

CSE 4392 SPECIAL TOPICS NATURAL LANGUAGE PROCESSING

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Expectation Maximization

2024 Spring

INTUITION OF EM

• Let's say I have 3 coins in my pocket,

- Coin 0 has probability λ of heads
- Coin 1 has probability p_1 of heads
- Coin 2 has probability p_2 of heads

• For each trial:

• First, I toss Coin 0

Quiz: Guess what are the estimated values of λ, p₁, p₂?

- If coin 0 turns up **heads**, I toss coin 1 three times
- If coin 0 turns up **tails**, I toss coin 2 three/times
- I don't tell you the results of the coin 0 toss, or whether coin 1 or coin 2 was tossed, but I tell you how many heads/tails are seen after each trial
- You see the following sequence: /

 $\langle H, H, H \rangle, \langle T, T, T \rangle, \langle H, H, H \rangle, \langle T, T, T \rangle, \langle H, H, H \rangle$

MAXIMAL LIKELIHOOD ESTIMATE

- Data points $x_1, x_2, ..., x_n$ from (finite or countable) set \mathcal{X} (x_i is a triplet of three tosses)
- Parameter vector θ
- Parameter space Ω
- We have a distribution $P(x \mid \theta)$ for any $\theta \in \Omega$, such that

$$\sum_{\substack{x \in \mathcal{X} \\ P(x \mid \theta) \ge 0, \forall x}} P(x \mid \theta) = 1$$

• Assume data points are drawn independently and identically distributed from a distribution $P(x | \theta^*)$ for some $\theta^* \in \Omega$

LOG LIKELIHOOD

o Probability distribution P (x | θ) for any θ ∈ Ω
o Likelihood of θ:

$$Likelihood(\theta) = P(x_1, x_2, ..., x_n \mid \theta) = \prod_{i=1}^{n} P(x_i \mid \theta)$$

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• Log likelihood of θ :

$$L(\theta) = \sum_{i=1}^{n} \log P(x_i | \theta)$$

EXAMPLE 1: COIN TOSSING

• $\mathcal{X} = \{H, T\}$. Our data set $x_1, x_2, ..., x_n$ is a sequence of heads and tails, e.g.,

НТНТННННТТТ

- Parameter vector θ is a single parameter, i.e. probability of coin showing heads
- Parameter space $\Omega = [0, 1]$

• Distribution
$$P(x | \theta) = \begin{cases} \theta \text{ if } x = H \\ 1 - \theta \text{ if } x = T \end{cases}$$

EXAMPLE 2: MARKOV CHAINS

- \mathcal{X} is the set of all possible state (or tag) sequences generated by an underlying generative process. Our sample is *n* sequences X_1, X_2, \dots, X_n , where $X_i \in \mathcal{X}$.
- θ_T is the vector of all transition $(s_i \rightarrow s_j)$ parameters. W.L.O.G., we assume there is a dummy start state ϕ and initial transition $\phi \rightarrow s_1$
- Let $T(\alpha) \subset T$ be all transition of the form $\alpha \to \beta$
- Ω is the set of $\theta \in [0,1]^{|S+1||S|}$ where S is the set of all states (tags), such that:

$$\forall \alpha \in S, \sum_{t \in T(\alpha)} \theta_t = 1$$

EXAMPLE 2: MARKOV CHAINS

Since θ_T is the vector of all transition parameters
We have:

$$P(X \mid \theta_T) = \prod_{t \in T} \theta_t^{Count(X,t)}$$

where Count(X, t) is the number of times transition t occures in sequence X.

• This gives:

$$\log(P(X|\theta_T)) = \sum_{t \in T} Count(X,t) \log \theta_t$$
$$L(\theta_T) = \sum_i \log P(X_i|||\theta_T) = \sum_i \sum_{t \in T} Count(X,t) \log \theta_t$$

MLE FOR MARKOV CHAINS

• We use θ for θ_T for simplicity

• To solve for $\theta_{MLE} = \arg \max_{\theta \in \Omega} L(\theta)$

• We solve θ in

$$\frac{\partial L(\theta)}{\partial \theta} = 0$$

with appropritate probability constraints

• Therefore:

$$\theta_{t} = \frac{\sum_{i} Count(X_{i}, t)}{\sum_{i} \sum_{t' \in T(\alpha)} Count(X_{i}, t')}$$

where *t* is a transition of the form $\alpha \rightarrow \beta$ for some β , $T(\alpha)$ is all the transitions originating from α .

MODELS WITH HIDDEN VARIABLES

- Suppose we have two sets \mathcal{X} and \mathcal{Y} , and a joint distribution $P(x, y \mid \theta)$
- If we have **fully-observable data**, (x_i, y_i) pairs, then

$$L(\theta) = \sum_{i} \log P(x_i, y_i \mid \theta)$$

• If we have **partially-observable data**, *x_i* examples only, then

$$L(\theta) = \sum_{i} \log P(x_i | \theta)$$
$$= \sum_{i} \log \sum_{y \in \mathcal{Y}} P(x_i, y | \theta)$$

- This is unsupervised learning, very similar to clustering.
- We will use an interative algorithm to infer θ like k-means

EXPECTATION-MAXIMILATION

• If we have **partially-observable data**, *x_i* examples only, then

$$L(\theta) = \sum_{i} \log \sum_{y \in \mathcal{Y}} P(x_i, y \mid \theta)$$

• The EM (Expectation Maximization) algorithm is a method for finding

$$\theta_{MLE} = \arg \max_{\theta} L(\theta) = \arg \max_{\theta} \sum_{i} \log \sum_{y \in \mathcal{Y}} P(x_i, y \mid \theta)$$

• In the three-coin example:

- $\mathcal{Y} = \{H, T\}$ (possible outcomes of coin 0)
- $\mathcal{X} = \{HHH, TTT, HTT, THH, HHT, TTH, HTH, THT\}$

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$$\theta = \{\lambda, p_1, p_2\}$$

• And $P(x, y | \theta) = P(y | \theta) P(x | y, \theta)$

where

$$P(y | \theta) = \begin{cases} \lambda \text{ if } y = H\\ 1 - \lambda \text{ if } y = T \end{cases}$$

$$h \text{ is number } t \text{ is number } t$$

h is num of heads in *x t* is num of tails in *x*

and

$$P(x | y, \theta) = \begin{cases} p_1^h (1 - p_1)^t & \text{if } y = H \\ p_2^h (1 - p_2)^t & \text{if } y = T \end{cases}$$

• Calculate various probabilities:

one H and two T from THT

$$P(x = THT, y = H | \theta) = \lambda p_1 (1 - p_1)^2$$

$$P(x = THT, y = T | \theta) = (1 - \lambda) p_2 (1 - p_2)^2$$

 $P(x = THT | \theta) = P(x = THT, y = H | \theta) + P(x = THT, y = T | \theta)$ = $\lambda p_1 (1 - p_1)^2 + (1 - \lambda) p_2 (1 - p_2)^2$

$$P(y = H | x = THT, \theta) = \frac{P(x = THT, y = H | \theta)}{P(x = THT | \theta)}$$
(Bayes rule)
$$= \frac{\lambda p_1 (1 - p_1)^2}{\lambda p_1 (1 - p_1)^2 + (1 - \lambda) p_2 (1 - p_2)^2}$$

• Suppose fully observed data looks like: $(\langle HHH \rangle, H), (\langle TTT \rangle, T), (\langle HHH \rangle, H), (\langle TTT \rangle, T), (\langle HHH \rangle, H)$

• In this case, the maximum likelihood estimates of the parameters are:

$$\lambda = \frac{3}{\frac{5}{9}}$$
$$p_1 = \frac{1}{\frac{9}{9}} = 1$$
$$p_2 = \frac{1}{\frac{9}{6}} = 0$$

• Partial observed data might look like: $\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle$

• How do you estimate the MLE parameters?

• Partial observed data might look like: $\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle$

• If the current parameters are λ , p_1 , p_2

 $P(y = H | x = \langle HHH \rangle) = \frac{P(\langle HHH \rangle, H)}{P(\langle HHH \rangle, H) + P(\langle HHH \rangle, T)}$ $\frac{\lambda p_1^3}{\lambda p_1^3 + (1-\lambda)p_2^3}$ $P(y = H | x = \langle TTT \rangle) = \frac{P(\langle TTT \rangle, H)}{P(\langle TTT \rangle, H) + P(\langle TTT \rangle, T)}$ $= \frac{\lambda(1-p_1)^3}{\lambda(1-p_1)^3 + (1-\lambda)(1-p_2)^3}$

• If the current parameters are λ , p_1 , p_2

 $P(y = H | x = \langle HHH \rangle) = \frac{P(\langle HHH \rangle, H)}{P(\langle HHH \rangle, H) + P(\langle HHH \rangle, T)}$ $= \frac{\lambda p_1^3}{\lambda p_1^3 + (1 - \lambda) p_2^3}$ $P(y = H | x = \langle TTT \rangle) = \frac{P(\langle TTT \rangle, H)}{P(\langle TTT \rangle, H) + P(\langle TTT \rangle, T)}$ $= \frac{\lambda (1 - p_1)^3}{\lambda (1 - p_1)^3 + (1 - \lambda)(1 - p_2)^3}$

• If $\lambda = 0.3$, $p_1 = 0.3$, $p_2 = 0.6$ $P(y = H | x = \langle HHH \rangle) = 0.0508$ $P(y = H | x = \langle TTT \rangle) = 0.6967$

• After filling in hidden variables for each example, the partially observed data looks like this:

 $\begin{array}{ll} (\langle \mathrm{HHH}\rangle, H) & P(y=\mathrm{H} \mid \mathrm{HHH}) = 0.0508 \\ (\langle \mathrm{HHH}\rangle, T) & P(y=\mathrm{T} \mid \mathrm{HHH}) = 0.9492 \end{array}$ sum to 1 ((TTT), H) P(y = H | TTT) = 0.6967sum to 1 ((TTT), T) = P(y = T | TTT) = 0.3033 - $((HHH), H) \quad P(y = H | HHH) = 0.0508$ sum to 1 $(\langle \text{HHH} \rangle, T)$ $P(y = T \mid \text{HHH}) = 0.9492$ - $((\text{TTT}), H) \qquad P(y = H | \text{TTT}) = 0.6967$ sum to 1 ((TTT), T) = P(y = T | TTT) = 0.3033 - $\begin{array}{ll} (\langle \mathrm{HHH} \rangle, H) & P(y = \mathrm{H} \mid \mathrm{HHH}) = 0.0508 \\ (\langle \mathrm{HHH} \rangle, T) & P(y = \mathrm{T} \mid \mathrm{HHH}) = 0.9492 \end{array} \right] \text{ sum to } 1$

• New estimates:

 $\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle$

$$(\langle \text{HHH} \rangle, H) \qquad P(y = \text{H} \mid \text{HHH}) = 0.0508$$

$$(\langle \text{HHH} \rangle, T) \qquad P(y = \text{T} \mid \text{HHH}) = 0.9492$$

$$(\langle \text{TTT} \rangle, H) \qquad P(y = \text{H} \mid \text{TTT}) = 0.6967$$

$$(\langle \text{TTT} \rangle, T) \qquad P(y = \text{T} \mid \text{TTT}) = 0.3033$$
...
how many
heads in X_i ?
$$\lambda = \frac{3 \times 0.0508 + 2 \times 0.6967}{5} = 0.3092$$
out of 5 coin 0 tosses
how may are heads?
$$p_1 = \frac{3 \times 3 \times 0.0508 + 0 \times 2 \times 0.6967}{3 \times 3 \times 0.0508 + 3 \times 2 \times 0.6967} = 0.0987$$

$$p_2 = \frac{3 \times 3 \times 0.9492 + 0 \times 2 \times 0.3033}{3 \times 3 \times 0.9492 + 3 \times 2 \times 0.3033} = 0.8244$$
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SUMMARY OF THREE COINS EXAMPLE

• Begins with λ =0.3, p_1 = 0.3, p_2 = 0.6

• Fill in hidden variables using:

$$P(y = H | x = \langle HHH \rangle) = 0.0508$$

 $P(y = H | x = \langle TTT \rangle) = 0.6967$

• Re-estimate parameters to be $\lambda{=}0.3092,\,p_1=0.0987,\,p_2=0.8244$

EM INTERATIONS

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Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4	\tilde{p}_5
0	0.3000	0.3000	0.6000	0.0508	0.6967	0.0508	0.6967	0.0508
1	0.3092	0.0987	0.8244	0.0008	0.9837	0.0008	0.9837	0.0008
2	0.3940	0.0012	0.9893	0.0000	1.0000	0.0000	1.0000	0.0000
3	0.4000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000

 $P(y = H \mid X_i)$

• Coin example for $\langle\langle HHH\rangle, \langle TTT\rangle, \langle HHH\rangle, \langle TTT\rangle, \langle HHH\rangle \rangle$

- λ is now 0.4, indicating that coin 0 has a probability 0.4 of selecting the tail-biased coin (coin 1)
- θ (parameters) are like the cluster centers in k-means

EM INTERATIONS

Iteration	λ	p_1	p_2	\tilde{p}_1	$ ilde{p}_2$	\tilde{p}_3	$ ilde{P}_4$
0	0.3000	0.3000	0.6000	0.0508	0.6967	0.0508	0.6967
1	0.3738	0.0680	0.7578	0.0004	0.9714	0.0004	0.9714
2	0.4859	0.0004	0.9722	0.0000	1.0000	0.0000	1.0000
3	0.5000	0.0000	1.0000	0.0000	1.0000	0.0000	1.0000

- Coin example for $x = \{\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle \}$.
- This solution of $\lambda = 0.5$, $p_1 = 0$, and $p_2 = 1$ is intuitively correct: the coin tosser has two coins, one which always shows heads, and another which always shows tails, and is picking between them with equal probability.
- Posterior probabilities $\overline{p_i}$ show that we are certain that coin 1 (tail-biased) generate x_2 and x_4 , whereas coin 2 generated x_1 and x_3 .

INITIALIZATION MATTERS

Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4
0	0.3000	0.7000	0.7000	0.3000	0.3000	0.3000	0.3000
1	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
2	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
3	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
4	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
5	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000
6	0.3000	0.5000	0.5000	0.3000	0.3000	0.3000	0.3000

• Coin example for $x = \{\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle \}$.

• In this case, EM is stuck in a "**saddle point**", or *local optimal*.

INTIALIZATION MATTERS

Iteration	λ	p_1	p_2	\tilde{p}_1	\tilde{p}_2	\tilde{p}_3	\tilde{p}_4
0	0.3000	0.7001	0.7000	0.3001	0.2998	0.3001	0.2998
1	0.2999	0.5003	0.4999	0.3004	0.2995	0.3004	0.2995
2	0.2999	0.5008	0.4997	0.3013	0.2986	0.3013	0.2986
3	0.2999	0.5023	0.4990	0.3040	0.2959	0.3040	0.2959
4	0.3000	0.5068	0.4971	0.3122	0.2879	0.3122	0.2879
5	0.3000	0.5202	0.4913	0.3373	0.2645	0.3373	0.2645
6	0.3009	0.5605	0.4740	0.4157	0.2007	0.4157	0.2007
7	0.3082	0.6744	0.4223	0.6447	0.0739	0.6447	0.0739
8	0.3593	0.8972	0.2773	0.9500	0.0016	0.9500	0.0016
9	0.4758	0.9983	0.0477	0.9999	0.0000	0.9999	0.0000
10	0.4999	1.0000	0.0001	1.0000	0.0000	1.0000	0.0000
11	0.5000	1.0000	0.0000	1.0000	0.0000	1.0000	0.0000

Coin example for $x = \{\langle HHH \rangle, \langle TTT \rangle, \langle HHH \rangle, \langle TTT \rangle \}$.

• Just modify p_1 a bit, EM is able to skip the saddle point and reach global optimum.

THE EM ALGORTHM

- θ^t is the parameter vector at the t^{th} iteration.
- Choose θ^0 at random (or using some smart heuristics)
- Iterative procedure defined as:

$$\theta^{t} = \arg \max_{\theta} Q(\theta, \theta^{t-1})$$

where

$$Q(\theta, \theta^{t-1}) = \sum_{i} \sum_{y \in \mathcal{Y}} P(y | x_i, \theta^{t-1}) \log P(x_i, y | \theta)$$

THE EM ALGORITHM

• (E-step): Compute *expected* counts.

$$\overline{Count}(r) = \sum_{i=1}^{n} \sum_{y} P(y | x_i, \theta^{t-1}) Count(x_i, y, r)$$

for every paramter θ_r , e.g.,

$$\overline{Count}(DT \to NN) = \sum_{i} \sum_{y} P(S \mid O_i, \theta^{t-1}) Count(O_i, S, \theta_{DT \to NN})$$

• (M-step): Re-estimate parameters using expected counts to *maximize* likelihood.

e.g.,

$$\theta_{DT \to NN} = \frac{\overline{Count}(DT \to NN)}{\sum_{\beta} \overline{Count}(DT \to \beta)}$$

THE EM ALGORITHM

- Intuition: Fill in hidden variables according to $P(y \mid x_i, \theta)$
- EM is guaranteed to converge to a local maximum, or saddle-point, of the likelihood function
- In general, if

$$\arg\max_{\theta} \sum_{i} \log P(x_i, y_i \mid \theta)$$

has a simple analytic solution, then

$$\arg\max_{\theta} \sum_{i} \sum_{y} P(y \mid x_{i}, \theta) \log P(x_{i}, y \mid \theta)$$

also has a simple solution.

EXAMPLE: EM FOR HMM

- We observe only word sequences X_1, X_2, \dots, X_n (no tags)
- θ is the vector of all transition parameters (include initial state distribution as a special case, $\phi \rightarrow s$
- ϕ is the vector of all emission parameters
- Initialize parameters θ^0 and ϕ^0

EXAMPLE: EM FOR HMM

Initialize parameters θ⁰ and φ⁰
E-step:

i=1 Y

 θ_k has nothing to do with X_i

$$\overline{Count}(\theta_k) = \sum_{i=1}^n \sum_Y P(Y|X_i, \theta^{t-1}, \phi^{t-1}) Count(X_i, Y, \theta_k)$$
$$= \sum_{i=1}^n \sum_Y P(Y|X_i, \theta^{t-1}, \phi^{t-1}) Count(Y, \theta_k)$$
$$\overline{Count}(\phi_k) = \sum_{i=1}^n \sum_Y P(Y|X_i, \theta^{t-1}, \phi^{t-1}) Count(X_i, Y, \phi_k)$$

EXAMPLE: EM FOR HMM

• M-step:

$$\theta_k^t = \frac{\overline{Count}(\theta_k)}{\sum_{\theta' \in M(\theta_k)} \overline{Count}(\theta')}$$

where $M(\theta_k)$ is the set of all transitions $(a \rightarrow b, \text{ for all } b)$ that share the same previous state as the k^{th} transition $(a \rightarrow c, \text{ for some } c)$

$$\phi_k^t = \frac{\overline{Count}(\phi_k)}{\sum_{\phi' \in M'(\phi_k)} \overline{Count}(\phi')}$$

where $M'(\phi_k)$ is the set of all emissions $(a \to x, \text{ for all } x)$ that share the same previous state as the k^{th} emission $(a \to x', \text{ for some } x')$.

Efficient EM?

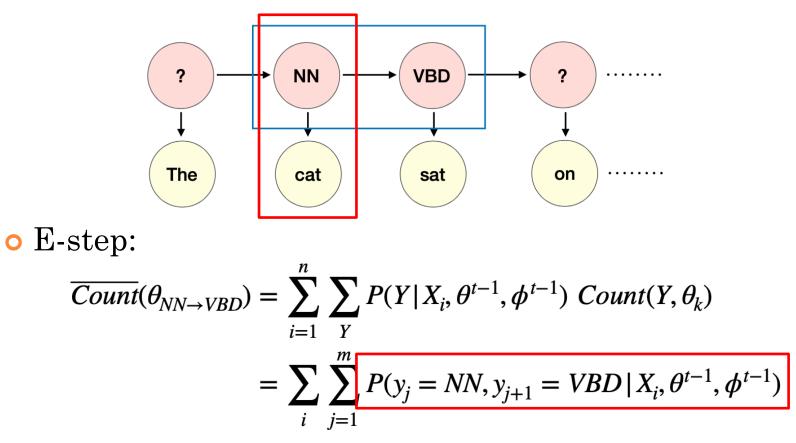
• E-step:

$$\overline{Count}(\theta_k) = \sum_{i=1}^n \sum_{Y} P(Y|X_i, \theta^{t-1}, \phi^{t-1}) Count(Y, \theta_k)$$
$$\overline{Count}(\phi_k) = \sum_{i=1}^n \sum_{Y} P(Y|X_i, \theta^{t-1}, \phi^{t-1}) Count(X_i, Y, \phi_k)$$

• Can't enumerate all possible Y's!

Quiz: How many possible Y's are there? Assume your own parameters before computing the answer.

EFFICIENT EM?



where m is the length of sequence X_i .

Similary,
$$\overline{Count}(\phi_{NN \to cat}) = \sum_{i} \sum_{j:X_{ij} = cat} P(y_j = NN | X_i, \theta^{t-1}, \phi^{t-1})$$

FORWARD-BACKWARD ALGORITHM

• Define:

α_s(j) = P(x₁,...,x_{j-1}, y_j = s | θ, φ) (forward probability)
β_s(j) = P(x_j,...,x_m|y_j = s, θ, φ) (backward probability)
Observation likelihood:

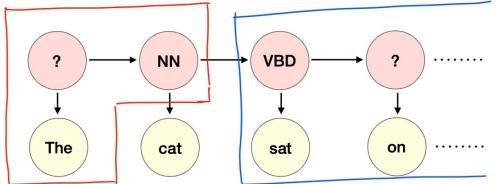
$$Z = P(x_1, \dots, x_m | \theta, \phi) = \sum_s \alpha_s(j) \beta_s(j) \ \forall j \in 1, \dots, m$$

o Thus,

$$P(y_j = s | X, \theta, \phi) = \frac{\alpha_s(j)\beta_s(j)}{Z}$$

$$P(y_j = s, y_{j+1} = s' | X, \theta, \phi) = \frac{\alpha_s(j) \ \theta_{s \to s'} \ \phi_{s \to x_j} \ \beta_{s'} \ (j+1)}{Z}$$





$$\alpha_{NN}(2) \qquad \beta_{VBD}(3)$$

$$P(y_j = s | X, \theta, \phi) = \frac{\alpha_s(j)\beta_s(j)}{Z}$$

$$P(y_j = s, y_{j+1} = s' | X, \theta, \phi) = \frac{\alpha_s(j) \ \theta_{s \to s'} \ \phi_{s \to x_j} \ \beta_{s'} \ (j+1)}{Z}$$

Now we can estimate:

$$\overline{Count}(\theta_{s \to s'}) = \sum_{i} \sum_{j=1}^{m} P(y_j = s, y_{j+1} = s' | X_i, \theta, \phi)$$
$$\overline{Count}(\phi_{s \to o}) = \sum_{i} \sum_{j:X_{ij} = o} P(y_j = s | X_i, \theta, \phi)$$

DYNAMIC PROGRAMMING

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Dynamic Programming

$$\begin{aligned} \alpha_s(j) &= P(y_j = s, x_1, \dots, x_{j-1}) \\ &= \sum_{s'} P(y_{j-1} = s', x_1, \dots, x_{j-2}) \ P(x_{j-1} \mid y_{j-1} = s') \ P(y_j = s \mid y_{j-1} = s') \\ &= \sum_{s'} \alpha_{s'} \ (j-1) \ \phi_{s' \to x_{j-1}} \ \theta_{s' \to s} \end{aligned}$$

Similarly,

$$\beta_{s}(j) = \phi_{s \to x_{j}} \sum_{s'} \beta_{s'} (j+1) \quad \theta_{s \to s'}$$

Time complexity: $O(|S|^2 \cdot m)$