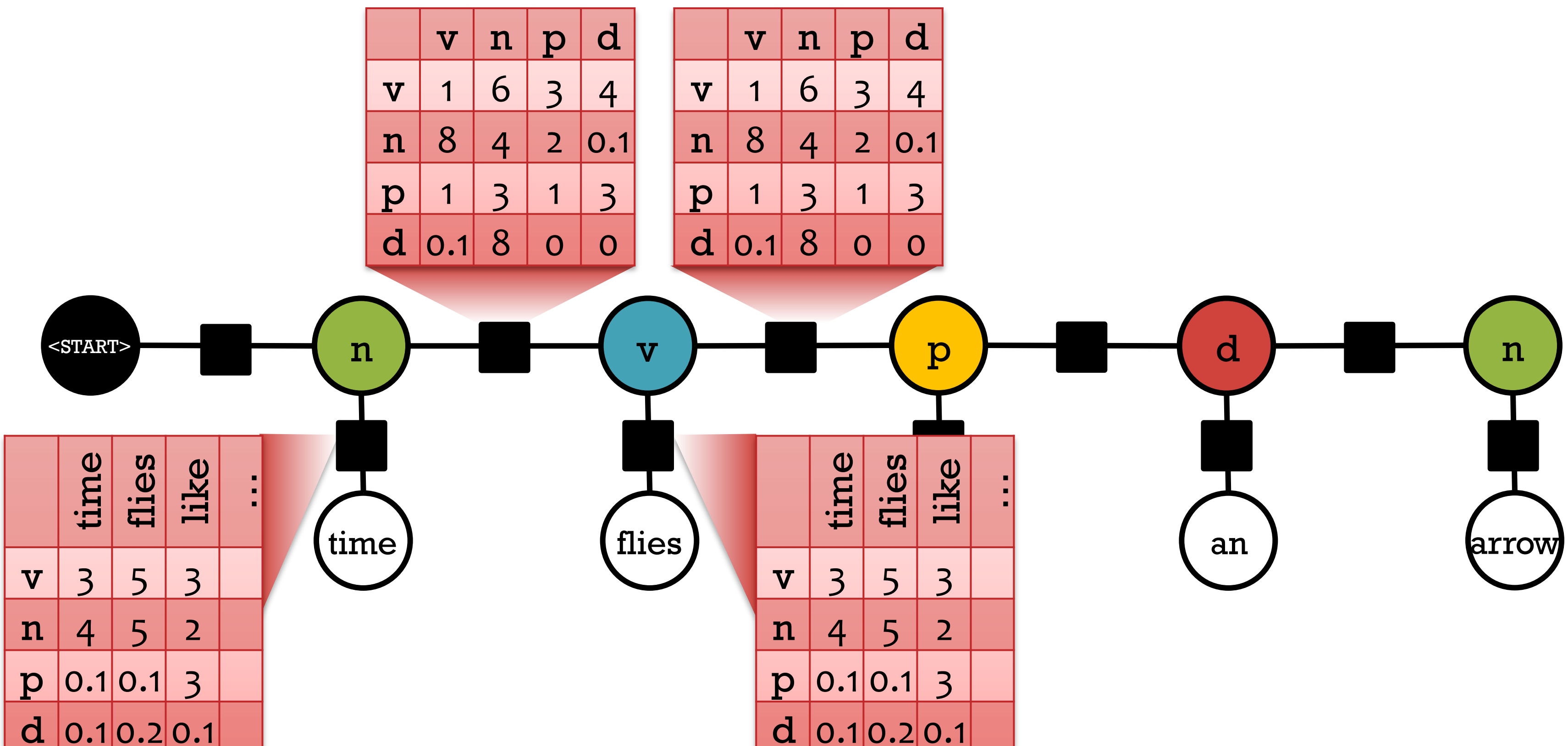
Factors have local opinions (≥ 0)

Each black box looks at *some* of the tags X_i and words W_i

$$p(\text{n, v, p, d, n, time, flies, like, an, arrow}) \quad = \quad ?$$



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Global probability = product of local opinions

Each black box looks at *some* of the tags X_i and words W_i

$$p(\text{n, v, p, d, n, time, flies, like, an, arrow}) = \frac{1}{Z}(4 * 8 * 5 * 3 * \ldots)$$

	v	n	p	d
v	1	6	3	4
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	v	n	p	d
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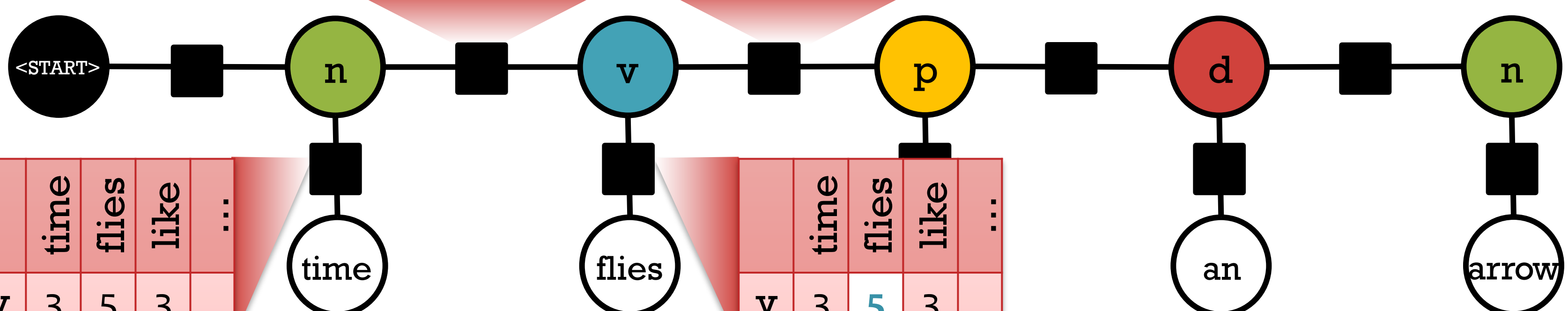
Uh-oh! The probabilities of the various assignments sum up to Z > 1.

So divide them all by Z.



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Markov Random Field (MRF)

Joint distribution over tags X_i and words W_i
The individual factors aren't *necessarily* probabilities.

$$p(\text{n, v, p, d, n, time, flies, like, an, arrow}) = \frac{1}{Z}(4 * 8 * 5 * 3 * \ldots)$$

	v	n	p	d
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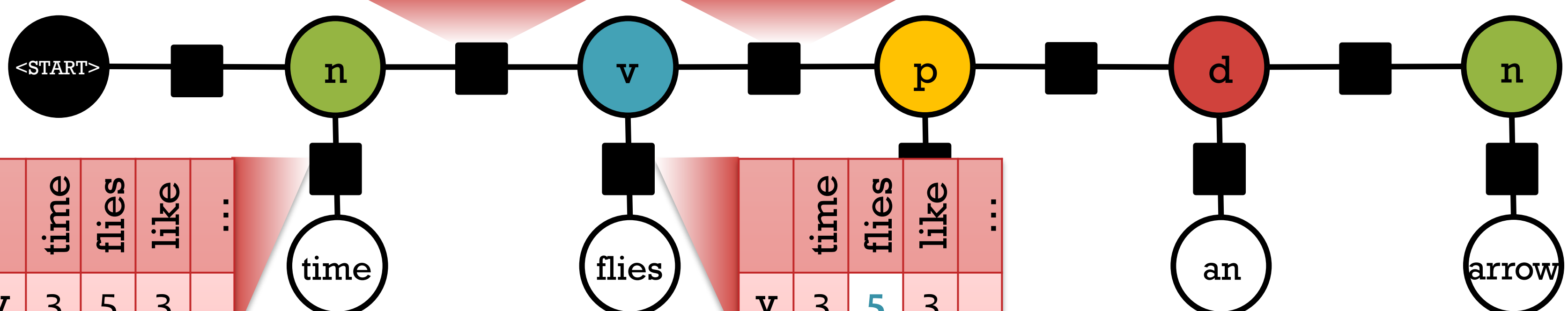

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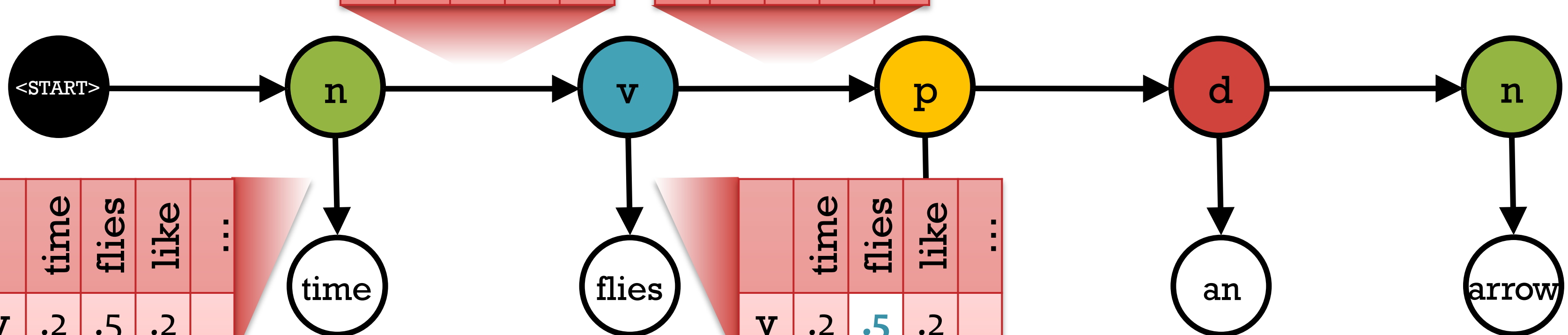
Bayesian Networks

But sometimes we *choose* to make them probabilities.
Constrain each row of a factor to sum to one. Now $Z = 1$.

$$p(\text{n, v, p, d, n, time, flies, like, an, arrow}) = \cancel{\frac{1}{Z}}(.3 * .8 * .2 * .5 * \ldots)$$

	v	n	p	d
v	.1	.4	.2	.3
n	.8	.1	.1	0
p	.2	.3	.2	.3
d	.2	.8	0	0

	v	n	p	d
v	.1	.4	.2	.3
n	.8	.1	.1	0
p	.2	.3	.2	.3
d	.2	.8	0	0



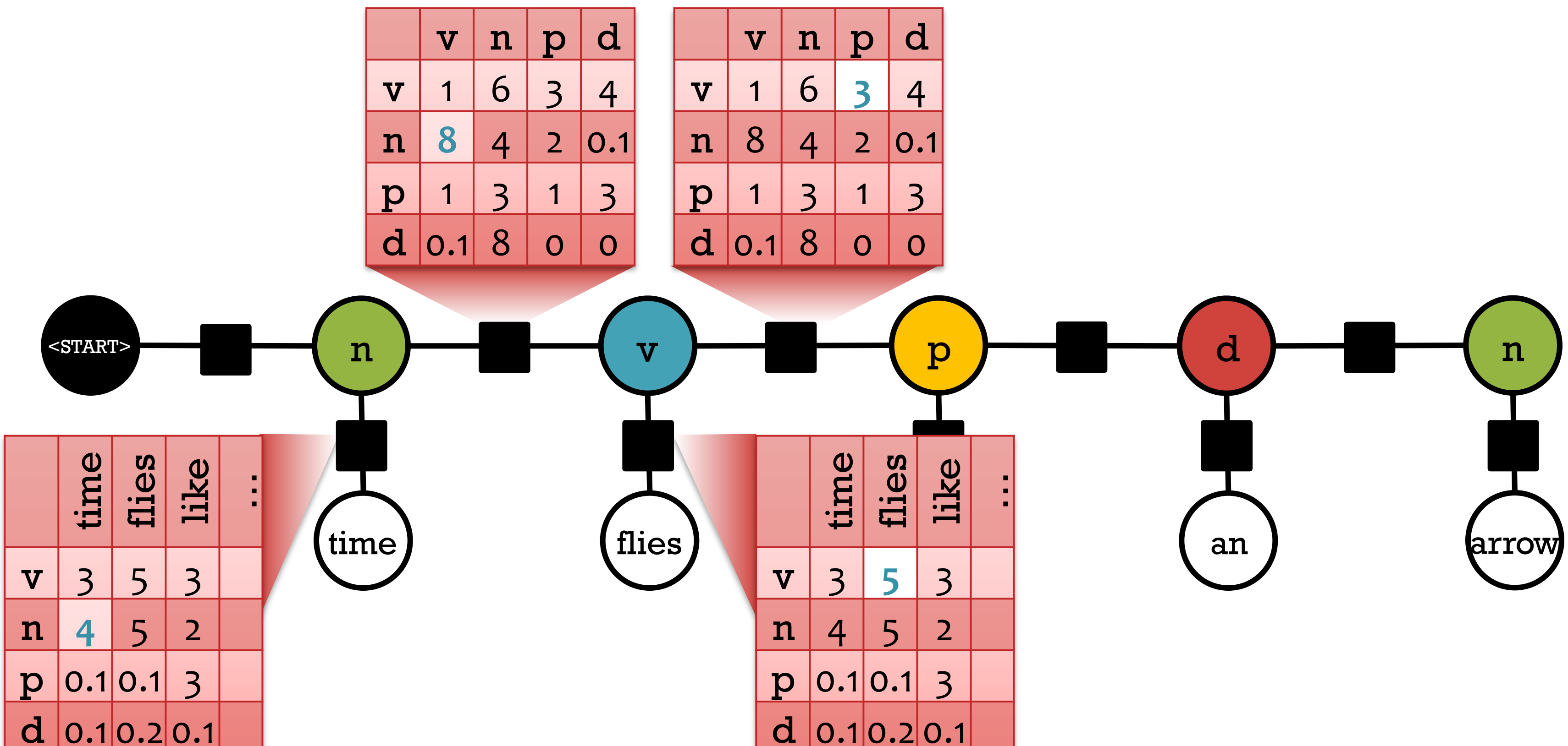
	time	flies	like	…
v	.2	.5	.2	
n	.3	.4	.2	
p	.1	.1	.3	
d	.1	.2	.1	

	time	flies	like	…
v	.2	.5	.2	
n	.3	.4	.2	
p	.1	.1	.3	
d	.1	.2	.1	

Markov Random Field (MRF)

Joint distribution over tags X_i <u>and</u> words W_i

$$p(\text{n, v, p, d, n, time, flies, like, an, arrow}) = \frac{1}{Z}(4 * 8 * 5 * 3 * \ldots)$$



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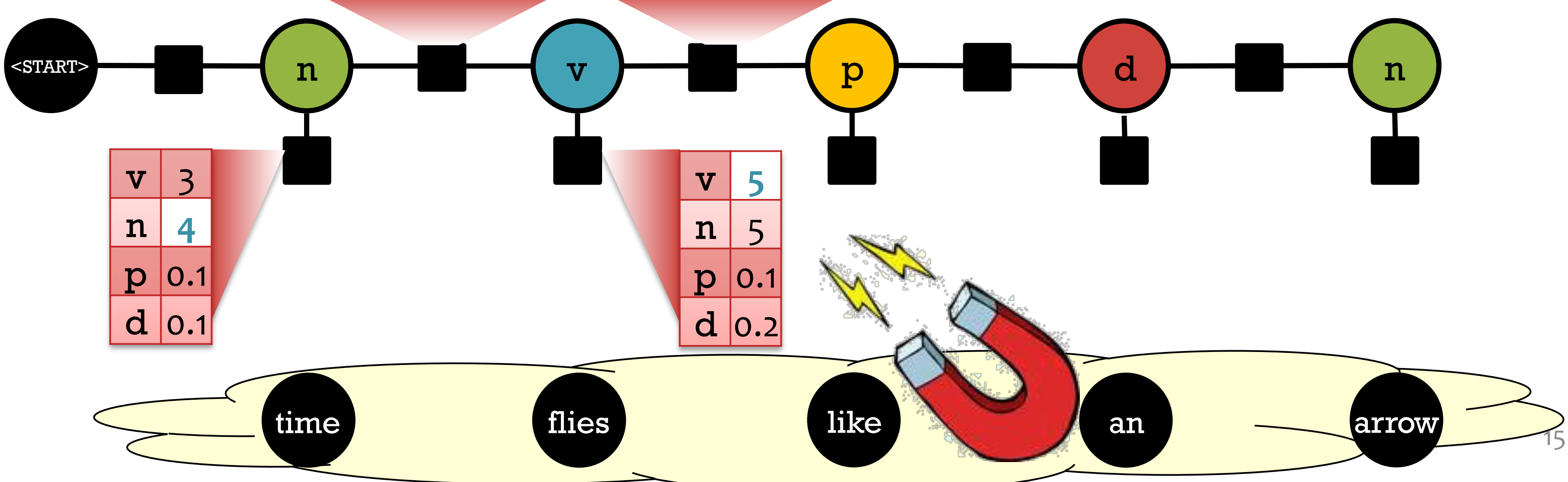
Conditional Random Field (CRF)

Conditional distribution over tags X_i given words w_i.
The factors and Z are now specific to the sentence w.

$$p(\text{n, v, p, d, n, time, flies, like, an, arrow}) \quad = \quad \frac{1}{Z}(4 * 8 * 5 * 3 * \ldots)$$



	v	n	p	d
v	1	6	3	4
n	8	4	2	0.1
p	1	3	1	3
d	0.1	8	0	0

	v	n	p	d
v	1	6	3	4
n	8	4	2	0.1
p	1	3	1	3
d	0.1	8	0	0

v	3
n	4
p	0.1
d	0.1

v	5
n	5
p	0.1
d	0.2

How General Are Factor Graphs?

- Factor graphs can be used to describe
  - Markov Random Fields (undirected graphical models)
    - i.e., log-linear models over a tuple of variables
  - Conditional Random Fields
  - Bayesian Networks (directed graphical models)

- *Inference* treats all of these interchangeably.
  - Convert your model to a factor graph first.
  - Pearl (1988) gave key strategies for *exact* inference:
    - **Belief propagation**, for inference on *acyclic* graphs
    - **Junction tree algorithm**, for making *any* graph acyclic (by merging variables and factors: blows up the runtime)

Factor Graph Notation

- Variables:

$$\mathcal{X} = \{X_1, \ldots, X_i, \ldots, X_n\}$$

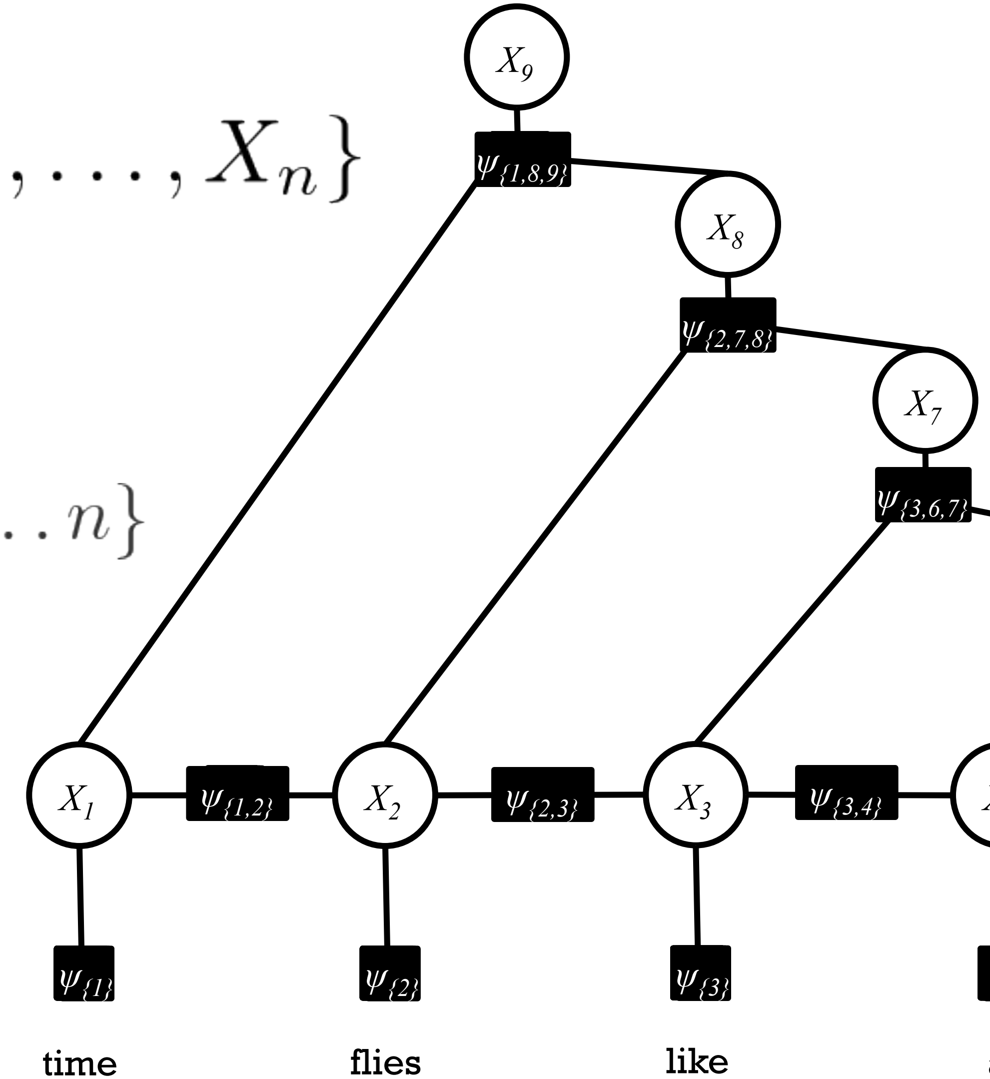
- Factors:

$$\psi_\alpha, \psi_\beta, \psi_\gamma, \ldots$$

where $\alpha, \beta, \gamma, \ldots \subseteq \{1, \ldots n\}$

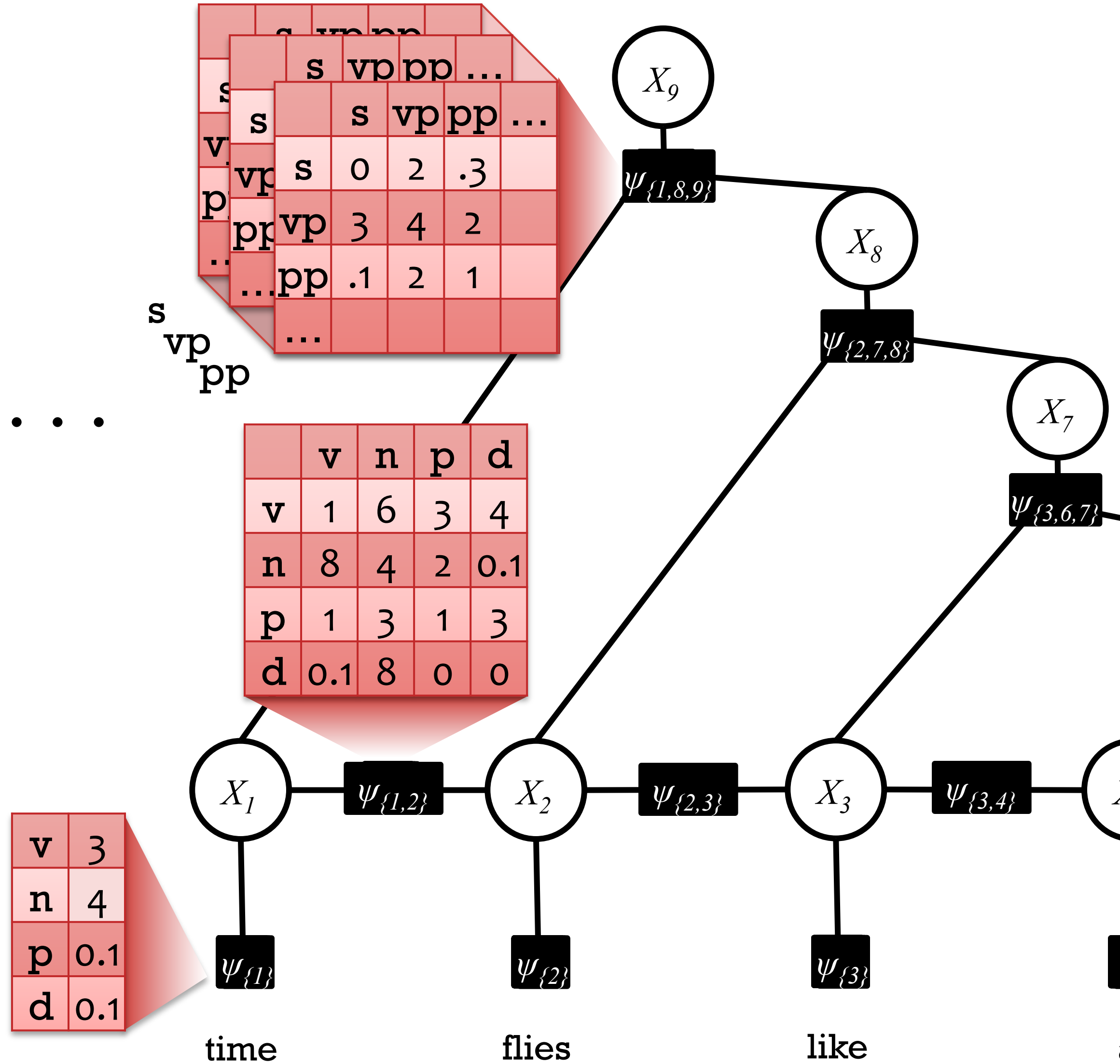
Joint Distribution

$$p(\boldsymbol{x}) = \frac{1}{Z} \prod_{\alpha} \psi_\alpha(\boldsymbol{x}_\alpha)$$



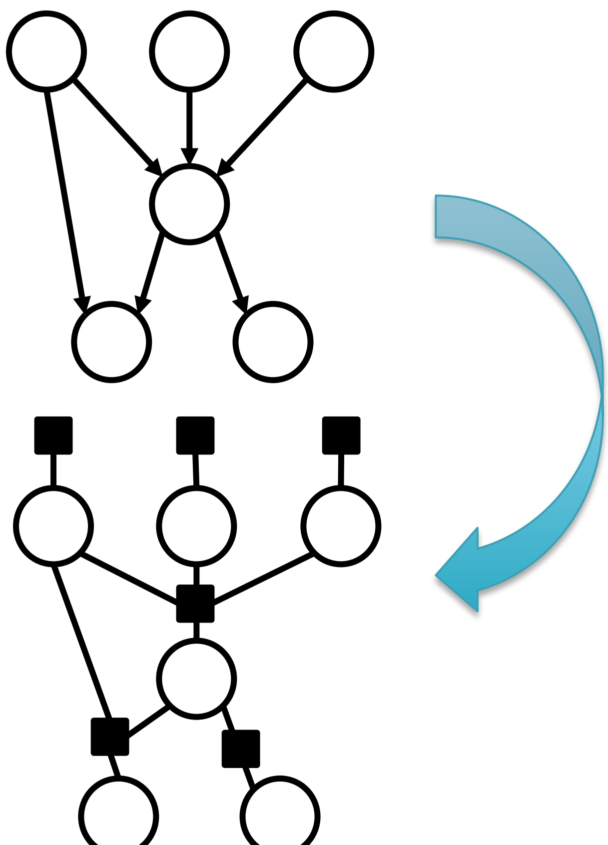
Factors are Tensors

- Factors:
  $$\psi_\alpha, \psi_\beta, \psi_\gamma, \ldots$$

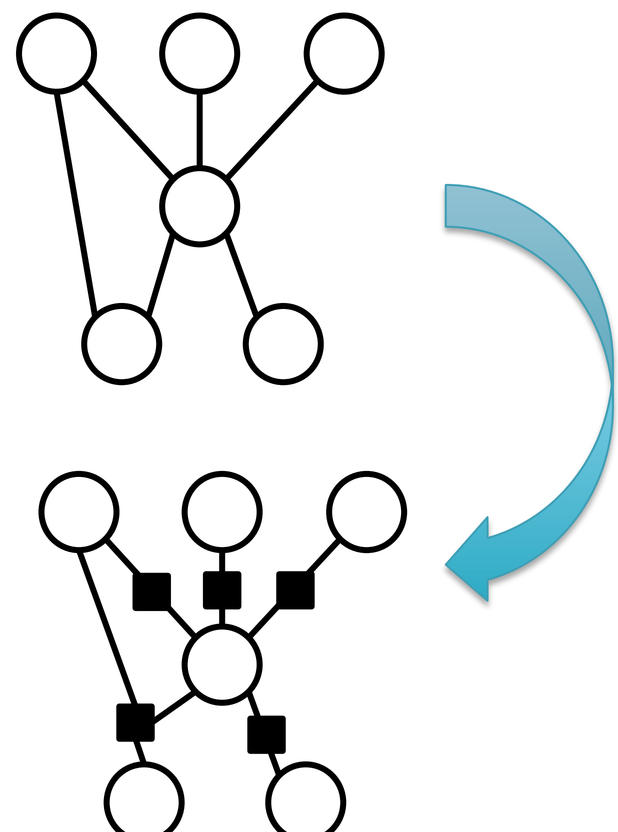


Converting to Factor Graphs

Each conditional and marginal distribution in a **directed GM** becomes a factor



Each clique in an **undirected GM** becomes a factor

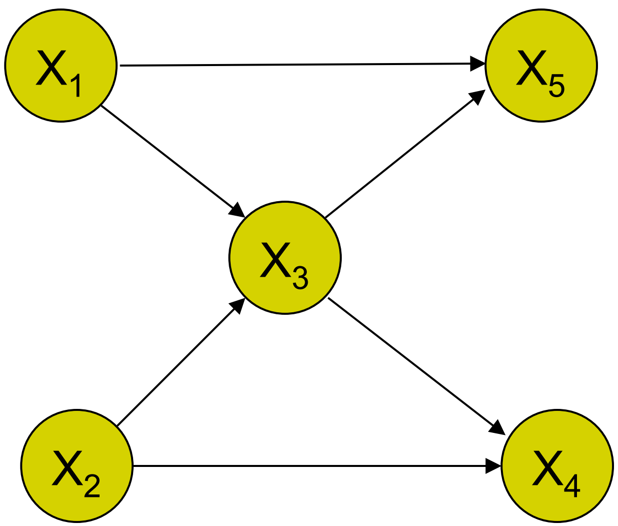


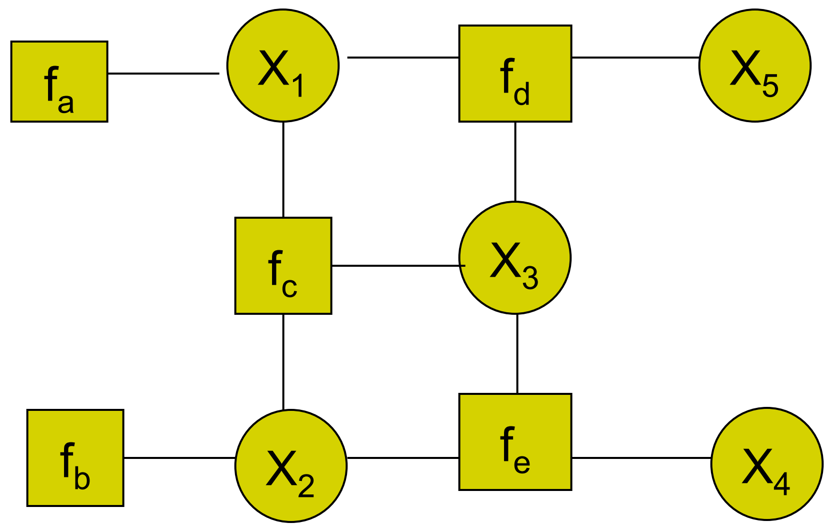
Equivalence of directed and undirected trees

- Any undirected tree can be converted to a directed tree by choosing a root node and directing all edges away from it
- A directed tree and the corresponding undirected tree make the same conditional independence assertions
- Parameterizations are essentially the same.
  - Undirected tree: $$p(x) = \frac{1}{Z}\left(\prod_{i \in V} \psi(x_i) \prod_{(i,j) \in E} \psi(x_i, x_j)\right)$$
  - Directed tree: $$p(x) = p(x_r) \prod_{(i,j) \in E} p(x_j | x_i)$$
  - Equivalence: $$\psi(x_r) = p(x_r); \quad \psi(x_i, x_j) = p(x_j | x_i);$$ $$Z = 1, \quad \psi(x_i) = 1$$

Factor Graph Examples

- Example 1



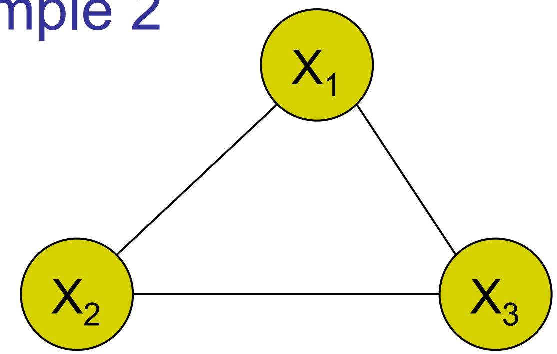


$$P(X_1) \quad P(X_2) \quad P(X_3|X_1,X_2) \quad P(X_5|X_1,X_3) \quad P(X_4|X_2,X_3)$$

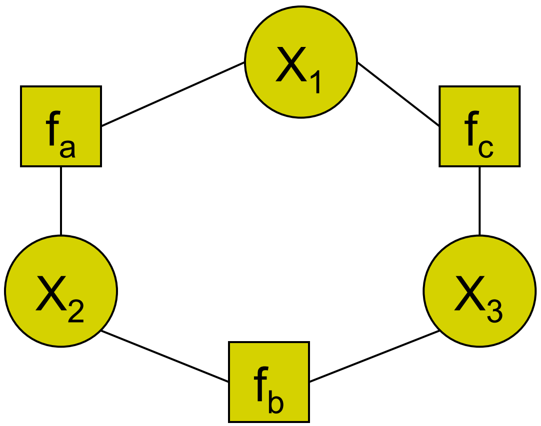
$$f_a(X_1) \quad f_b(X_2) \quad f_c(X_3,X_1,X_2) \quad f_d(X_5,X_1,X_3) \quad f_e(X_4,X_2,X_3)$$

Factor Graph Examples

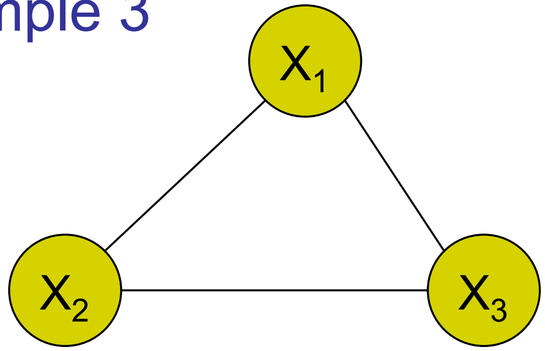
- Example 2



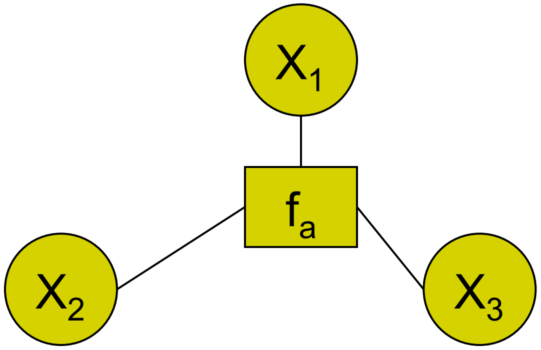
$$\psi(x_1,x_2,x_3) = f_a(x_1,x_2)f_b(x_2,x_3)f_c(x_3,x_1)$$



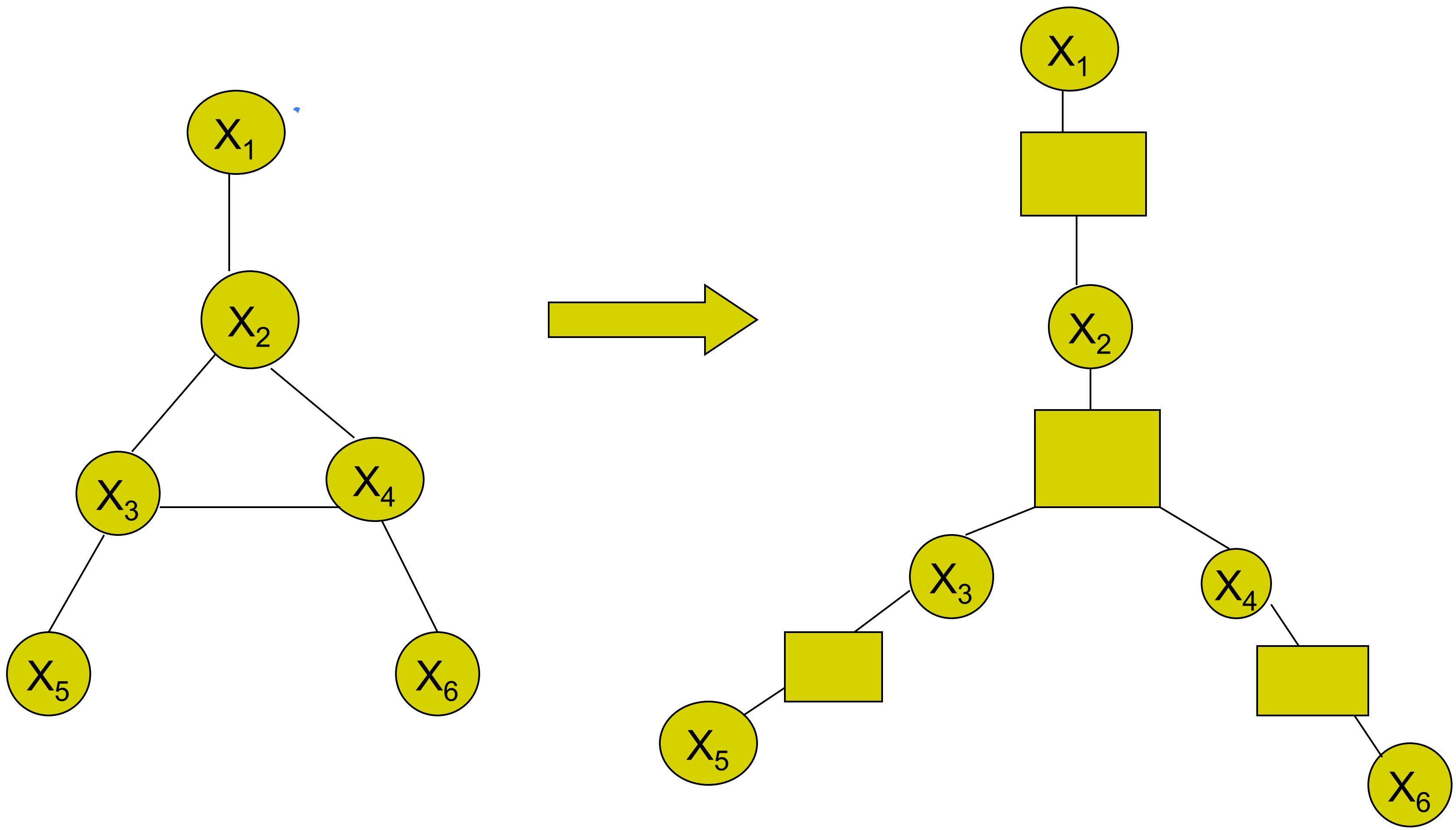
- Example 3



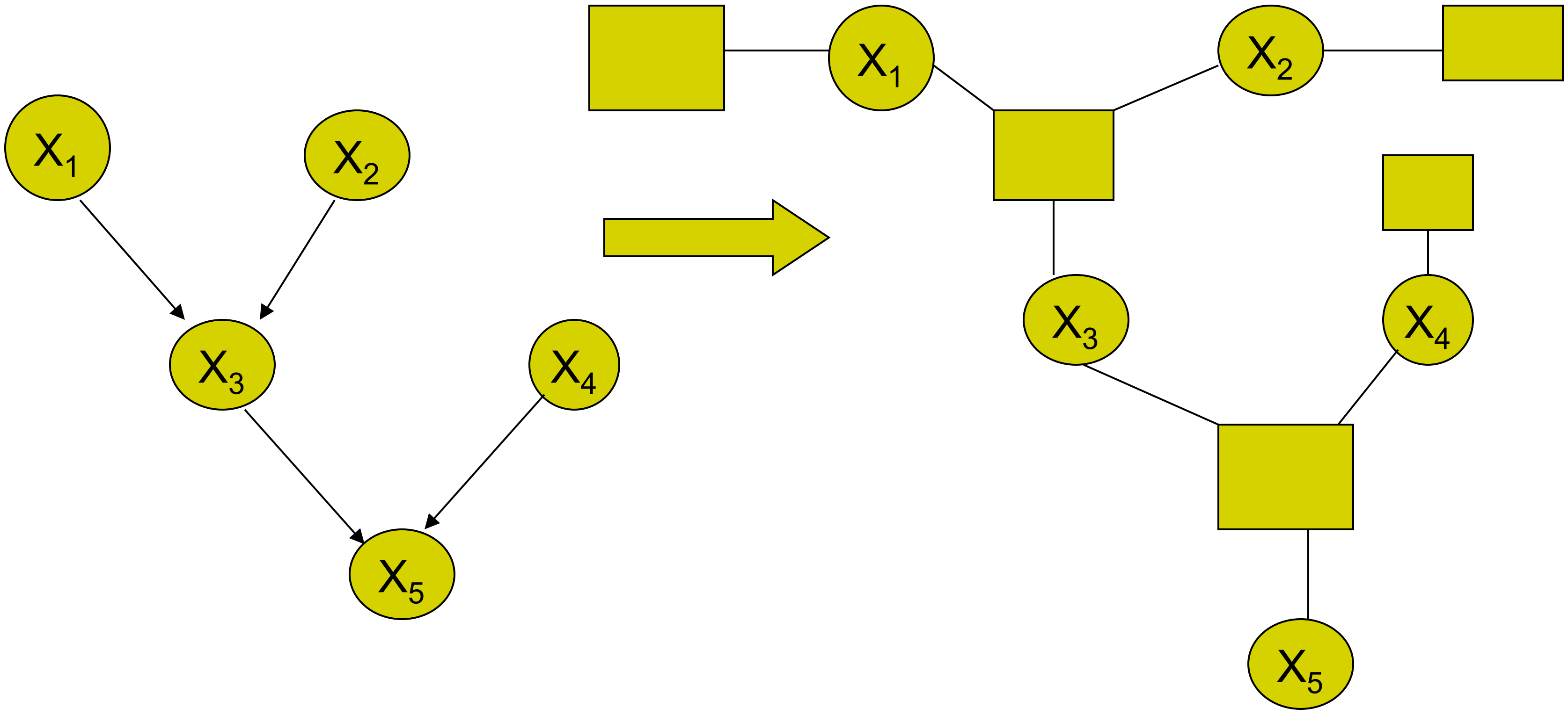
$$\psi(x_1,x_2,x_3) = f_a(x_1,x_2,x_3)$$



Tree-like Undirected GMs to Factor Trees

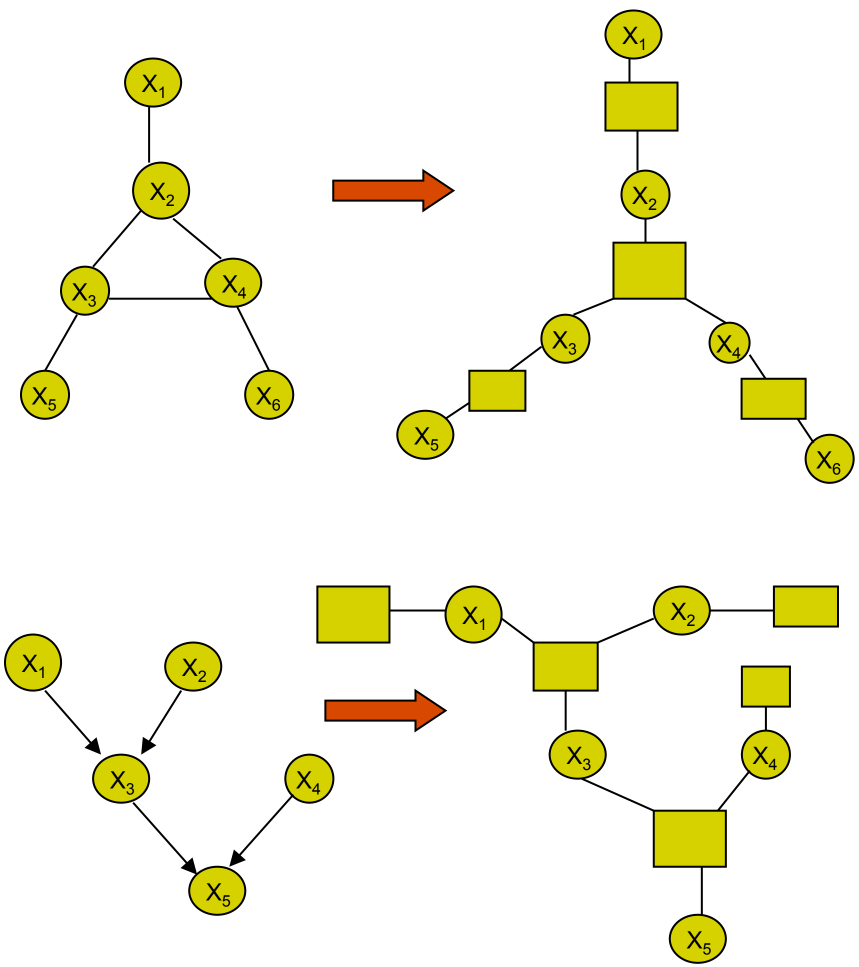


Poly-trees to Factor trees



Why factor graphs?

- Because FG turns tree-like graphs to factor trees,
- Trees are a data-structure that guarantees correctness of BP !



Exact Inference

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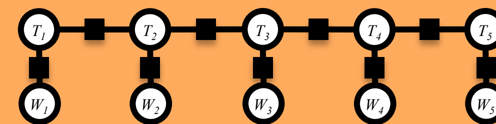

3. Objective

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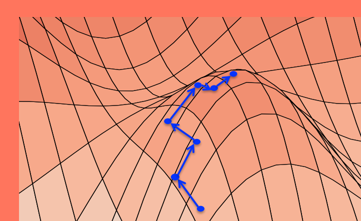

Goals for Today's Lecture

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2. Perform exact inference on factor graphs with two algorithms: **Elimination** and **Sum-Product Belief Propagation**

Model

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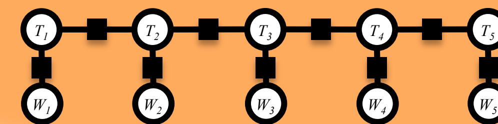

Objective

$$\ell(\theta; \mathcal{D}) = \sum_{n=1}^{N} \log p(\boldsymbol{x}^{(n)} \mid \boldsymbol{\theta})$$

5. Inference

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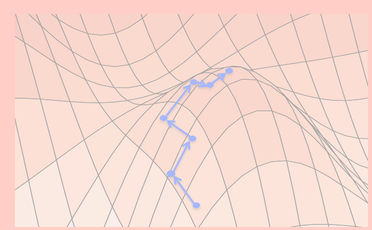


5. Inference

Three Tasks: **(All three are NP-Hard in the general case)**

1. Marginal Inference
Compute marginals of variables and cliques

$$p(x_i) = \sum_{\boldsymbol{x}' : x'_i = x_i} p(\boldsymbol{x}' \mid \boldsymbol{\theta}) \qquad \Big| \qquad p(\boldsymbol{x}_C) = \sum_{\boldsymbol{x}' : \boldsymbol{x}'_C = \boldsymbol{x}_C} p(\boldsymbol{x}' \mid \boldsymbol{\theta})$$

2. Partition Function
Compute the normalization constant

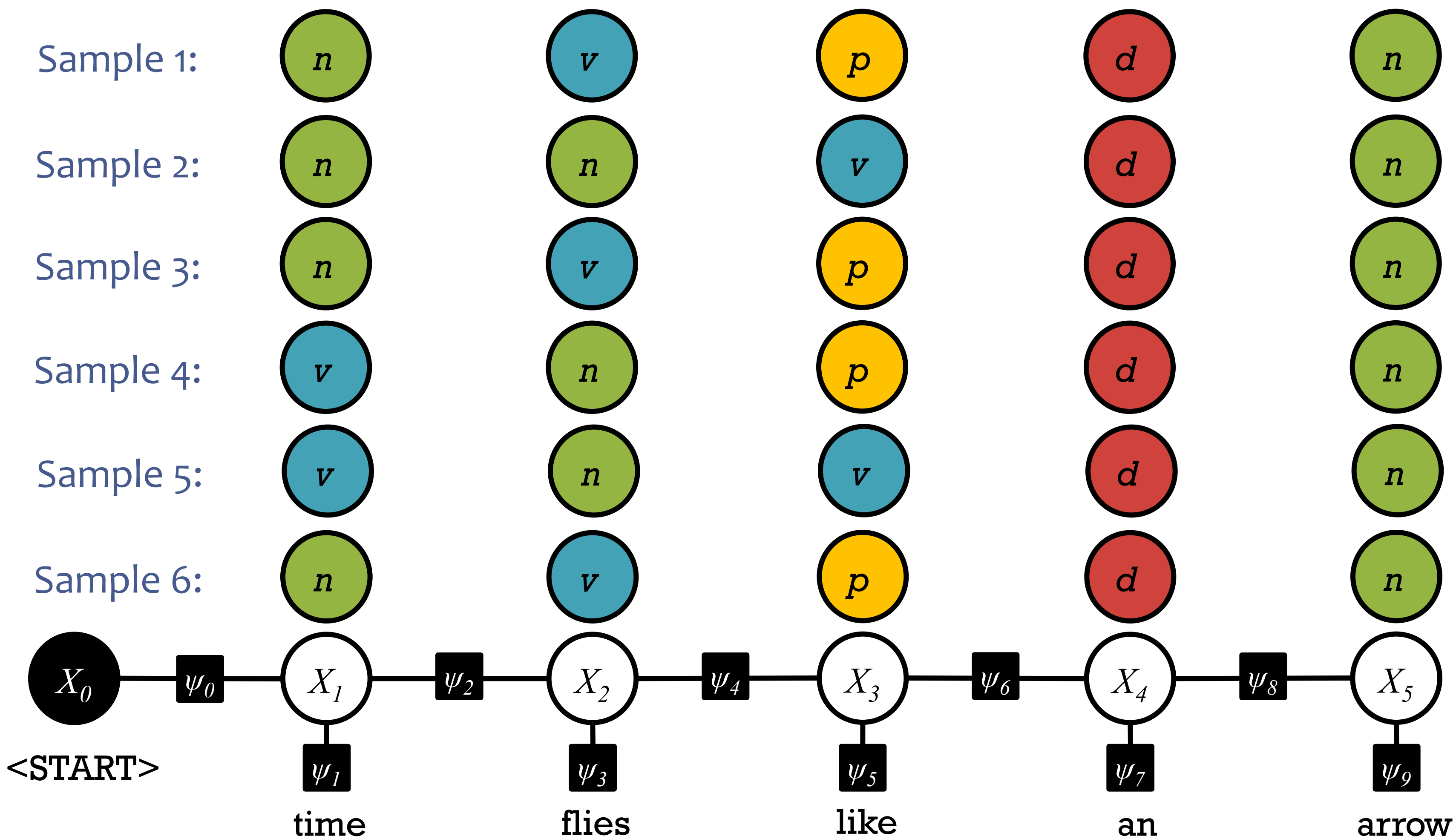
$$Z(\boldsymbol{\theta}) = \sum_{\boldsymbol{x}} \prod_{C \in \mathcal{C}} \psi_C(\boldsymbol{x}_C)$$

3. MAP Inference
Compute variable assignment with highest probability

$$\hat{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\text{argmax}} \; p(\boldsymbol{x} \mid \boldsymbol{\theta})$$

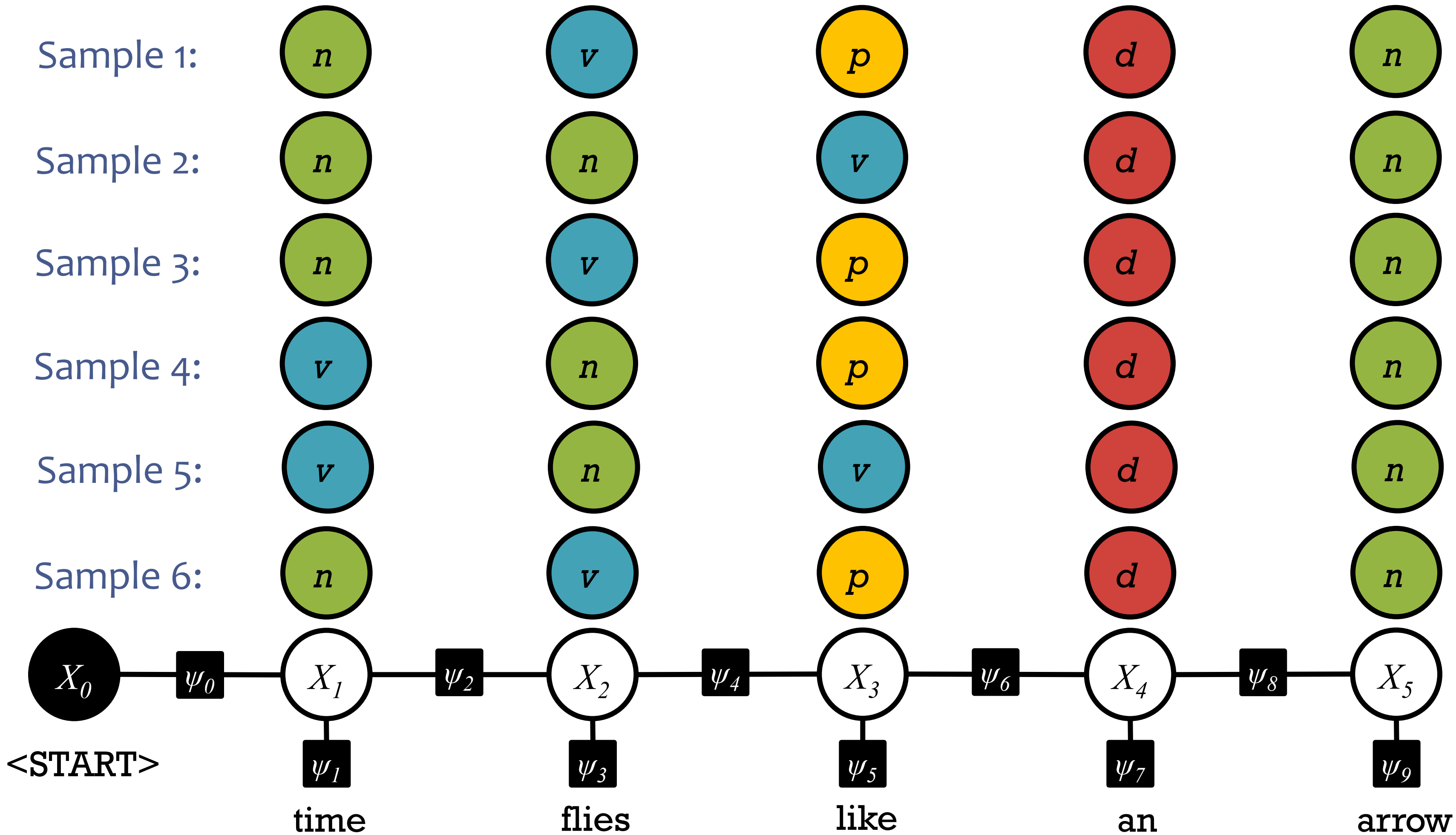
Marginals by Sampling on Factor Graph

Suppose we took many samples from the distribution over taggings: $p(\boldsymbol{x}) = \frac{1}{Z} \prod_{\alpha} \psi_\alpha(\boldsymbol{x}_\alpha)$

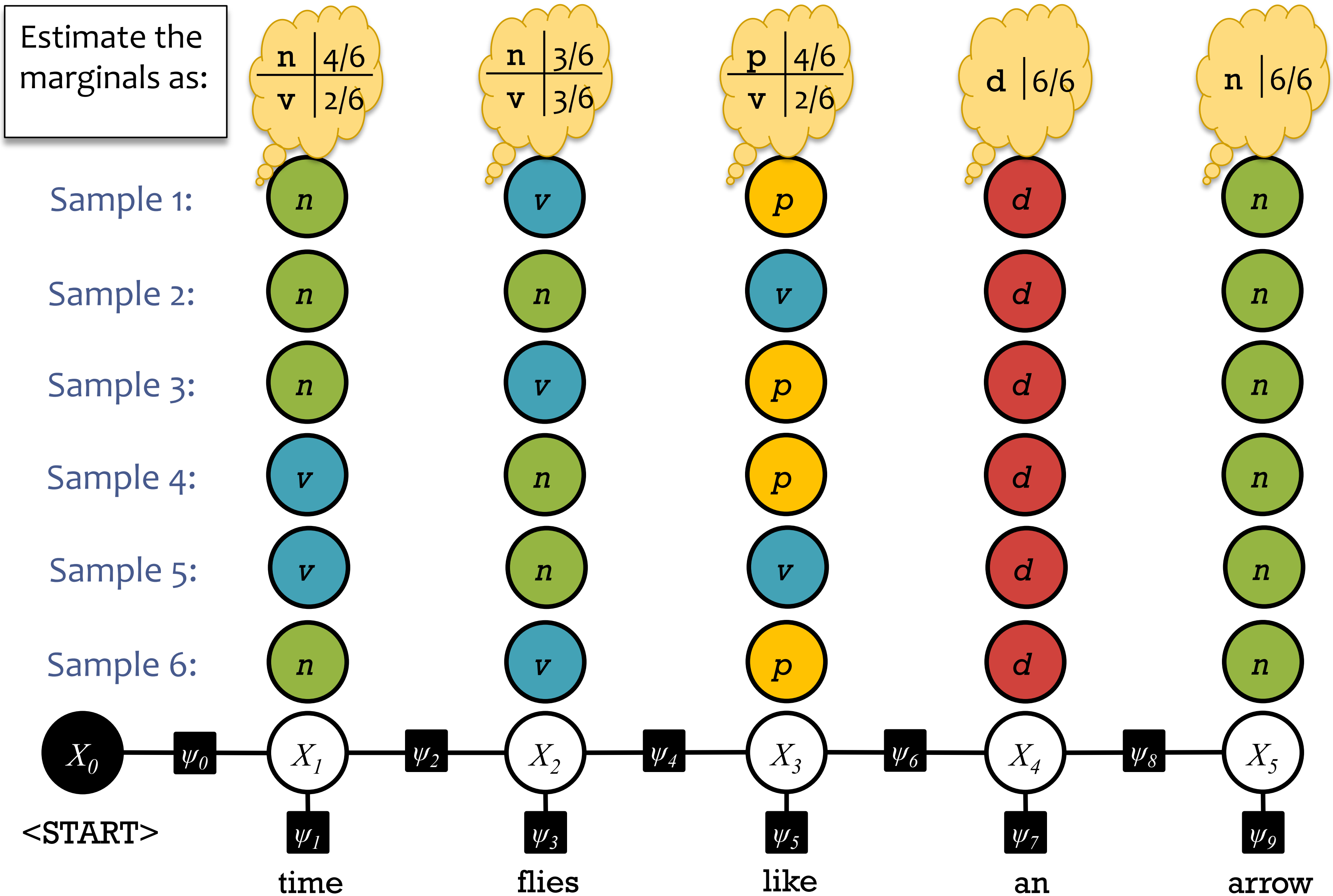


Marginals by Sampling on Factor Graph

The marginal $p(X_i = x_i)$ gives the probability that variable X_i takes value x_i in a random sample



Marginals by Sampling on Factor Graph



How do we get marginals without sampling?

That's what Belief Propagation is all about!

Why not just sample?

- Sampling one joint assignment is *also* NP-hard in general.
  - In practice: Use MCMC (e.g., Gibbs sampling) as an anytime algorithm.
  - So draw an approximate sample fast, or run longer for a "good" sample.

- Sampling finds the high-probability values x_i efficiently.
  But it takes too many samples to see the low-probability ones.
  - How do you find p("The quick brown fox …") under a language model?
    - Draw random sentences to see how often you get it? Takes a *long* time.
    - Or multiply factors (trigram probabilities)? That's what BP would do.

Simple and general exact inference for graphical models

VARIABLE ELIMINATION

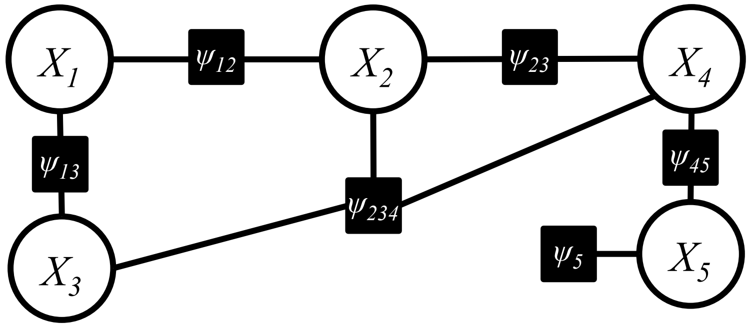
The Variable Elimination Algorithm

For all i, suppose the **range** of X_i is $\{0, 1, 2\}$.

Let $k=3$ denote the **size of the range**.

The distribution **factorizes** as:

$$p(\boldsymbol{x}) = \psi_{12}(x_1, x_2)\psi_{13}(x_1, x_3)\psi_{24}(x_2, x_4)$$
$$\psi_{234}(x_2, x_3, x_4)\psi_{45}(x_4, x_5)\psi_5(x_5)$$



Naively, we compute the **partition function** as:

$$Z = \sum_{x_1} \sum_{x_2} \sum_{x_3} \sum_{x_4} \sum_{x_5} p(\boldsymbol{x})$$

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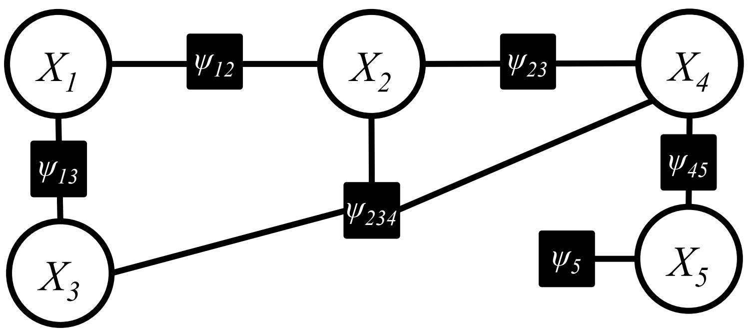

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$$Z = \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4}\sum_{x_5} p(\boldsymbol{x})$$

$p(\boldsymbol{x})$ can be represented as a joint probability table with 3^5 entries:

x_1	x_2	x_3	x_4	x_5	$p(\boldsymbol{x})$
0	0	0	0	0	0.019517693
0	0	0	0	1	0.017090249
0	0	0	0	2	0.014885825
0	0	0	1	0	0.024117638
0	0	0	1	1	0.000925849
0	0	0	1	2	0.028112576
0	0	0	2	0	0.028050205
0	0	0	2	1	0.004812689
0	0	0	2	2	0.007987737
0	0	1	0	0	0.028433687
0	0	1	0	1	0.037073469
0	0	1	0	2	0.013558227
0	0	1	1	0	0.019479016
0	0	1	1	1	0.012312901
0	0	1	1	2	0.023439775
0	0	1	2	0	0.038206131
0	0	1	2	1	0.038996005
0	0	1	2	2	0.041458783
0	0	2	0	0	0.044616806
0	0	2	0	1	0.020846989
0	0	2	0	2	0.03006475
0	0	2	1	0	0.048436964
0	0	2	1	1	0.02854376
0	0	2	1	2	0.029191506
0	0	2	2	0	0.031531118
0	0	2	2	1	0.005132392
0	0	2	2	2	0.032027091
…	…	…	…	…	…

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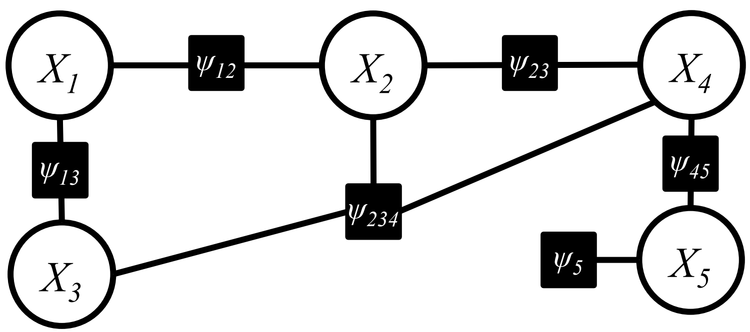

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0	0	0	1	1	0.000925849
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0	0	2	0	0	0.044616806
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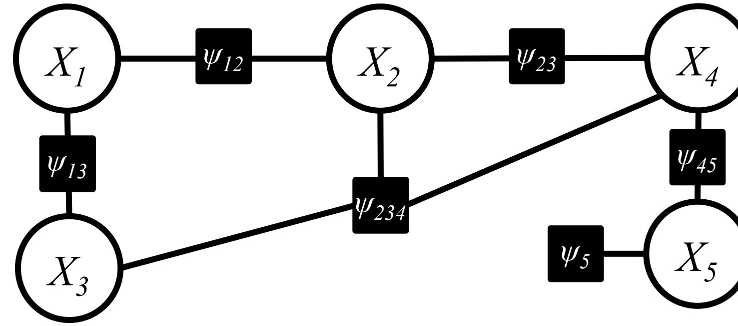
0	0	2	0	2	0.03006475
0	0	2	1	0	0.048436964
0	0	2	1	1	0.02854376

Naïve computation of Z requires 3^5 additions.

Can we do better?

The Variable Elimination Algorithm

Instead, capitalize on the factorization of $p(\mathbf{x})$.



$$Z = \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4}\sum_{x_5} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)\psi_{45}(x_4,x_5)\psi_5(x_5)$$

$$= \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)\underbrace{\sum_{x_5}\psi_{45}(x_4,x_5)\psi_5(x_5)}$$

Only 3^2 additions are needed to marginalize out x_5.

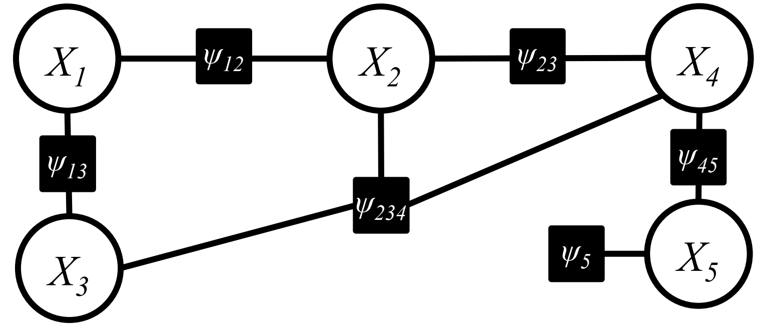
We denote the **marginal's table** by $m_5(x_4)$.

This "factor" is a much smaller table with 3^2 entries:

x_4	x_5	$p(\mathbf{x})$
0	0	0.019517693
0	1	0.017090249
0	2	0.014885825
1	0	0.024117638
1	1	0.000925849
1	2	0.028112576
2	0	0.028050205
2	1	0.004812689
2	2	0.007987737

The Variable Elimination Algorithm

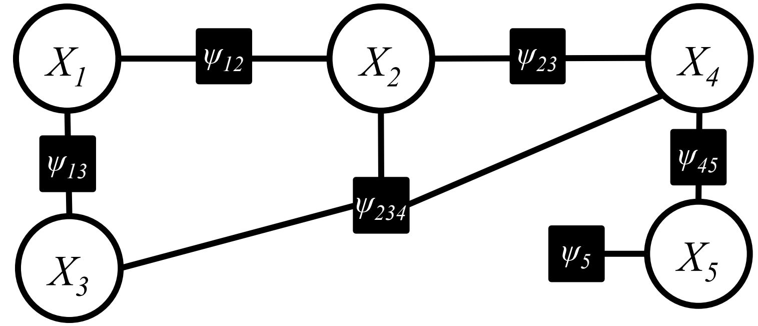
Instead, capitalize on the factorization of *p*(***x***).



$$
\begin{aligned}
Z &= \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4}\sum_{x_5} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)\psi_{45}(x_4,x_5)\psi_5(x_5) \\
&= \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4) \sum_{x_5} \psi_{45}(x_4,x_5)\psi_5(x_5) \\
&= \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4) m_5(x_4)
\end{aligned}
$$

$$\boxed{m_5(x_4) \triangleq \sum_{x_5} \psi_{45}(x_4,x_5)\psi_5(x_5)}$$

The Variable Elimination Algorithm



Instead, capitalize on the factorization of $p(\mathbf{x})$.

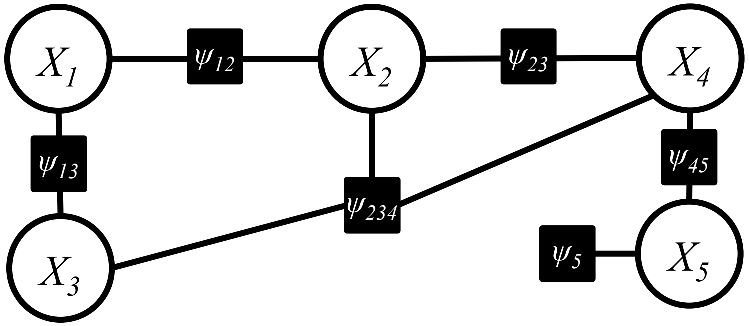
$$
\begin{aligned}
Z &= \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4}\sum_{x_5} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)\psi_{45}(x_4,x_5)\psi_5(x_5) \\
&= \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4} \psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4) \sum_{x_5} \psi_{45}(x_4,x_5)\psi_5(x_5) \\
&= \sum_{x_1}\sum_{x_2}\sum_{x_3}\sum_{x_4} \underbrace{\psi_{12}(x_1,x_2)\psi_{13}(x_1,x_3)\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4) m_5(x_4)}
\end{aligned}
$$

This "factor" is still a 3^4 table so apply the same trick again.

$$\boxed{m_5(x_4) \triangleq \sum_{x_5} \psi_{45}(x_4,x_5)\psi_5(x_5)}$$

The Variable Elimination Algorithm

Instead, capitalize on the factorization of $p(\mathbf{x})$.



$$
\begin{aligned}
Z &= \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)\sum_{x_3}\psi_{13}(x_1,x_3)\sum_{x_4}\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)\sum_{x_5}\psi_{45}(x_4,x_5)\psi_5(x_5)\\
&= \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)\sum_{x_3}\psi_{13}(x_1,x_3)\sum_{x_4}\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)m_5(x_4)\\
&= \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)\sum_{x_3}\psi_{13}(x_1,x_3)m_4(x_2,x_3)\\
&= \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)m_3(x_1,x_2)\\
&= \sum_{x_1}m_2(x_1)
\end{aligned}
$$

3^2 additions

3^3 additions

3^3 additions

3^2 additions

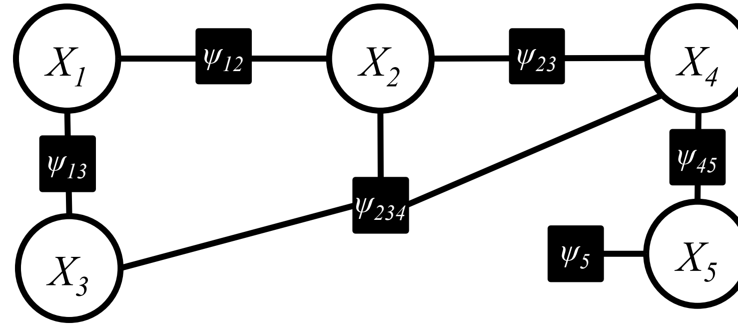
3 additions

Naïve solution requires $3^5=243$ additions.

Variable elimination only requires $3+3^2+3^3+3^3+3^2 = 75$ additions.

The Variable Elimination Algorithm

The same trick can be used to compute **marginal probabilities.** Just choose the variable elimination order such that the query variables are last.



$$\begin{aligned}
p(x_1) &= \frac{1}{Z} \sum_{x_2} \psi_{12}(x_1, x_2) \sum_{x_3} \psi_{13}(x_1, x_3) \sum_{x_4} \psi_{24}(x_2, x_4) \psi_{234}(x_2, x_3, x_4) \sum_{x_5} \psi_{45}(x_4, x_5) \psi_5(x_5) \\
&= \frac{1}{Z} \sum_{x_2} \psi_{12}(x_1, x_2) \sum_{x_3} \psi_{13}(x_1, x_3) \sum_{x_4} \psi_{24}(x_2, x_4) \psi_{234}(x_2, x_3, x_4) m_5(x_4) \\
&= \frac{1}{Z} \sum_{x_2} \psi_{12}(x_1, x_2) \sum_{x_3} \psi_{13}(x_1, x_3) m_4(x_2, x_3) \\
&= \frac{1}{Z} \sum_{x_2} \psi_{12}(x_1, x_2) m_3(x_1, x_2) \\
&= \frac{1}{Z} m_2(x_1)
\end{aligned}$$

3^2 additions

3^3 additions

3^3 additions

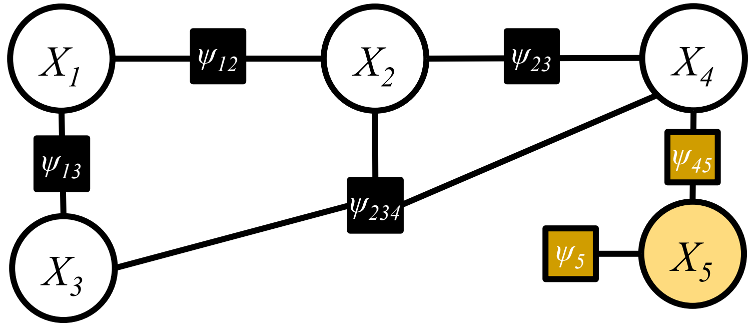
3^2 additions

3 different values on LHS

For directed graphs, Z = 1.

For undirected graphs, if we compute each (unnormalized) value on the LHS, we can sum them to get Z.

The Variable Elimination Algorithm



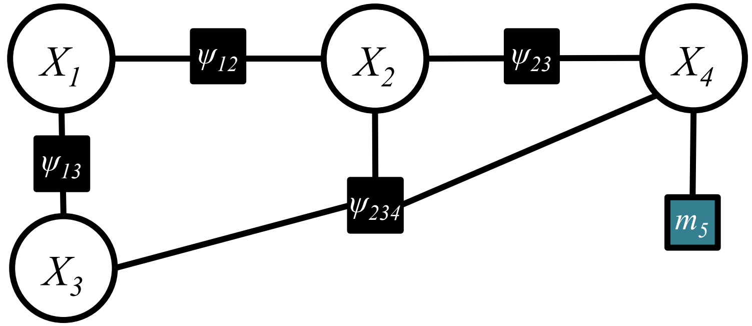
$$Z = \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)\sum_{x_3}\psi_{13}(x_1,x_3)\sum_{x_4}\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)\sum_{x_5}\psi_{45}(x_4,x_5)\psi_5(x_5)$$

$$= \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)\sum_{x_3}\psi_{13}(x_1,x_3)\sum_{x_4}\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)m_5(x_4)$$

$$= \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)\sum_{x_3}\psi_{13}(x_1,x_3)m_4(x_2,x_3)$$

In a factor graph, variable **elimination** corresponds to replacement of a subgraph with a factor.

The Variable Elimination Algorithm



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\begin{aligned}
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&= \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)\sum_{x_3}\psi_{13}(x_1,x_3)\sum_{x_4}\psi_{24}(x_2,x_4)\psi_{234}(x_2,x_3,x_4)m_5(x_4) \\
&= \sum_{x_1}\sum_{x_2}\psi_{12}(x_1,x_2)\sum_{x_3}\psi_{13}(x_1,x_3)m_4(x_2,x_3)
\end{aligned}
$$

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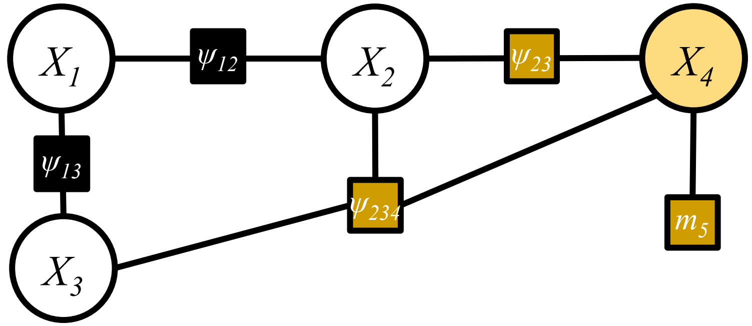

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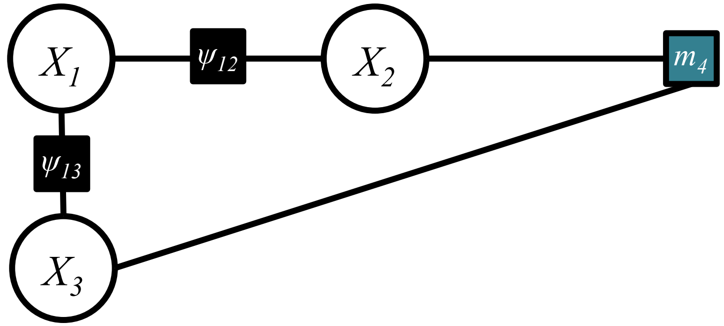
The Variable Elimination Algorithm



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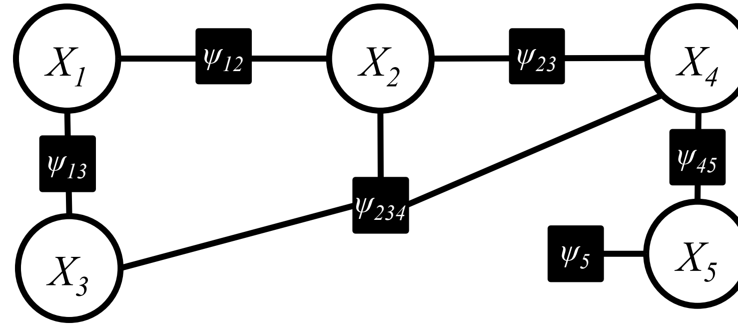
In a factor graph, variable **elimination** corresponds to replacement of a subgraph with a factor.

Variable Elimination Complexity

Instead, capitalize on the factorization of $p(\boldsymbol{x})$.



Naïve solution is $O(k^n)$

Variable elimination is $O(nk^r)$

where
n = # of variables
k = max # values a variable can take
r = # variables participating in largest "intermediate" table

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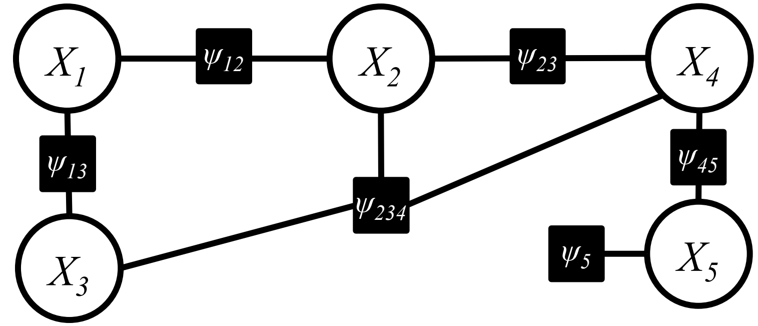

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where
- n = # of variables
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Variable Elimination Complexity

- The graph elimination process we saw has an analogous interpretation on undirected graphical models, where instead of adding a few factor we add a new clique.
- The overall complexity is determined by the number of the largest elimination clique.

  - What is the largest elimination clique? – a pure graph theoretic question
  - **Tree-width** *t*: one less than the smallest achievable value of the cardinality of the largest elimination clique, ranging over all possible elimination ordering
  - “good” elimination orderings lead to **small cliques** and hence reduce complexity (what will happen if we eliminate "e" first in the above graph?)
  - Find the best elimination ordering of a graph --- NP-hard

  → Inference is NP-hard

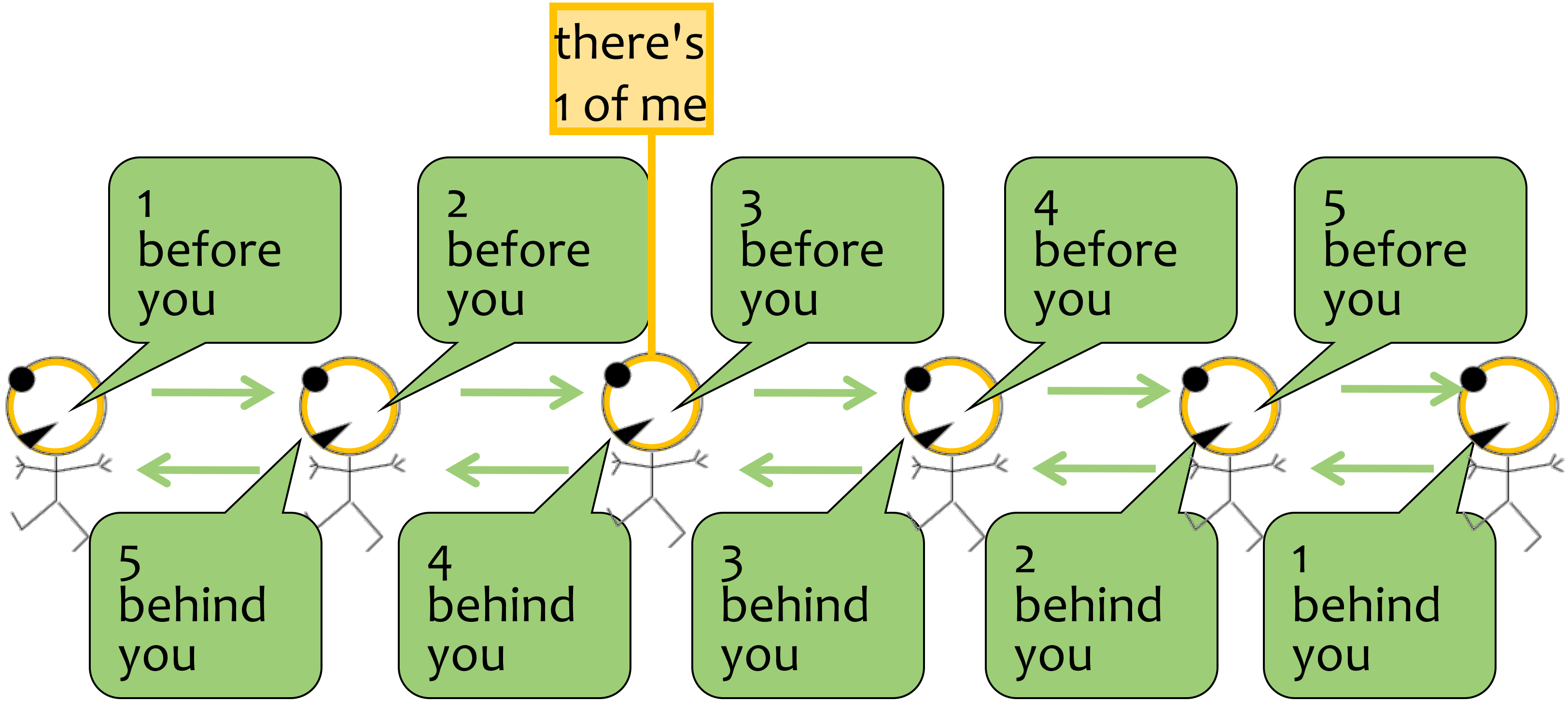
  - But there often exist "obvious" optimal or near-opt elimination ordering

Exact marginal inference for factor trees

SUM-PRODUCT BELIEF PROPAGATION

Great Ideas in ML: Message Passing

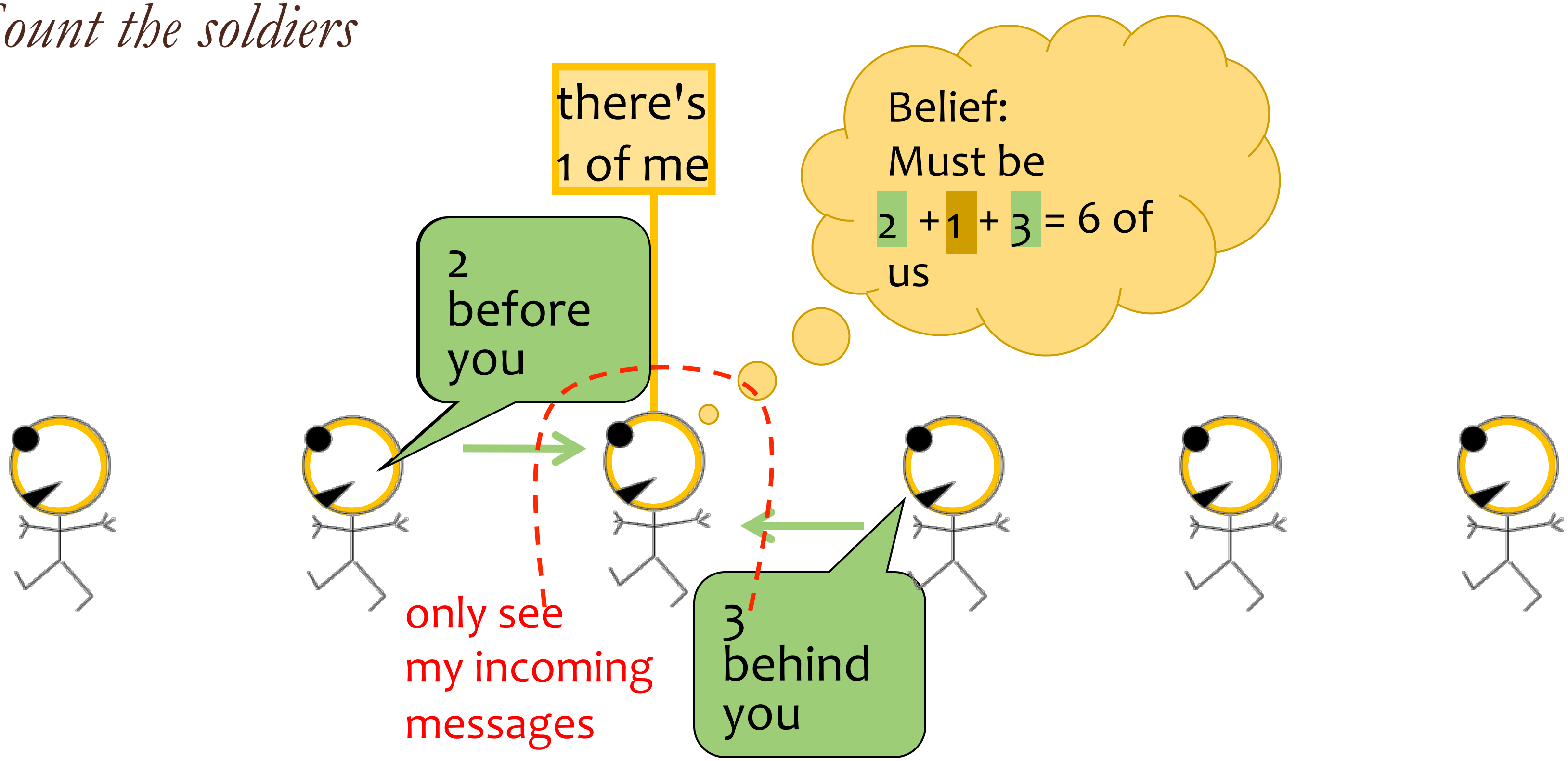
Count the soldiers



adapted from MacKay (2003) textbook

Great Ideas in ML: Message Passing

Count the soldiers



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Great Ideas in ML: Message Passing

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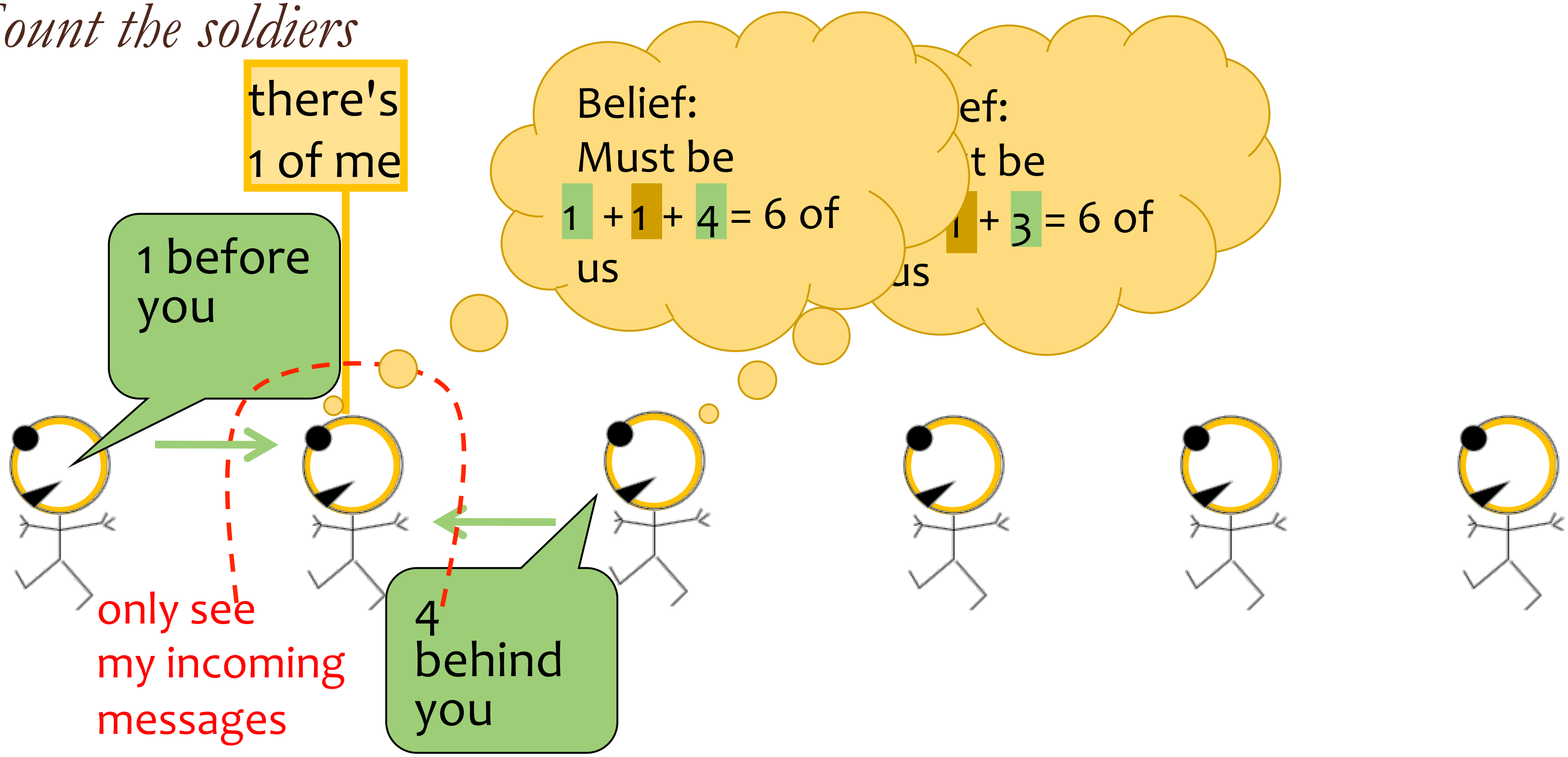

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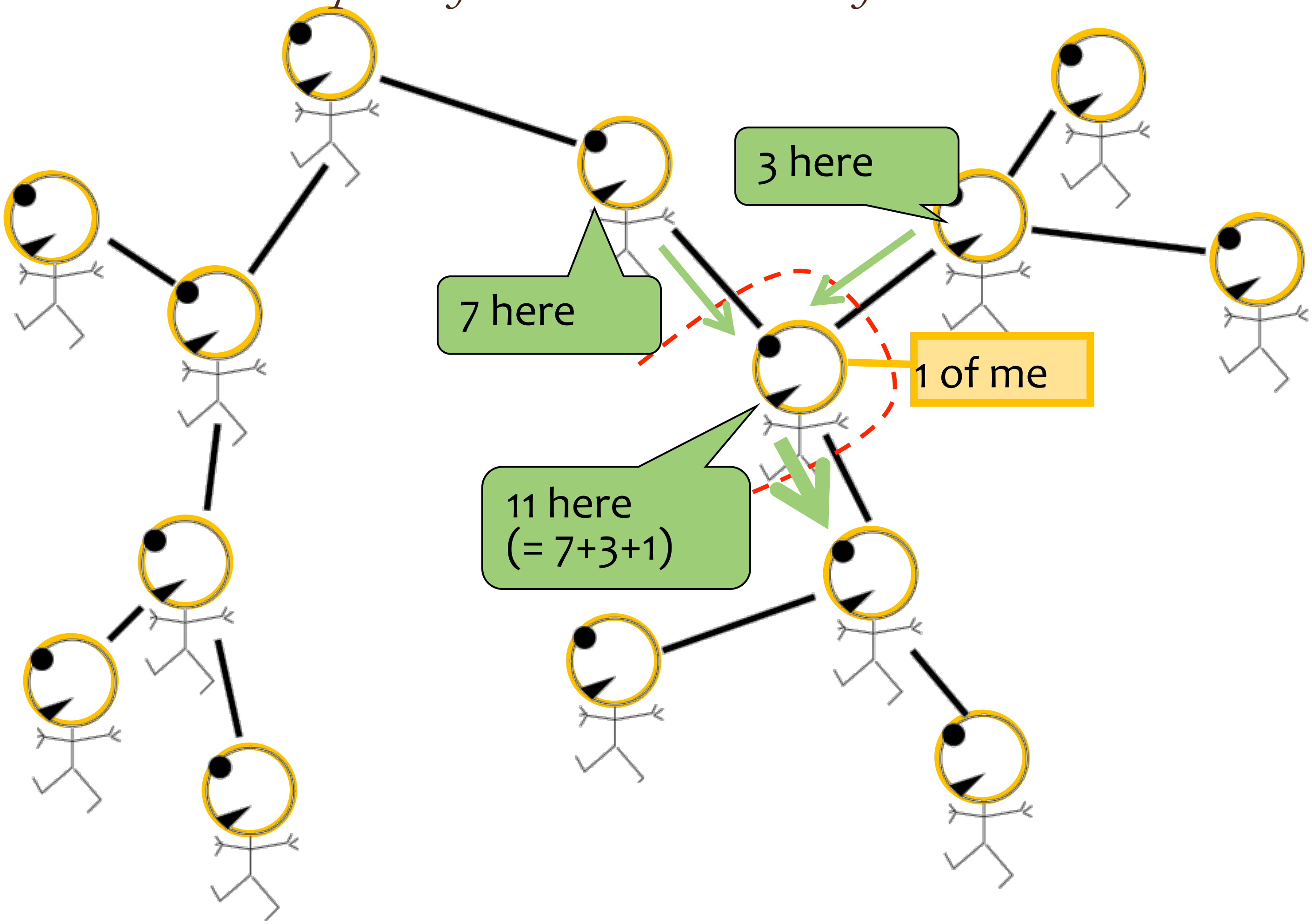
Great Ideas in ML: Message Passing

Each soldier receives reports from all branches of tree



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Great Ideas in ML: Message Passing

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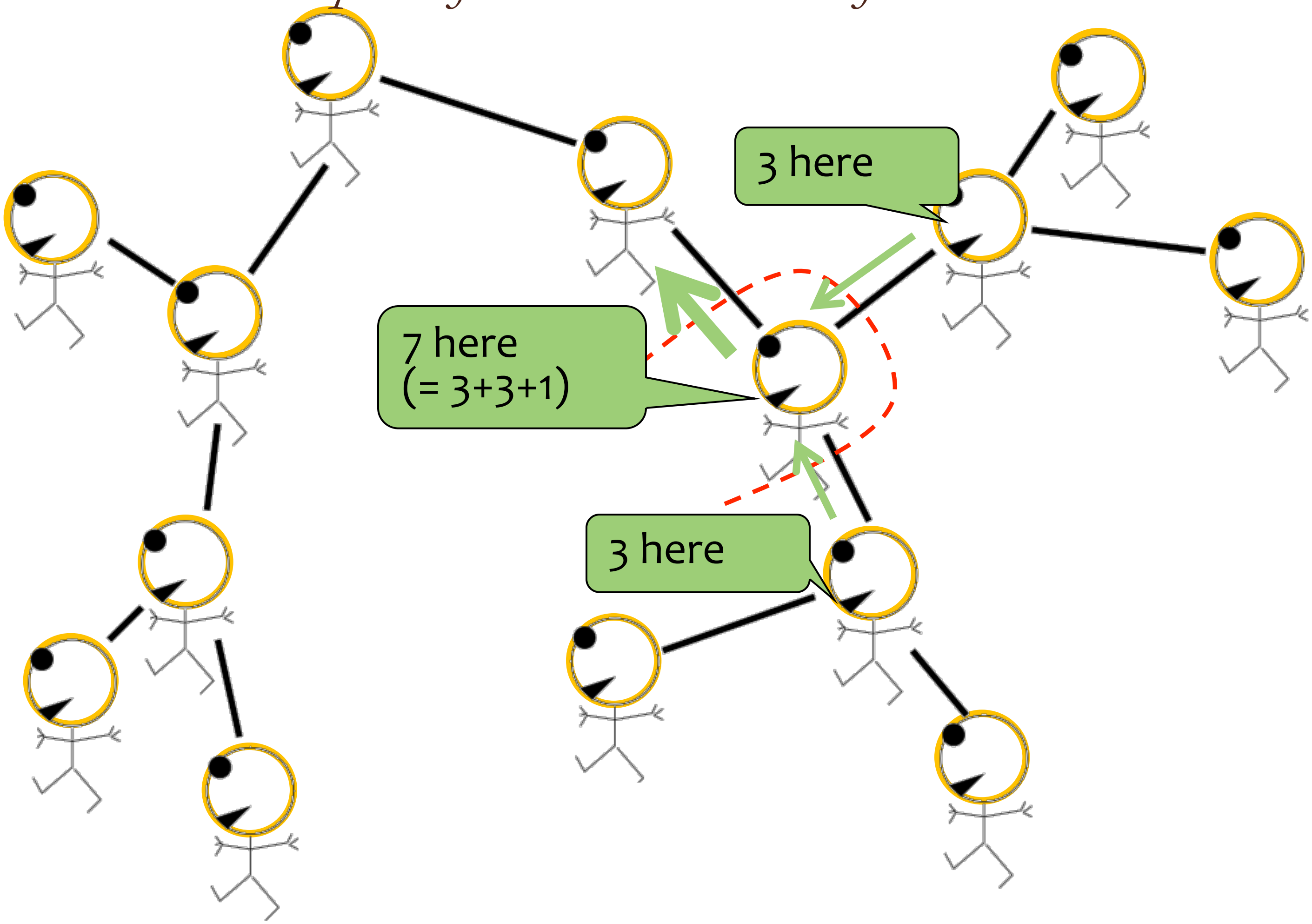

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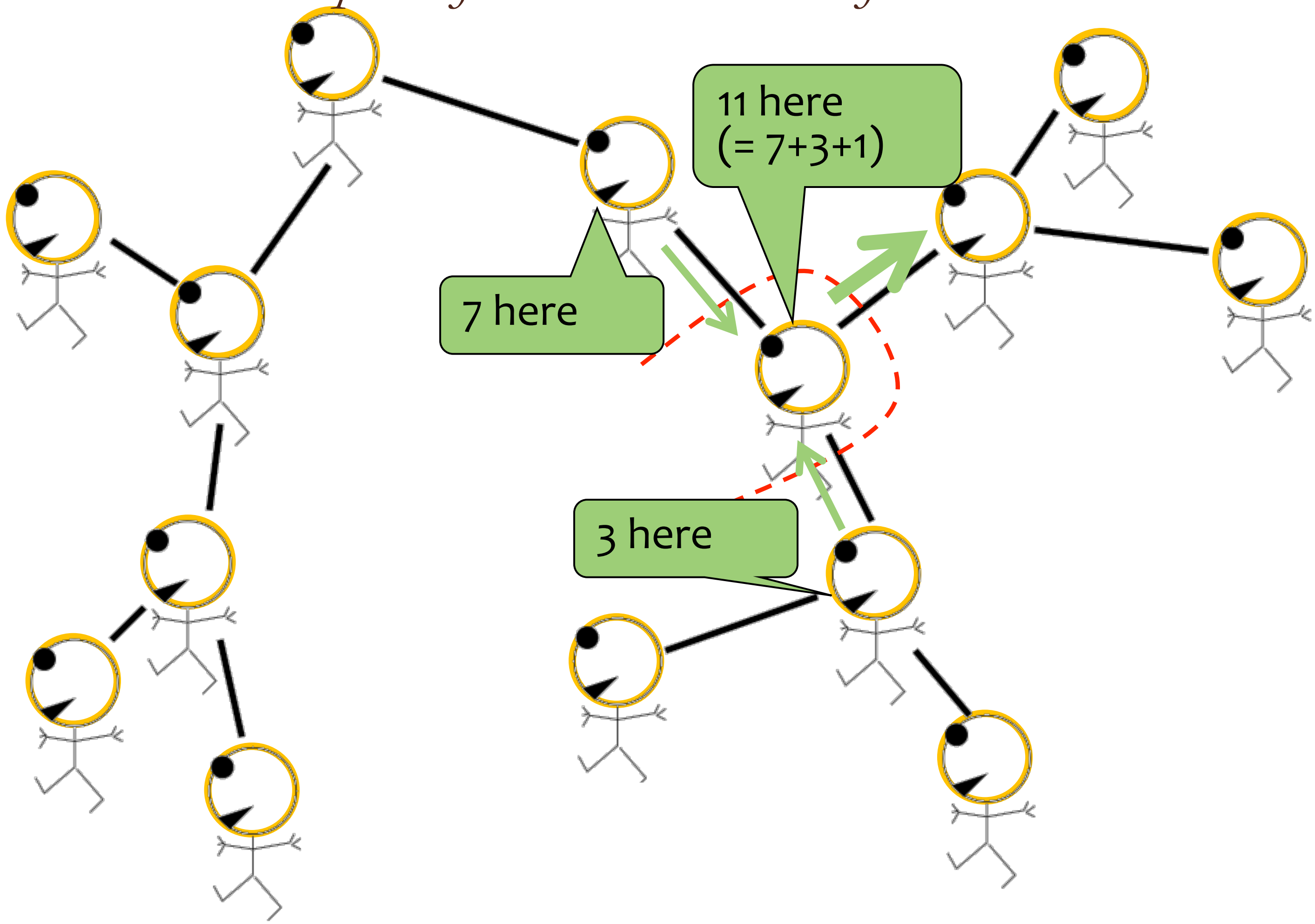
Great Ideas in ML: Message Passing

Each soldier receives reports from all branches of tree



adapted from MacKay (2003) textbook

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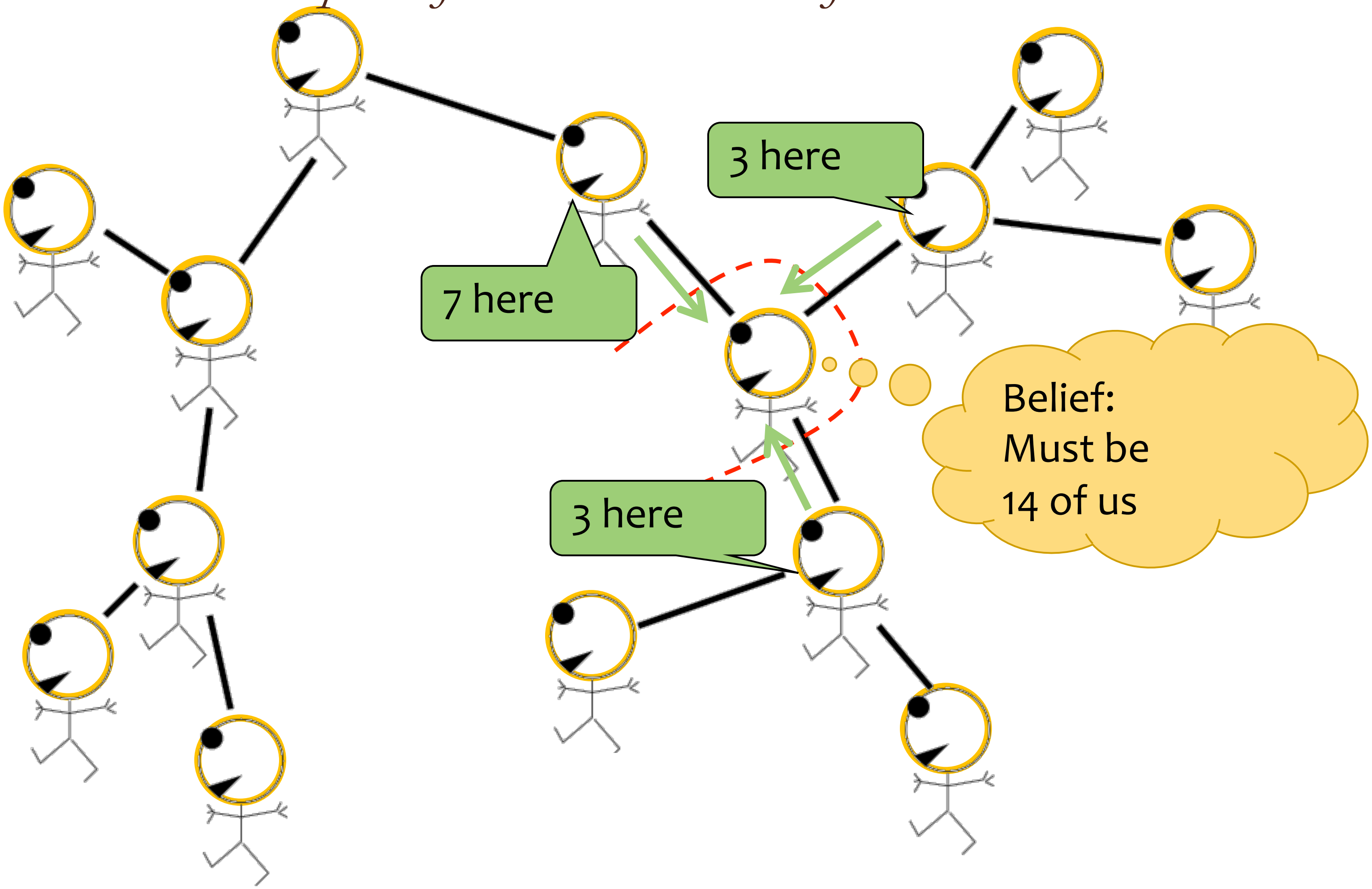

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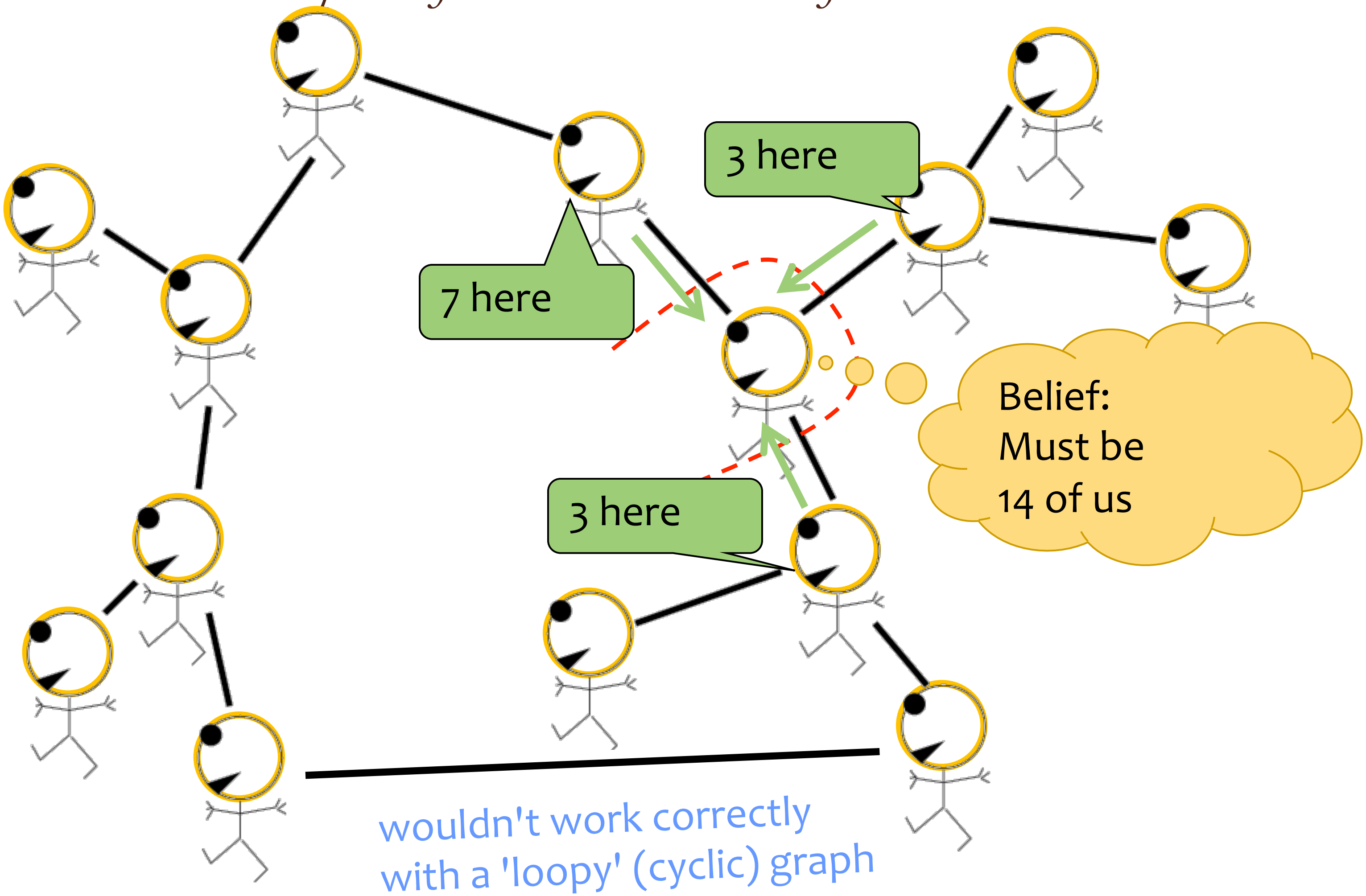

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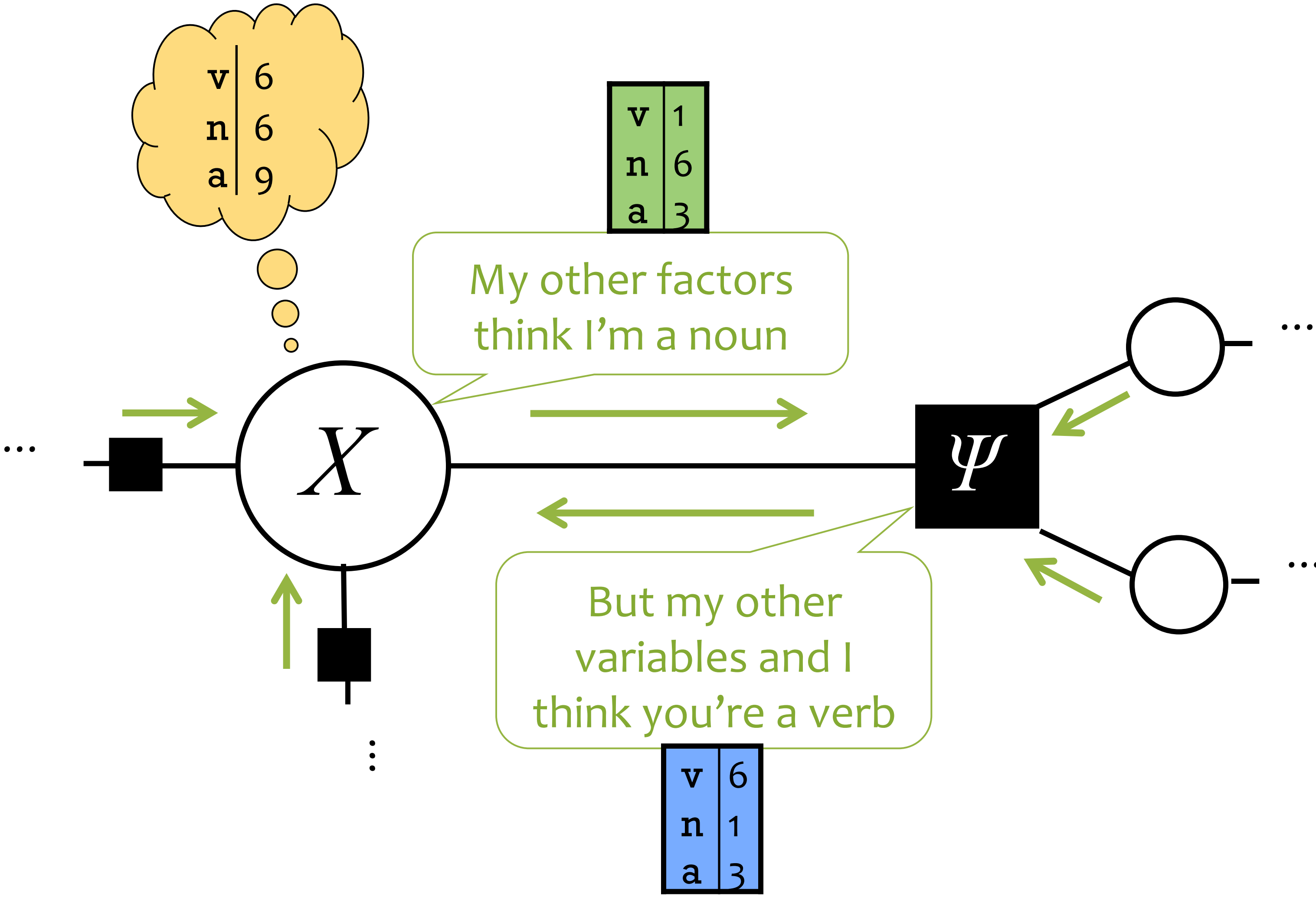
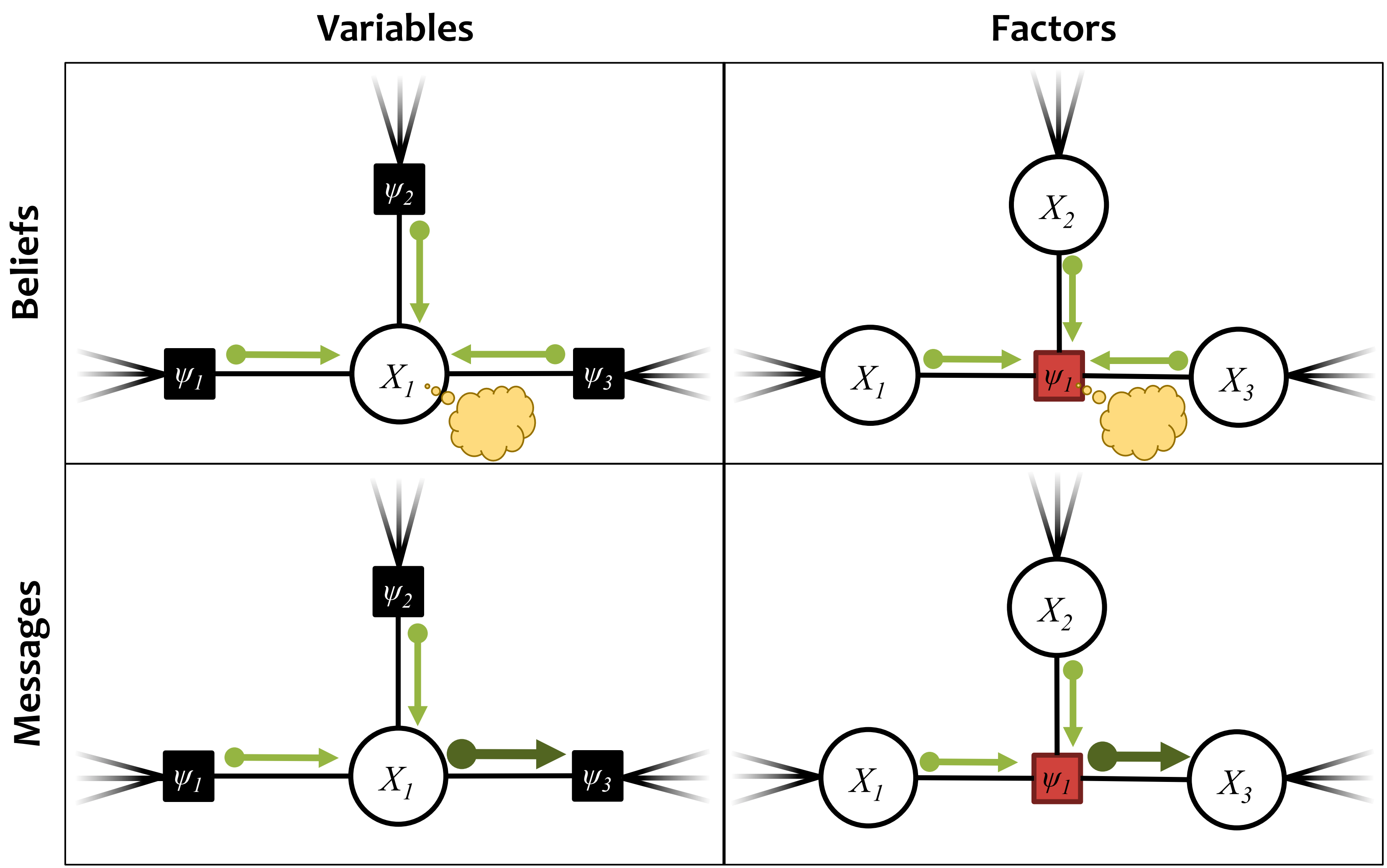
Message Passing in Belief Propagation



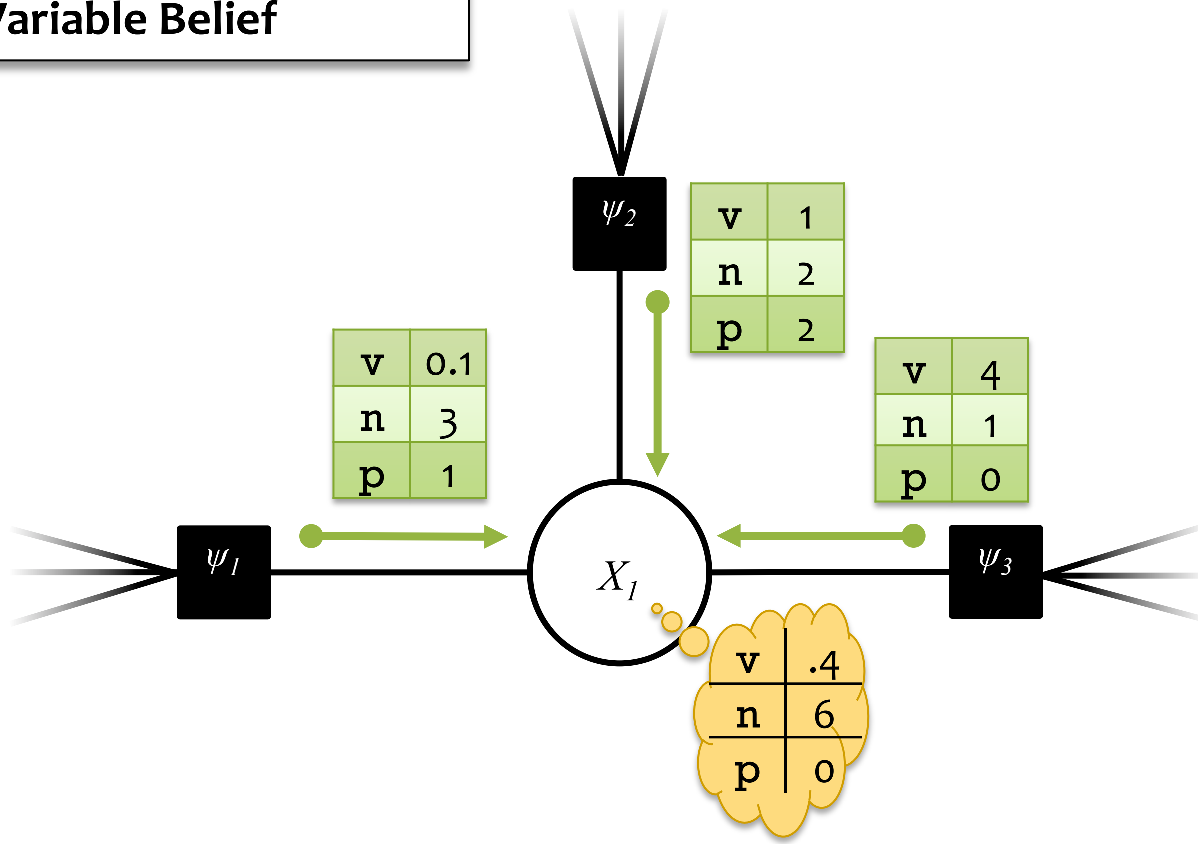
Both of these messages judge the possible values of variable X.
Their product = belief at X = product of all 3 messages to X.

Sum-Product Belief Propagation



Sum-Product Belief Propagation

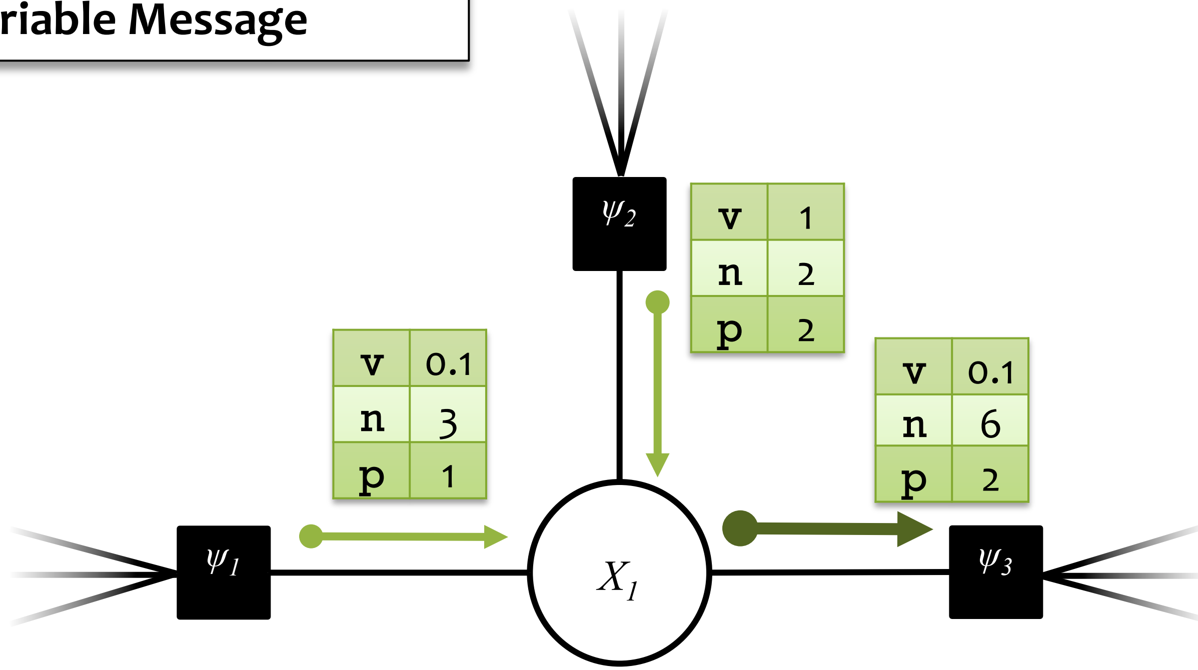
Variable Belief



$$b_i(x_i) = \prod_{\alpha \in \mathcal{N}(i)} \mu_{\alpha \to i}(x_i)$$

Sum-Product Belief Propagation

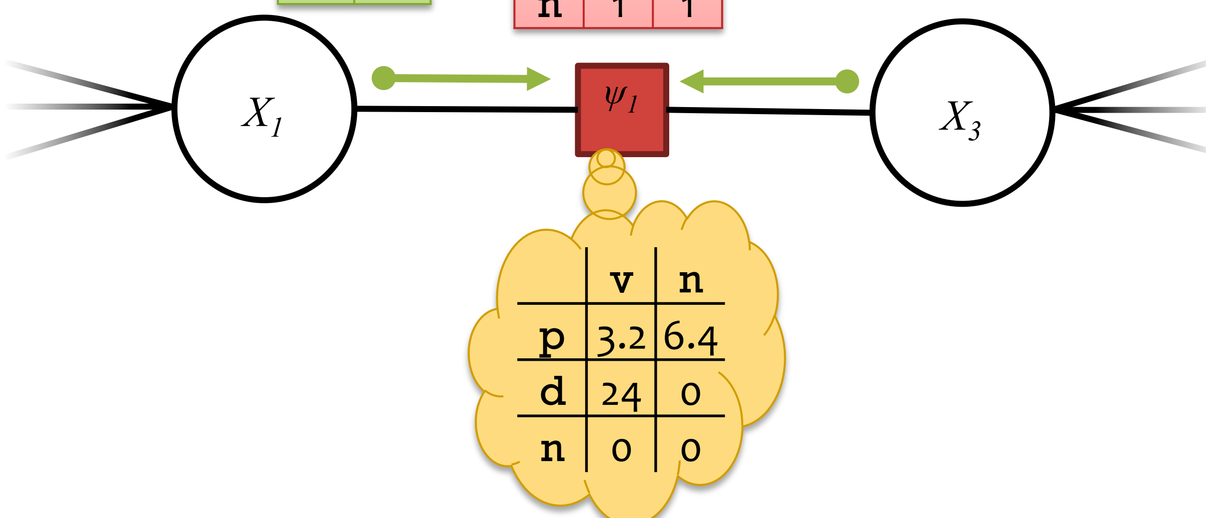
Variable Message



$$\mu_{i \to \alpha}(x_i) = \prod_{\alpha \in \mathcal{N}(i) \setminus \alpha} \mu_{\alpha \to i}(x_i)$$

Sum-Product Belief Propagation

Factor Belief



p	4
d	1
n	0

	v	n
p	0.1	8
d	3	0
n	1	1

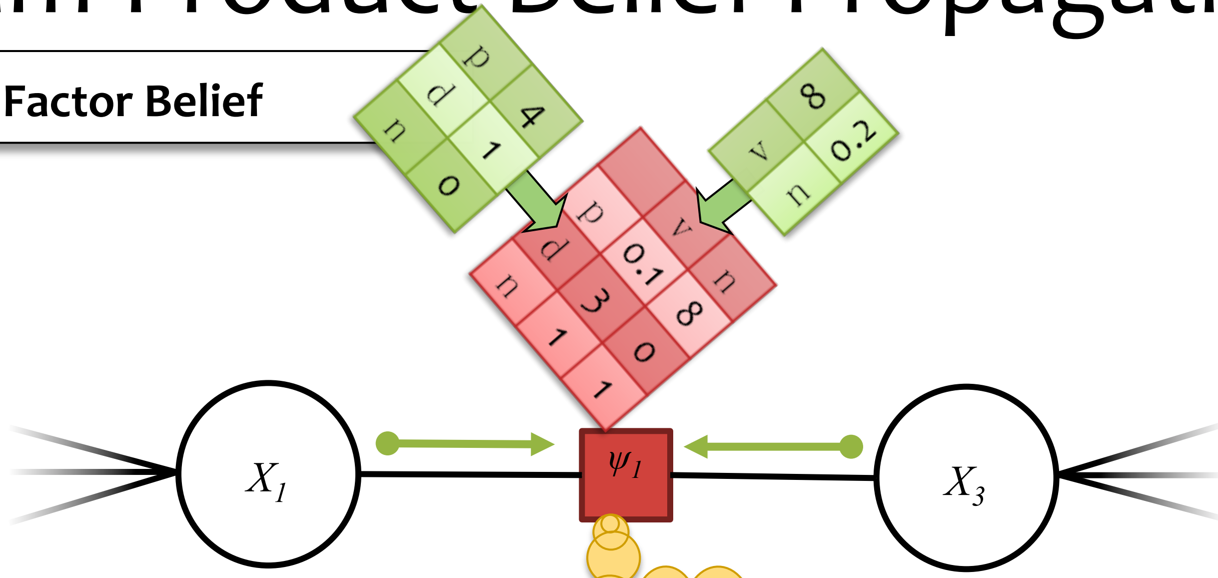
v	8
n	0.2

	v	n
p	3.2	6.4
d	24	0
n	0	0

$$b_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) = \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{i \in \mathcal{N}(\alpha)} \mu_{i \to \alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])$$

Sum-Product Belief Propagation

Factor Belief



	v	n
p	3.2	6.4
d	24	0
n	0	0

$$b_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) = \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{i \in \mathcal{N}(\alpha)} \mu_{i \to \alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])$$

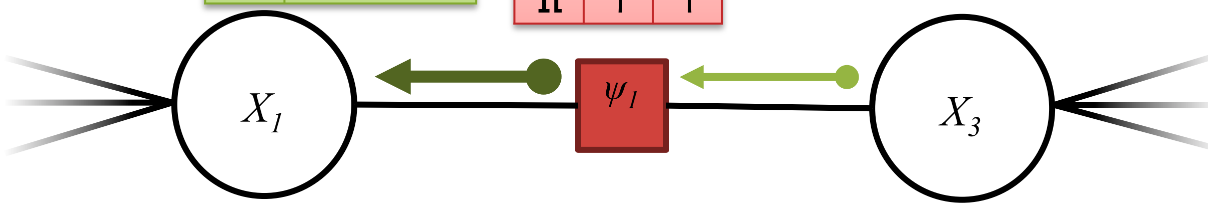
Sum-Product Belief Propagation

Factor Message

p	0.8 + 0.16
d	24 + 0
n	8 + 0.2

	v	n
p	0.1	8
d	3	0
n	1	1

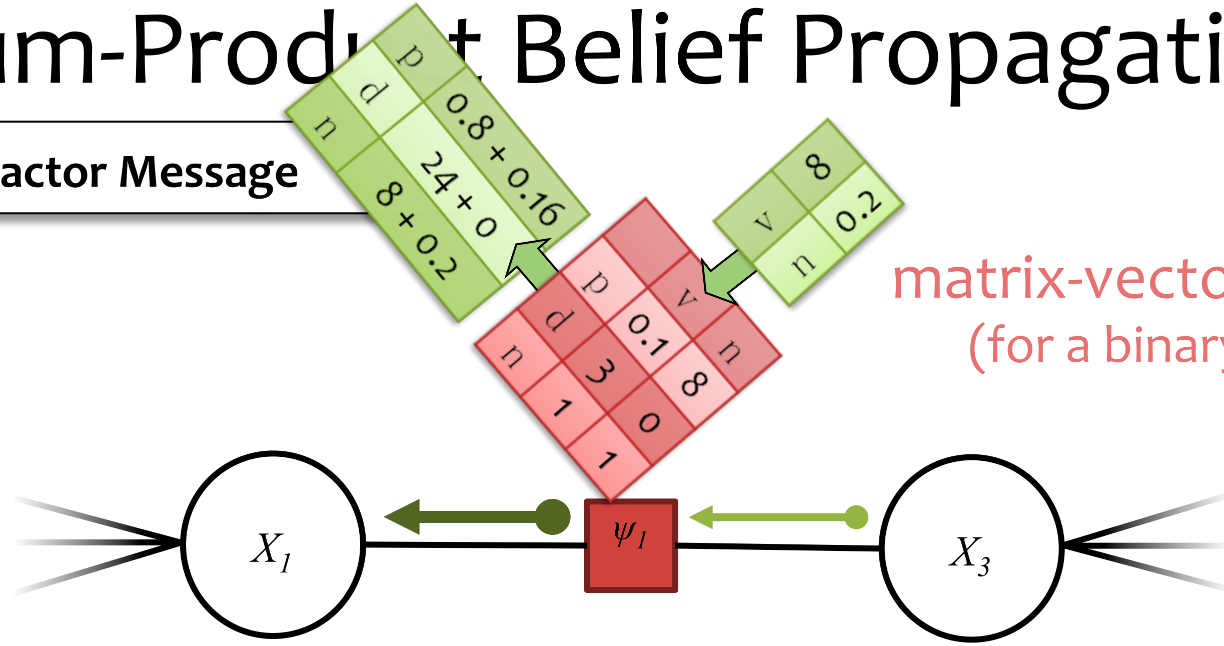
v	8
n	0.2



$$\mu_{\alpha \to i}(x_i) = \sum_{\boldsymbol{x}_{\boldsymbol{\alpha}} : \boldsymbol{x}_{\boldsymbol{\alpha}}[i] = x_i} \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{j \in \mathcal{N}(\alpha) \setminus i} \mu_{j \to \alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])$$

Sum-Product Belief Propagation

Factor Message



matrix-vector product
(for a binary factor)

$$\mu_{\alpha \to i}(x_i) = \sum_{\boldsymbol{x}_{\boldsymbol{\alpha}} : \boldsymbol{x}_{\boldsymbol{\alpha}}[i] = x_i} \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{j \in \mathcal{N}(\alpha) \setminus i} \mu_{j \to \alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])$$

Sum-Product Belief Propagation

Input: a factor graph with no cycles
Output: exact marginals for each variable and factor

Algorithm:

1. Initialize the messages to the uniform distribution.

$$\boxed{\mu_{i \to \alpha}(x_i) = 1} \quad \boxed{\mu_{\alpha \to i}(x_i) = 1}$$

2. Choose a root node.
3. Send messages from the **leaves** to the **root**.
   Send messages from the **root** to the **leaves**.

$$\boxed{\mu_{i \to \alpha}(x_i) = \prod_{\alpha \in \mathcal{N}(i) \setminus \alpha} \mu_{\alpha \to i}(x_i)} \quad \boxed{\mu_{\alpha \to i}(x_i) = \sum_{\boldsymbol{x}_{\boldsymbol{\alpha}} : \boldsymbol{x}_{\boldsymbol{\alpha}}[i] = x_i} \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{j \in \mathcal{N}(\alpha) \setminus i} \mu_{j \to \alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])}$$

4. Compute the beliefs (unnormalized marginals).

$$\boxed{b_i(x_i) = \prod_{\alpha \in \mathcal{N}(i)} \mu_{\alpha \to i}(x_i)} \quad \boxed{b_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) = \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{i \in \mathcal{N}(\alpha)} \mu_{i \to \alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])}$$

5. Normalize beliefs and return the **exact** marginals.

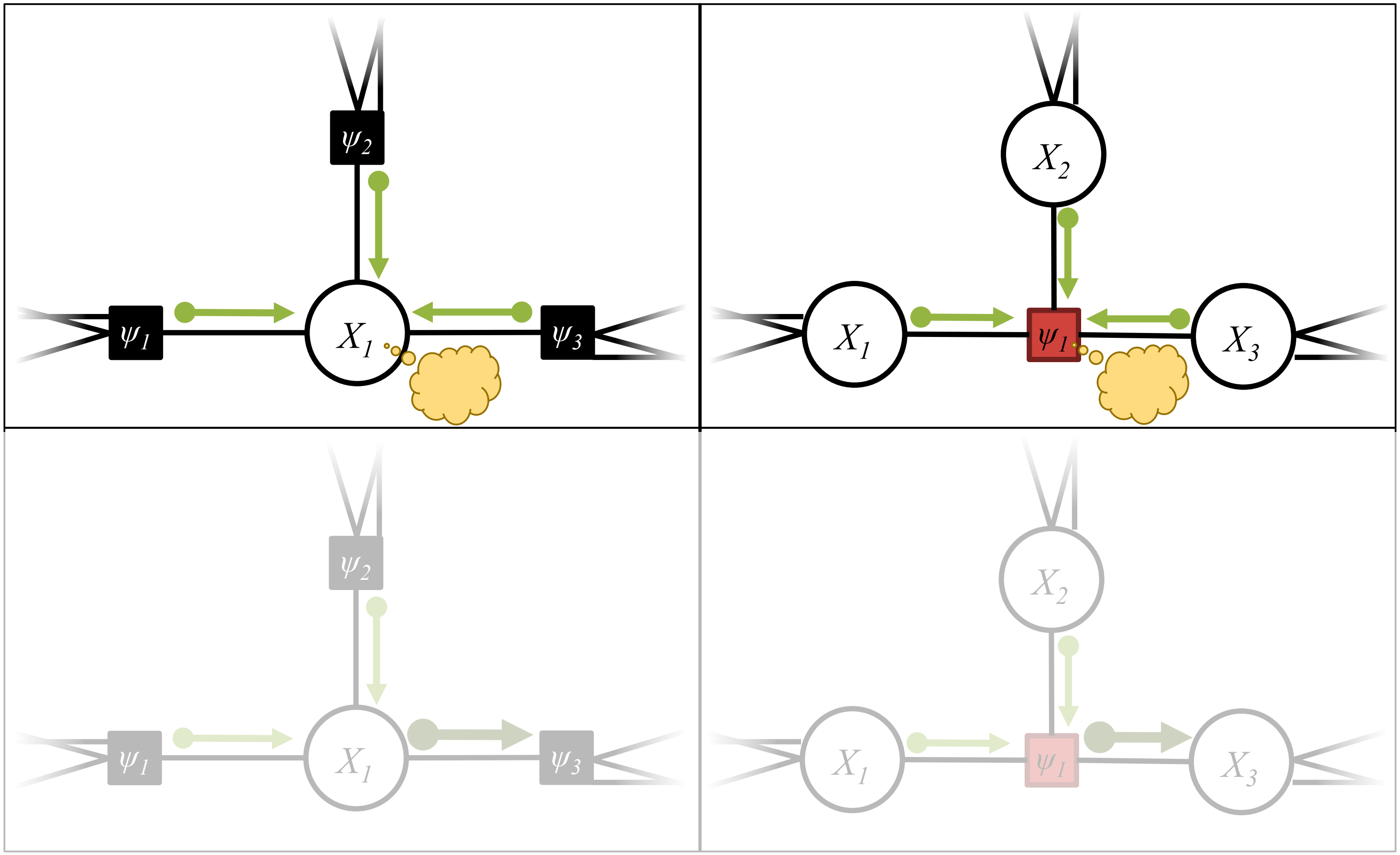
$$\boxed{p_i(x_i) \propto b_i(x_i)} \quad \boxed{p_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \propto b_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}})}$$

Sum-Product Belief Propagation

Variables | **Factors**

Beliefs

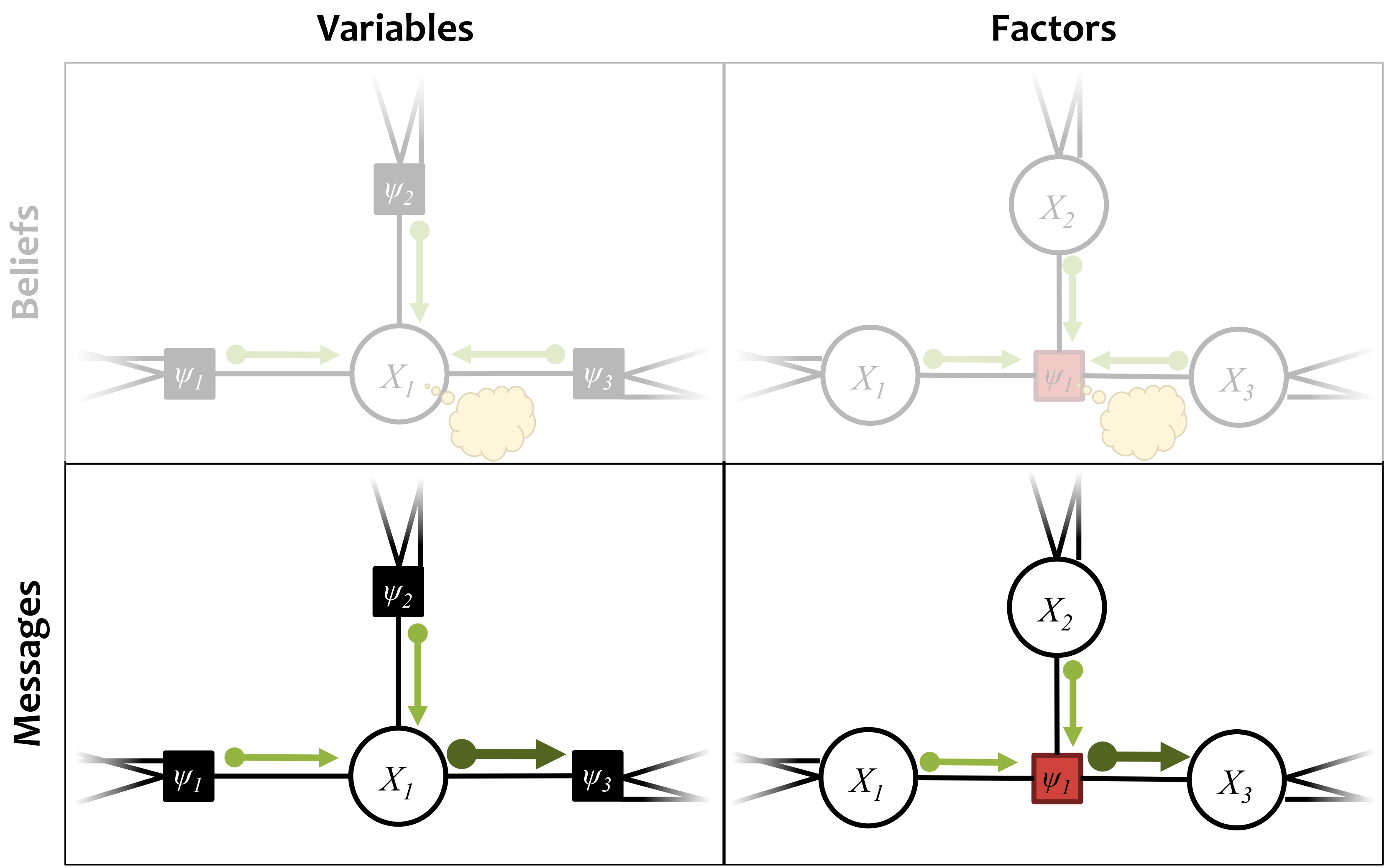
Messages



$$b_i(x_i) = \prod_{\alpha \in \mathcal{N}(i)} \mu_{\alpha \to i}(x_i)$$

$$b_\alpha(\boldsymbol{x_\alpha}) = \psi_\alpha(\boldsymbol{x_\alpha}) \prod_{i \in \mathcal{N}(\alpha)} \mu_{i \to \alpha}(\boldsymbol{x_\alpha}[i])$$

Sum-Product Belief Propagation



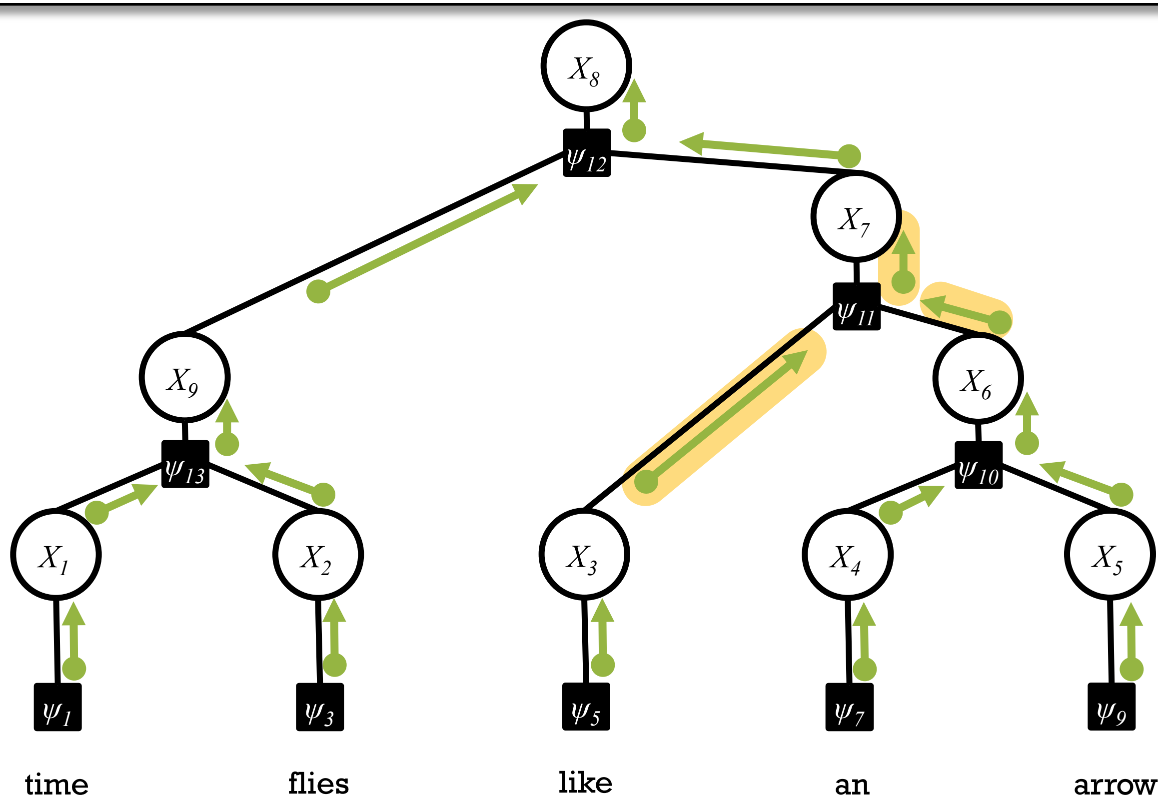
$$\mu_{i\to\alpha}(x_i) = \prod_{\alpha\in\mathcal{N}(i)\backslash\alpha} \mu_{\alpha\to i}(x_i)$$

$$\mu_{\alpha\to i}(x_i) = \sum_{\boldsymbol{x}_{\boldsymbol{\alpha}}:\boldsymbol{x}_{\boldsymbol{\alpha}}[i]=x_i} \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{j\in\mathcal{N}(\alpha)\backslash i} \mu_{j\to\alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])$$

(Acyclic) Belief Propagation

In a factor graph with no cycles:
1. Pick any node to serve as the root.
2. Send messages from the **leaves** to the **root**.
3. Send messages from the **root** to the **leaves**.

A node computes an outgoing message along an edge only after it has received incoming messages along all its other edges.



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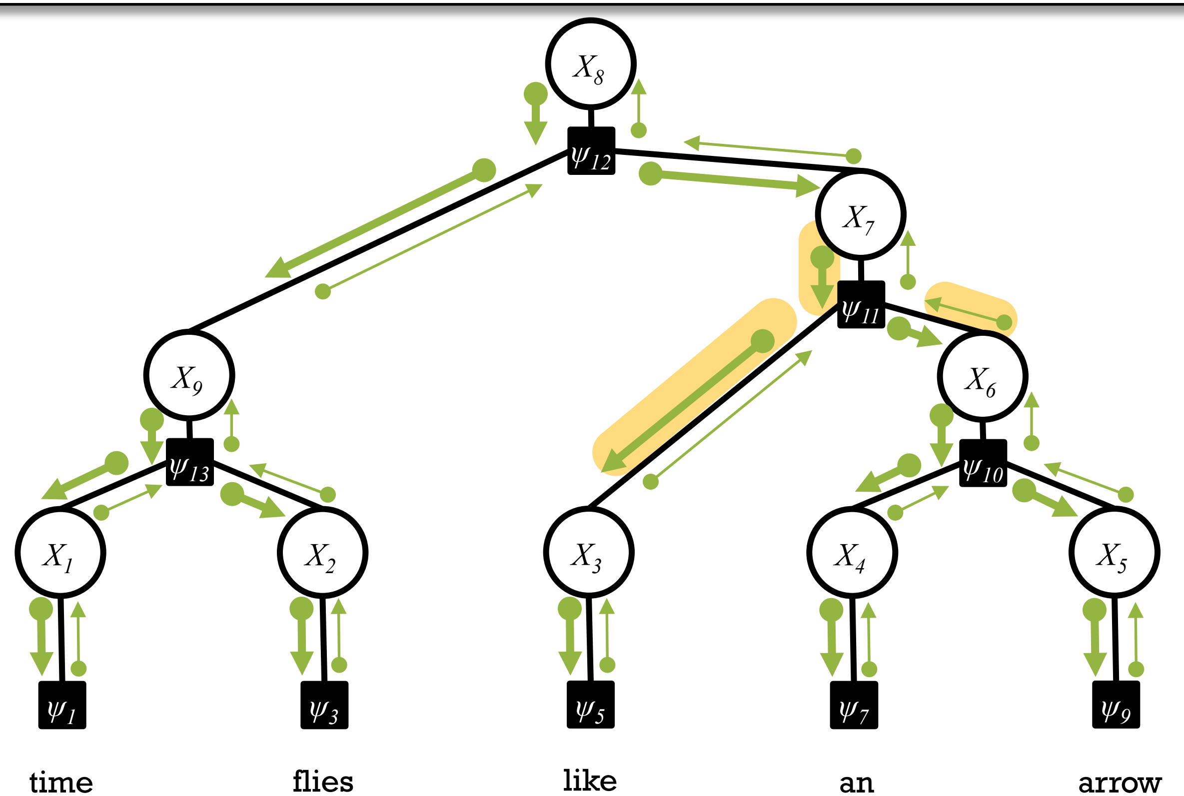
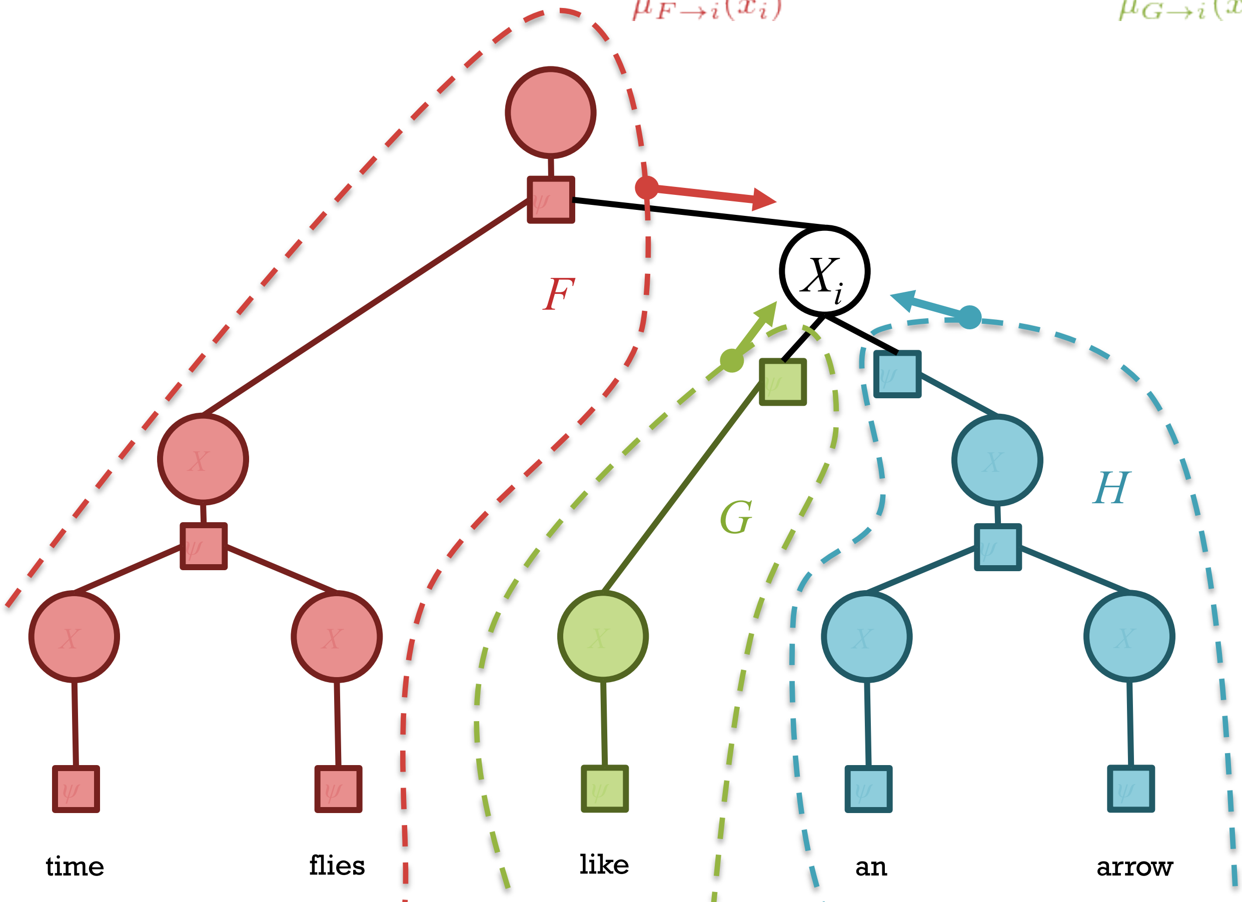


Acyclic BP as Dynamic Programming

$$p(X_i = x_i) \propto b_i(x_i) = \sum_{\boldsymbol{x}:\boldsymbol{x}[i]=x_i} \prod_{\alpha} \psi_\alpha(\boldsymbol{x}_\alpha)$$

$$= \underbrace{\left(\sum_{\boldsymbol{x}:\boldsymbol{x}[i]=x_i} \prod_{\alpha \subseteq F} \psi_\alpha(\boldsymbol{x}_\alpha) \right)}_{\mu_{F\to i}(x_i)} \underbrace{\left(\sum_{\boldsymbol{x}:\boldsymbol{x}[i]=x_i} \prod_{\alpha \subseteq G} \psi_\alpha(\boldsymbol{x}_\alpha) \right)}_{\mu_{G\to i}(x_i)} \underbrace{\left(\sum_{\boldsymbol{x}:\boldsymbol{x}[i]=x_i} \prod_{\alpha \subseteq H} \psi_\alpha(\boldsymbol{x}_\alpha) \right)}_{\mu_{H\to i}(x_i)}$$



Subproblem:
Inference using just the factors in subgraph H

Figure adapted from Burkett & Klein (2012)

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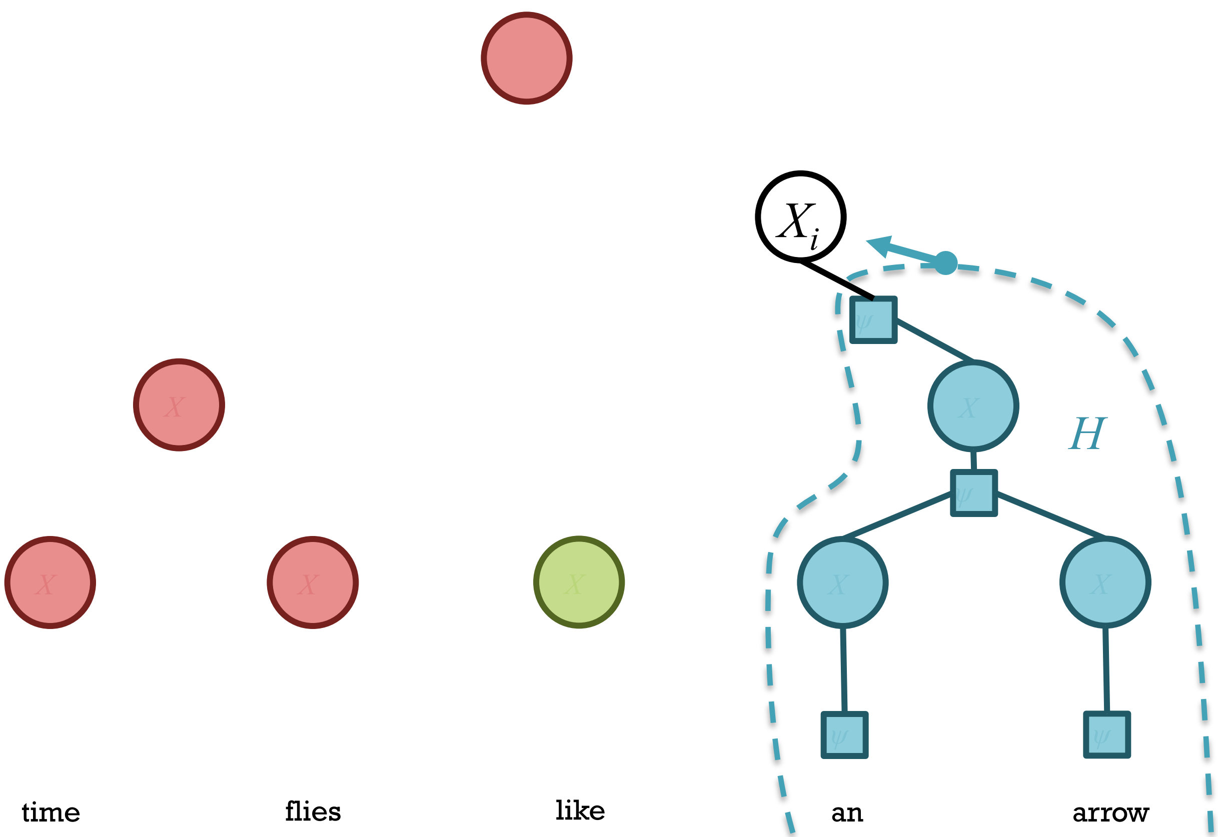

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The marginal of X_i in that smaller model is the message sent to X_i from subgraph H

*Message **to** a variable*

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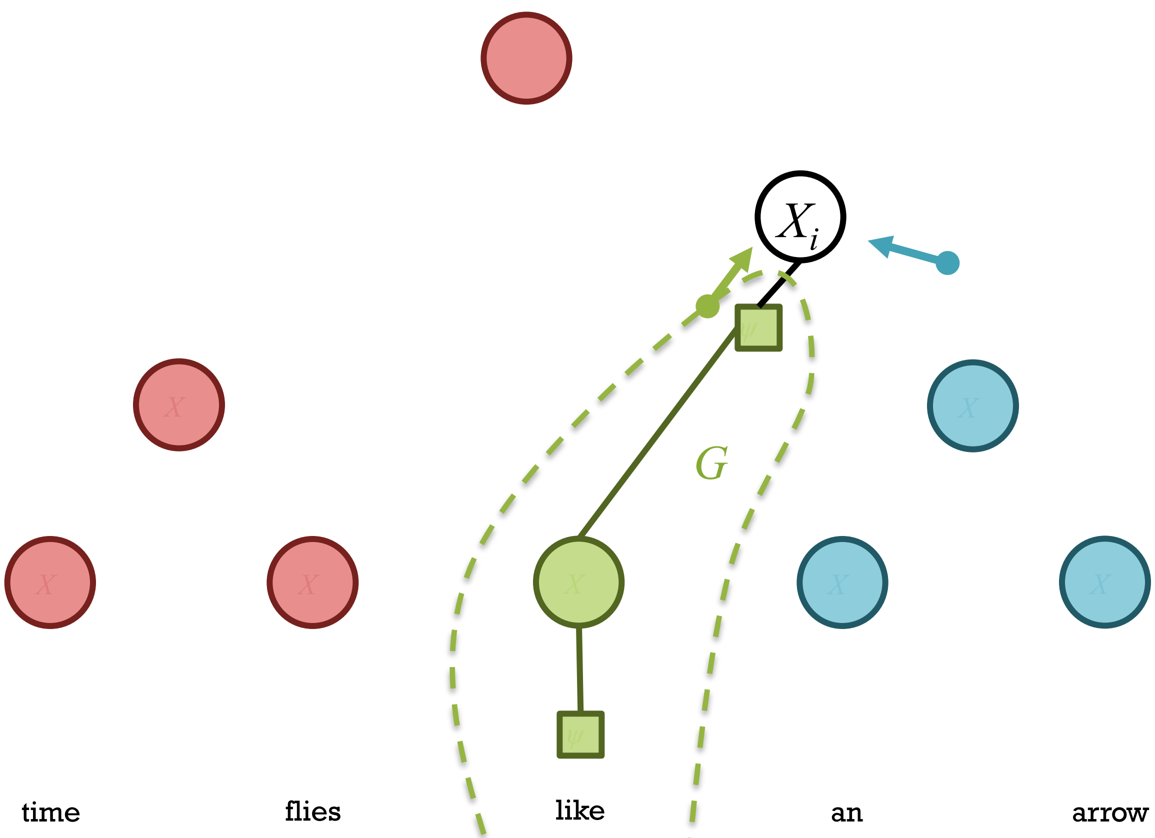

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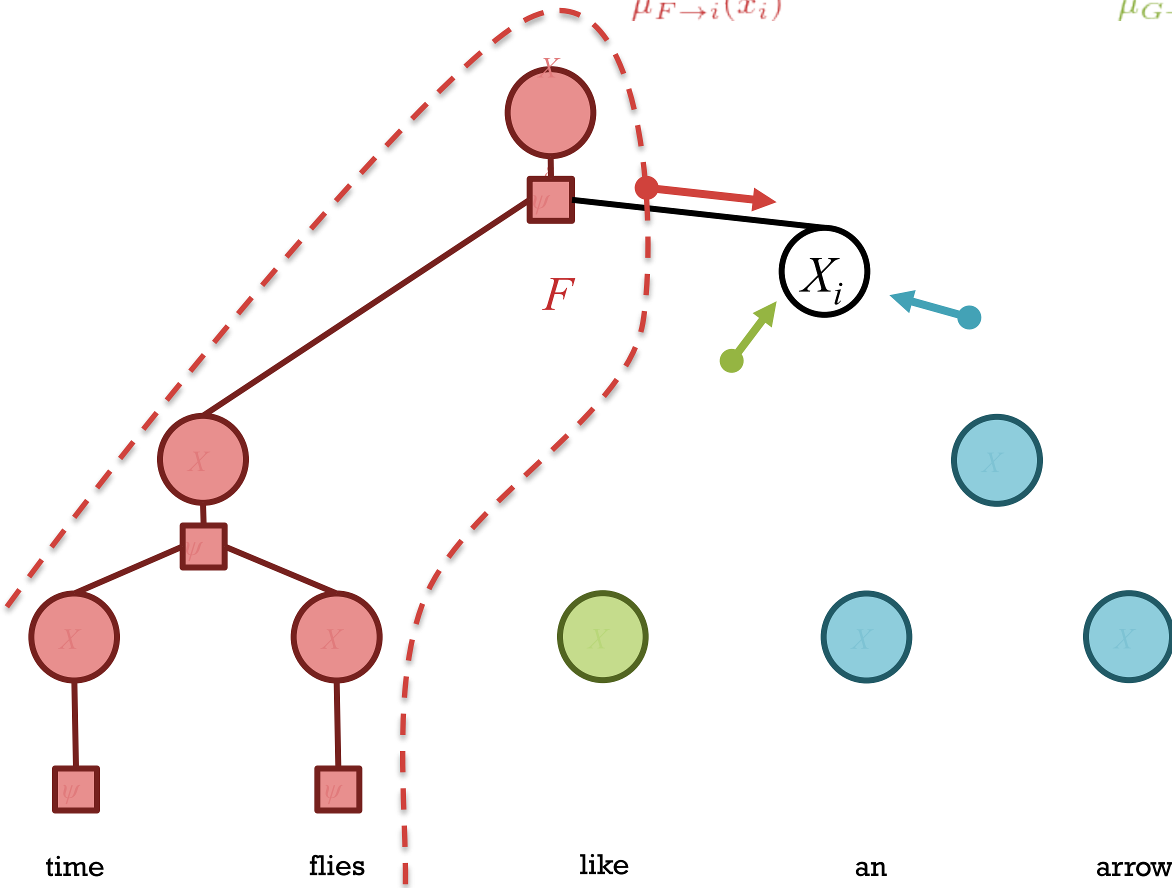

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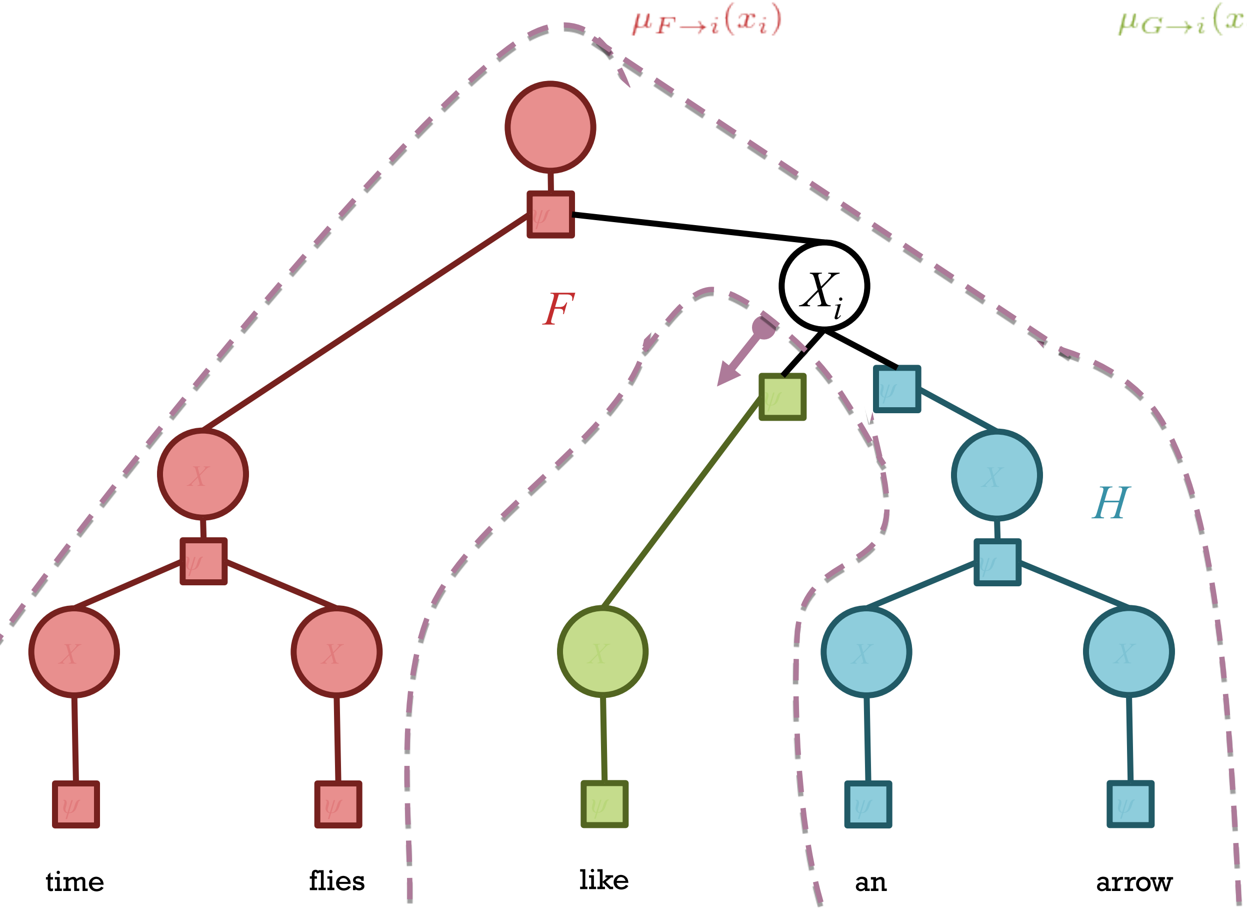


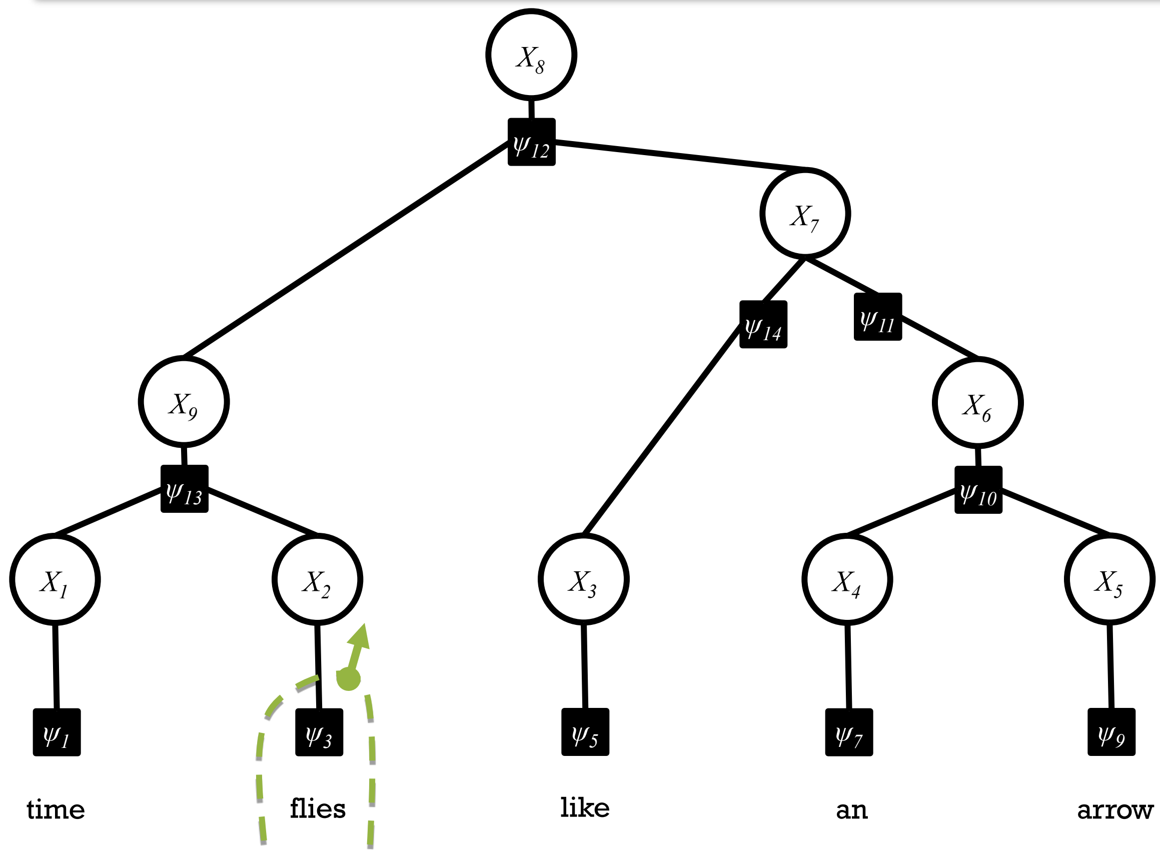
Subproblem:
Inference using just the factors in subgraph $F \cup H$

The marginal of X_i in that smaller model is the message sent by X_i <u>out of</u> subgraph $F \cup H$

***Message from** a variable*

Acyclic BP as Dynamic Programming

- If you want the **marginal** $p_i(x_i)$ where X_i has degree k, you can think of that summation as a **product of k marginals** computed on smaller subgraphs.
- Each subgraph is obtained by **cutting** some edge of the tree.
- The message-passing algorithm uses **dynamic programming** to compute the marginals on all such subgraphs, working from **smaller to bigger**. So you can compute all the marginals.



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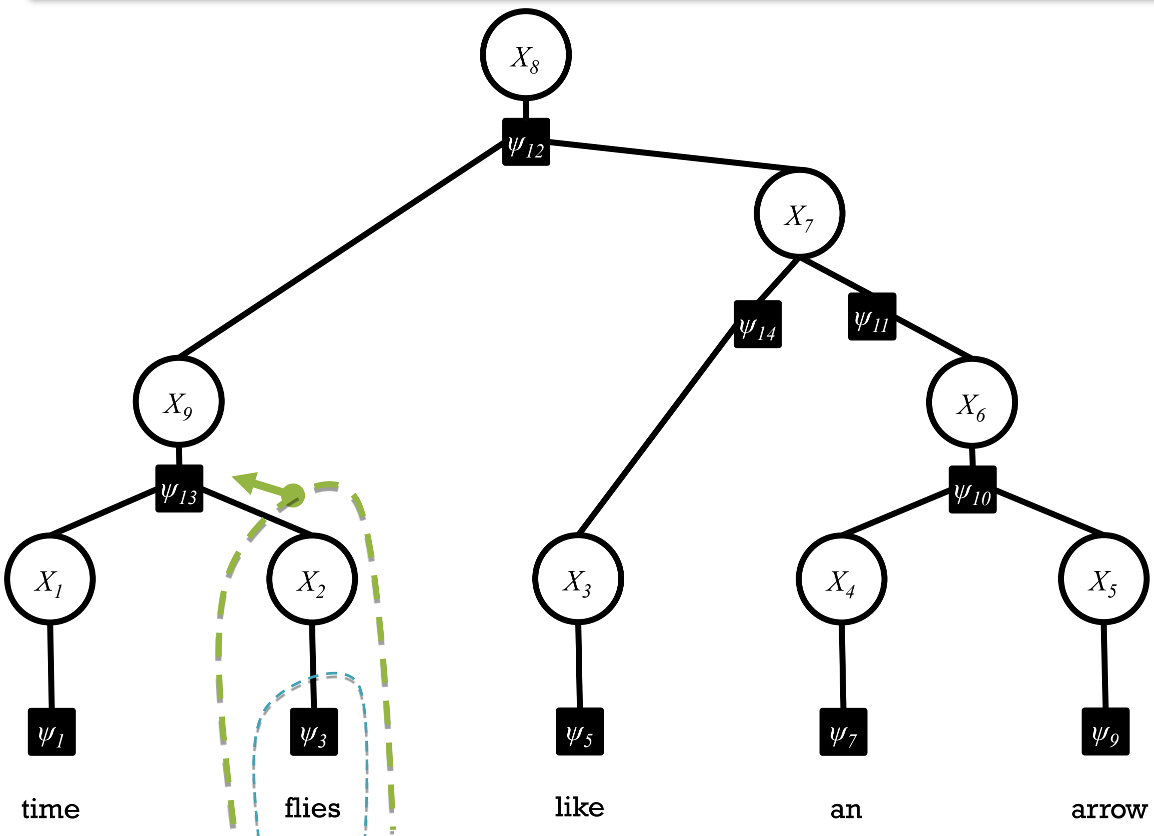

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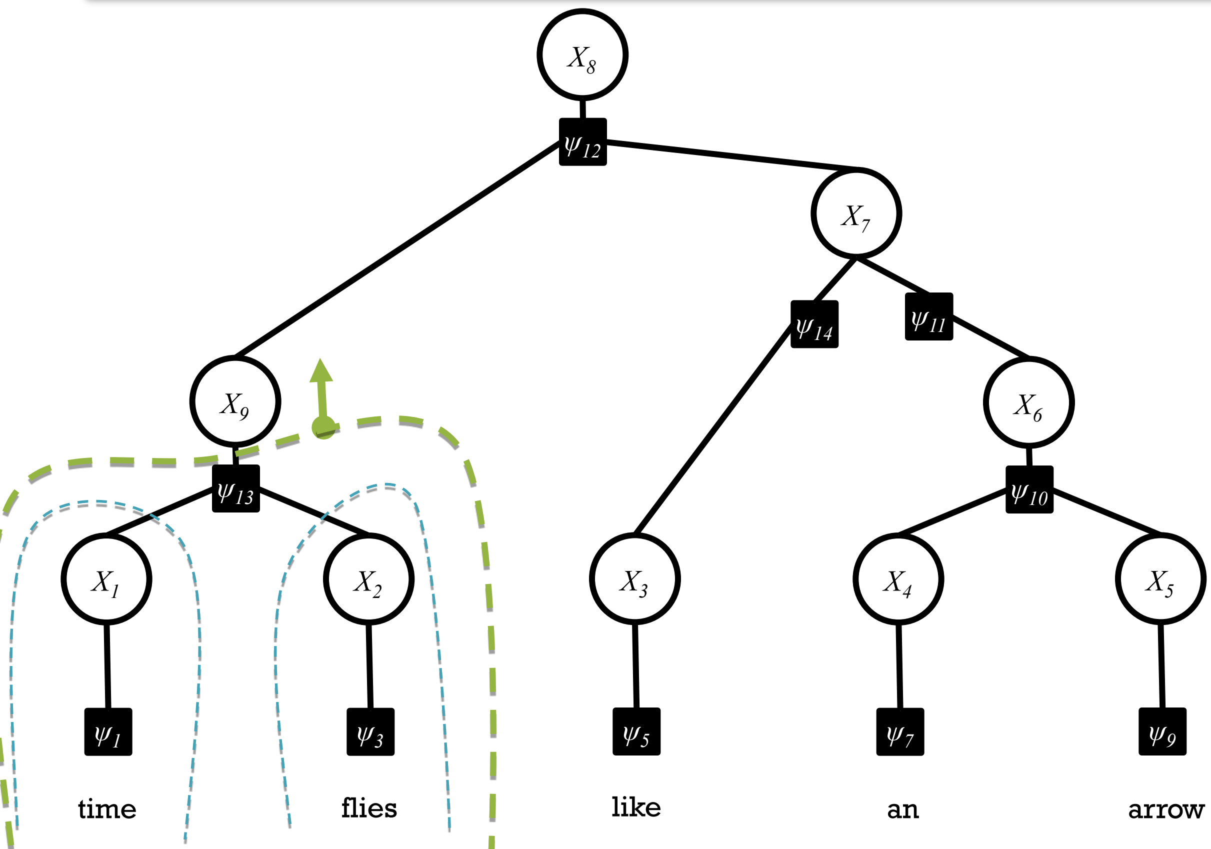

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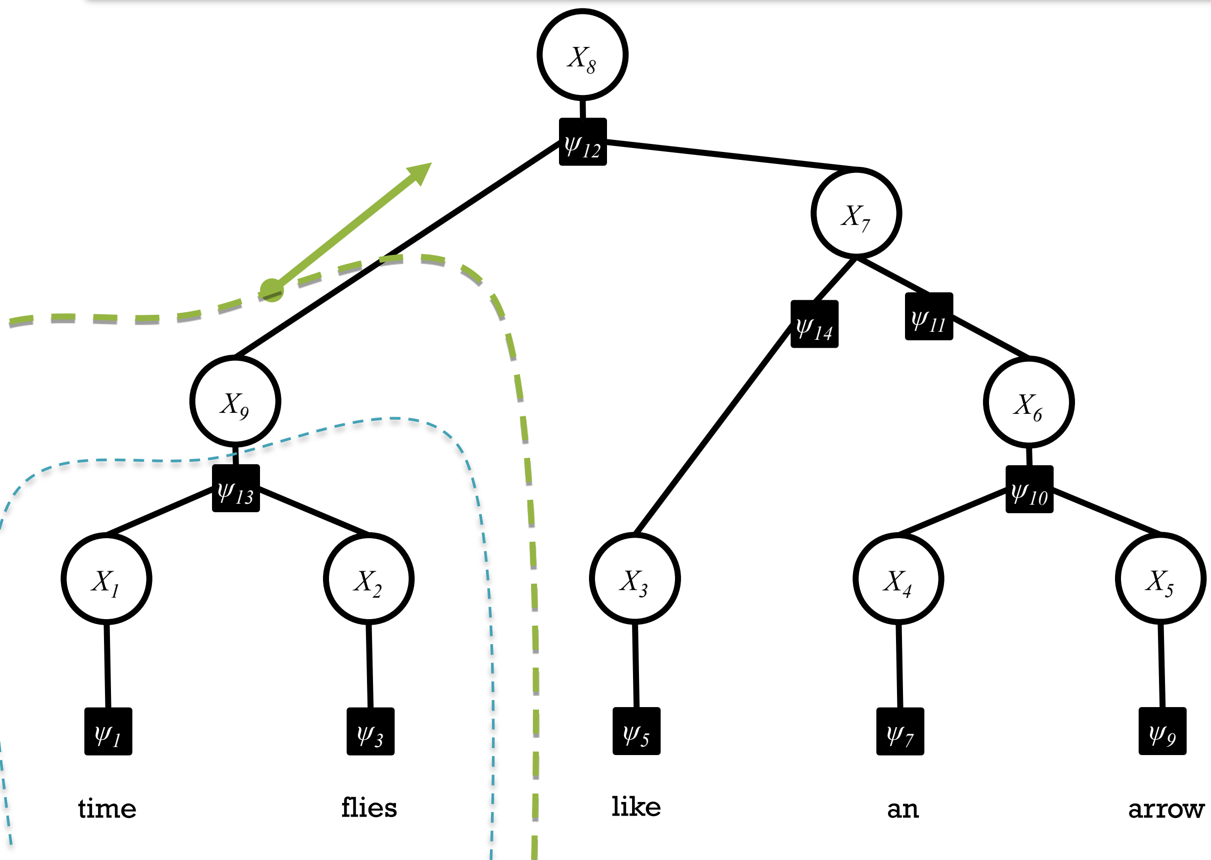

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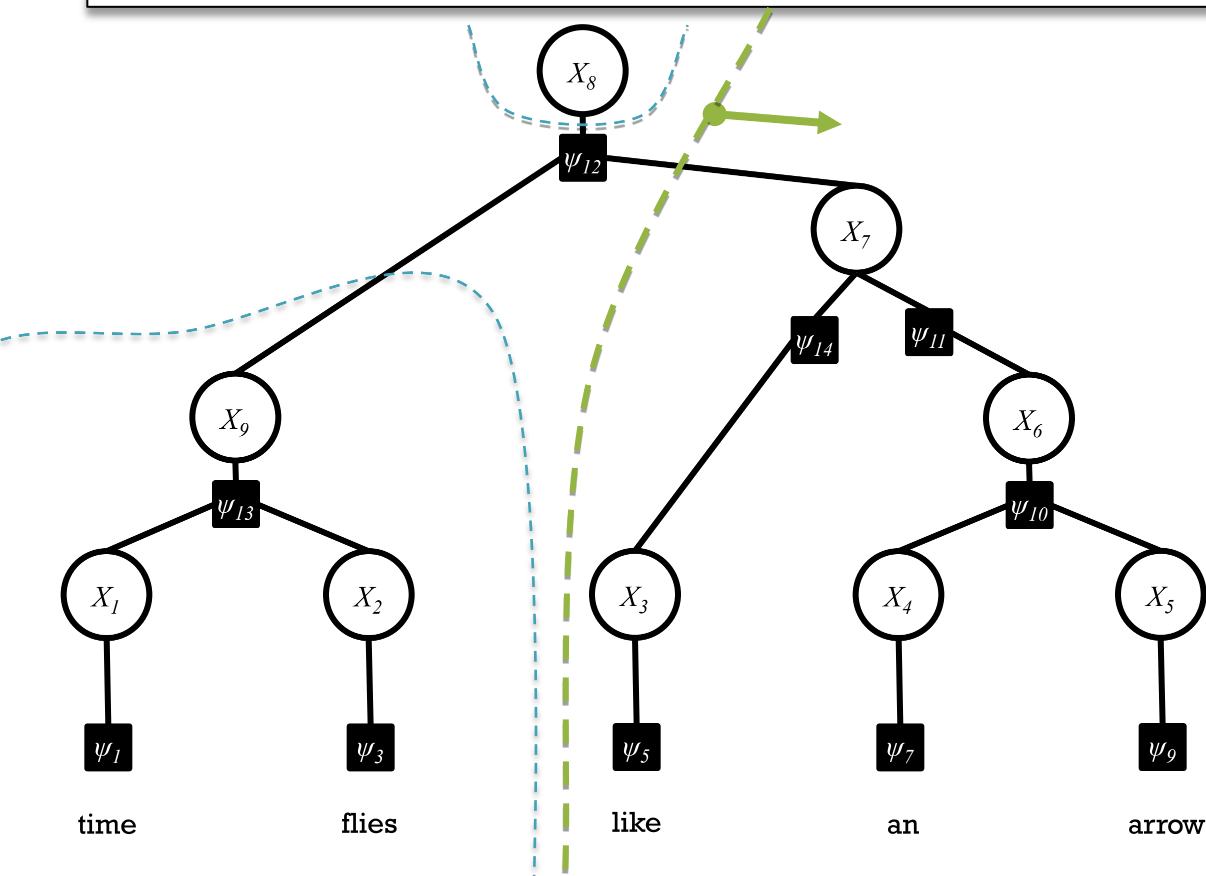

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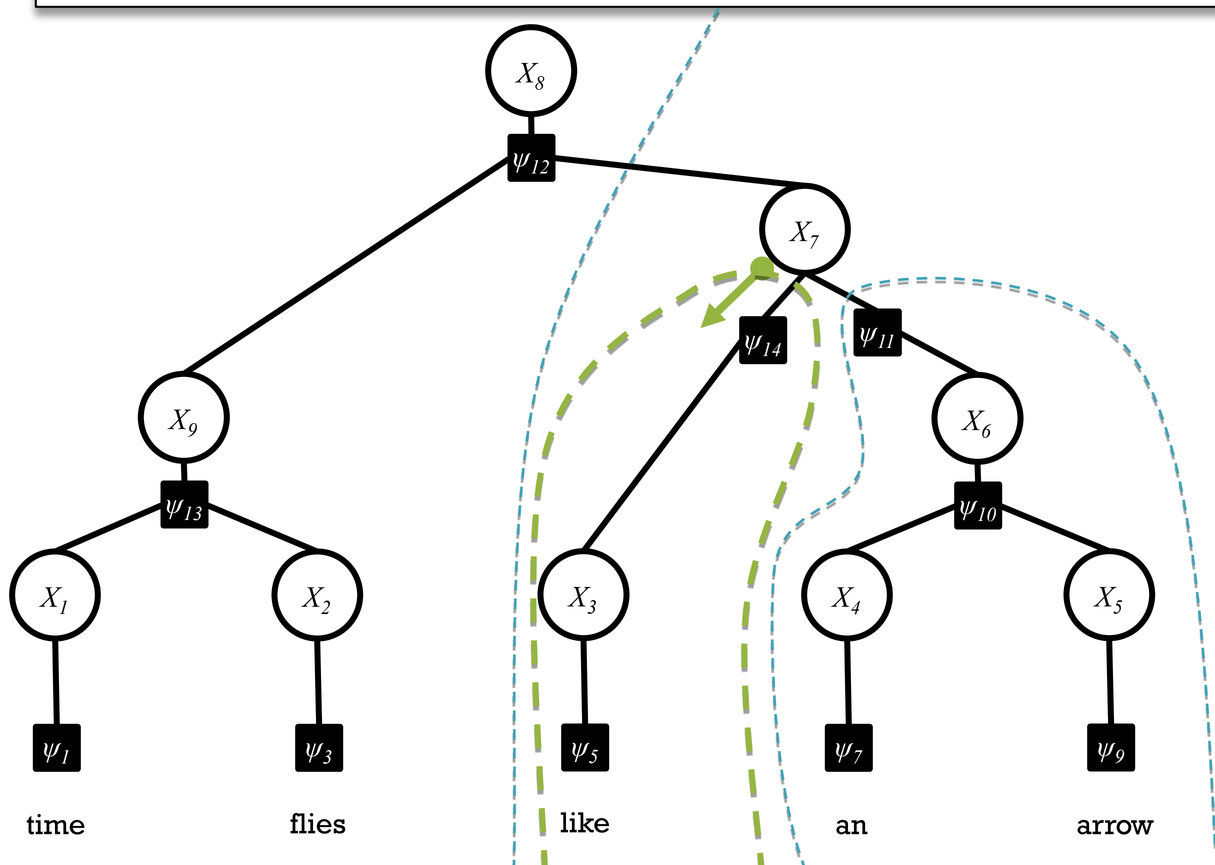

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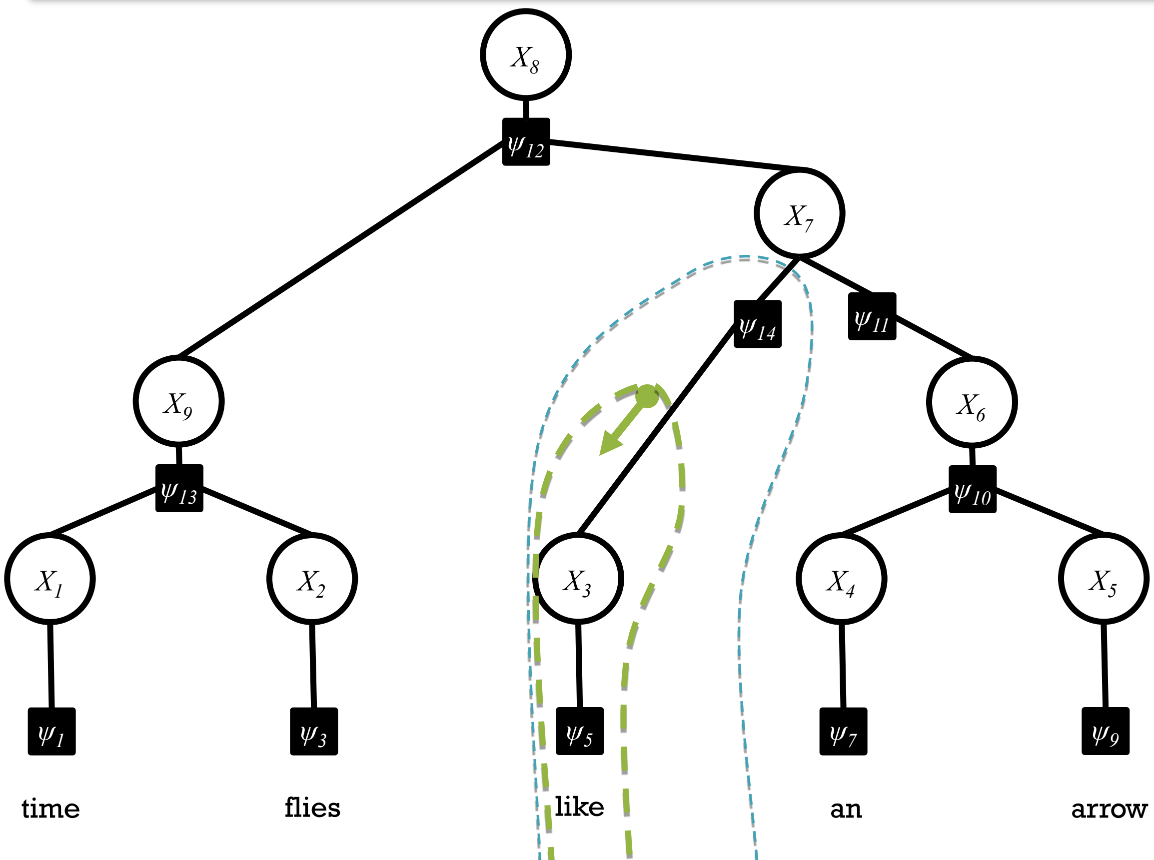

Exact MAP inference for factor trees

MAX-PRODUCT BELIEF PROPAGATION

Max-product Belief Propagation

- **Sum-product BP** can be used to compute the marginals, $p_i(X_i)$
- **Max-product BP** can be used to compute the most likely assignment, $\boldsymbol{X}^* = \mathrm{argmax}_{\boldsymbol{X}}\, p(\boldsymbol{X})$

Max-product Belief Propagation

- Change the sum to a max:

$$\mu_{i \to \alpha}(x_i) = \prod_{\alpha \in \mathcal{N}(i) \setminus \alpha} \mu_{\alpha \to i}(x_i)$$

$$\mu_{\alpha \to i}(x_i) = \sum_{\boldsymbol{x}_{\boldsymbol{\alpha}} : \boldsymbol{x}_{\boldsymbol{\alpha}}[i] = x_i} \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{j \in \mathcal{N}(\alpha) \setminus i} \mu_{j \to \alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])$$

- **Max-product BP** computes **max-marginals**
  - The max-marginal $b_i(x_i)$ is the (unnormalized) probability of the MAP assignment under the constraint $X_i = x_i$.
  - For an acyclic graph, the MAP assignment (assuming there are no ties) is given by:

$$x_i^* = \arg\max_{x_i} b_i(x_i)$$

Max-product Belief Propagation

- Change the sum to a max:

$$\mu_{i \to \alpha}(x_i) = \prod_{\alpha \in \mathcal{N}(i) \setminus \alpha} \mu_{\alpha \to i}(x_i)$$

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Deterministic Annealing

Motivation: Smoothly transition from sum-product to max-product

1. Incorporate inverse temperature parameter into each factor:

Annealed Joint Distribution

$$p(\boldsymbol{x}) = \frac{1}{Z} \prod_{\alpha} \psi_{\alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}})^{\frac{1}{T}}$$

2. Send messages as usual for sum-product BP
3. Anneal T from 1 to 0:

$T = 1$	Sum-product
$T \rightarrow 0$	Max-product

4. Take resulting beliefs to power T

Semirings

- Sum-product +/* and max-product max/* are commutative semirings
- We can run BP with any such commutative semiring

$$\boxed{\mu_{i\to\alpha}(x_i) = \prod_{\alpha\in\mathcal{N}(i)\setminus\alpha} \mu_{\alpha\to i}(x_i)}$$

$$\boxed{\mu_{\alpha\to i}(x_i) = \sum_{\boldsymbol{x}_{\boldsymbol{\alpha}}:\boldsymbol{x}_{\boldsymbol{\alpha}}[i]=x_i} \psi_\alpha(\boldsymbol{x}_{\boldsymbol{\alpha}}) \prod_{j\in\mathcal{N}(\alpha)\setminus i} \mu_{j\to\alpha}(\boldsymbol{x}_{\boldsymbol{\alpha}}[i])}$$

- In practice, multiplying many small numbers together can yield underflow
  - instead of using +/*, we use log-add/+
  - Instead of using max/*, we use max/+

Exact inference for linear chain models

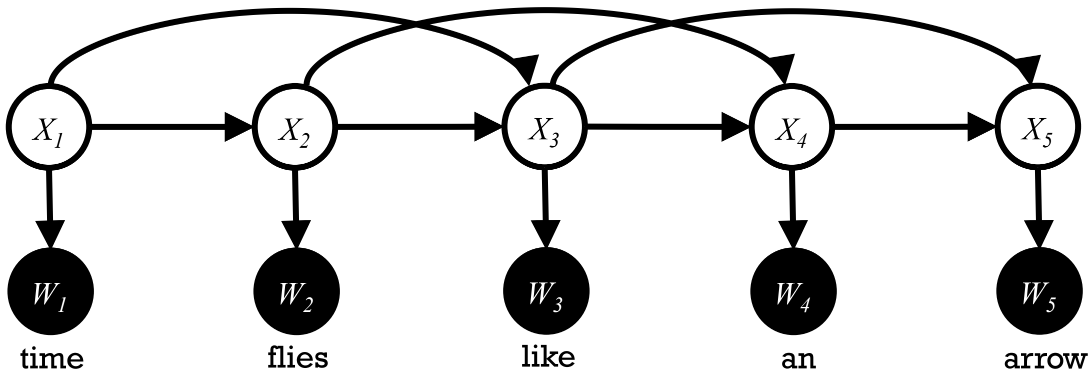
FORWARD-BACKWARD AND VITERBI ALGORITHMS

Forward-Backward Algorithm

- Sum-product BP on an HMM is called the **forward-backward algorithm**
- Max-product BP on an HMM is called the **Viterbi algorithm**

Forward-Backward Algorithm

Trigram HMM is not a tree, even when converted to a factor graph



Forward-Backward Algorithm

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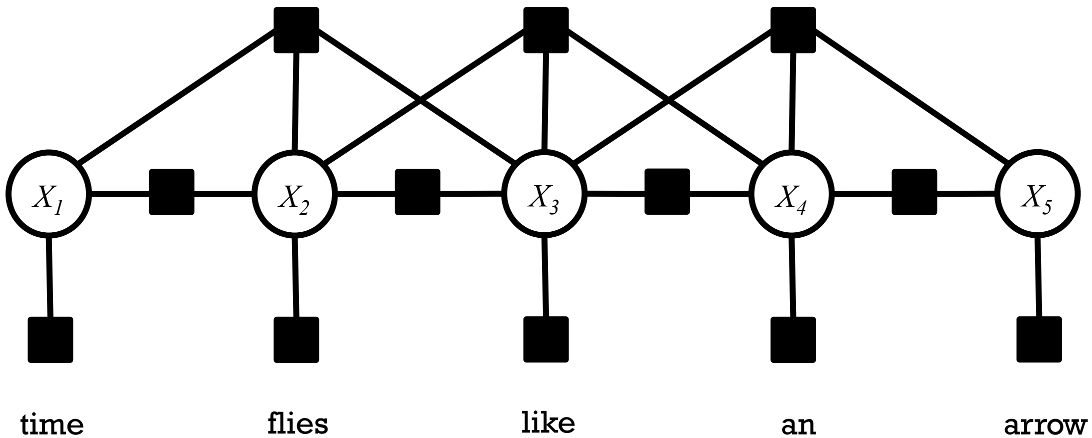
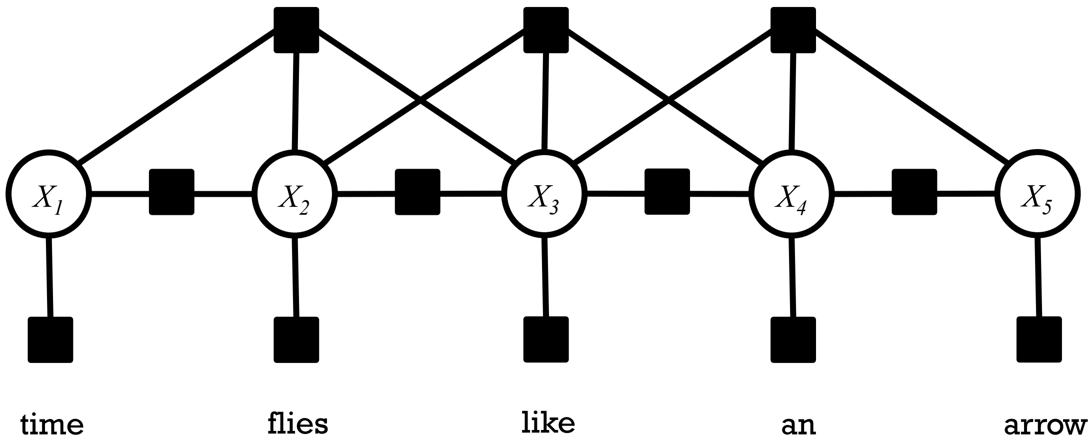


Forward-Backward Algorithm

Trigram HMM is not a tree, even when converted to a factor graph



Trick: (See also Sha & Pereira (2003))

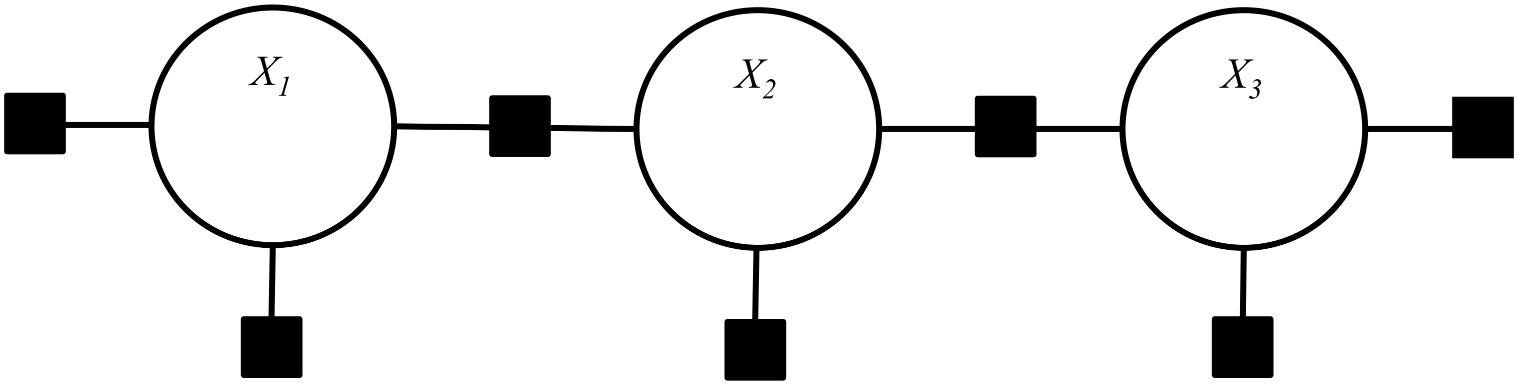
- Replace each variable domain with its cross product
  e.g. {B,I,O} → {BB, BI, BO, IB, II, IO, OB, OI, OO}
- Replace each pair of variables with a single one. For all i, $y_{i,i+1} = (x_i, x_{i+1})$
- Add features with weight -∞ that disallow illegal configurations between pairs of the new variables
  e.g. **legal** = BI and IO **illegal** = II and OO
- This is effectively a special case of the junction tree algorithm

Summary

1. **Factor Graphs**
   - Alternative representation of directed / undirected graphical models
   - Make the cliques of an undirected GM explicit
2. **Variable Elimination**
   - Simple and general approach to exact inference
   - Just a matter of being clever when computing sum-products
3. **Sum-product Belief Propagation**
   - Computes all the marginals and the partition function in only twice the work of Variable Elimination
4. **Max-product Belief Propagation**
   - Identical to sum-product BP, but changes the semiring
   - Computes: max-marginals, probability of MAP assignment, and (with backpointers) the MAP assignment itself.

EXTRA SLIDES ON FORWARD BACKWARD AS SUM-PRODUCT BP

CRF Tagging Model



find

preferred

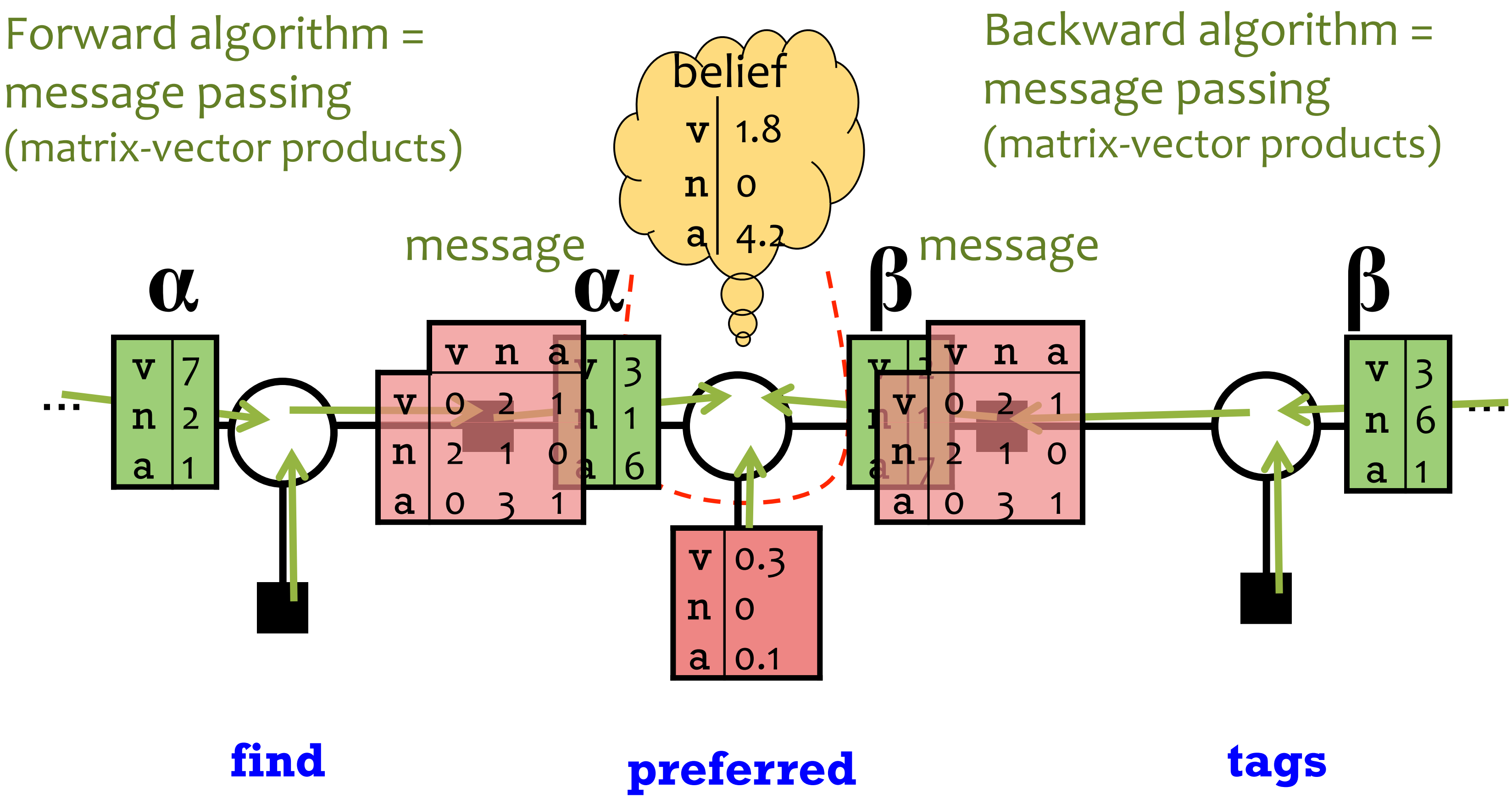
tags

Could be verb or noun

Could be adjective or verb

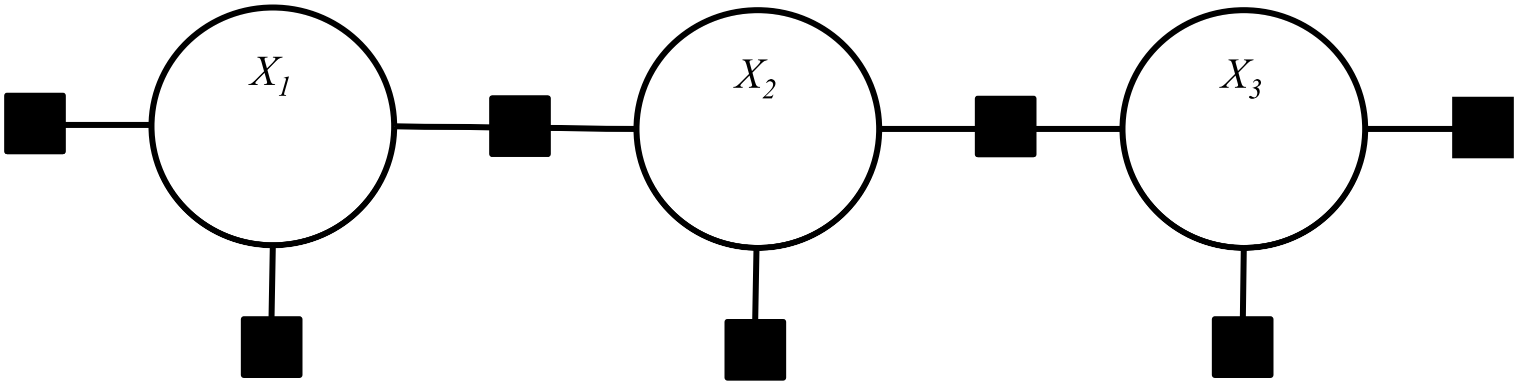
Could be noun or verb

CRF Tagging by Belief Propagation



- Forward-backward is a message passing algorithm.
- It’s the simplest case of belief propagation.

So Let's Review Forward-Backward …



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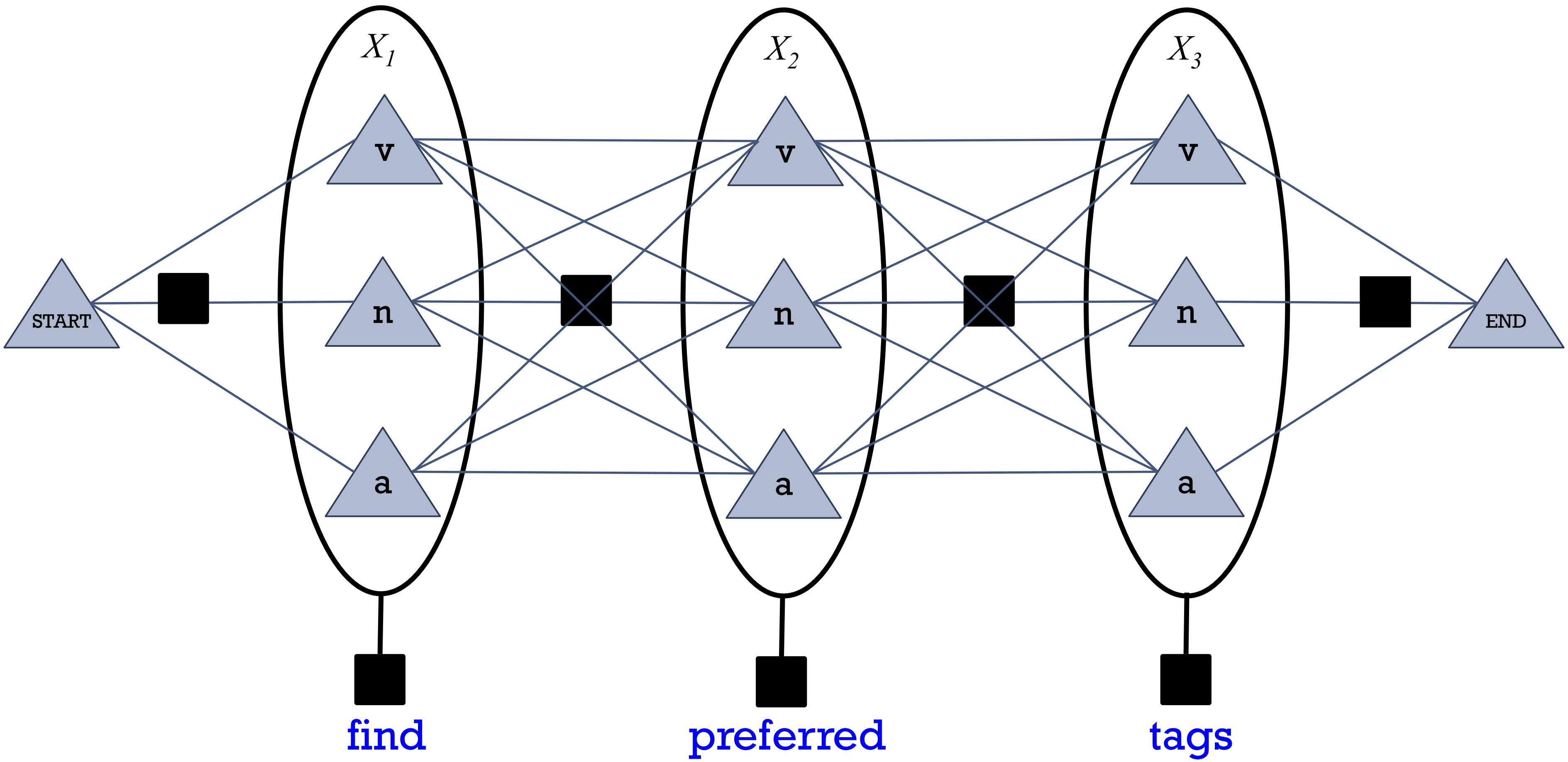
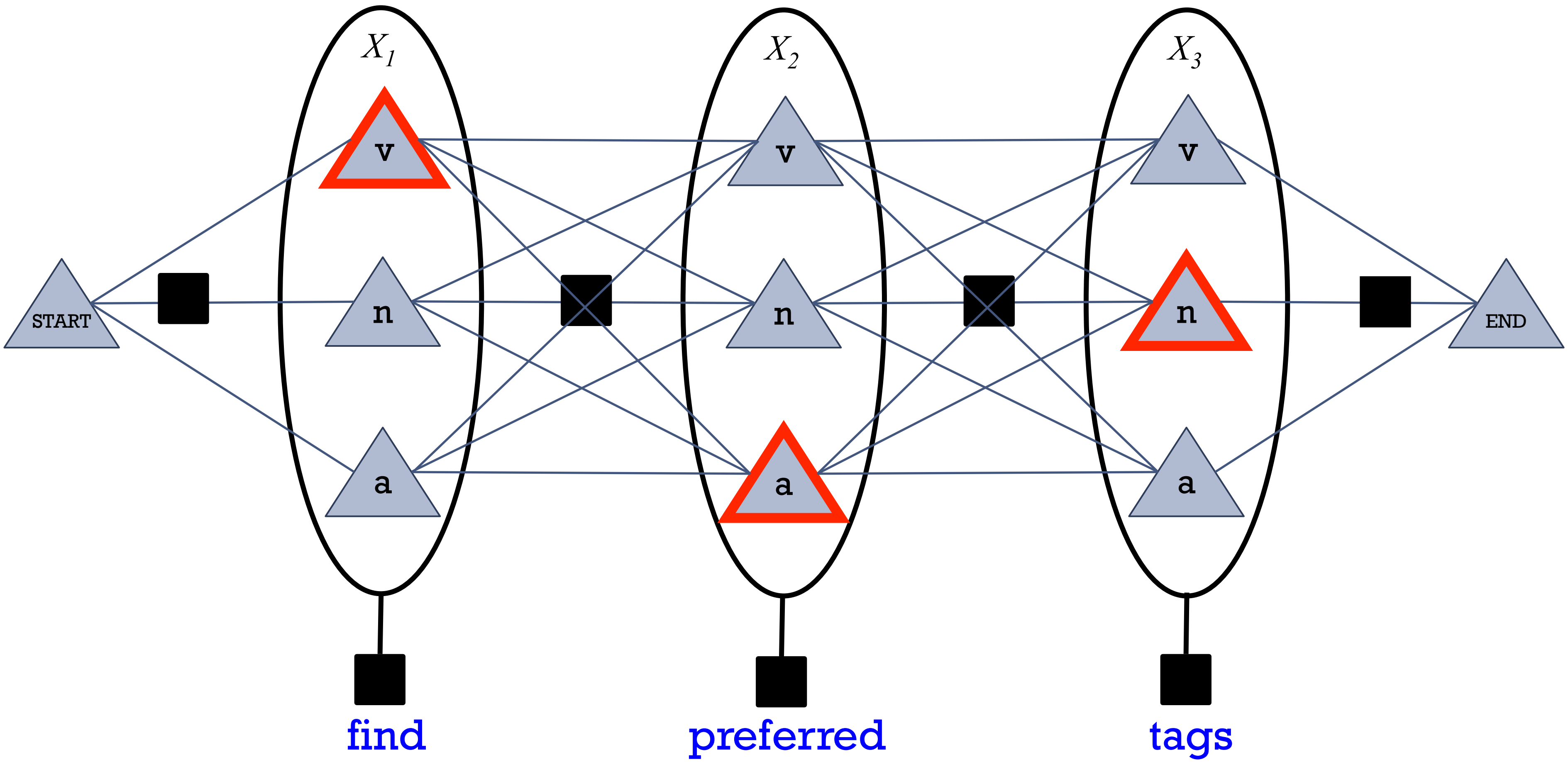


- Show the possible *values* for each variable

So Let's Review Forward-Backward …



- Let's show the possible *values* for each variable
- One possible assignment

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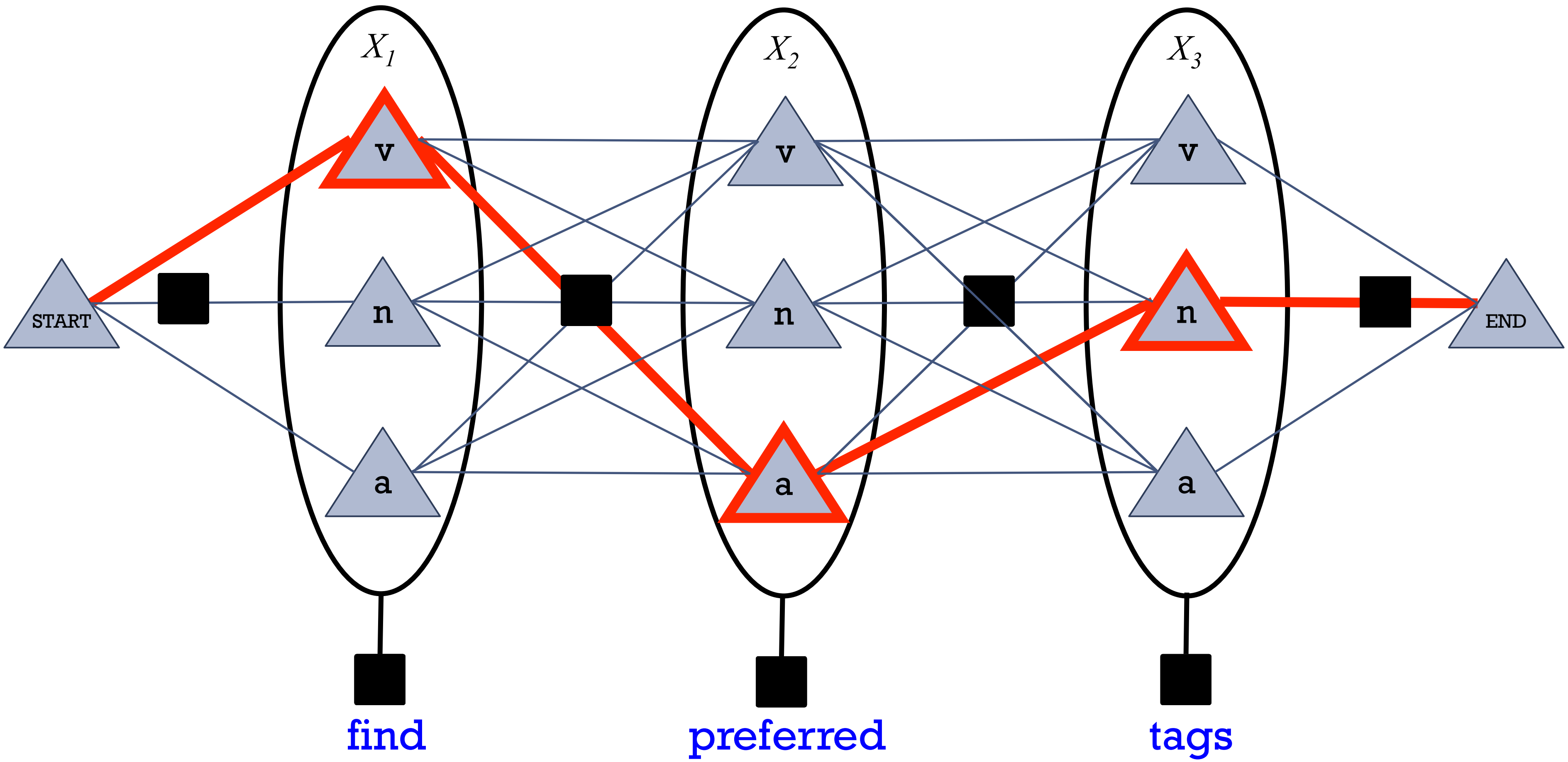
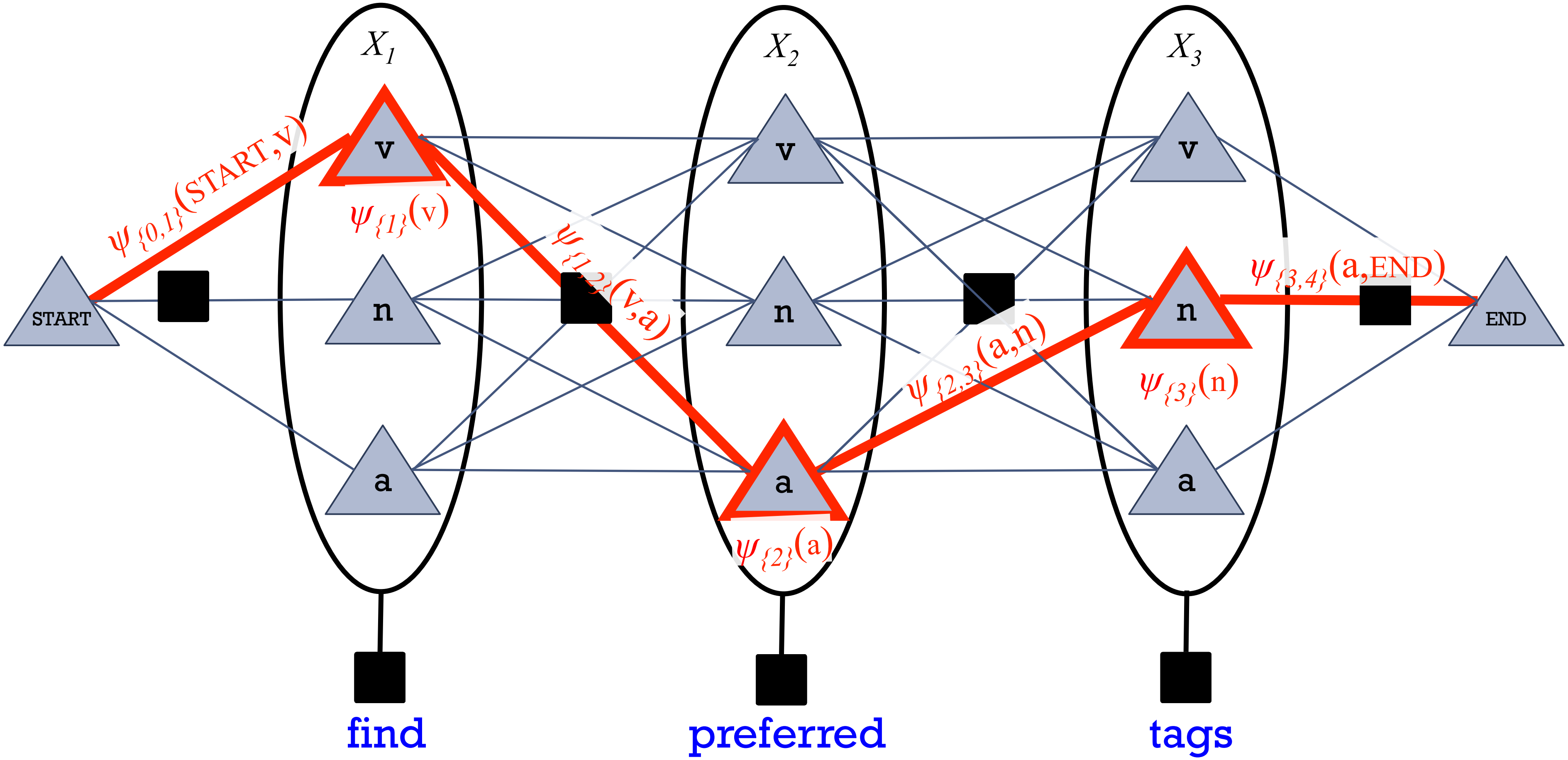


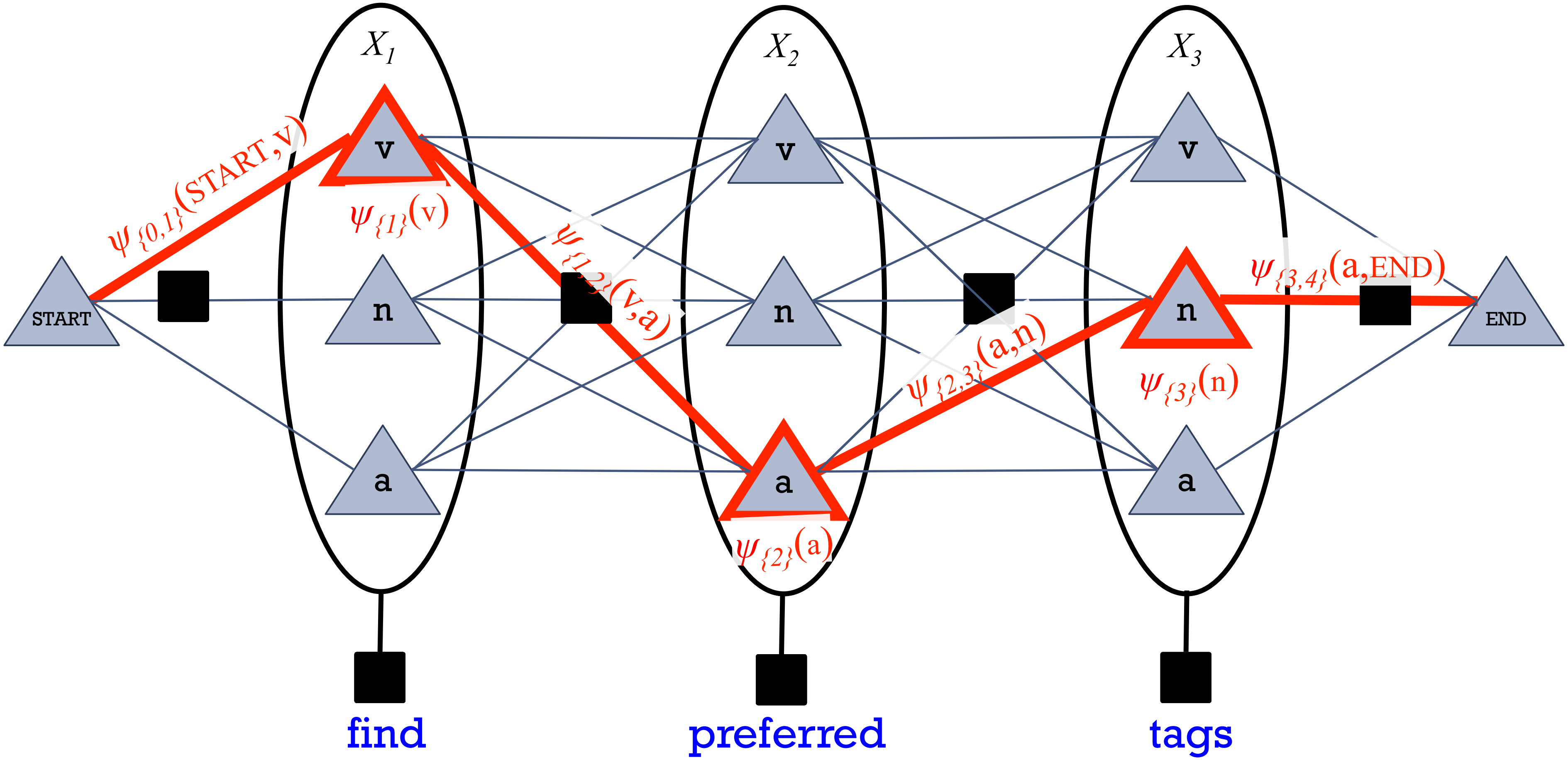
- Let's show the possible *values* for each variable
- One possible assignment
- And what the 7 factors think of it …

Viterbi Algorithm: Most Probable Assignment



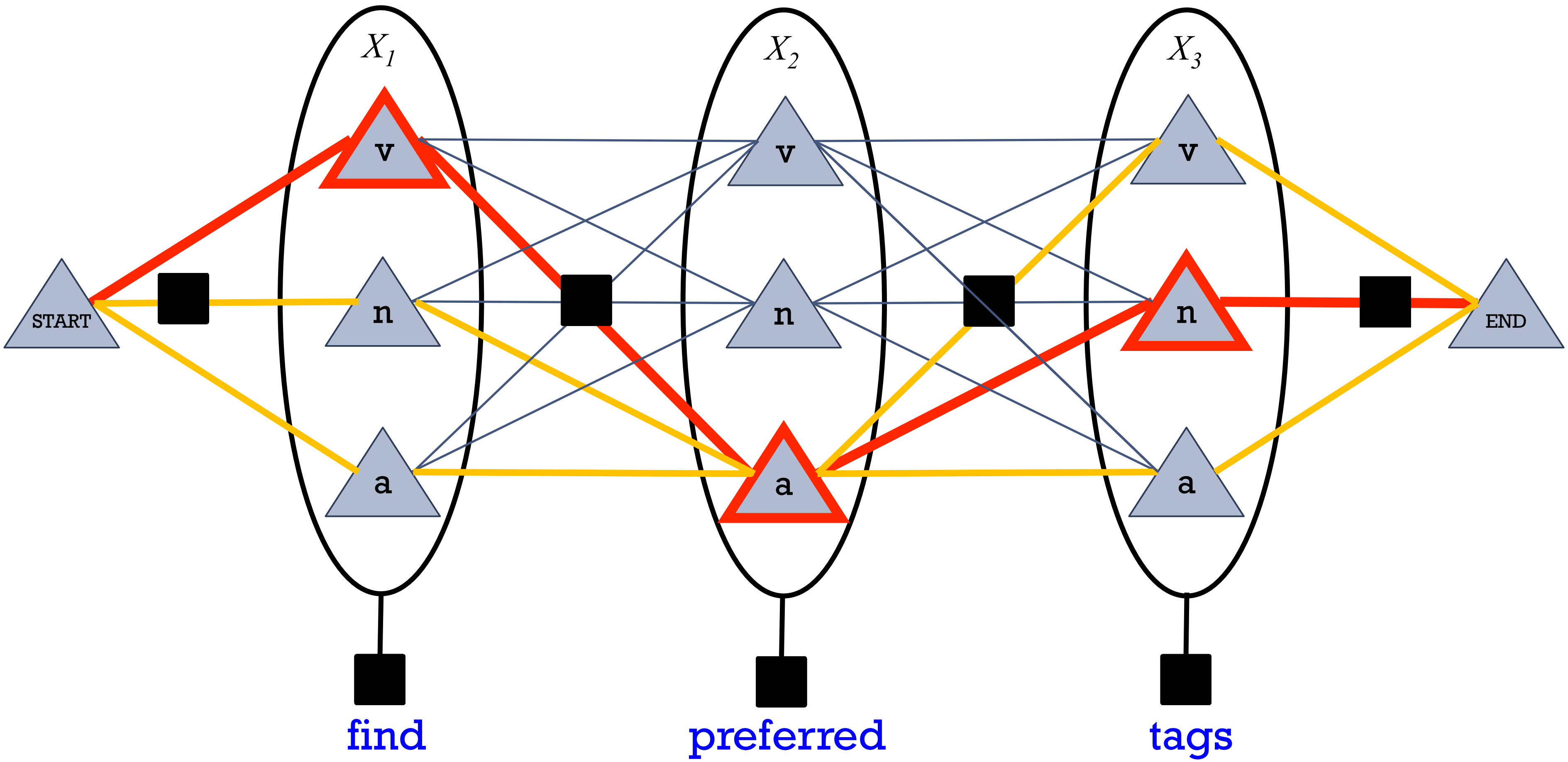
- So p(**v a n**) = (1/Z) * product of 7 numbers
- Numbers associated with edges and nodes of path
- Most probable assignment = **path with highest product**

Viterbi Algorithm: Most Probable Assignment



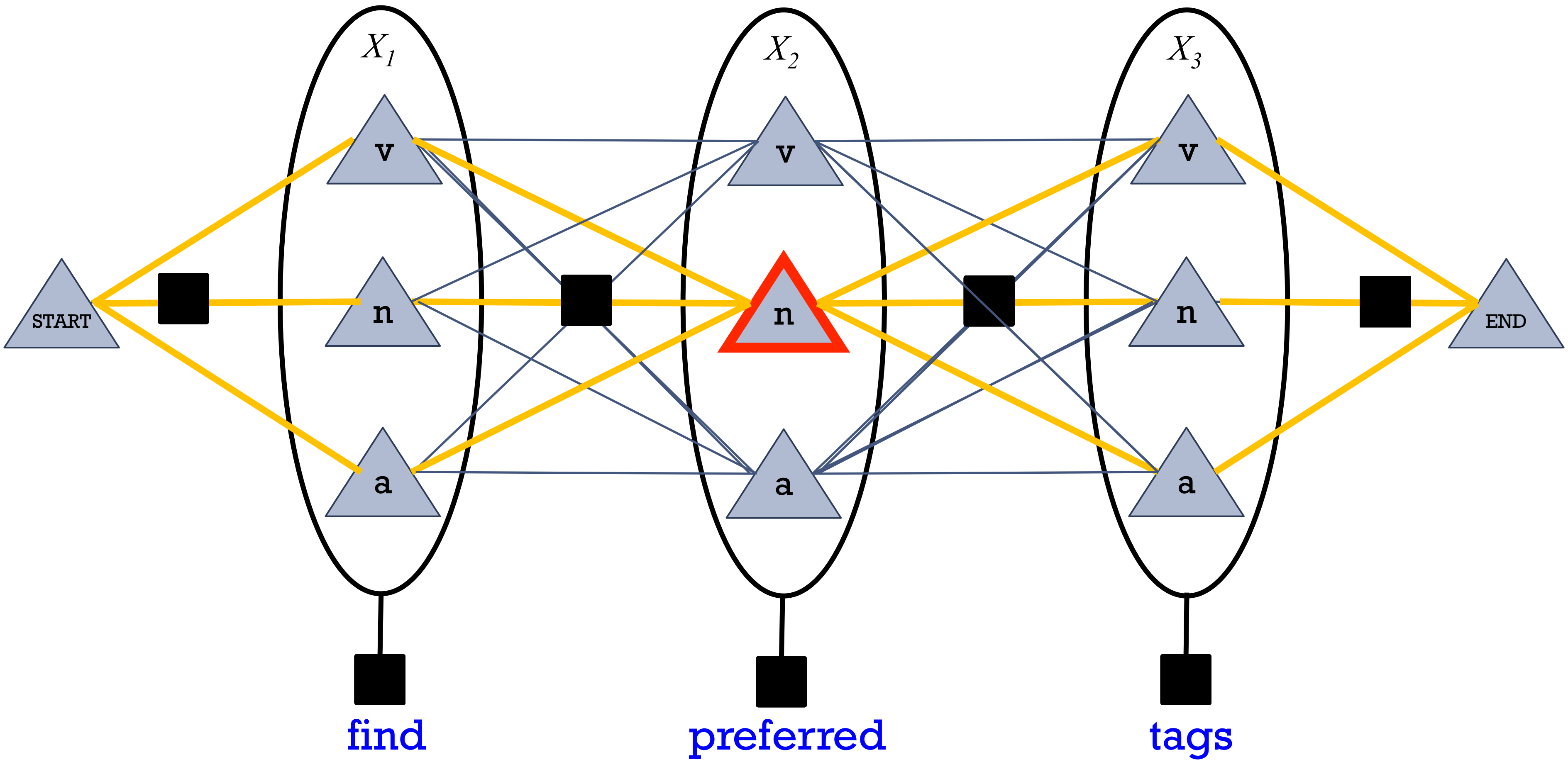
- So p(**v a n**) = (1/Z) * product weight of one path

Forward-Backward Algorithm: Finds Marginals



- So p(**v a n**) = (1/Z) * product weight of one path
- Marginal probability $p(X_2 = a)$
  = (1/Z) * total weight of *all* paths through a

Forward-Backward Algorithm: Finds Marginals



- So p(**v a n**) = (1/Z) * product weight of one path
- Marginal probability $p(X_2 = a)$
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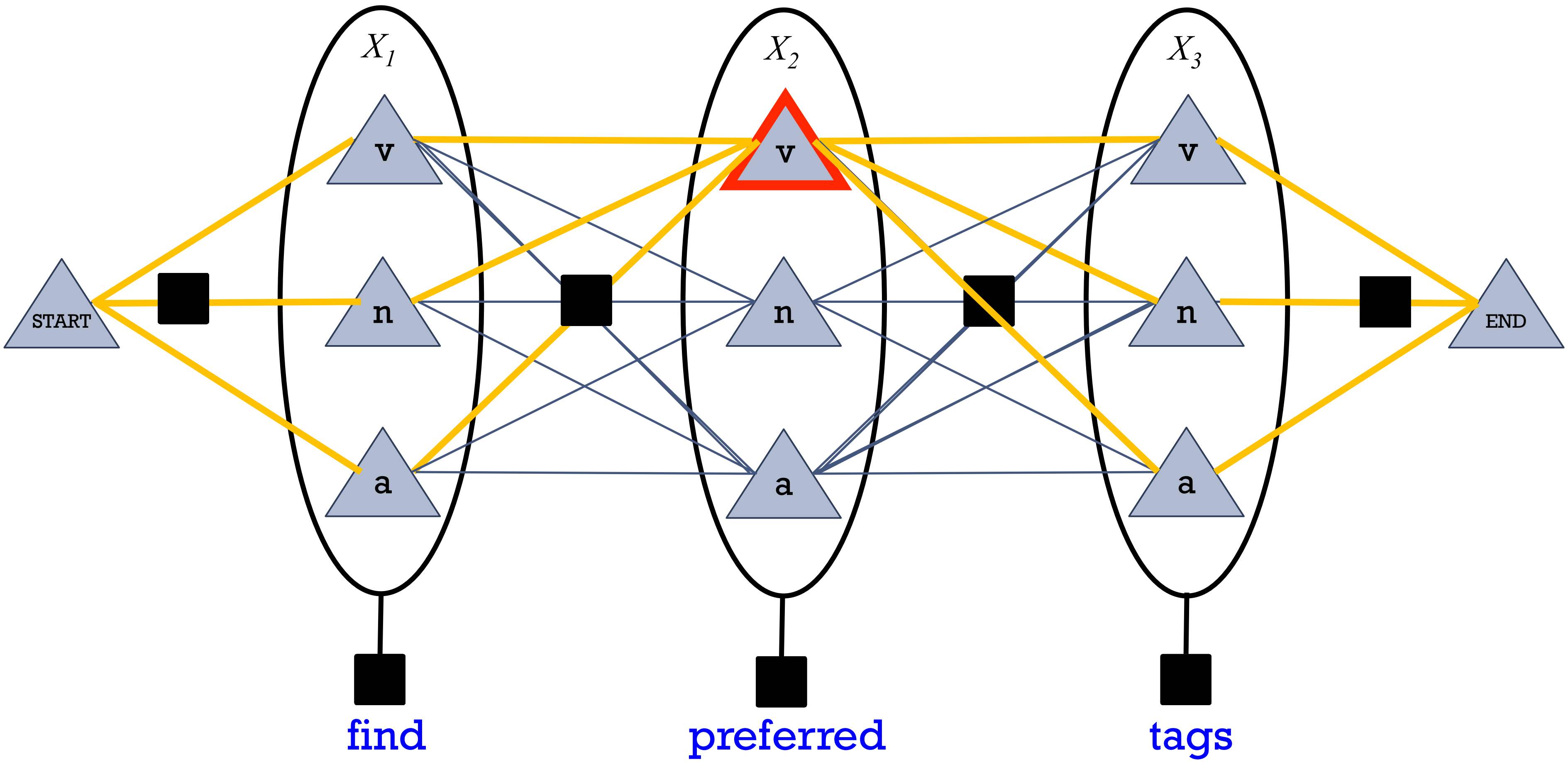
Forward-Backward Algorithm: Finds Marginals



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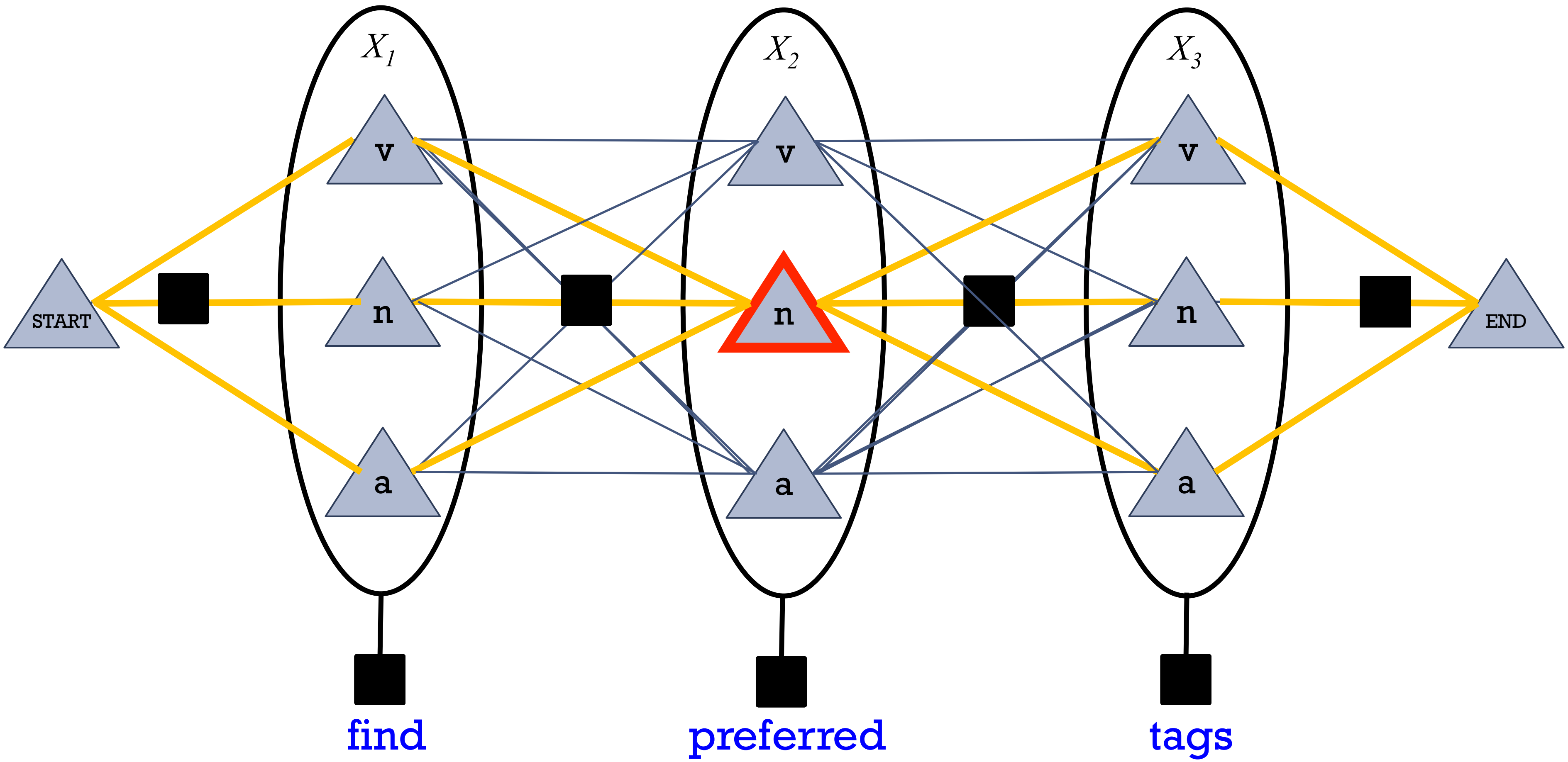
Forward-Backward Algorithm: Finds Marginals



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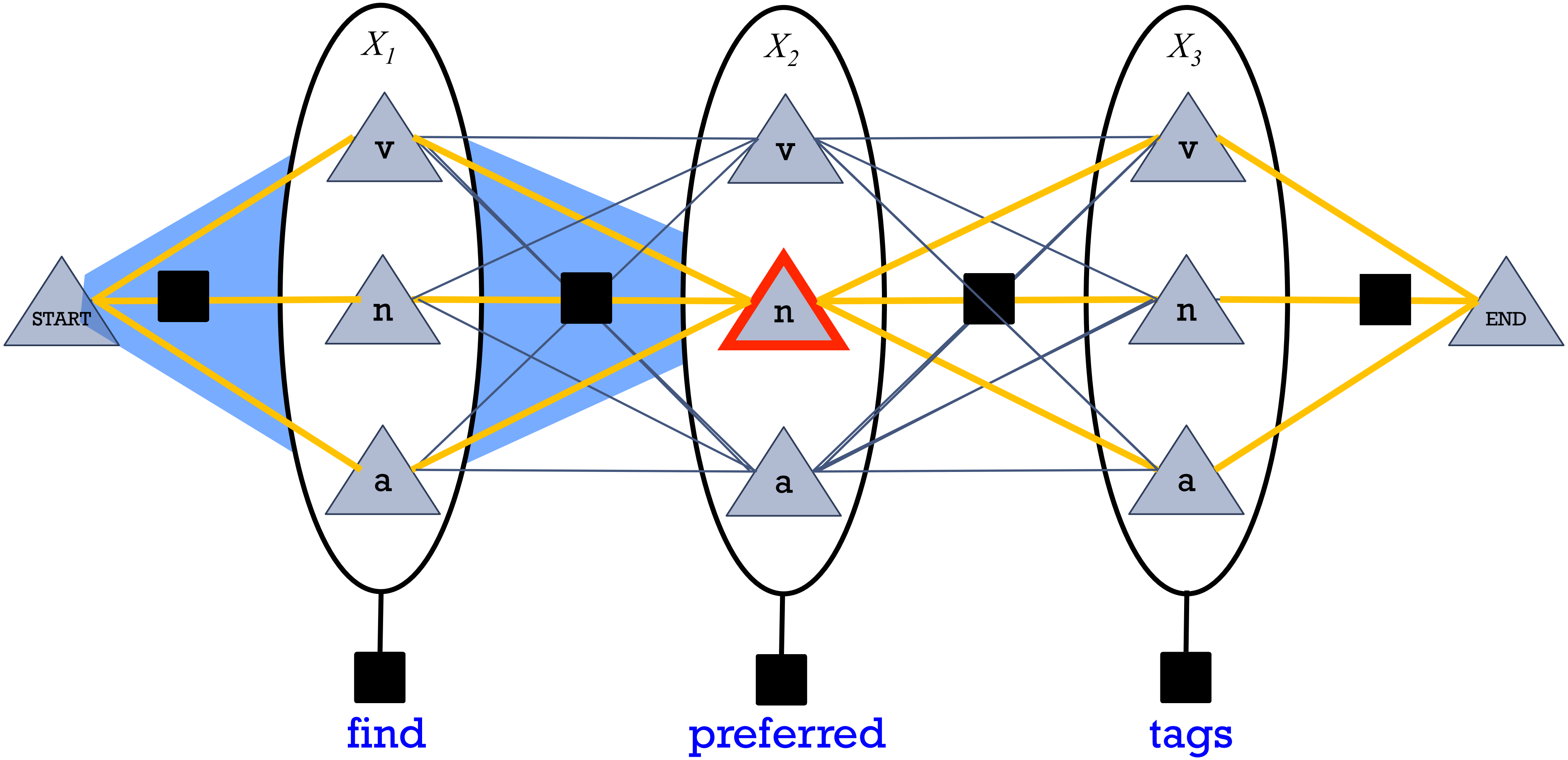
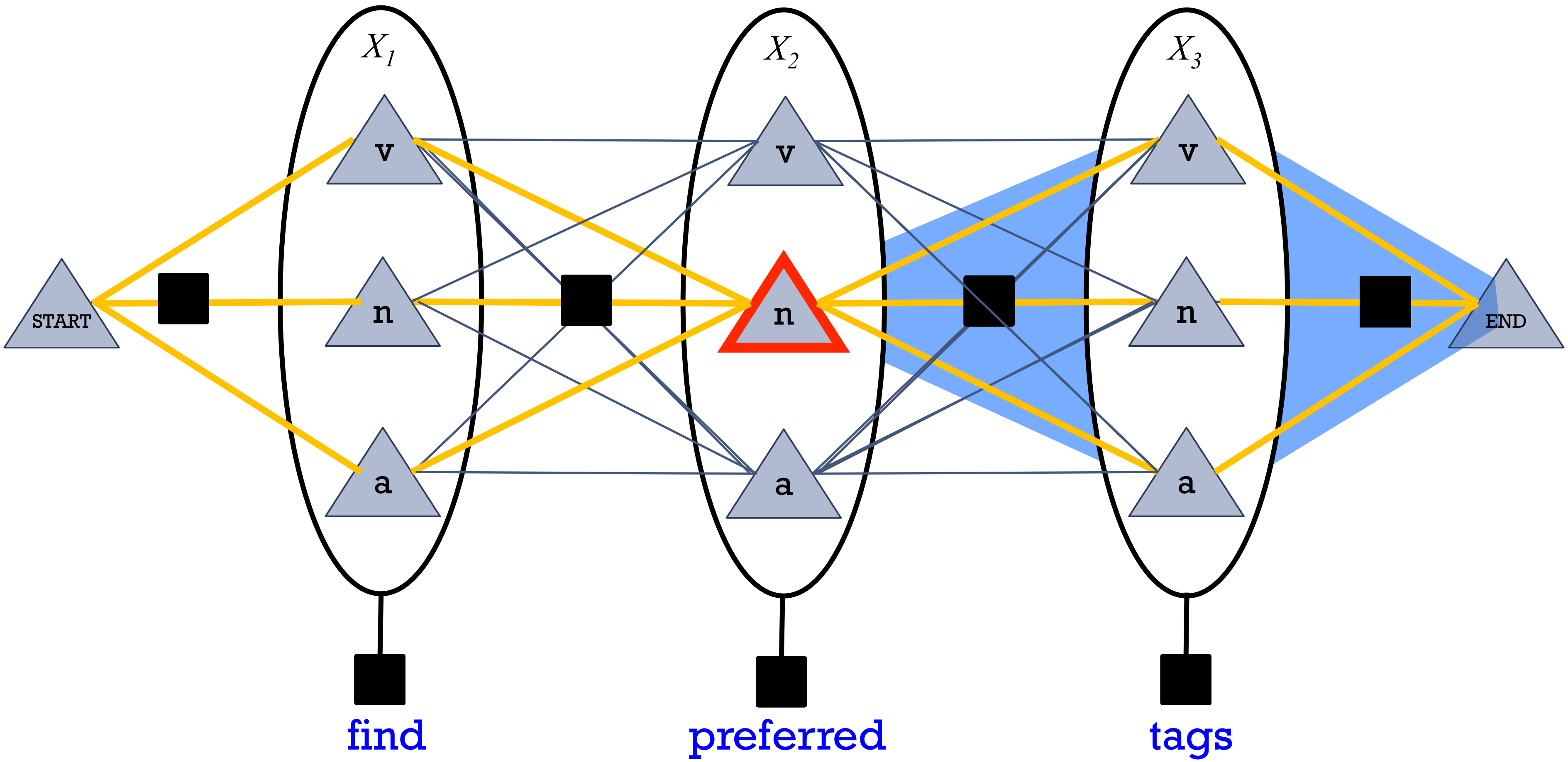
Forward-Backward Algorithm: Finds Marginals



$\alpha_2(\mathbf{n})$ = total weight of these path *prefixes*

(found by dynamic programming: matrix-vector products)

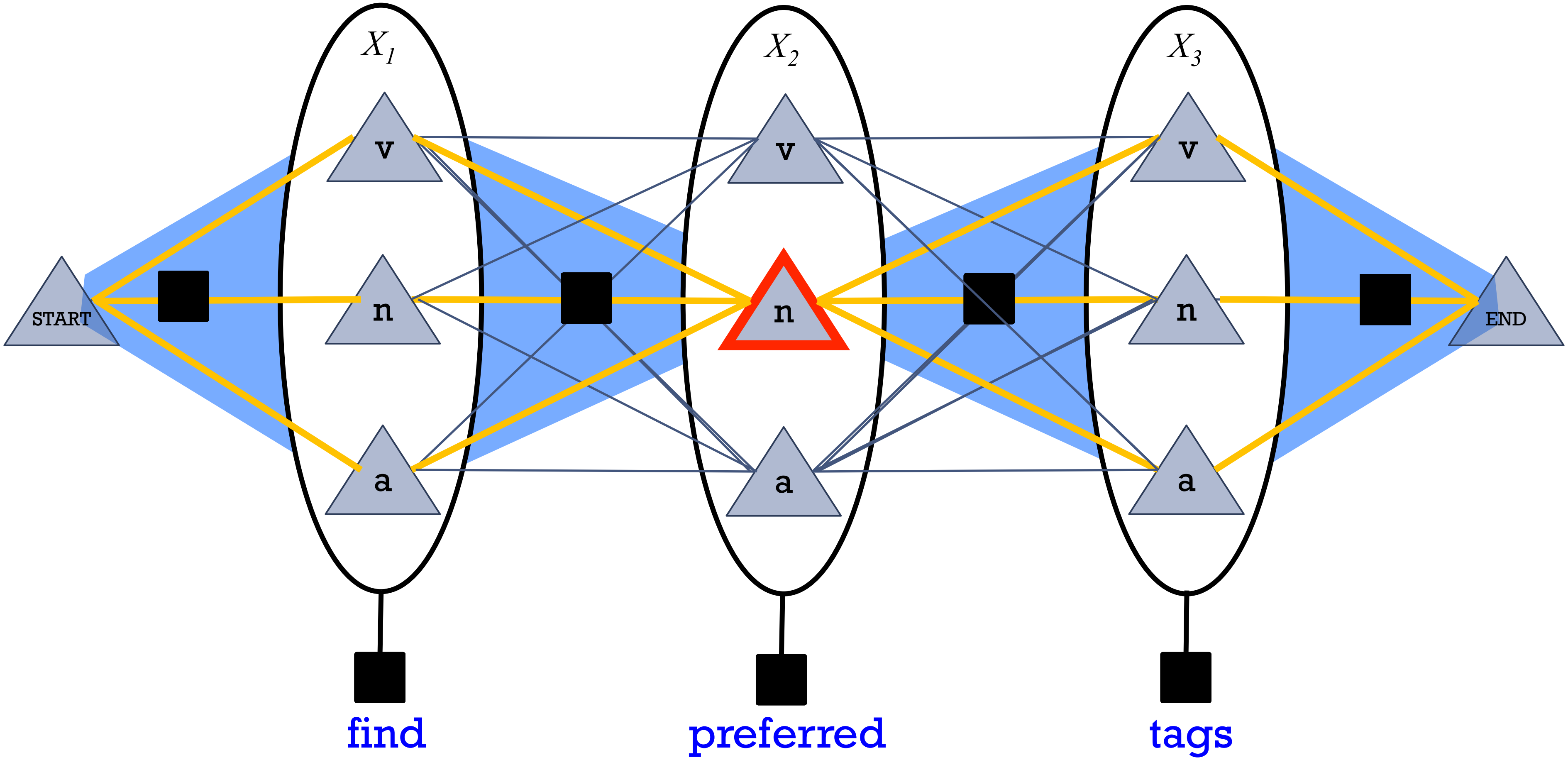
Forward-Backward Algorithm: Finds Marginals



$\beta_2(\mathbf{n})$ = total weight of these path *suffixes*

(found by dynamic programming: matrix-vector products)

Forward-Backward Algorithm: Finds Marginals



$\alpha_2(\mathbf{n})$ = total weight of these path *prefixes* (a + b + c)

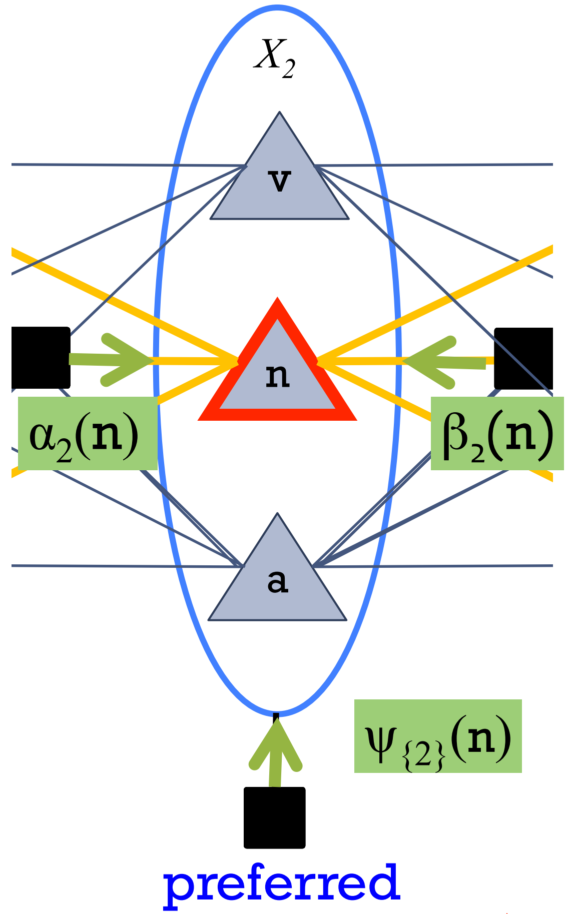
$\beta_2(\mathbf{n})$ = total weight of these path *suffixes* (x + y + z)

Product gives ax+ay+az+bx+by+bz+cx+cy+cz = total weight of paths

Forward-Backward Algorithm: Finds Marginals

Oops! The weight of a path through a state also includes a weight at that state.
So $\alpha(\mathbf{n})\cdot\beta(\mathbf{n})$ isn't enough.

The extra weight is the opinion of the unigram factor at this variable.

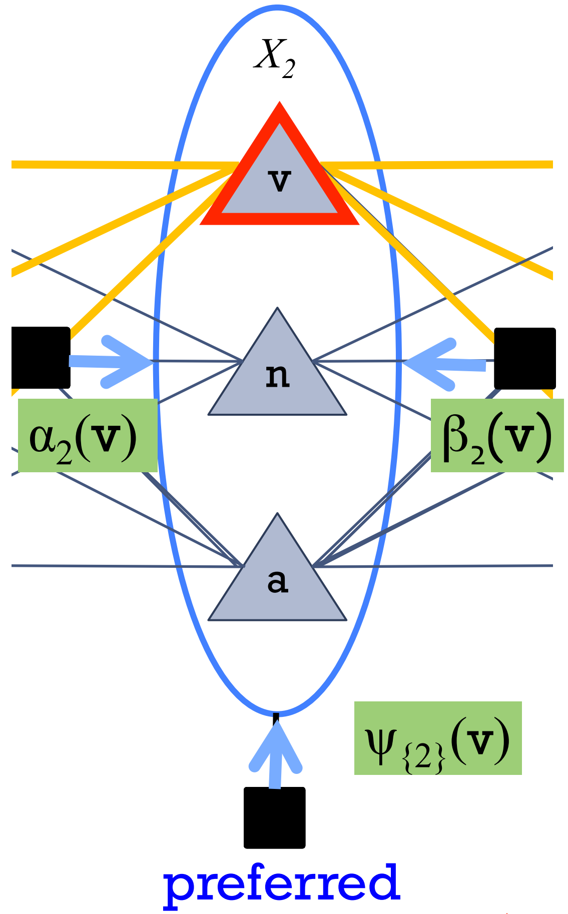


"belief that $X_2 = \mathbf{n}$"

total weight of *all* paths through n

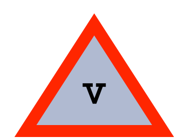
$= \alpha_2(\mathbf{n})\ \psi_{\{2\}}(\mathbf{n})\ \beta_2(\mathbf{n})$

Forward-Backward Algorithm: Finds Marginals



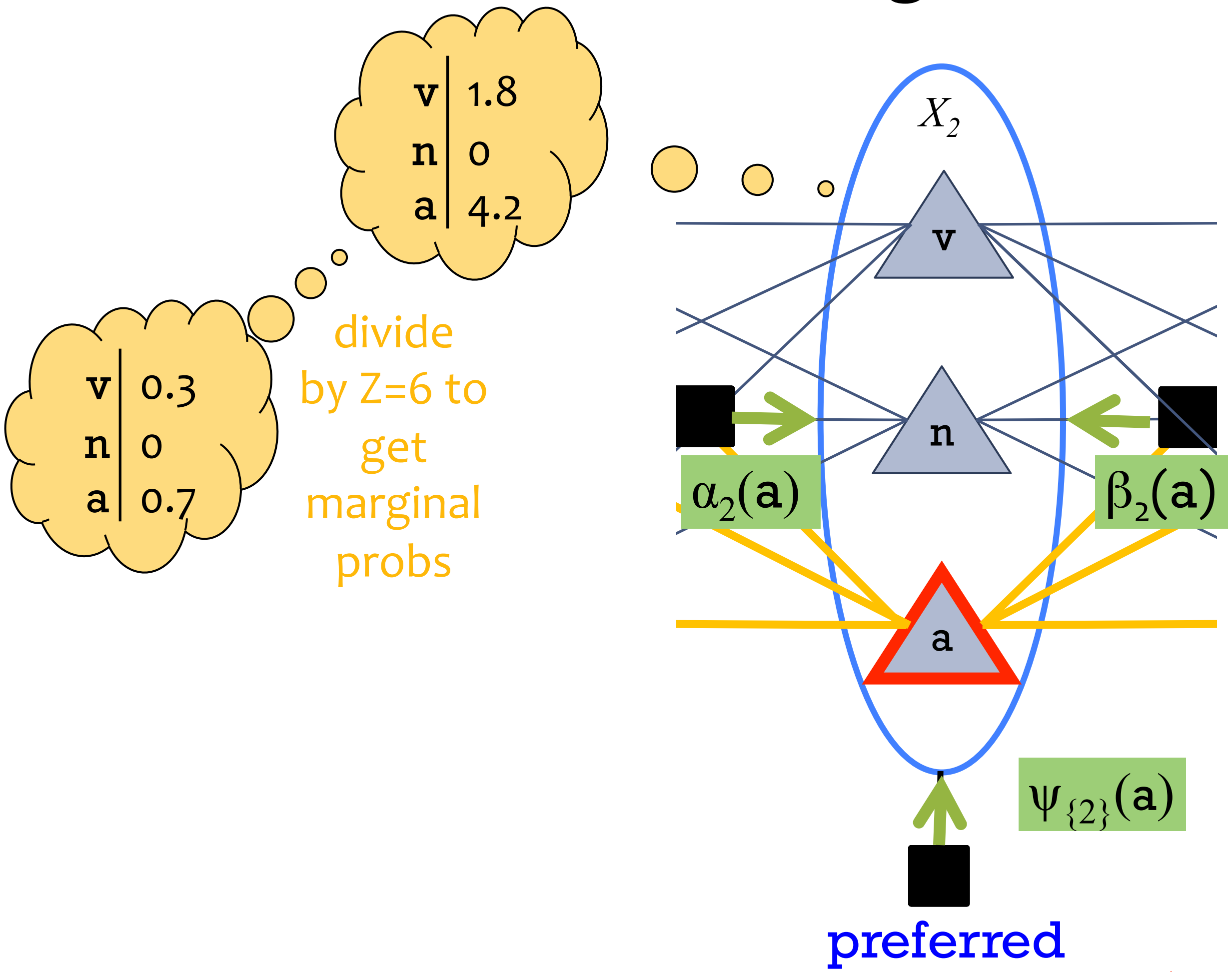
"belief that $X_2 = \mathbf{v}$"

"belief that $X_2 = \mathbf{n}$"

total weight of *all* paths through 

$= \alpha_2(\mathbf{v})\ \psi_{\{2\}}(\mathbf{v})\ \beta_2(\mathbf{v})$

Forward-Backward Algorithm: Finds Marginals



"belief that X_2 = **v**"

"belief that X_2 = **n**"

"belief that X_2 = **a**"

---

sum = Z
(total probability of *all* paths)

total weight of *all* paths through a

= $\alpha_2(\mathtt{a})$ $\psi_{\{2\}}(\mathtt{a})$ $\beta_2(\mathtt{a})$