



10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Hidden Markov Models

Matt Gormley
Lecture 23
April 4, 2018

Reminders

- **Homework 6: PAC Learning / Generative Models**
 - Out: Wed, Mar 28
 - Due: Wed, Apr 04 at 11:59pm
- **Homework 7: HMMs**
 - Out: Wed, Apr 04
 - Due: Mon, Apr 16 at 11:59pm

HMM Outline

- **Motivation**
 - Time Series Data
- **Hidden Markov Model (HMM)**
 - Example: Squirrel Hill Tunnel Closures [courtesy of Roni Rosenfeld]
 - Background: Markov Models
 - From Mixture Model to HMM
 - History of HMMs
 - Higher-order HMMs
- **Training HMMs**
 - (Supervised) Likelihood for HMM
 - Maximum Likelihood Estimation (MLE) for HMM
 - EM for HMM (aka. Baum-Welch algorithm)
- **Forward-Backward Algorithm**
 - Three Inference Problems for HMM
 - Great Ideas in ML: Message Passing
 - Example: Forward-Backward on 3-word Sentence
 - Derivation of Forward Algorithm
 - Forward-Backward Algorithm
 - Viterbi algorithm



Last Lecture

This Lecture

SUPERVISED LEARNING FOR HMMS

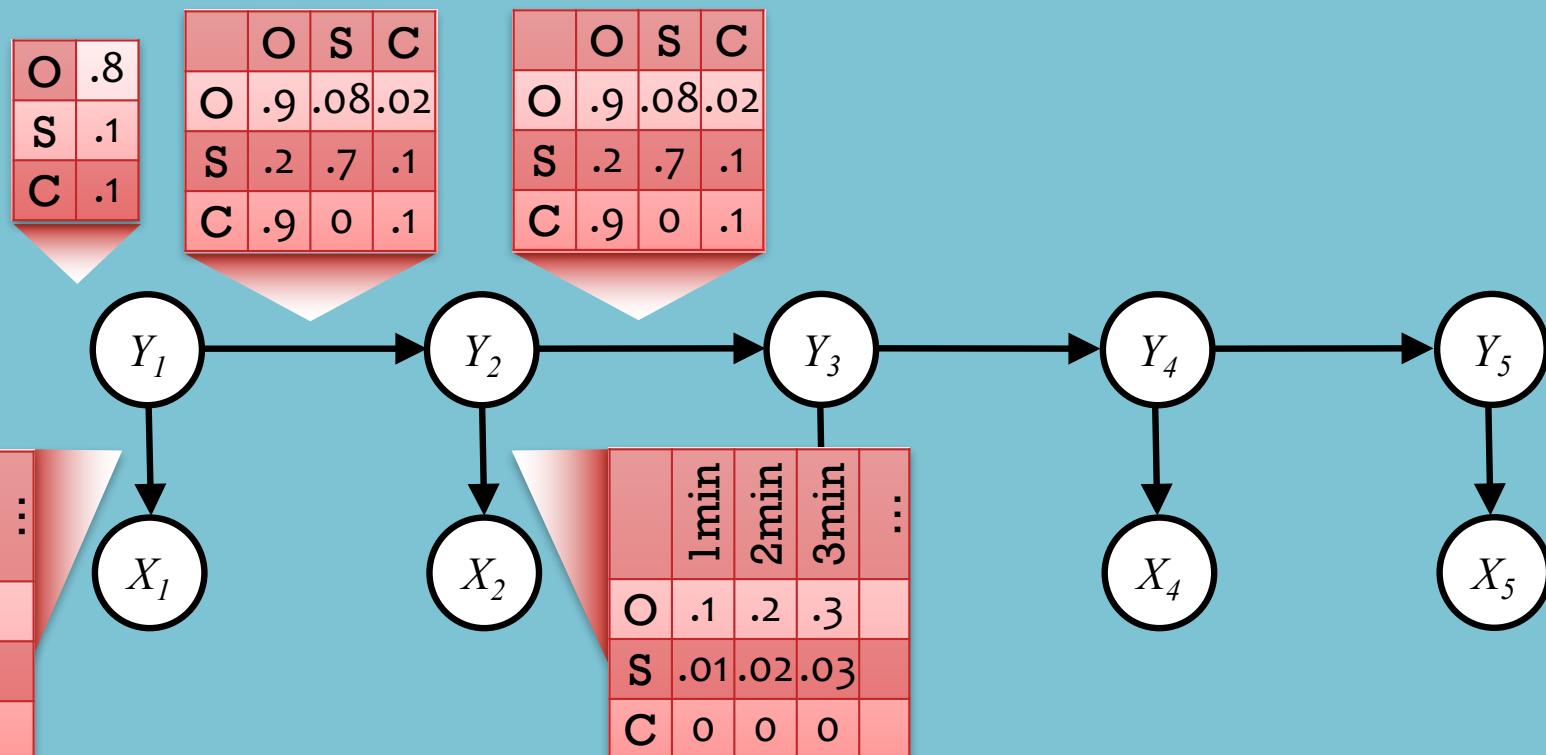
Hidden Markov Model

HMM Parameters:

Emission matrix, \mathbf{A} , where $P(X_t = k|Y_t = j) = A_{j,k}, \forall t, k$

Transition matrix, \mathbf{B} , where $P(Y_t = k|Y_{t-1} = j) = B_{j,k}, \forall t, k$

Initial probs, \mathbf{C} , where $P(Y_1 = k) = C_k, \forall k$



Hidden Markov Model

HMM Parameters:

Emission matrix, \mathbf{A} , where $P(X_t = k|Y_t = j) = A_{j,k}, \forall t, k$

Transition matrix, \mathbf{B} , where $P(Y_t = k|Y_{t-1} = j) = B_{j,k}, \forall t, k$

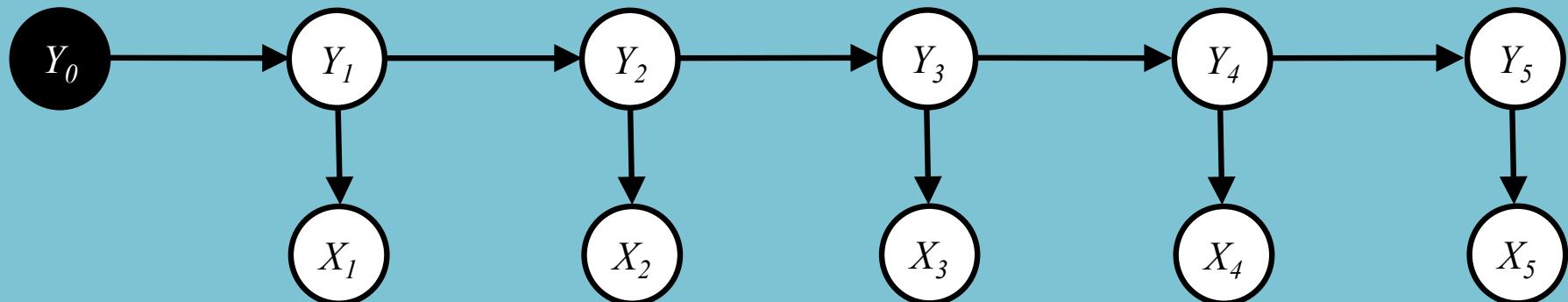
Assumption: $y_0 = \text{START}$

Generative Story:

$Y_t \sim \text{Multinomial}(\mathbf{B}_{Y_{t-1}}) \quad \forall t$

$X_t \sim \text{Multinomial}(\mathbf{A}_{Y_t}) \quad \forall t$

For notational convenience, we fold the initial probabilities \mathbf{C} into the transition matrix \mathbf{B} by our assumption.

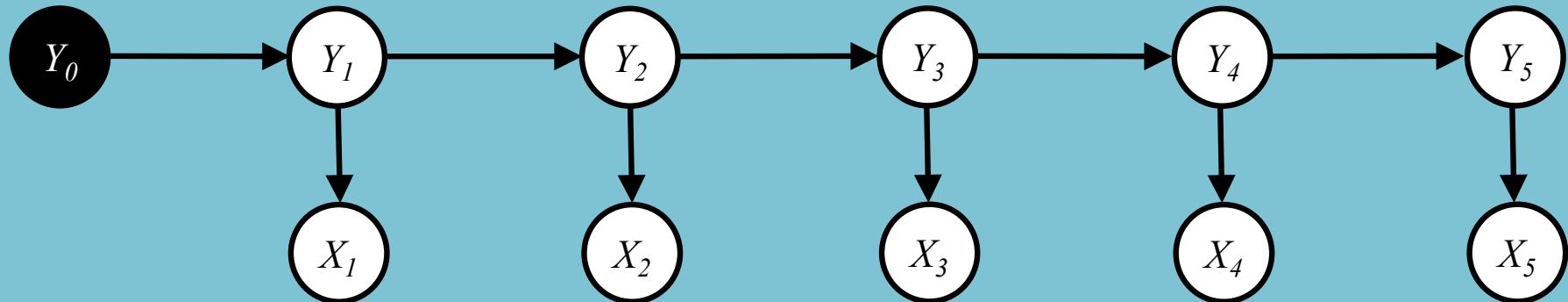


Hidden Markov Model

Joint Distribution:

$y_0 = \text{START}$

$$\begin{aligned} p(\mathbf{x}, \mathbf{y}|y_0) &= \prod_{t=1}^T p(x_t|y_t)p(y_t|y_{t-1}) \\ &= \prod_{t=1}^T A_{y_t, x_t} B_{y_{t-1}, y_t} \end{aligned}$$



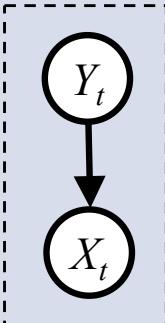
Training HMMs

Whiteboard

- (Supervised) Likelihood for an HMM
- Maximum Likelihood Estimation (MLE) for HMM

Supervised Learning for HMMs

Learning an HMM decomposes into solving two (independent) Mixture Models



Data:

$D = \{(\vec{x}^{(i)}, \vec{y}^{(i)})\}_{i=1}^N$

$$\vec{x} = [x_1, \dots, x_T]^T$$

$$\vec{y} = [y_1, \dots, y_T]^T$$

Likelihood:

$$\begin{aligned} l(A, B, C) &= \sum_{i=1}^N \log p(\vec{x}^{(i)}, \vec{y}^{(i)} | A, B, C) \\ &= \sum_{i=1}^N \left[\underbrace{\log p(y_1^{(i)} | C)}_{\text{initial}} + \underbrace{\left(\sum_{t=2}^T \log p(y_t^{(i)} | y_{t-1}^{(i)}, B) \right)}_{\text{transition}} + \underbrace{\left(\sum_{t=1}^T \log p(x_t^{(i)} | y_t^{(i)}, A) \right)}_{\text{emission}} \right] \end{aligned}$$

MLE:

$$\hat{A}, \hat{B}, \hat{C} = \underset{A, B, C}{\operatorname{argmax}} l(A, B, C)$$

$$\Rightarrow \hat{C} = \underset{C}{\operatorname{argmax}} \sum_{i=1}^N \log p(y_1^{(i)} | C)$$

$$\hat{B} = \underset{B}{\operatorname{argmax}} \sum_{i=1}^N \sum_{t=2}^T \log p(y_t^{(i)} | y_{t-1}^{(i)}, B)$$

$$\hat{A} = \underset{A}{\operatorname{argmax}} \sum_{i=1}^N \sum_{t=1}^T \log p(x_t^{(i)} | y_t^{(i)}, A)$$

} Can solve in closed form, which yields...

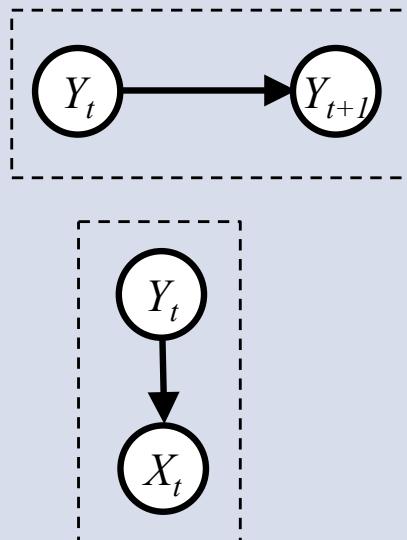
$$\hat{C}_k = \frac{\#(y_1^{(i)} = k)}{N} \quad \forall i, k$$

$$\hat{B}_{jk} = \frac{\#(y_t^{(i)} = k \text{ and } y_{t-1}^{(i)} = j)}{\#(y_{t-1}^{(i)} = j)} \quad \forall i, t > 1, j, k$$

$$\hat{A}_{jk} = \frac{\#(x_t^{(i)} = k \text{ and } y_t^{(i)} = j)}{\#(y_t^{(i)} = j)} \quad \forall i, t, j, k$$

Supervised Learning for HMMs

Learning an HMM decomposes into solving two (independent) Mixture Models



$$D = \{(\vec{x}^{(i)}, \vec{y}^{(i)})\}_{i=1}^N$$

$$\begin{aligned} \text{Likelihood} &: \ell(A, B) = \sum_{i=1}^N \log p(\vec{x}^{(i)}, \vec{y}^{(i)}) \\ &= \sum_{i=1}^N \left[\sum_{t=1}^T \log p(y_t^{(i)} | y_{t-1}^{(i)}, B) + \log p(x_t^{(i)} | y_t^{(i)}, A) \right] \end{aligned}$$

$$\text{MLE: } \hat{A}, \hat{B} = \arg \max \ell(A, B)$$

$$\hat{A} = \arg \max \sum_{i=1}^N \left[\sum_{t=1}^T \log p(x_t^{(i)} | y_t^{(i)}, A) \right]$$

$$\hat{B} = \arg \max \sum_{i=1}^N \left[\sum_{t=1}^T \log p(y_t^{(i)} | y_{t-1}^{(i)}, B) \right]$$

A can solve in closed form to get...

$$\hat{B}_{jk} = \frac{\#(y_t^{(i)} = k \text{ and } y_{t-1}^{(i)} = j)}{\#(y_{t-1}^{(i)} = j)}$$

$$\hat{A}_{jk} = \frac{\#(x_t^{(i)} = k \text{ and } y_t^{(i)} = j)}{\#(y_t^{(i)} = j)}$$

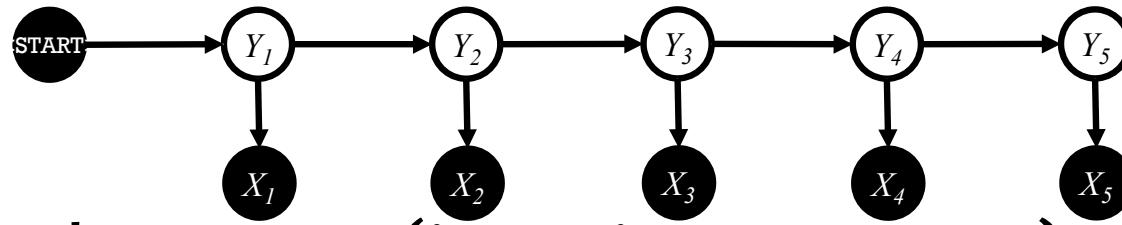
HMMs: History

- Markov chains: Andrey Markov (1906)
 - Random walks and Brownian motion
- Used in Shannon's work on information theory (1948)
- Baum-Welsh learning algorithm: late 60's, early 70's.
 - Used mainly for speech in 60s-70s.
- Late 80's and 90's: David Haussler (major player in learning theory in 80's) began to use HMMs for modeling biological sequences
- Mid-late 1990's: Dayne Freitag/Andrew McCallum
 - Freitag thesis with Tom Mitchell on IE from Web using logic programs, grammar induction, etc.
 - McCallum: multinomial Naïve Bayes for text
 - With McCallum, IE using HMMs on CORA
- ...

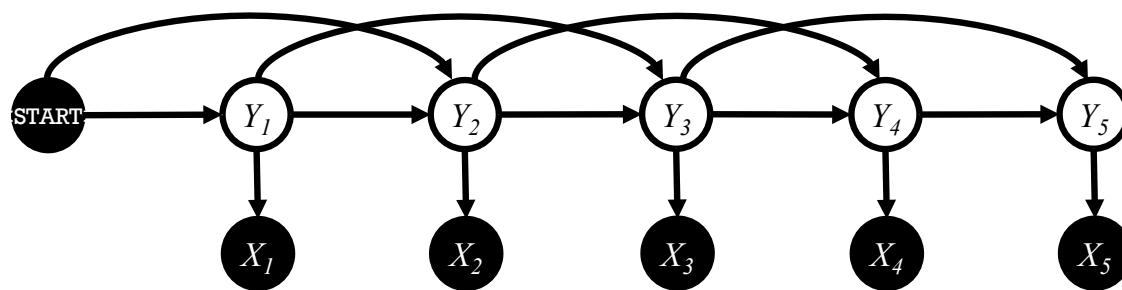


Higher-order HMMs

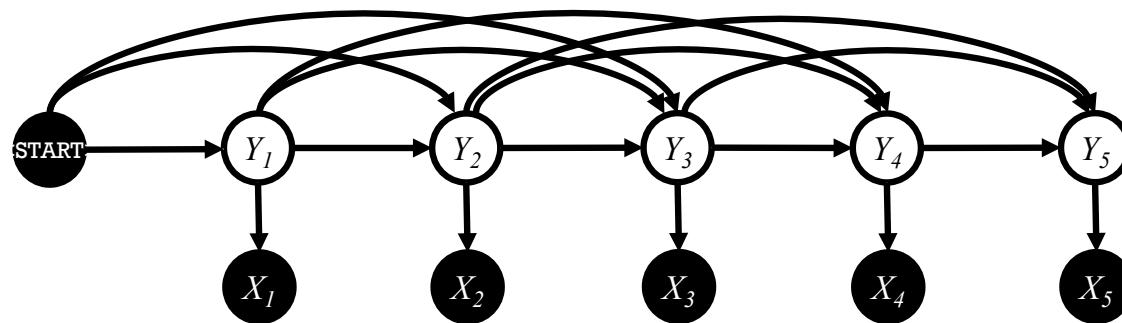
- 1st-order HMM (i.e. bigram HMM)



- 2nd-order HMM (i.e. trigram HMM)



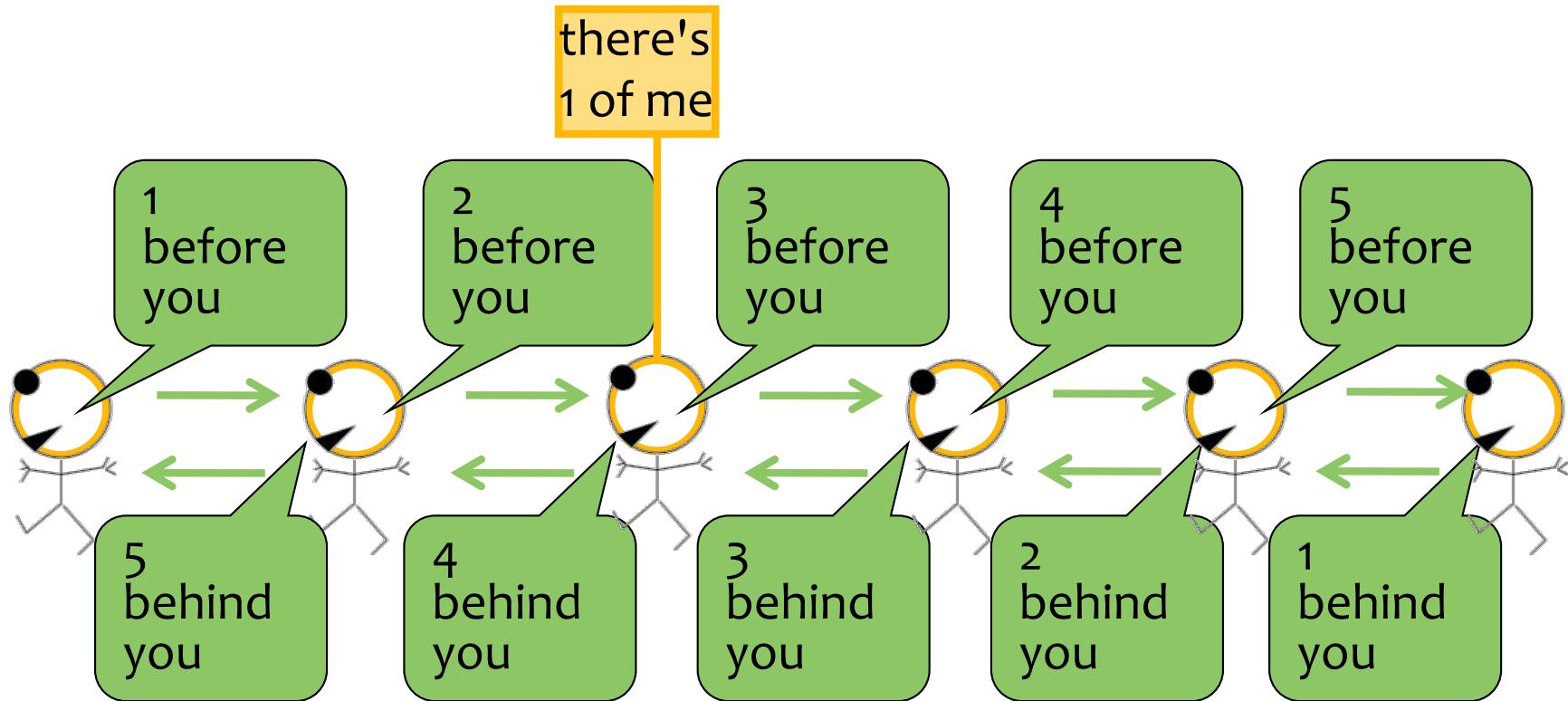
- 3rd-order HMM



BACKGROUND: MESSAGE PASSING

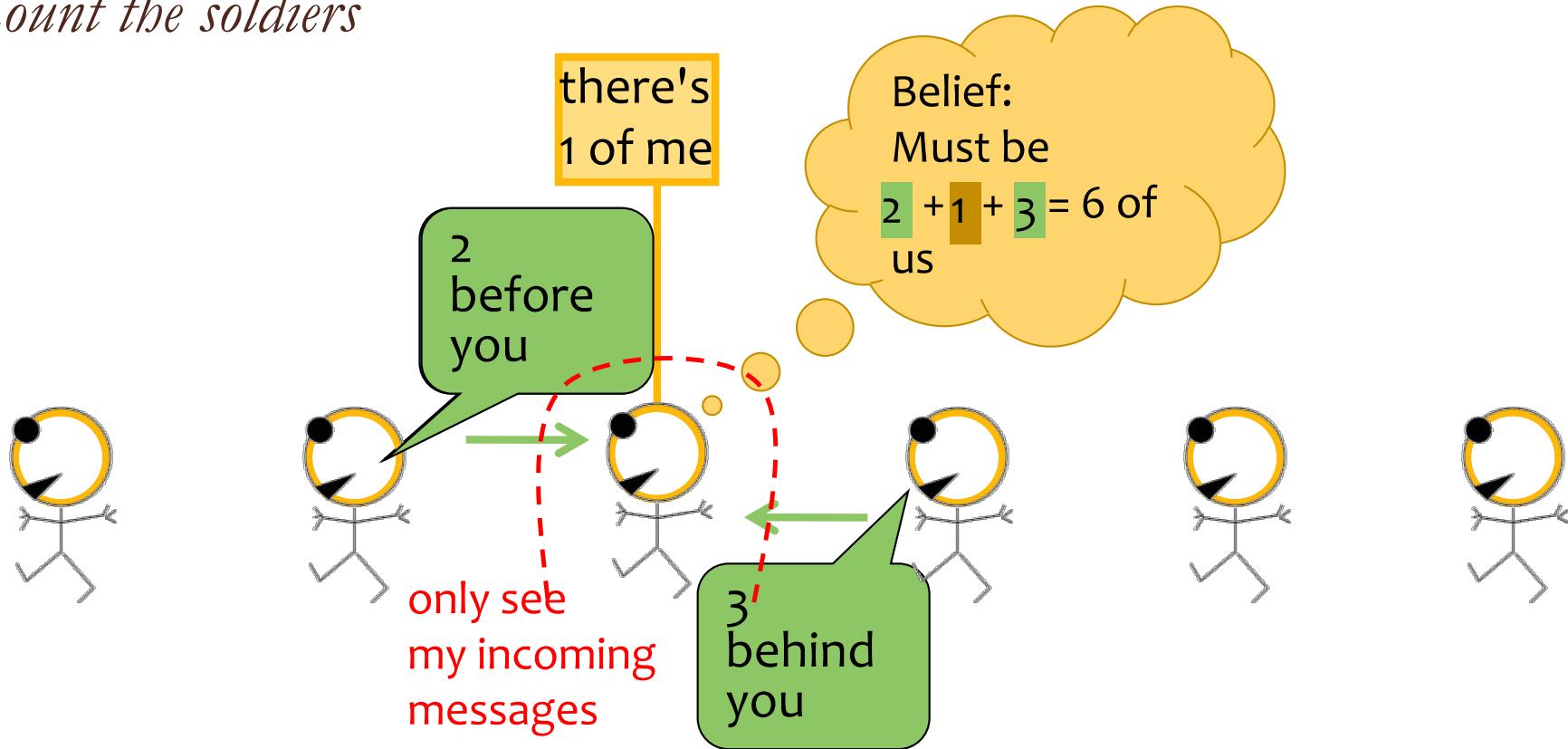
Great Ideas in ML: Message Passing

Count the soldiers



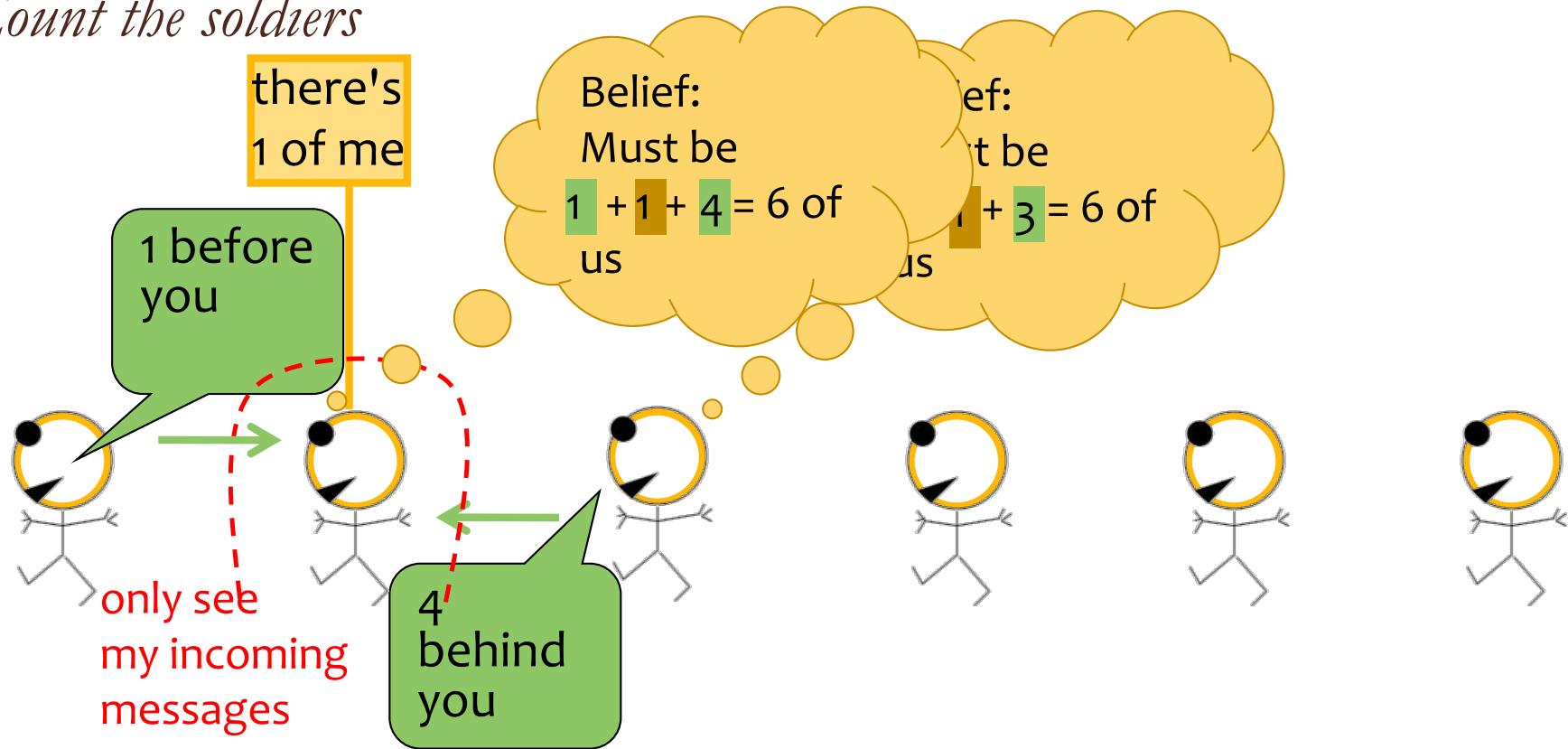
Great Ideas in ML: Message Passing

Count the soldiers



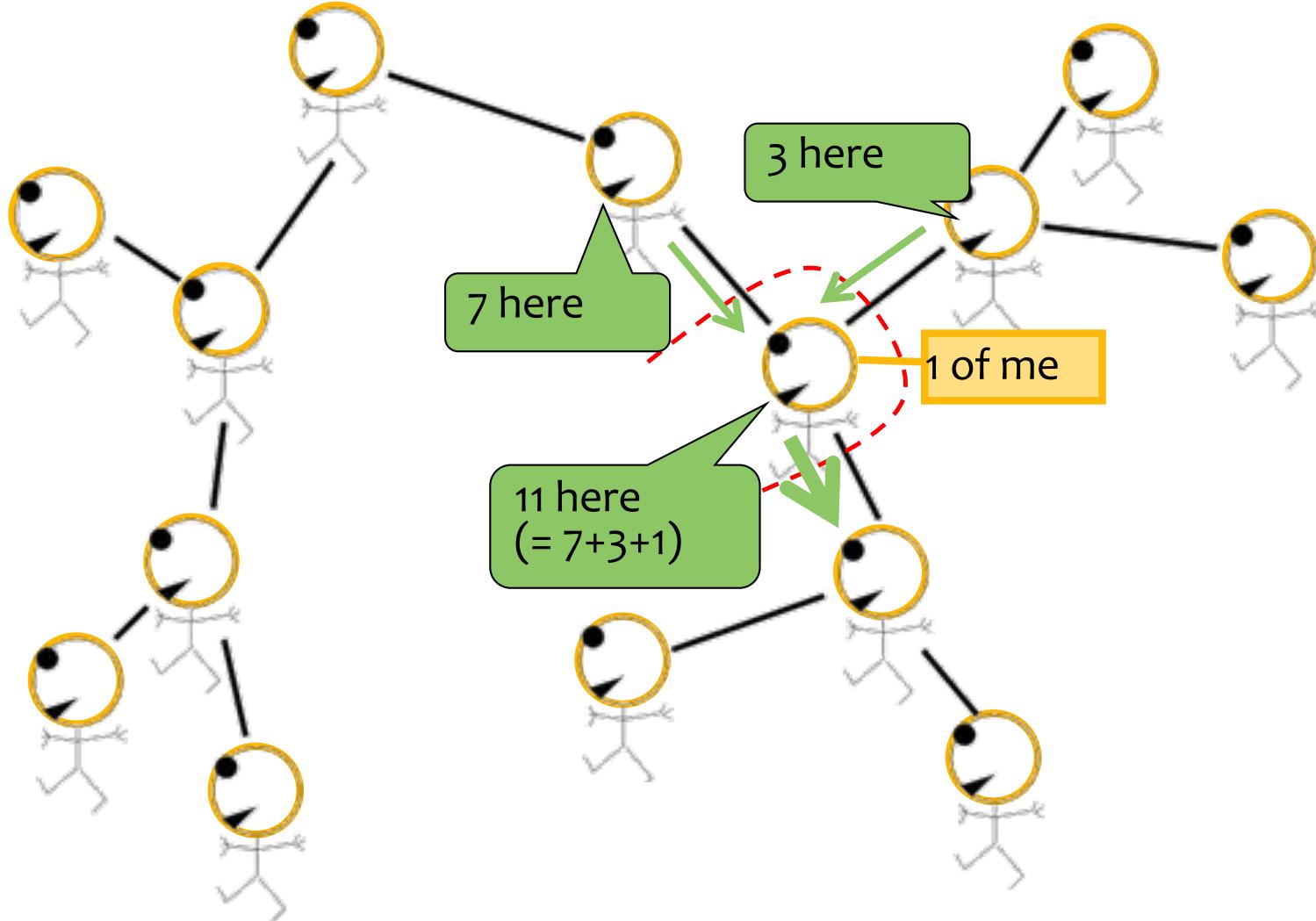
Great Ideas in ML: Message Passing

Count the soldiers



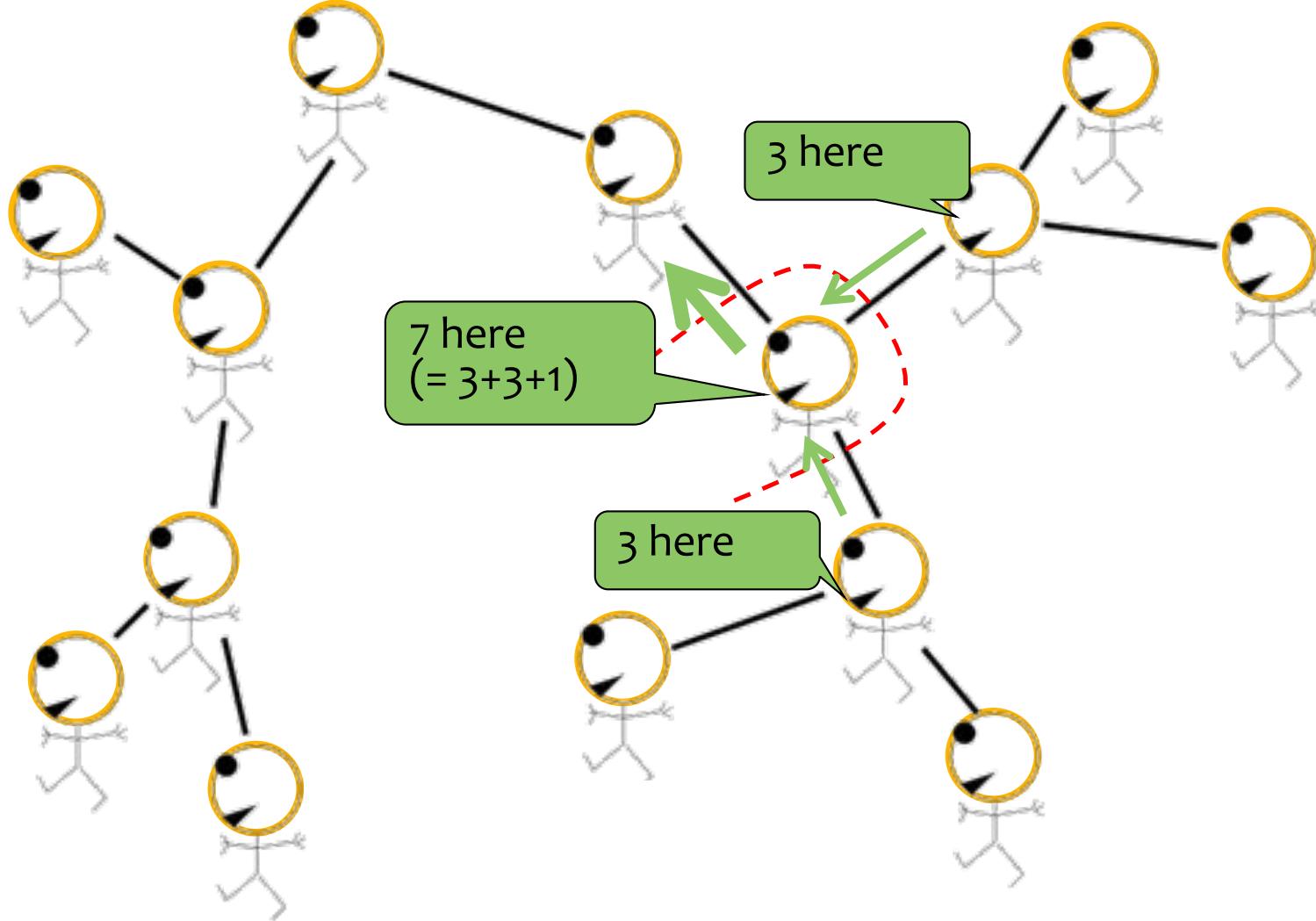
Great Ideas in ML: Message Passing

Each soldier receives reports from all branches of tree



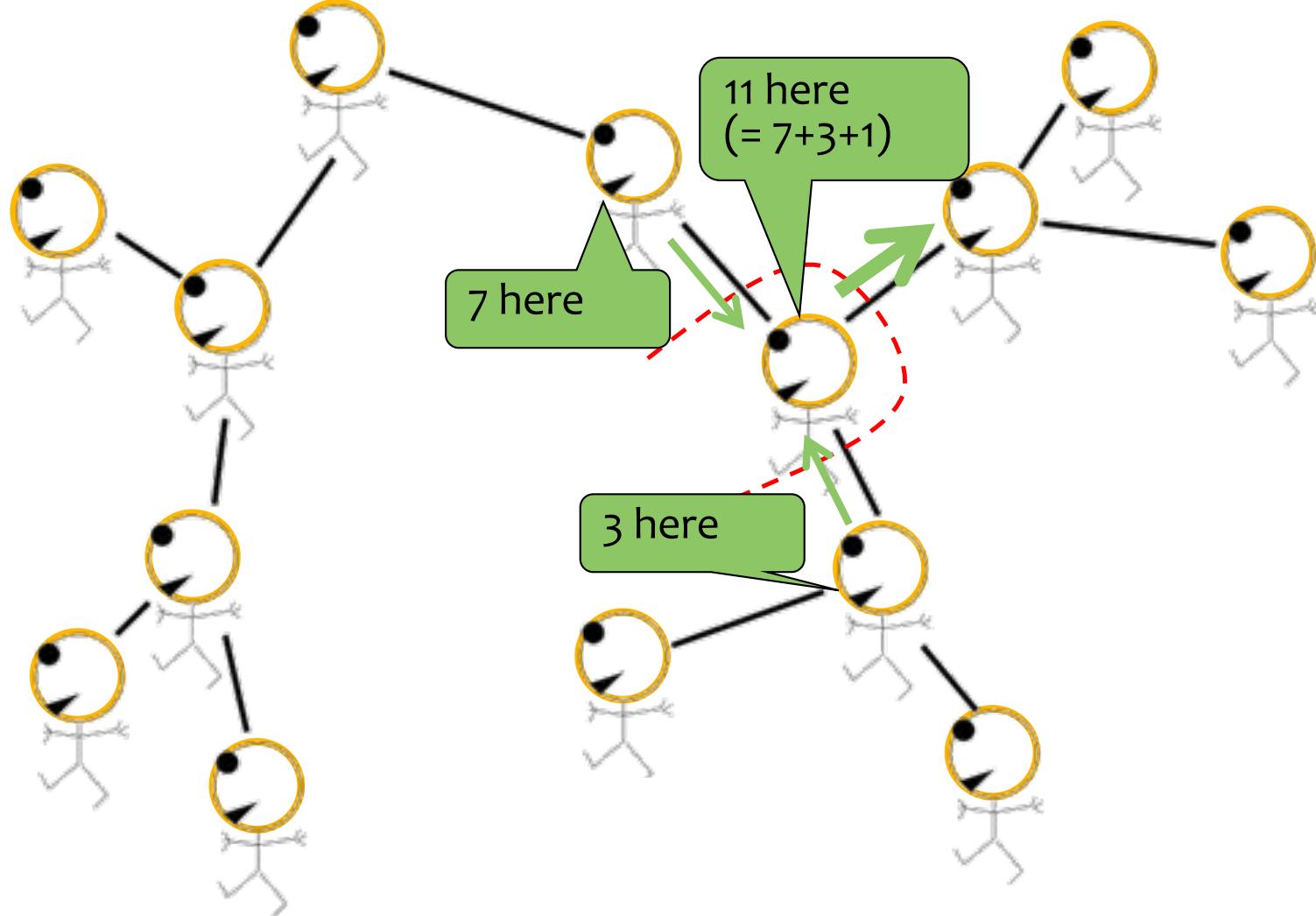
Great Ideas in ML: Message Passing

Each soldier receives reports from all branches of tree



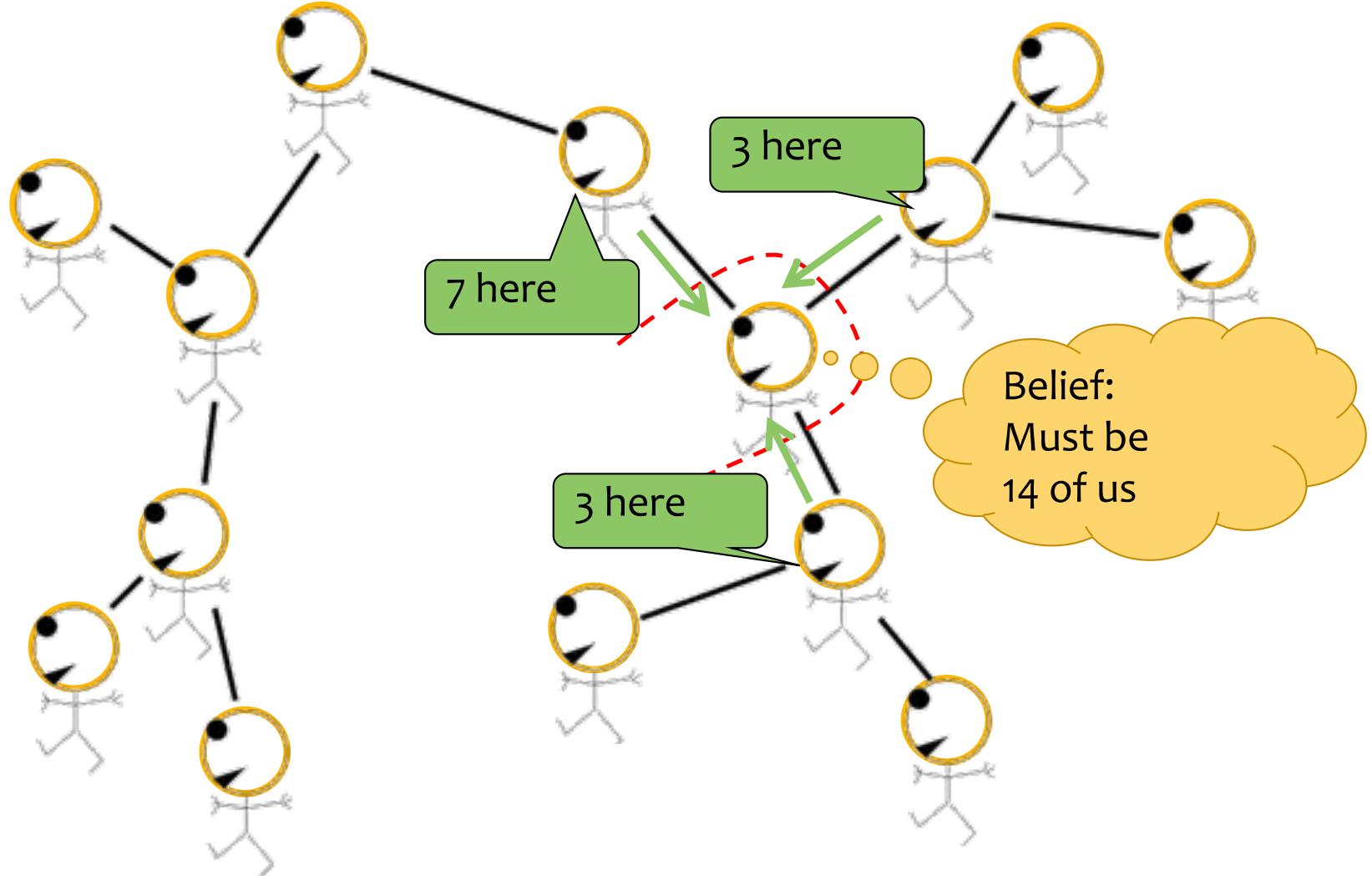
Great Ideas in ML: Message Passing

Each soldier receives reports from all branches of tree



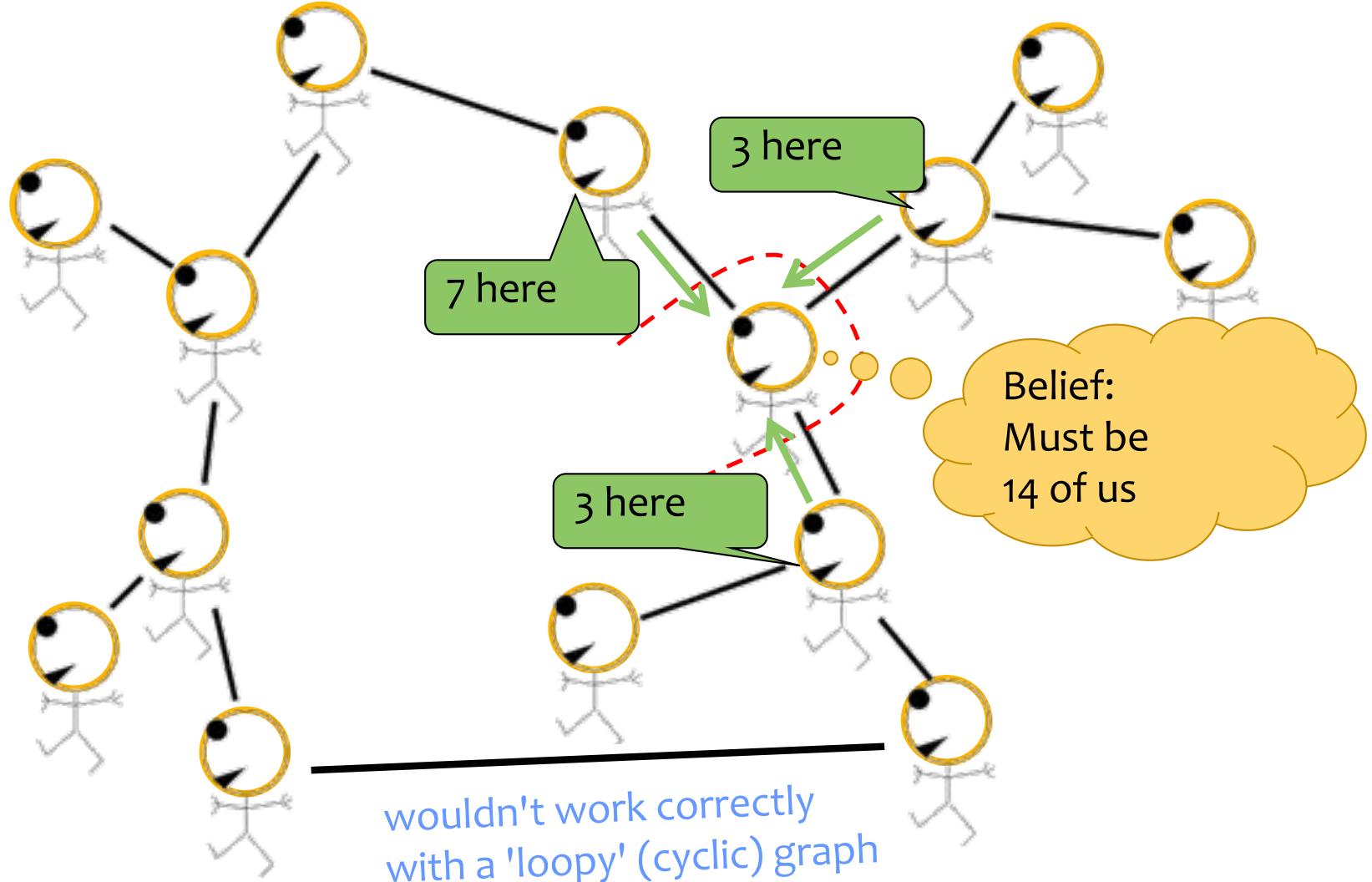
Great Ideas in ML: Message Passing

Each soldier receives reports from all branches of tree



Great Ideas in ML: Message Passing

Each soldier receives reports from all branches of tree



THE FORWARD-BACKWARD ALGORITHM

Inference for HMMs

Whiteboard

- Three Inference Problems for an HMM
 1. Evaluation: Compute the probability of a given sequence of observations
 2. Viterbi Decoding: Find the most-likely sequence of hidden states, given a sequence of observations
 3. Marginals: Compute the marginal distribution for a hidden state, given a sequence of observations

Dataset for Supervised Part-of-Speech (POS) Tagging

Data: $\mathcal{D} = \{\mathbf{x}^{(n)}, \mathbf{y}^{(n)}\}_{n=1}^N$

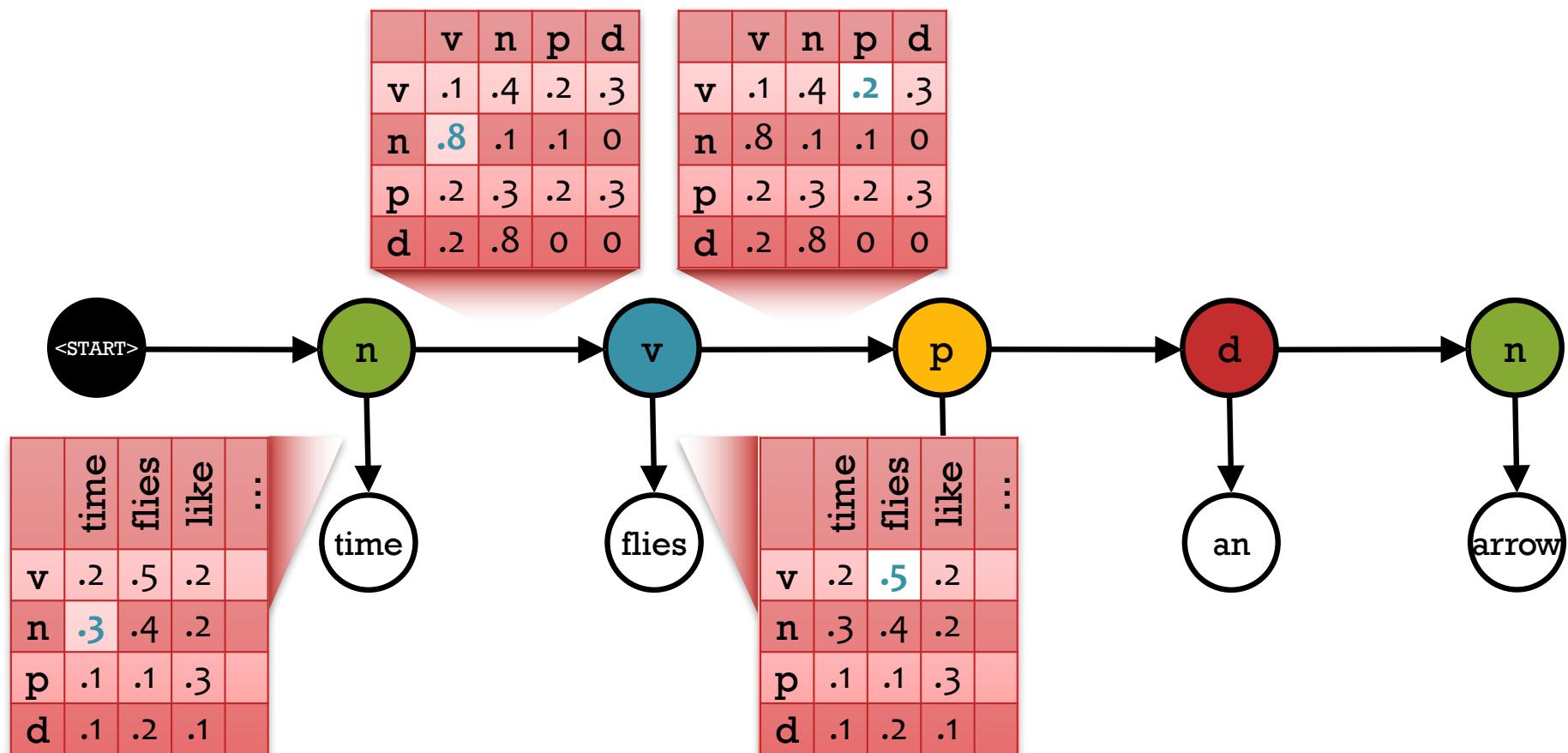
Sample 1:	n time	v flies	p like	d an	n arrow	$y^{(1)}$
Sample 2:	n time	n flies	v like	d an	n arrow	$y^{(2)}$
Sample 3:	n flies	v fly	p with	n their	n wings	$y^{(3)}$
Sample 4:	p with	n time	n you	v will	v see	$y^{(4)}$

The diagram illustrates a dataset for supervised POS tagging. It consists of four samples, each represented by a row of five tokens. Each token is shown in two circles: the top circle contains its part-of-speech tag (e.g., n for noun, v for verb, p for preposition), and the bottom circle contains its corresponding word (e.g., time, flies). To the right of the samples, vertical teal brackets group the tags and words respectively, labeled $y^{(1)}$, $x^{(1)}$, $y^{(2)}$, $x^{(2)}$, $y^{(3)}$, $x^{(3)}$, $y^{(4)}$, and $x^{(4)}$. Sample 1 shows the sequence: noun, verb, preposition, determiner, noun. Sample 2 shows: noun, noun, verb, determiner, noun. Sample 3 shows: noun, verb, preposition, noun, noun. Sample 4 shows: preposition, noun, noun, verb, verb.

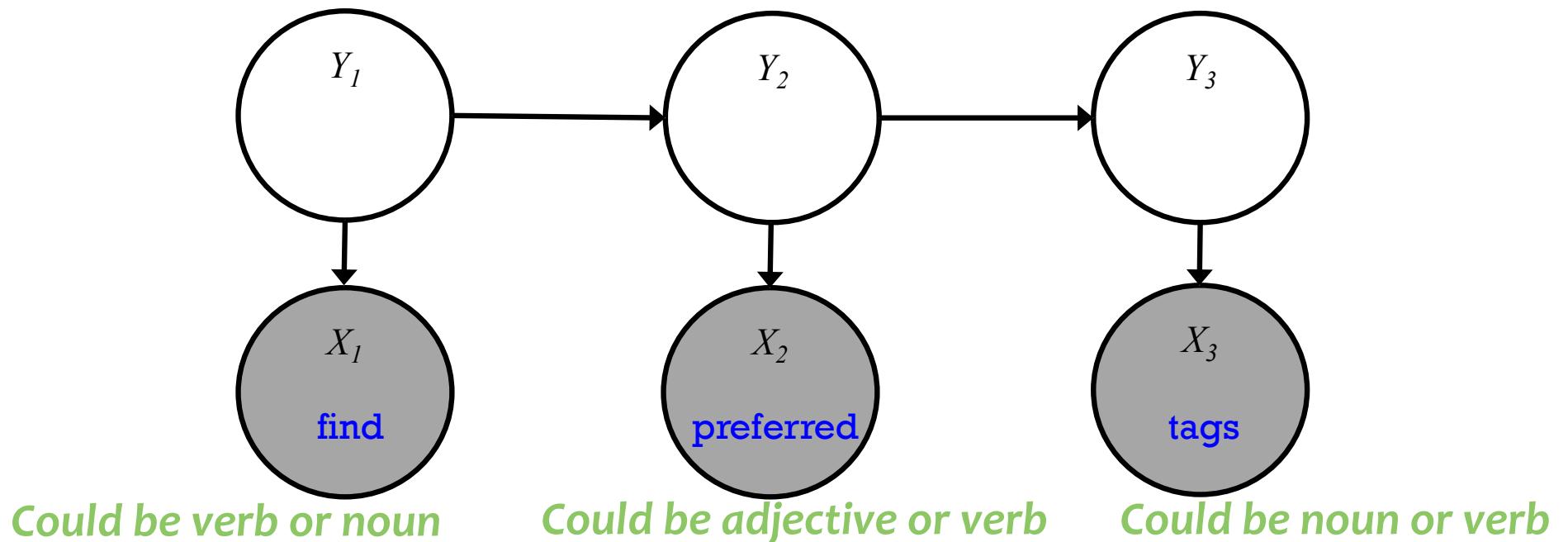
Hidden Markov Model

A Hidden Markov Model (HMM) provides a joint distribution over the sentence/tags with an assumption of dependence between adjacent tags.

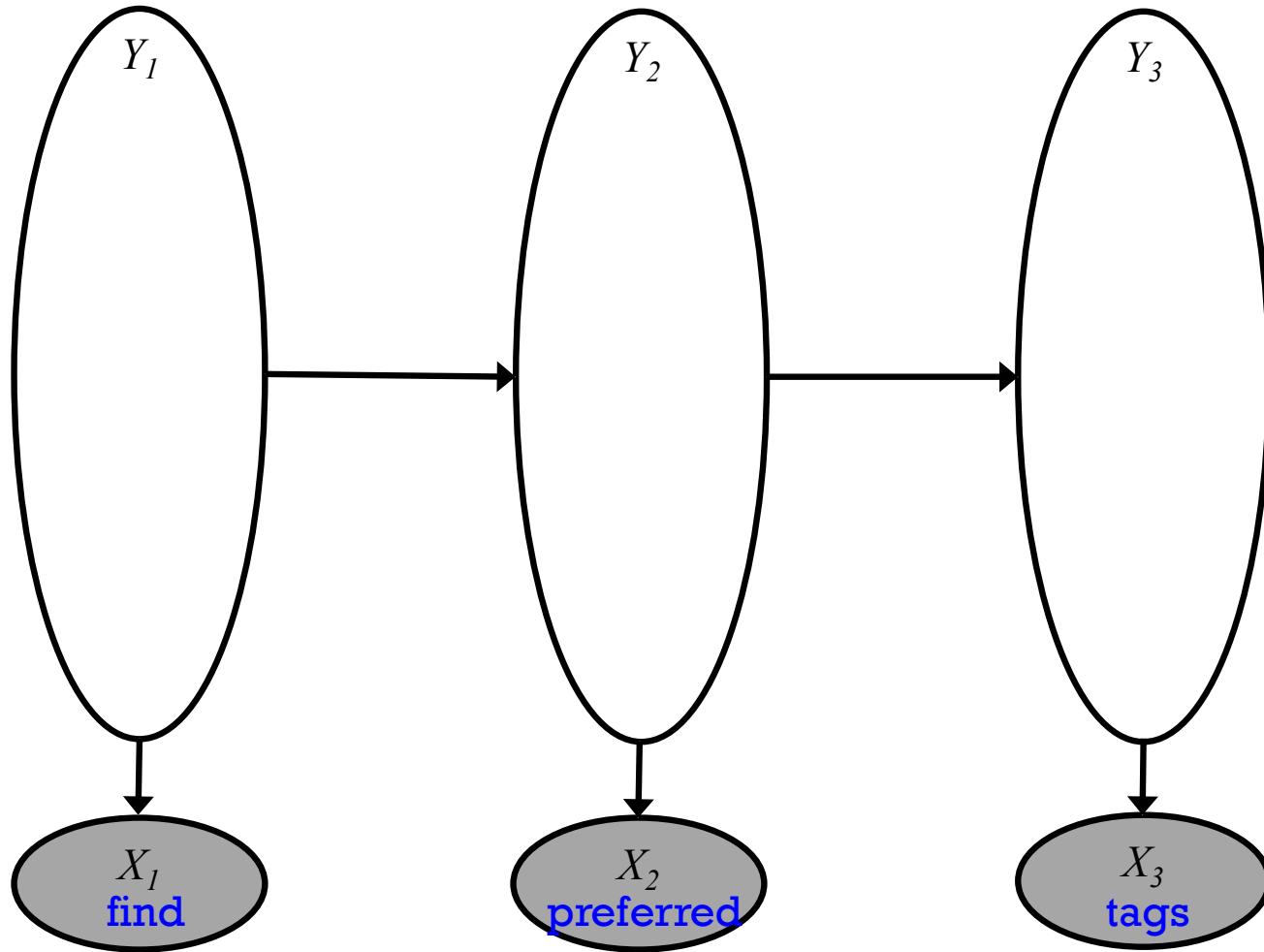
$$p(n, v, p, d, n, \text{time}, \text{flies}, \text{like}, \text{an}, \text{arrow}) = (.3 * .8 * .2 * .5 * \dots)$$



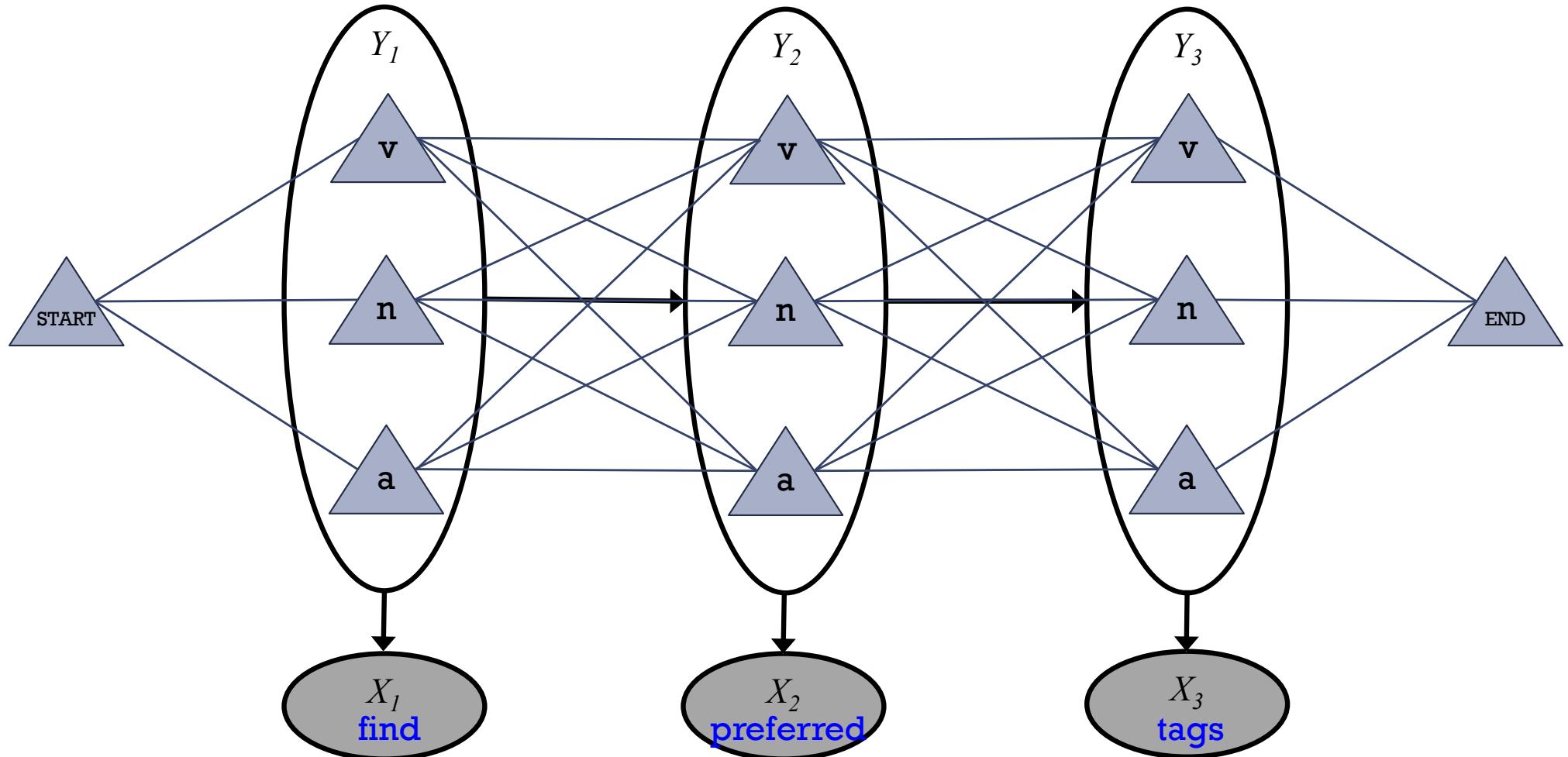
Forward-Backward Algorithm



Forward-Backward Algorithm

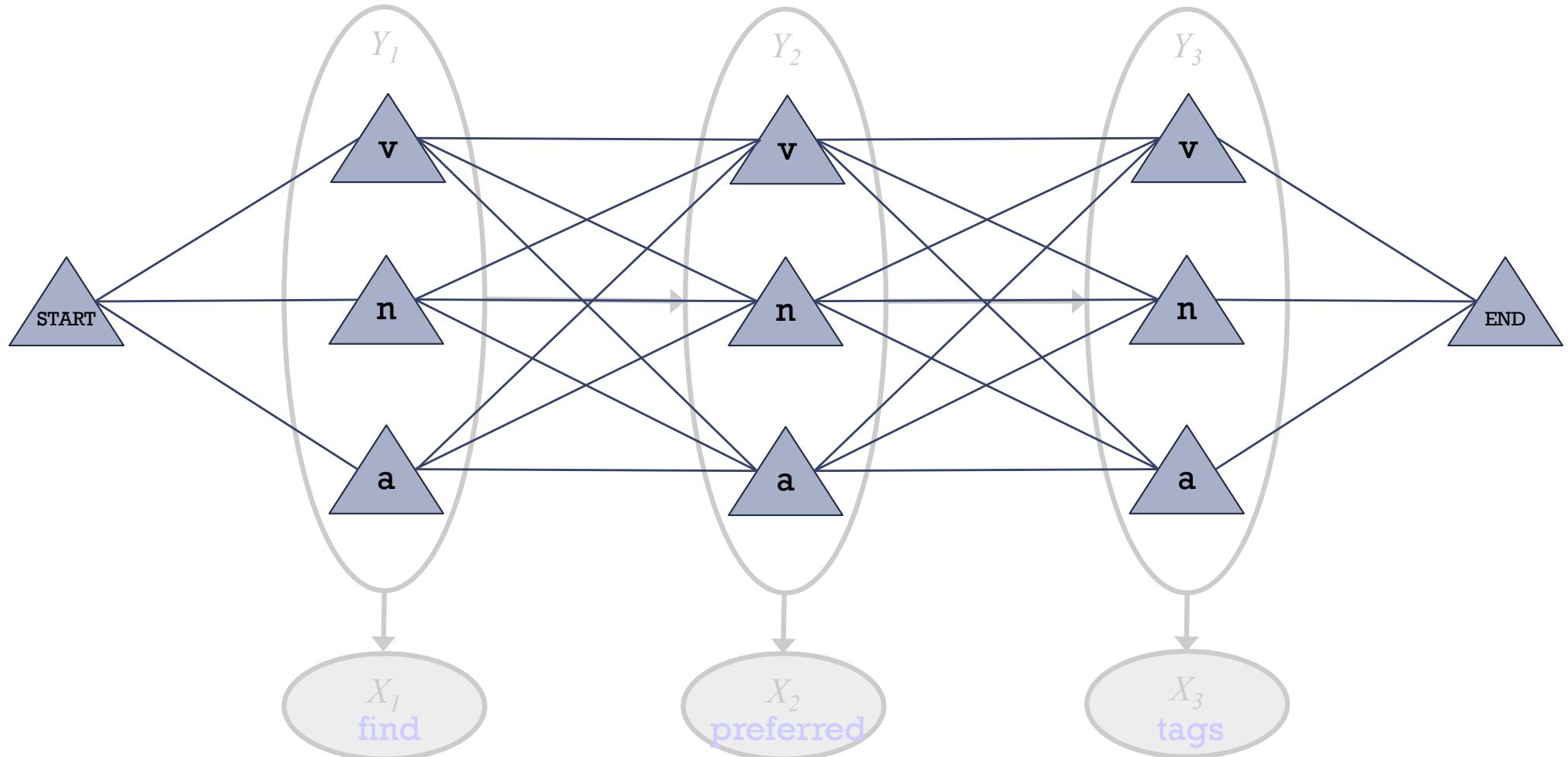


Forward-Backward Algorithm



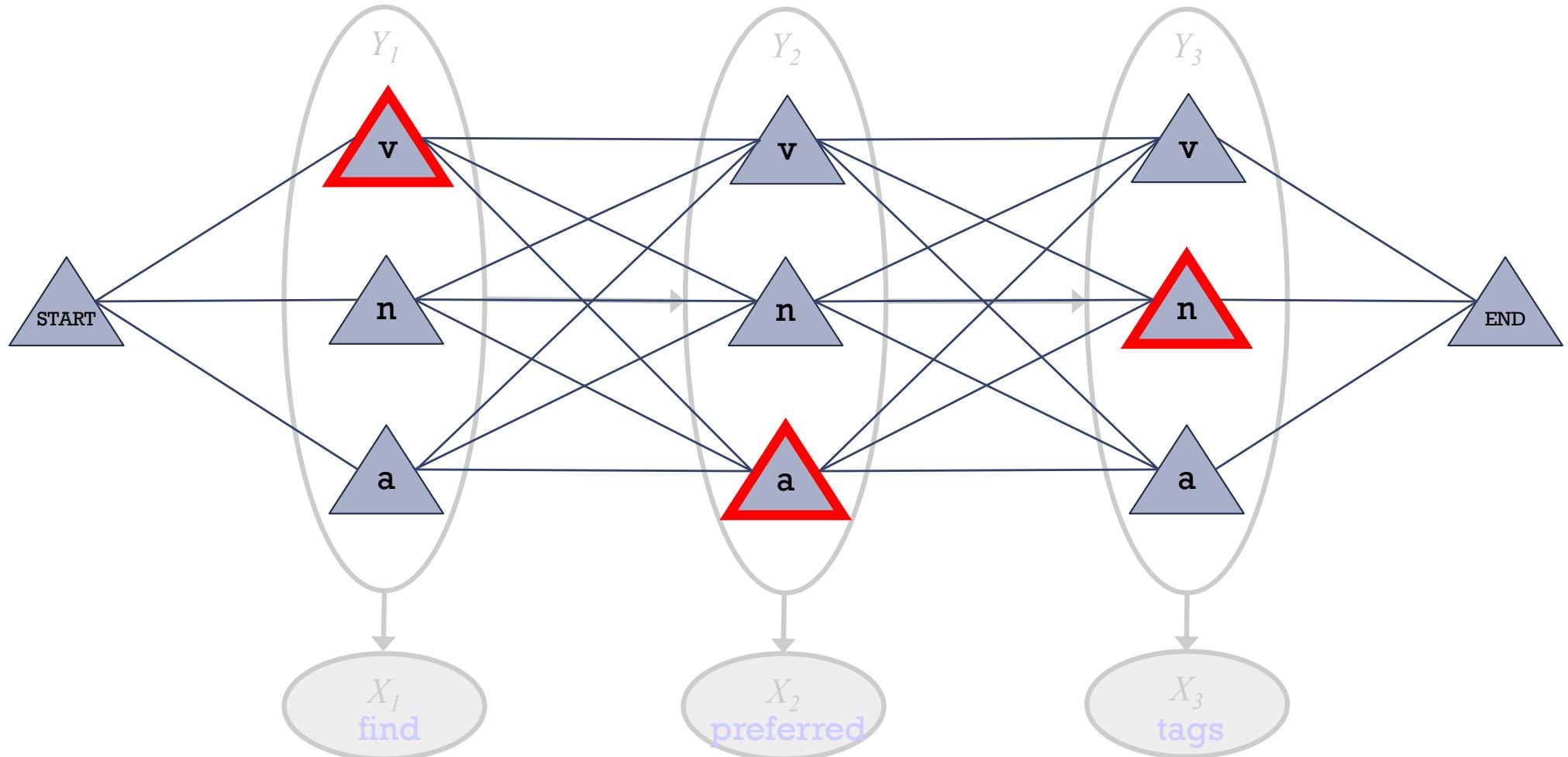
- Let's show the possible *values* for each variable

Forward-Backward Algorithm



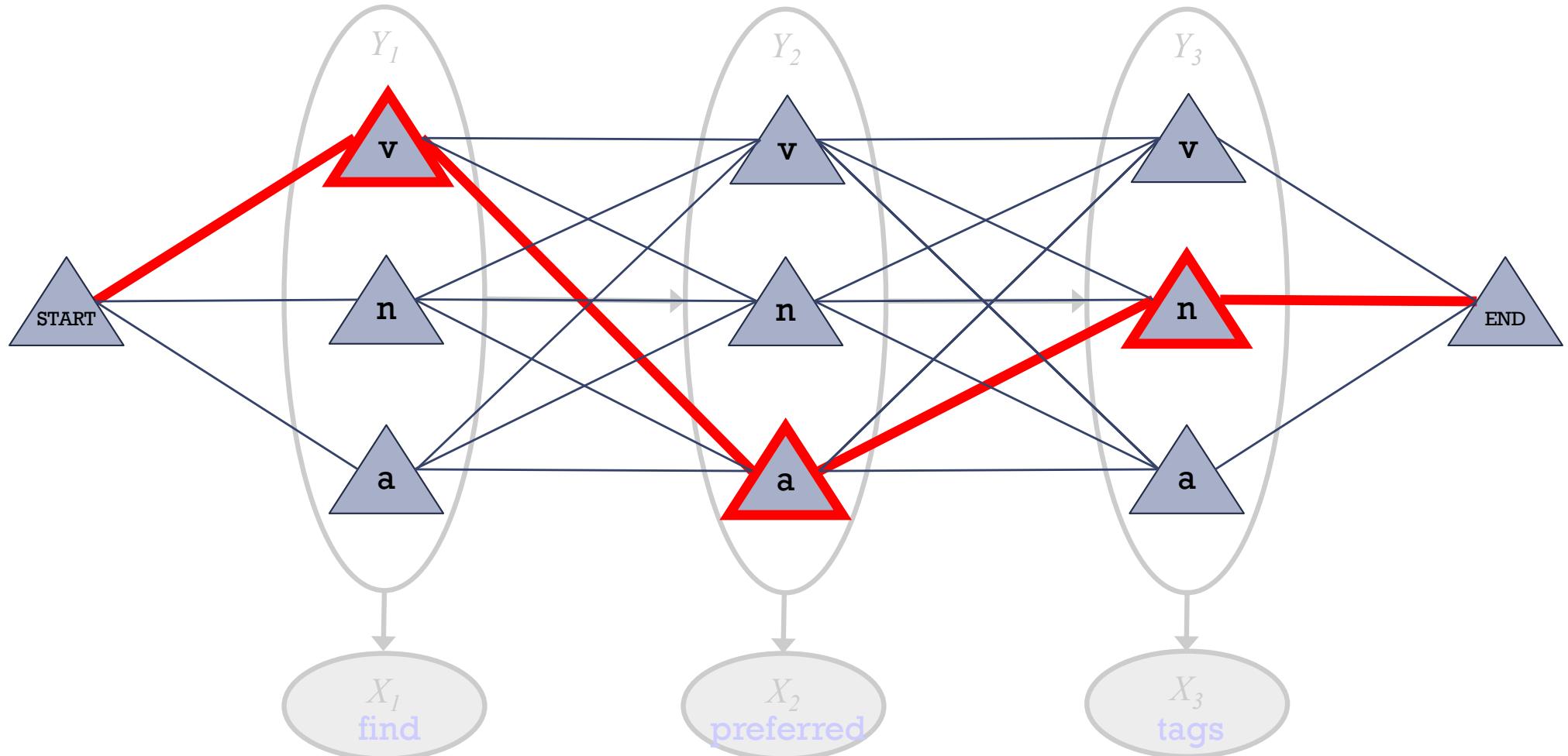
- Let's show the possible *values* for each variable

Forward-Backward Algorithm



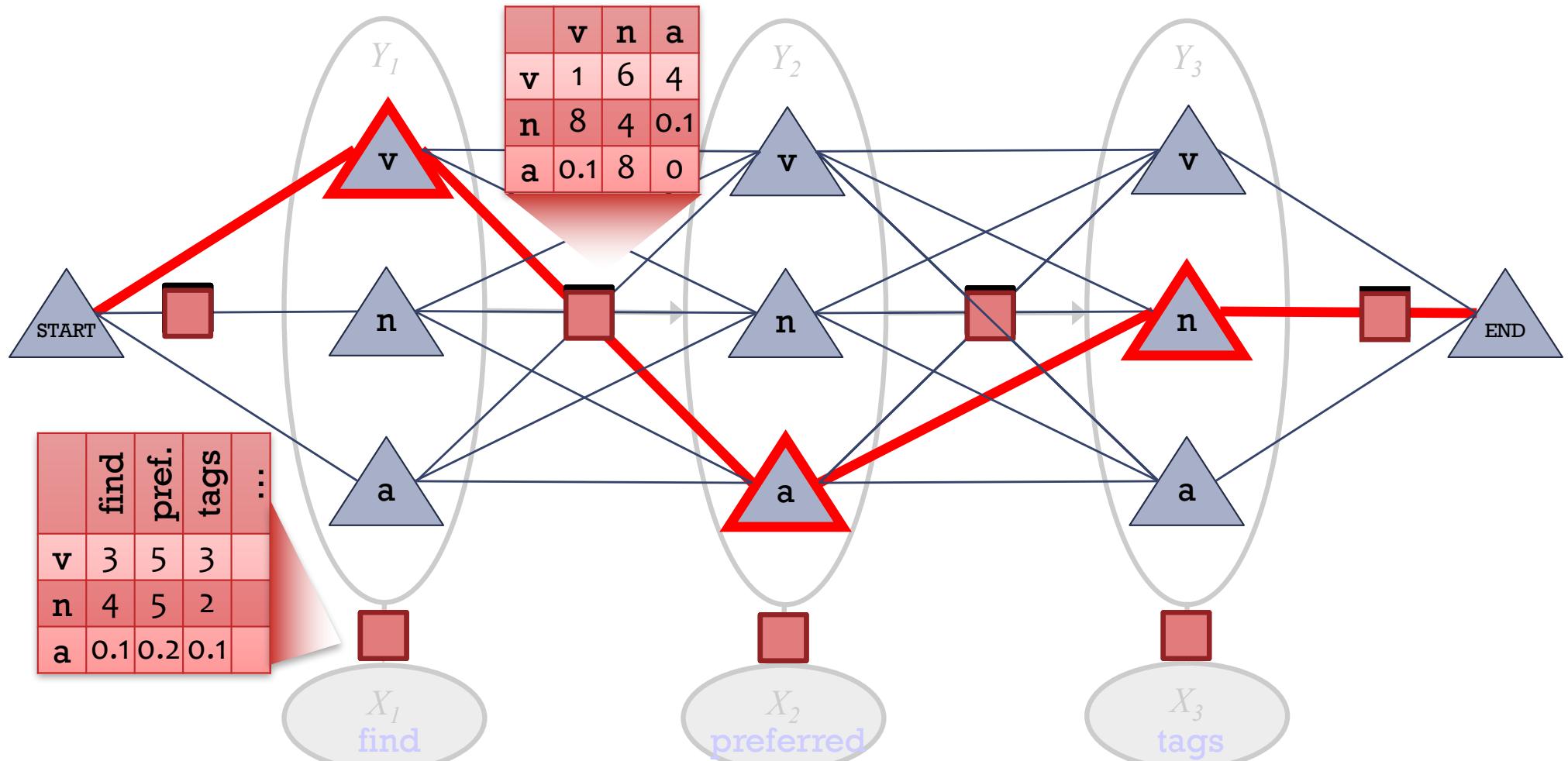
- Let's show the possible *values* for each variable
- One possible assignment

Forward-Backward Algorithm



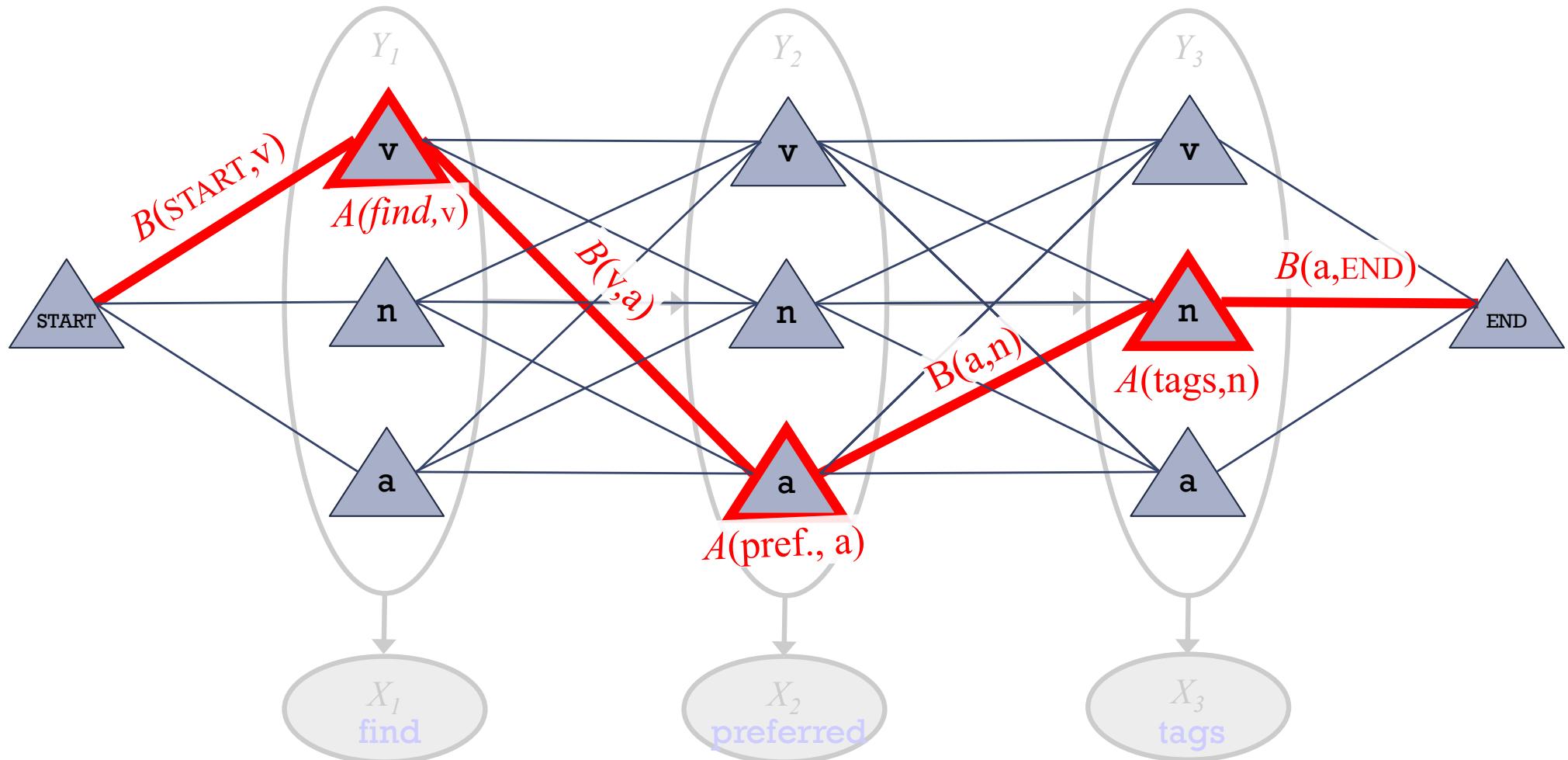
- Let's show the possible values for each variable
- One possible assignment
- And what the 7 transition / emission factors **think of it ...**

Forward-Backward Algorithm



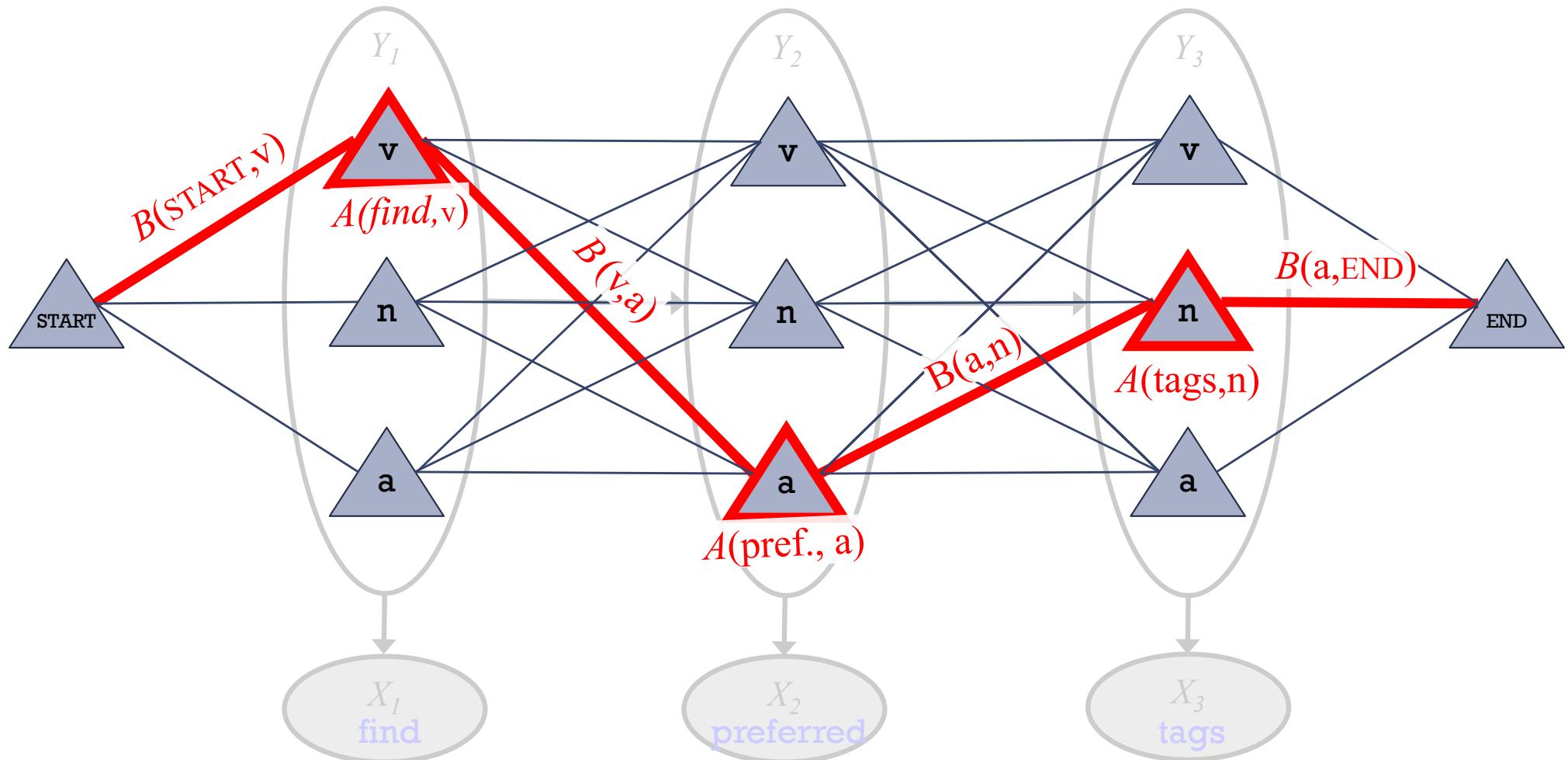
- Let's show the possible values for each variable
- One possible assignment
- And what the 7 transition / emission factors think of it ...

Viterbi Algorithm: Most Probable Assignment



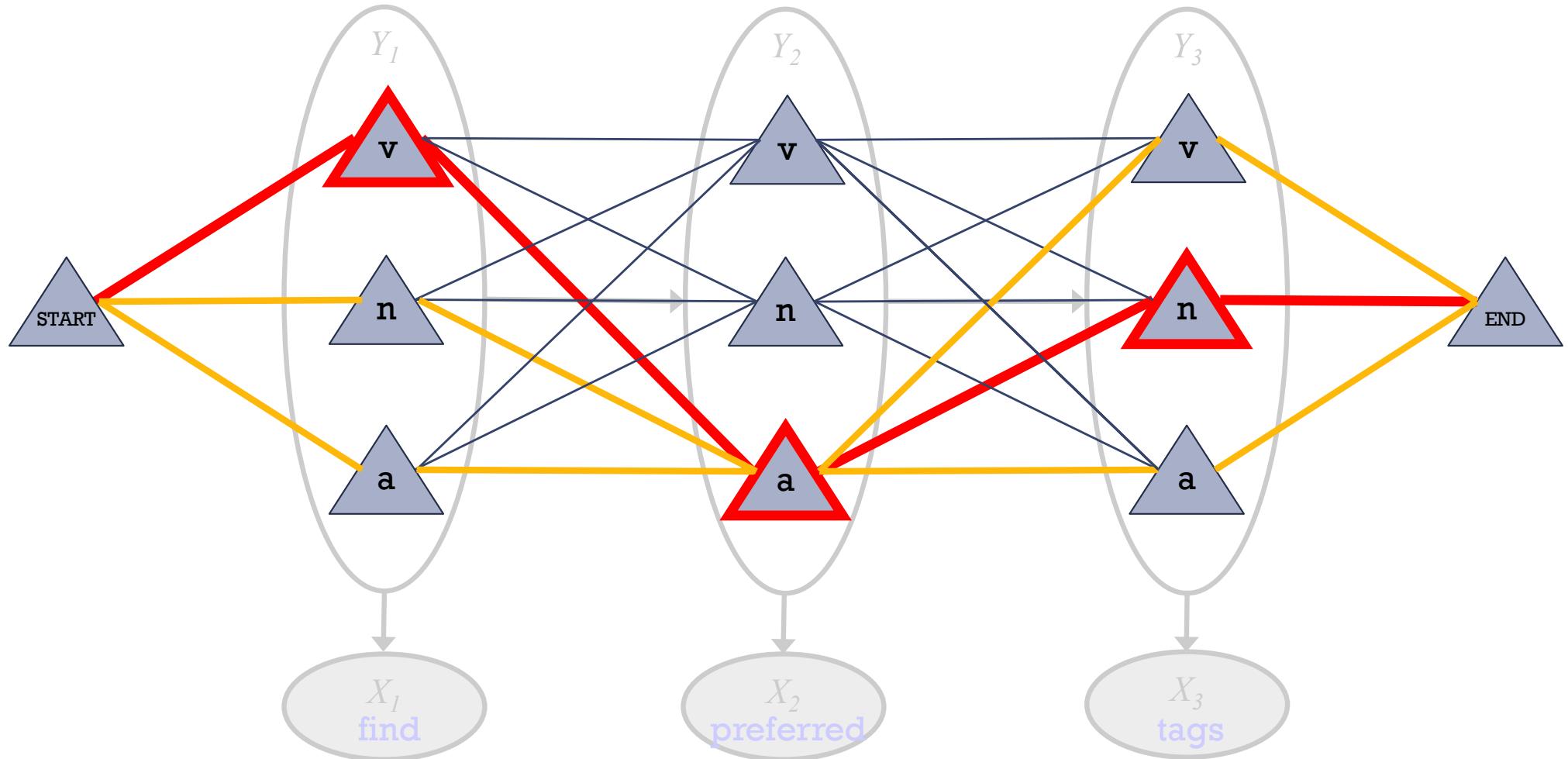
- So $p(v \ a \ n) = (1/Z) * \text{product of 7 numbers}$
- Numbers associated with edges and nodes of path
- Most probable assignment = **path with highest product**

Viterbi Algorithm: Most Probable Assignment

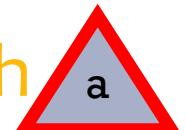


- So $p(v \ a \ n) = (1/Z) * \text{product weight of one path}$

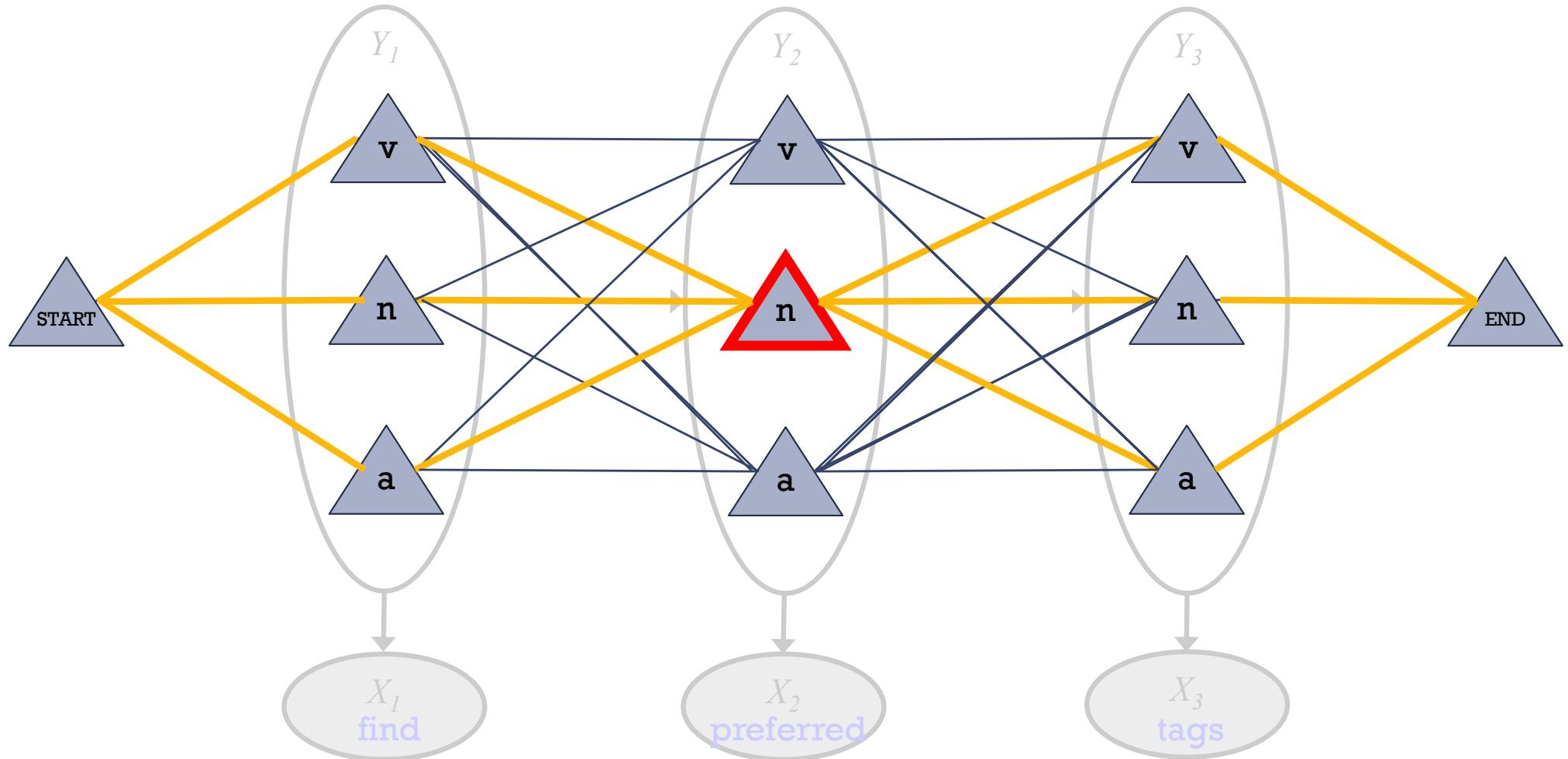
Forward-Backward Algorithm: Finds Marginals



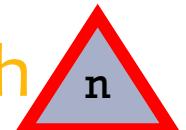
- So $p(v \ a \ n) = (1/Z) * \text{product weight of one path}$
- Marginal probability $p(Y_2 = a)$
 $= (1/Z) * \text{total weight of all paths through } a$



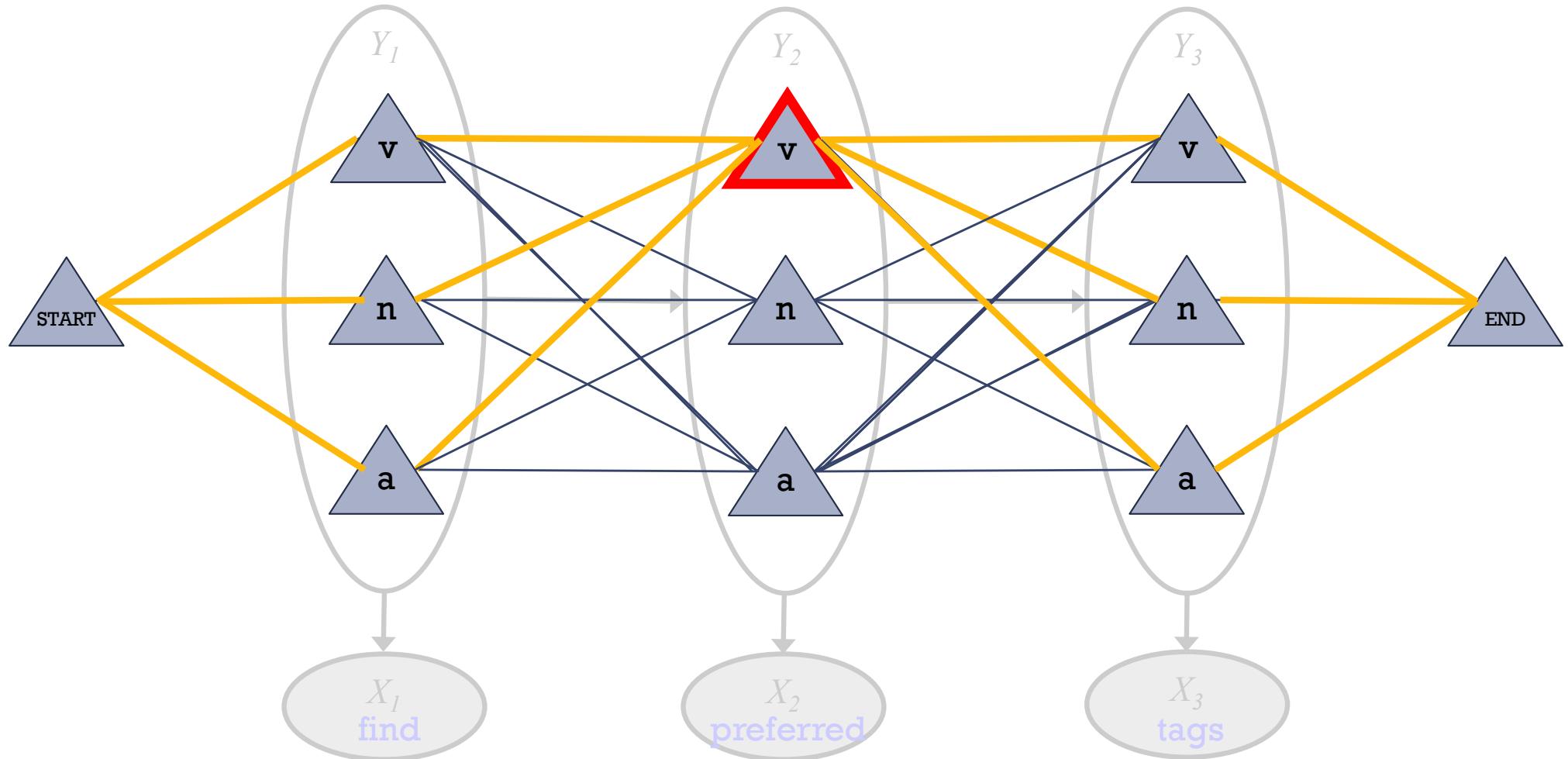
Forward-Backward Algorithm: Finds Marginals



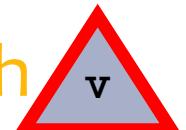
- So $p(v \ a \ n) = (1/Z) * \text{product weight of one path}$
- Marginal probability $p(Y_2 = n) = (1/Z) * \text{total weight of all paths through } n$



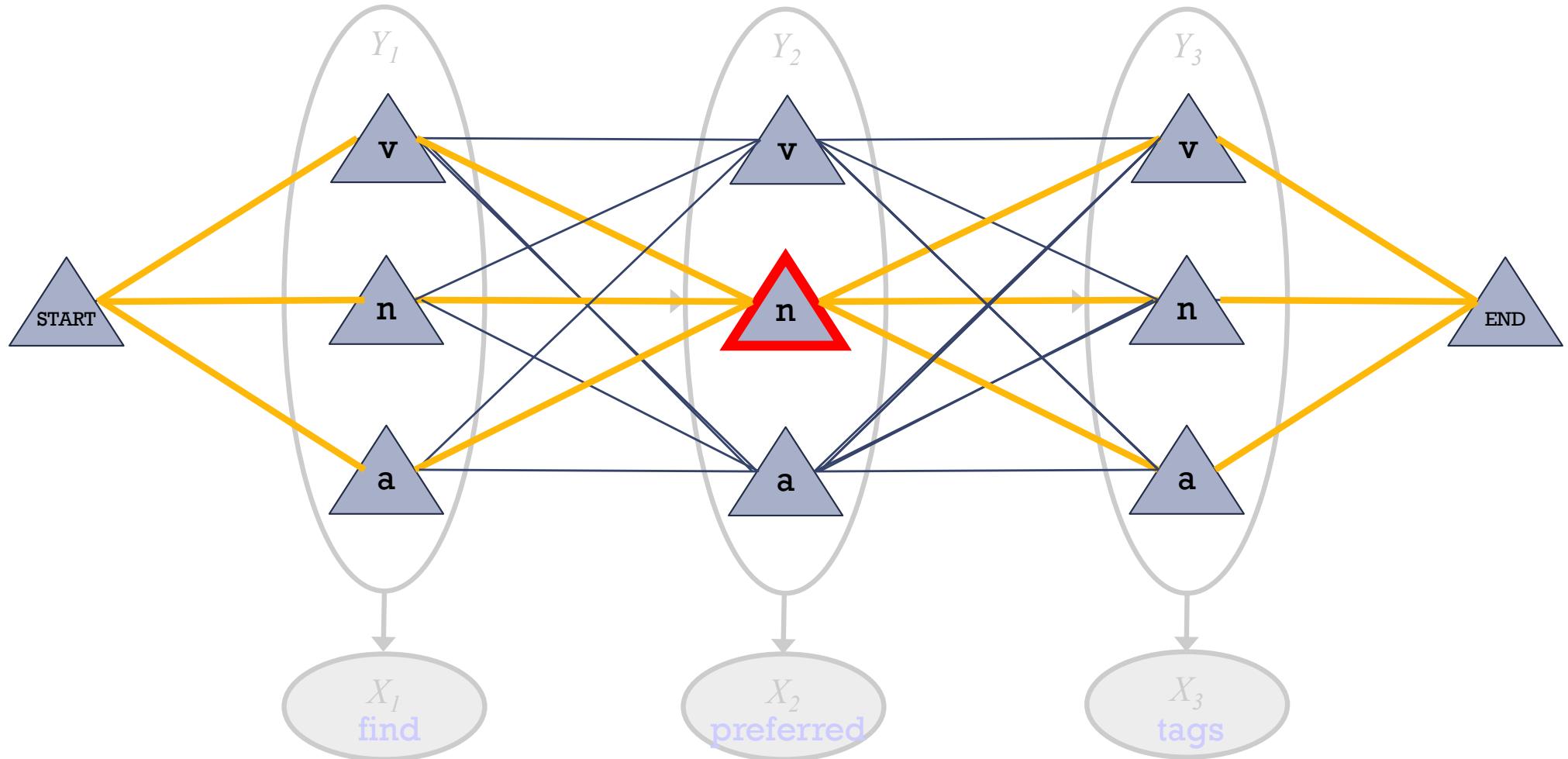
Forward-Backward Algorithm: Finds Marginals



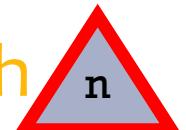
- So $p(v \ a \ n) = (1/Z) * \text{product weight of one path}$
- Marginal probability $p(Y_2 = v)$
 $= (1/Z) * \text{total weight of all paths through }$



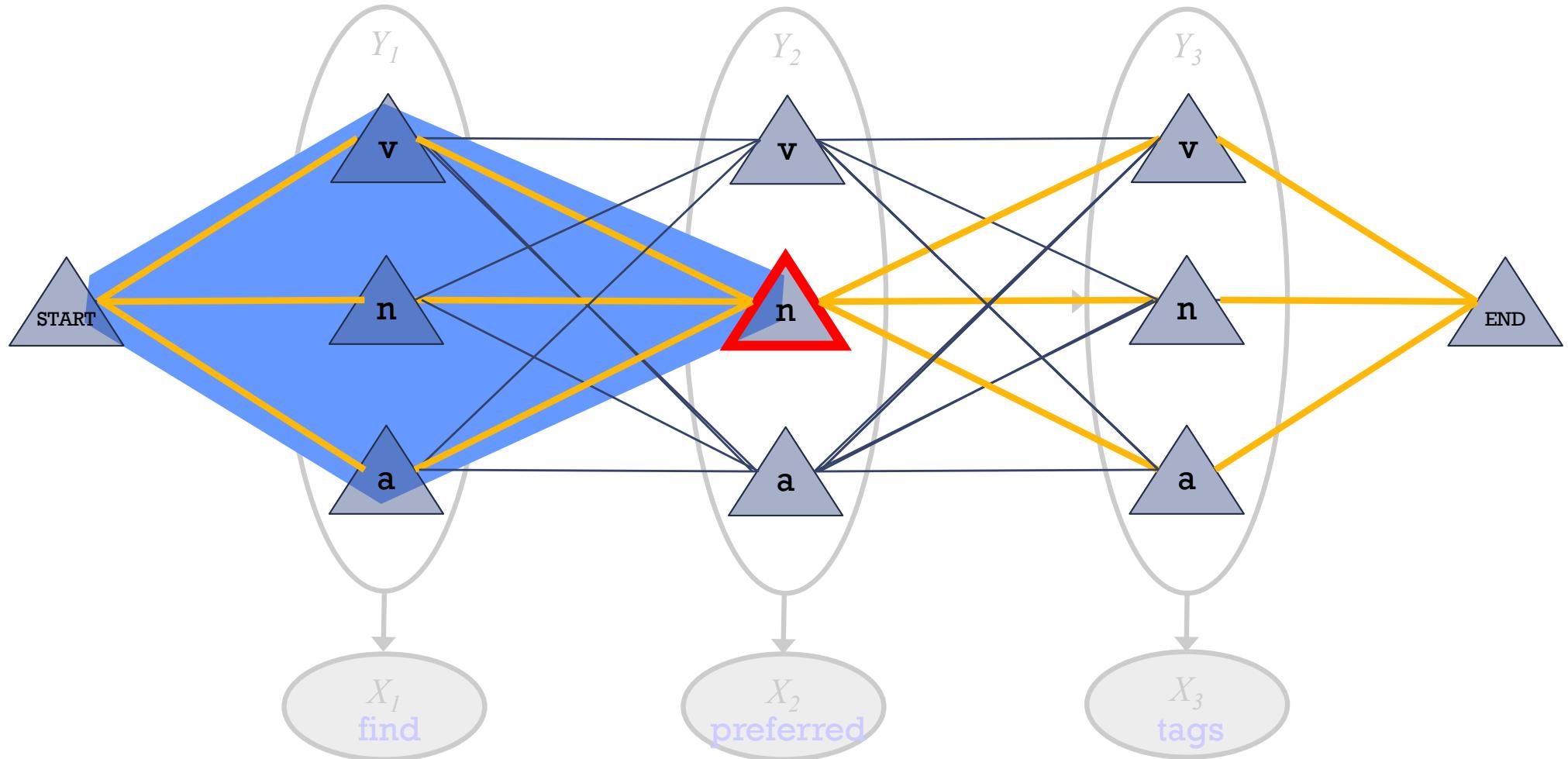
Forward-Backward Algorithm: Finds Marginals



- So $p(v \ a \ n) = (1/Z) * \text{product weight of one path}$
- Marginal probability $p(Y_2 = n)$
 $= (1/Z) * \text{total weight of all paths through } n$



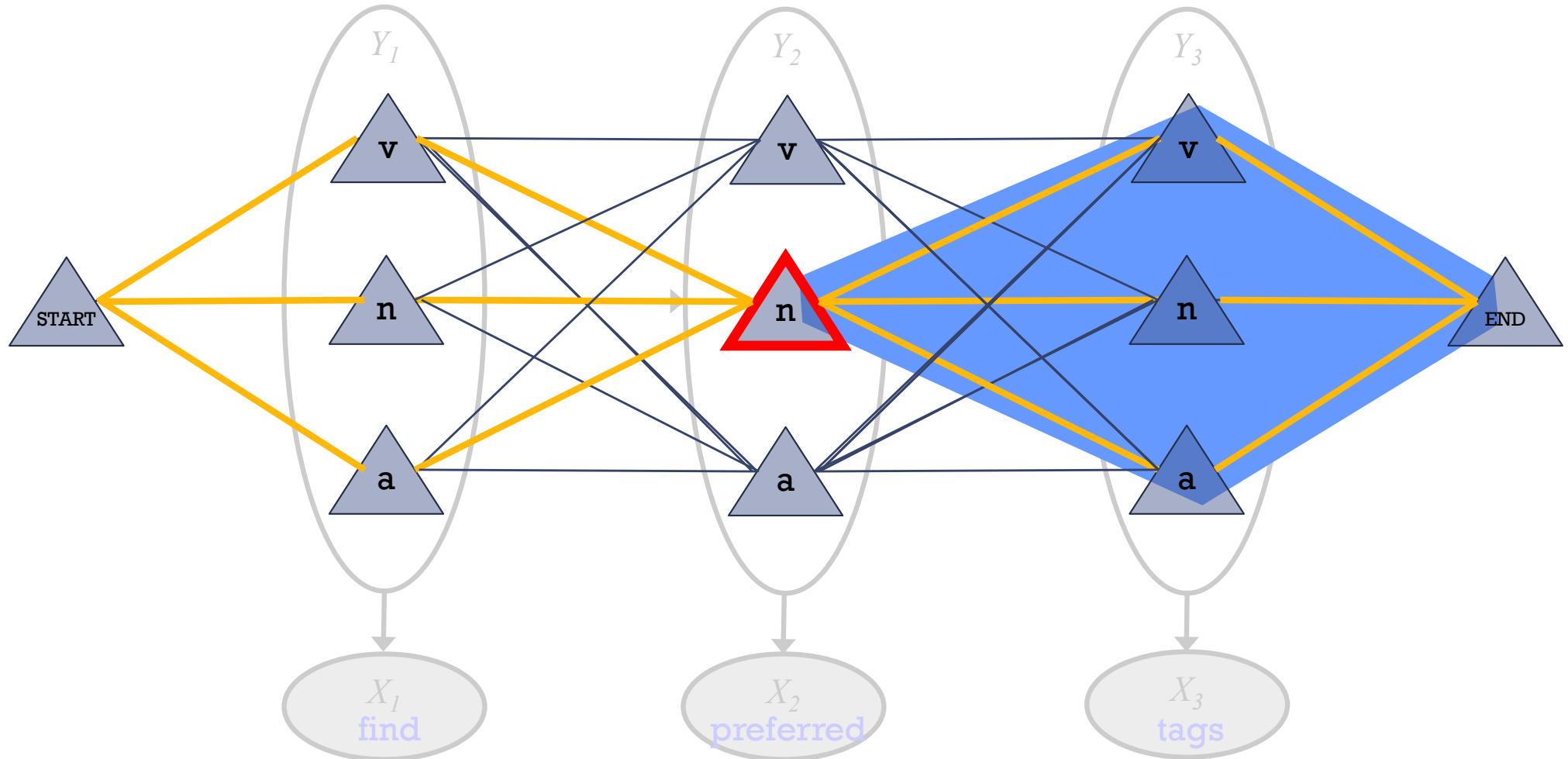
Forward-Backward Algorithm: Finds Marginals



$\alpha_2(n)$ = total weight of these path prefixes

(found by dynamic programming: matrix-vector products)

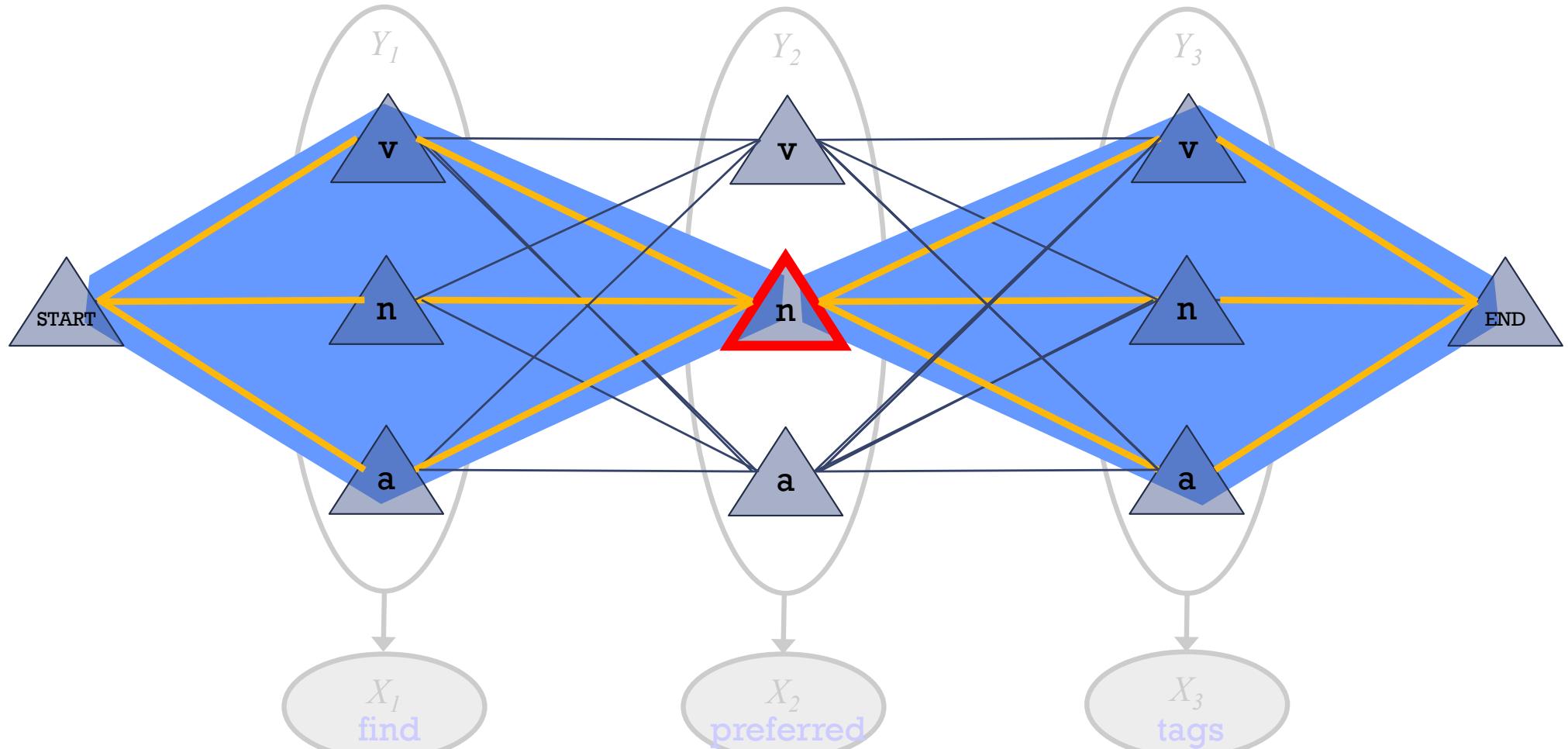
Forward-Backward Algorithm: Finds Marginals



$\beta_2(n)$ = total weight of these path suffixes

(found by dynamic programming: matrix-vector products)

Forward-Backward Algorithm: Finds Marginals



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

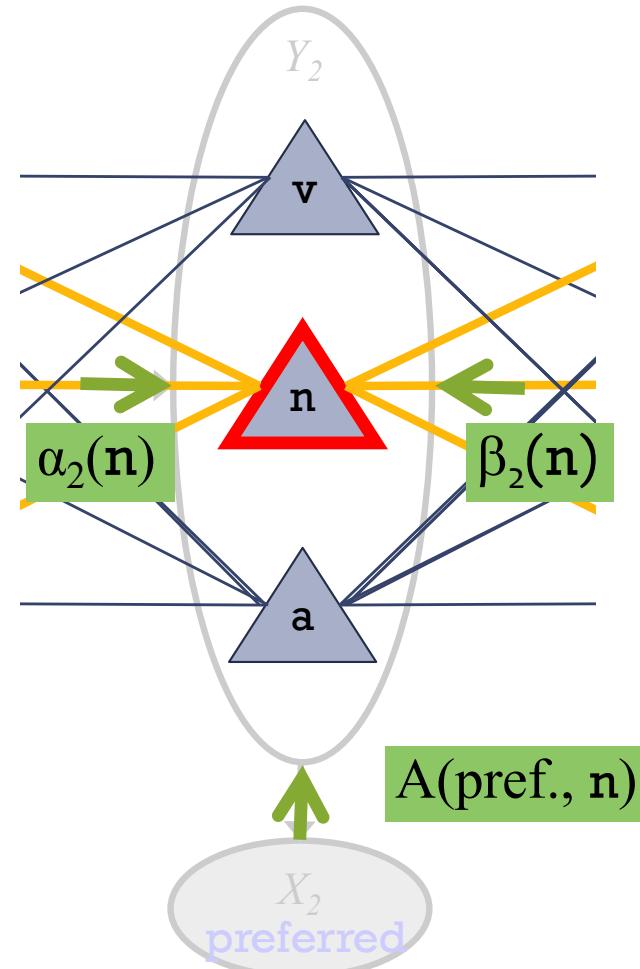
$\beta_2(n)$ = total weight of these path suffixes ($x + y + z$)

Product gives $ax+ay+az+bx+by+bz+cx+cy+cw$ = total weight of paths ⁴⁴

Forward-Backward Algorithm: Finds Marginals

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

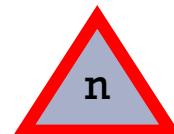
The extra weight is the opinion of the emission probability at this variable.



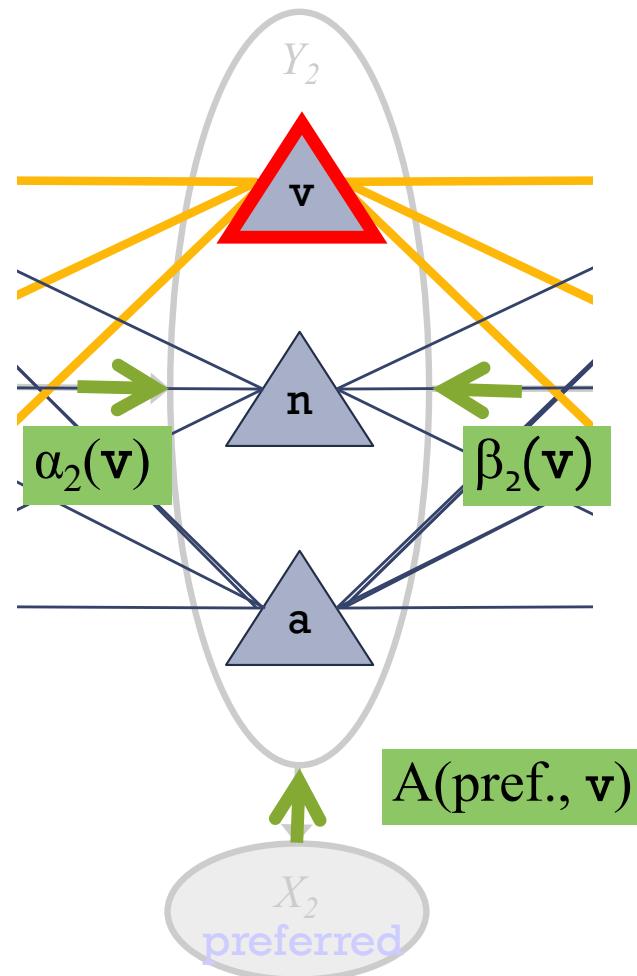
“belief that $Y_2 = n$ ”

total weight of **all** paths through

$$= \alpha_2(n) \ A(\text{pref.}, n) \ \beta_2(n)$$



Forward-Backward Algorithm: Finds Marginals

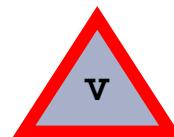


“belief that $Y_2 = v$ ”

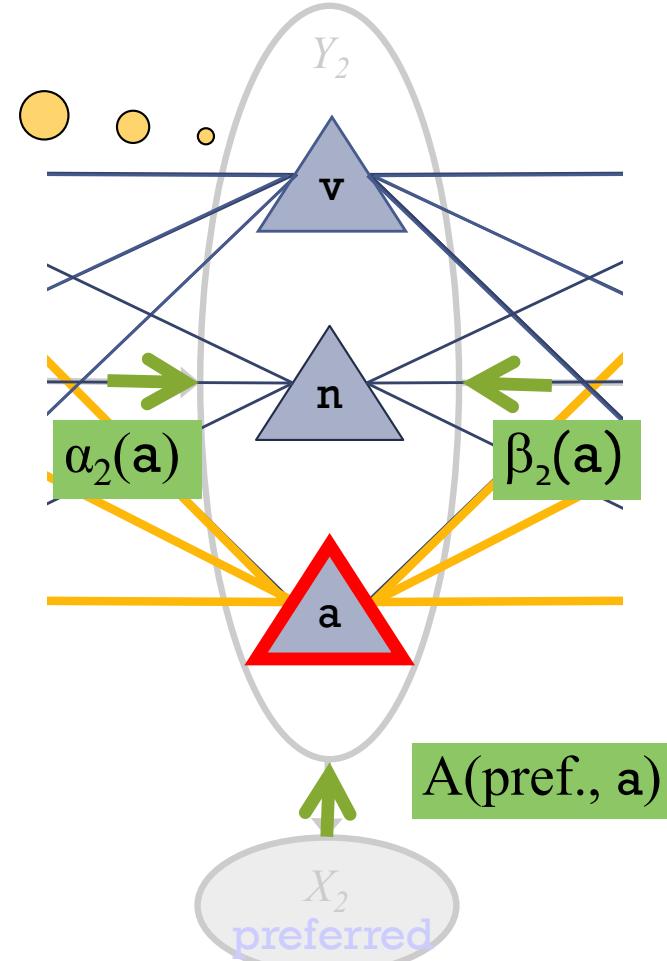
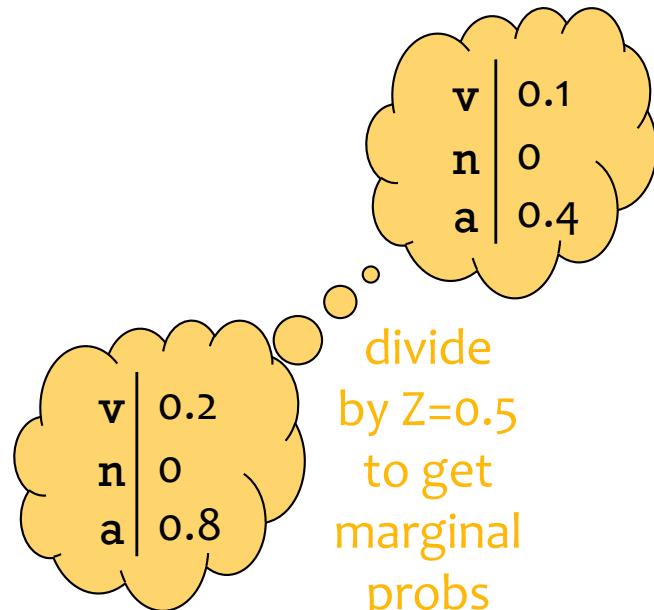
“belief that $Y_2 = n$ ”

total weight of **all paths through**

$$= \alpha_2(v) \quad A(\text{pref.}, v) \quad \beta_2(v)$$

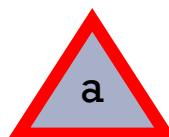


Forward-Backward Algorithm: Finds Marginals



total weight of **all** paths through

$$= \alpha_2(a) \quad A(\text{pref., } a) \quad \beta_2(a)$$



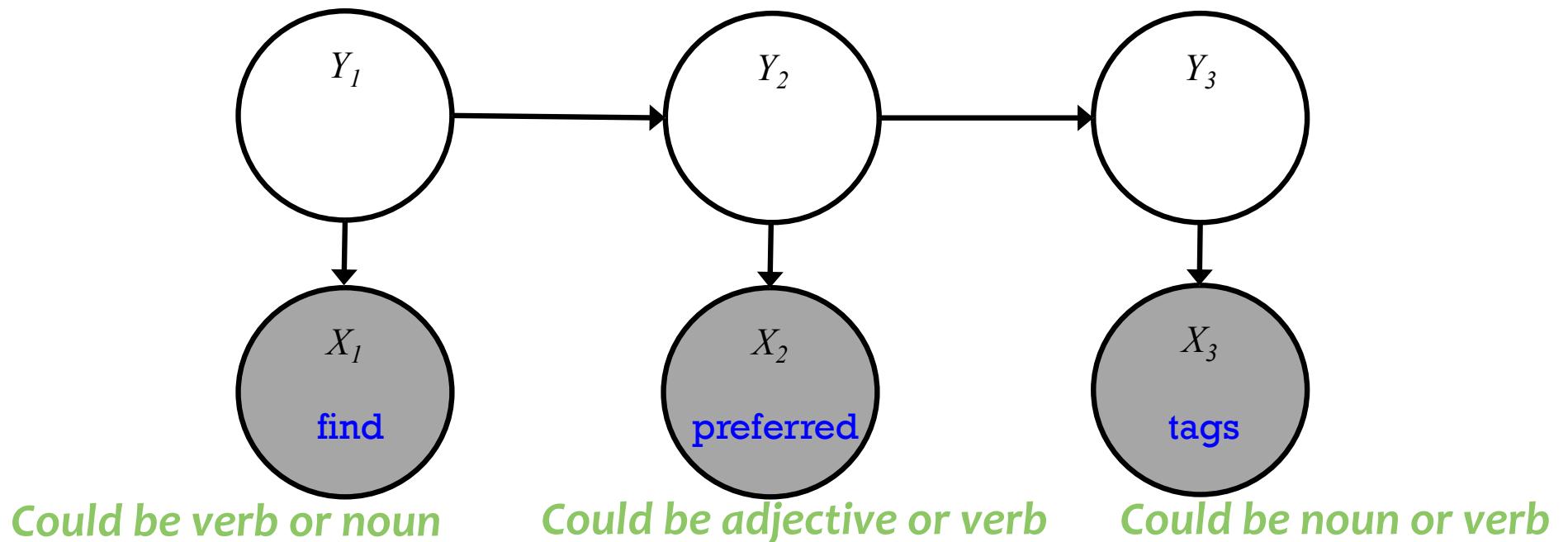
“belief that $Y_2 = v$ ”

“belief that $Y_2 = n$ ”

“belief that $Y_2 = a$ ”

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

Forward-Backward Algorithm



Inference for HMMs

Whiteboard

- Derivation of Forward algorithm
- Forward-backward algorithm
- Viterbi algorithm

Derivation of Forward Algorithm

Definition: $\alpha_t(k) \triangleq p(x_1, \dots, x_t, y_t = k)$

Derivation:

$$\begin{aligned}\alpha_T(\text{END}) &= p(x_1, \dots, x_T, y_T = \text{END}) \\ &= p(x_1, \dots, x_T | y_T) p(y_T) \quad \leftarrow \text{by def. of joint} \\ &= p(x_T | y_T) p(x_1, \dots, x_{T-1} | y_T) p(y_T) \quad \leftarrow \text{by cond. indep. of HMM} \\ &= p(x_T | y_T) p(x_1, \dots, x_{T-1}, y_T) \quad \leftarrow \text{by def. of joint} \\ &= p(x_T | y_T) \sum_{y_{T-1}} p(x_1, \dots, x_{T-1}, y_{T-1}, y_T) \quad \leftarrow \text{by def. of marginal} \\ &= p(x_T | y_T) \sum_{y_{T-1}} p(x_1, \dots, x_{T-1}, y_T | y_{T-1}) p(y_{T-1}) \quad \leftarrow \text{by def. of joint} \\ &= p(x_T | y_T) \sum_{y_{T-1}} \underbrace{p(x_1, \dots, x_{T-1} | y_{T-1})}_{\text{blue bracket}} p(y_T | y_{T-1}) p(y_{T-1}) \quad \leftarrow \text{by cond. indep. of HMM} \\ &= p(x_T | y_T) \sum_{y_{T-1}} \underbrace{p(x_1, \dots, x_{T-1}, y_{T-1})}_{\text{blue bracket}} p(y_T | y_{T-1}) \quad \leftarrow \text{by def. of joint} \\ &= p(x_T | y_T) \sum_{y_{T-1}} \alpha_{T-1}(y_{T-1}) p(y_T | y_{T-1}) \quad \leftarrow \text{by def. of } \alpha_t(k)\end{aligned}$$

Herein using "y_T" as shorthand for "y_T = END"

Forward-Backward Algorithm

Define: $\alpha_t(k) \triangleq p(x_1, \dots, x_t, y_t = k)$

$$\beta_t(k) \triangleq p(x_{t+1}, \dots, x_T | y_t = k)$$

Assume $y_0 = \text{START}$
 $y_{T+1} = \text{END}$

① Initialize $\alpha_0(\text{START}) = 1$ $\alpha_0(k) = 0 \quad \forall k \neq \text{START}$

$$\beta_{T+1}(\text{END}) = 1 \quad \beta_{T+1}(k) = 0 \quad \forall k \neq \text{END}$$

② For $t = 1, \dots, T$:

For $k = 1, \dots, K$:

$$\alpha_t(k) = p(x_t | y_t = k) \sum_{j=1}^K \alpha_{t-1}(j) p(y_t = k | y_{t-1} = j)$$

the alphas include the emission probabilities
so we don't multiply them in separately

③ For $t = T, \dots, 1$:

For $k = 1, \dots, K$:

$$\beta_t(k) = \sum_{j=1}^K p(x_{t+1} | y_{t+1} = j) \beta_{t+1}(j) p(y_{t+1} = j | y_t = k)$$

④ Compute $p(\vec{x}) = \alpha_{T+1}(\text{END})$

[Evaluation]

⑤ Compute $p(y_t = k | \vec{x}) = \frac{\alpha_t(k) \beta_t(k)}{p(\vec{x})}$

[Marginals]

Viterbi Algorithm

Define: $\omega_t(k) \triangleq \max_{y_1, \dots, y_{t-1}} p(x_1, \dots, x_t, y_1, \dots, y_{t-1}, y_t = k)$

"backpointers" $\rightarrow b_t(k) \triangleq \arg \max_{y_1, \dots, y_{t-1}} p(x_1, \dots, x_t, y_1, \dots, y_{t-1}, y_t = k)$

Assume $y_0 = \text{START}$

① Initialize $\omega_0(\text{START}) = 1$ $\omega_0(k) = 0 \quad \forall k \neq \text{START}$

② For $t = 1, \dots, T$:

For $k = 1, \dots, K$:

$$\omega_t(k) = \max_{j \in \{1, \dots, K\}} p(x_t | y_t = k) \omega_{t-1}(j) p(y_t = k | y_{t-1} = j)$$

$$b_t(k) = \arg \max_{j \in \{1, \dots, K\}} p(x_t | y_t = k) \omega_{t-1}(j) p(y_t = k | y_{t-1} = j)$$

③ Compute Most Probable Assignment

$$\hat{y}_T = b_{T+1}(\text{END})$$

For $t = T-1, \dots, 1$

$$\hat{y}_t = b_{t+1}(\hat{y}_{t+1})$$

[Decoding]

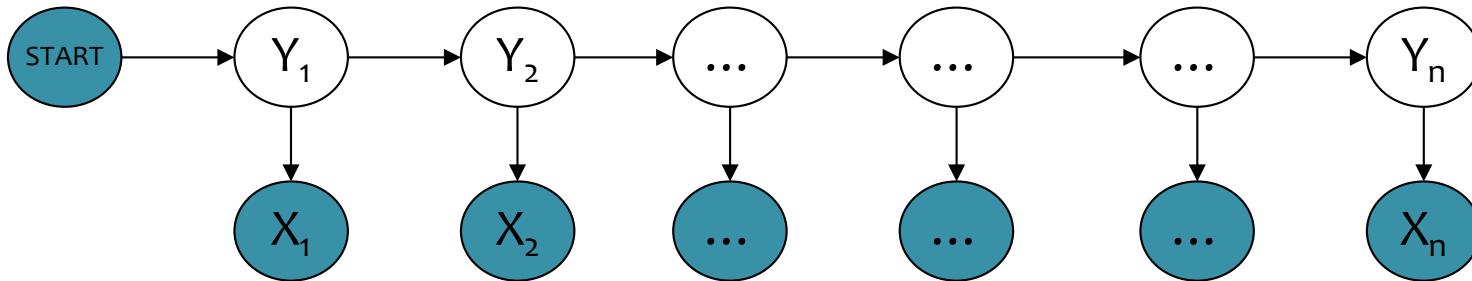
] follow the
"backpointers"

Inference in HMMs

What is the **computational complexity** of inference for HMMs?

- The **naïve** (brute force) computations for *Evaluation, Decoding, and Marginals* take **exponential time**, $O(K^T)$
- The **forward-backward** algorithm and **Viterbi** algorithm run in **polynomial time**, $O(T*K^2)$
 - Thanks to dynamic programming!

Shortcomings of Hidden Markov Models



- HMM models capture dependences between each state and **only its corresponding observation**
 - NLP example: In a sentence segmentation task, each segmental state may depend not just on a single word (and the adjacent segmental stages), but also on the (non-local) features of the whole line such as line length, indentation, amount of white space, etc.
- Mismatch between learning objective function and prediction objective function
 - HMM learns a joint distribution of states and observations $P(Y, X)$, but in a prediction task, we need the conditional probability $P(Y|X)$

MBR DECODING

Inference for HMMs

- Four
- Three Inference Problems for an HMM
 1. Evaluation: Compute the probability of a given sequence of observations
 2. Viterbi Decoding: Find the most-likely sequence of hidden states, given a sequence of observations
 3. Marginals: Compute the marginal distribution for a hidden state, given a sequence of observations
 4. MBR Decoding: Find the lowest loss sequence of hidden states, given a sequence of observations
(Viterbi decoding is a special case)

Minimum Bayes Risk Decoding

- Suppose we given a loss function $l(\hat{y}, y)$ and are asked for a single tagging
- How should we choose just one from our probability distribution $p(y|x)$?
- A minimum Bayes risk (MBR) decoder $h(x)$ returns the variable assignment with minimum **expected** loss under the model's distribution

$$\begin{aligned} h_{\theta}(x) &= \operatorname{argmin}_{\hat{y}} \mathbb{E}_{y \sim p_{\theta}(\cdot|x)} [\ell(\hat{y}, y)] \\ &= \operatorname{argmin}_{\hat{y}} \sum_y p_{\theta}(y | x) \ell(\hat{y}, y) \end{aligned}$$

Minimum Bayes Risk Decoding

$$h_{\theta}(x) = \operatorname{argmin}_{\hat{y}} \mathbb{E}_{y \sim p_{\theta}(\cdot | x)} [\ell(\hat{y}, y)]$$

Consider some example loss functions:

The **0-1 loss function** returns 1 only if the two assignments are identical and 0 otherwise:

$$\ell(\hat{y}, y) = 1 - \mathbb{I}(\hat{y}, y)$$

The MBR decoder is:

$$\begin{aligned} h_{\theta}(x) &= \operatorname{argmin}_{\hat{y}} \sum_y p_{\theta}(y | x) (1 - \mathbb{I}(\hat{y}, y)) \\ &= \operatorname{argmax}_{\hat{y}} p_{\theta}(\hat{y} | x) \end{aligned}$$

which is exactly the Viterbi decoding problem!

Minimum Bayes Risk Decoding

$$h_{\theta}(x) = \operatorname{argmin}_{\hat{y}} \mathbb{E}_{y \sim p_{\theta}(\cdot | x)} [\ell(\hat{y}, y)]$$

Consider some example loss functions:

The **Hamming loss** corresponds to accuracy and returns the number of incorrect variable assignments:

$$\ell(\hat{y}, y) = \sum_{i=1}^V (1 - \mathbb{I}(\hat{y}_i, y_i))$$

The MBR decoder is:

$$\hat{y}_i = h_{\theta}(x)_i = \operatorname{argmax}_{\hat{y}_i} p_{\theta}(\hat{y}_i \mid x)$$

This decomposes across variables and requires the variable marginals.

Learning Objectives

Hidden Markov Models

You should be able to...

1. Show that structured prediction problems yield high-computation inference problems
2. Define the first order Markov assumption
3. Draw a Finite State Machine depicting a first order Markov assumption
4. Derive the MLE parameters of an HMM
5. Define the three key problems for an HMM: evaluation, decoding, and marginal computation
6. Derive a dynamic programming algorithm for computing the marginal probabilities of an HMM
7. Interpret the forward-backward algorithm as a message passing algorithm
8. Implement supervised learning for an HMM
9. Implement the forward-backward algorithm for an HMM
10. Implement the Viterbi algorithm for an HMM
11. Implement a minimum Bayes risk decoder with Hamming loss for an HMM