#### Hidden Markov Models

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October 11, 2020

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#### Generative vs discriminative models

Generative modeling: (<br/>
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Discriminative modeling:  $P(\Im | X)$ 

Examples:

	generative	discriminative
classification	Naive Bayes	logistic regression
sequence labeling	HMM	CRF

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#### Generative modeling for sequence labeling



Task: given  $x = (x_1, \ldots, x_m) \in \mathcal{X}^m$ , predict  $y = (y_1, \ldots, y_m) \in \mathcal{Y}^m$ 

Three questions:

- Modeling: how to define a parametric joint distribution  $p(x, y; \theta)$ ?
- Learning: how to estimate the parameters  $\theta$  given observed data?
- lnference: how to efficiently find  $\arg \max_{y \in \mathcal{Y}^m} p(x, y; \theta)$  given x?

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Decompose the joint probability



$$=\prod_{i=1}^{m} p(x_i \mid y_i) \prod_{i=1}^{m} p(y_i \mid y_{i-1}) \quad \text{Markov assumption}$$

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#### Hidden Markov models

#### Hidden Markov model (HMM):

- Discrete-time, discrete-state Markov chain
- Hidden states  $z_i \in \mathcal{Y}$  (e.g. POS tags)
- Observations  $x_i \in \mathcal{X}$  (e.g. words)

$$p(x_{1:m}, y_{1:m}) = \prod_{i=1}^{m} \underbrace{p(x_i \mid y_i)}_{\text{emission probability}} \prod_{i=1}^{m} \underbrace{p(y_i \mid y_{i-1})}_{\text{transition probability}}$$

For sequence labeling:

Transition probabilities:  $p(y_i = t \mid y_{i-1} = t') = \theta_t \left( \frac{y_i^2 + 2y_i}{y_i + 2y_i} \right)$ Emission probabilities:  $p(x_i = w \mid y_i = t) = \gamma_{w \mid t} \left( \frac{y_i \mid y_i}{y_i + 2y_i} \right)$   $y_0 = x, y_m = \text{STOP}$ 

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# Learning: MLE

Data: 
$$\mathcal{D} = \{(x, y)\} (x \in \mathcal{X}^m, y \in \mathcal{Y}^m)$$
  
Task: estimate transition probabilities  $\theta_{t|t'}$  and emission probabilities  $\gamma_{w|t}$   
(# parameters?)

$$\begin{split} \ell(\theta, \gamma) &= \sum_{(x,y)\in\mathcal{D}} \left( \sum_{i=1}^{m} \log p(x_i \mid y_i) + \sum_{i=1}^{m} \log p(y_i \mid y_{i-1}) \right) \\ &\max_{\theta, \gamma} \sum_{(x,y)\in\mathcal{D}} \left( \sum_{i=1}^{m} \log \gamma_{x_i \mid y_i} + \sum_{i=1}^{m} \log \theta_{y_i \mid y_{i-1}} \right) \\ \text{s.t.} \quad &\sum_{w\in\mathcal{X}} \gamma_{w \mid t} = 1 \quad \forall w \in \mathcal{X} \\ &\sum_{t\in\mathcal{Y}\cup\{\text{STOP}\}} \theta_{t \mid t'} = 1 \quad \forall t' \in \mathcal{Y} \cup \{*\} \end{split}$$

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#### MLE solution

Count the occurrence of certain transitions and emissions in the data.

Transition probabilities:

$$\theta_{t|t'} = \frac{\Pr(NN)}{\sum_{a \in \mathcal{Y} \cup \{\text{STOP}\}} \operatorname{count}(t' \to t)}$$

Emission probabilities:

$$\gamma_{w|t} = \frac{\operatorname{count}(w, t)}{\sum_{w' \in \mathcal{X}} \operatorname{count}(w', t)}$$

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#### Inference

Task: given  $x \in \mathcal{X}^m$ , find the most likely  $y \in \mathcal{Y}^m$ 

$$\begin{aligned} \arg\max_{y\in\mathcal{Y}^m} \log p(x,y) \\ = \argmax_{y\in\mathcal{Y}^m} \sum_{i=1}^m \log p(x_i \mid y_i) + \sum_{i=1}^m \log p(y_i \mid y_{i-1}) \end{aligned}$$

Viterbi + backtracking:

$$\pi[j,t] = \max_{t' \in \mathcal{Y}} \left( \log p(x_j \mid t) + \log p(t \mid t') + \pi[j-1,t'] \right)$$

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# Naive Bayes with missing labels

Task:

- Assume data is generated from a Naive Bayes model.
- Observe  $\{x^{(i)}\}_{i=1}^{N}$  without labels.
- Estimate model parameters and the most likely labels.

ID   US		government	gene	lab	label
1	1	1	0	0	?
2	0	1	0	0	?
3	0	0	1	1	?
4	0	1	1	1	?
5	1	1	0	0	?

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# A chicken and egg problem

If we know the model parameters, we can predict labels easily. If we know the labels, we can estiamte the model parameters easily.

Idea: start with guesses of labels, then iteratively refine it.

ID	US	government		gene	lab	label
1	1	1		0	0	
2	0	1		0	0	
3	0	0		1	1	
4	0	1		1	1	
5	1	1		0	0	
		US	government		gene	lab
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# A chicken and egg problem

If we know the model parameters, we can predict labels easily. If we know the labels, we can estiamte the model parameters easily.

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# Algorithm: EM for NB

- 1. Initialization:  $\theta \leftarrow \text{random parameters}$
- 2. Repeat until convergence:
  - (i) Inference:

$$q(y \mid x^{(i)}) = p(y \mid x^{(i)}; \theta)$$

(ii) Update parameters:

$$\theta_{w|y} = \frac{\sum_{i=1}^{N} q(y \mid x^{(i)}) \mathbb{I}\left[w \text{ in } x^{i}\right]}{\sum_{i=1}^{N} q(y \mid x^{(i)})}$$

- With fully observed data,  $q(y | x^{(i)}) = 1$  if  $y^{(i)} = y$ .
- Similar to the MLE solution except that we're using "soft counts".
- What is the algorithm optimizing?

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### Objective: maximize marginal likelihood

Likelihood: 
$$L(\theta; D) = \prod_{x \in D} p(x; \theta)$$
 marginal prob  
Marginal likelihood:  $L(\theta; D) = \prod_{x \in D} \sum_{z \in Z} p(x, z; \theta)$ 

▶ Marginalize over the (discrete) latent variable  $z \in \mathcal{Z}$  (e.g. missing labels)

Maximum marginal log-likelihood estimator:

$$\hat{\theta} = \arg\max_{\theta \in \Theta} \sum_{x \in \mathcal{D}} \log \sum_{z \in \mathcal{Z}} p(x, z; \theta)$$

$$\lim_{\theta \in \Theta} p(x, z; \theta)$$

Goal: maximize log  $p(x; \theta)$ 

Challenge: in general not concave, hard to optimize

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#### Intuition

Problem: marginal log-likelihood is hard to optimize (only observing the words)

Observation: complete data log-likelihood is easy to optimize (observing both words and tags)

 $\max_{\theta} \log p(x, z; \theta)$ 

Idea: guess a distribution of the latent variables q(z) (soft tags)

Maximize the expected complete data log-likelihood:

$$\max_{\theta} \sum_{z \in \mathcal{Z}} q(z) \log p(x, z; \theta)$$

EM assumption: the expected complete data log-likelihood is easy to optimize (use soft counts)

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#### Lower bound of the marginal log-likelihood

$$\log p(x;\theta) = \log \sum_{z \in \mathbb{Z}} p(x,z;\theta)$$

$$= \log \sum_{z \in \mathbb{Z}} q(z) \frac{p(x,z;\theta)}{q(z)} = \log \mathbb{E}_{z} [p(x,z;\theta)]$$

$$\int ensen's \geq \sum_{z \in \mathbb{Z}} q(z) \log \frac{p(x,z;\theta)}{q(z)} = \mathbb{E}_{z} [\log p(x,z;\theta)]$$

$$\lim_{z \in \mathbb{Z}} q(z) \log \frac{p(x,z;\theta)}{q(z)} = \mathbb{E}_{z} [\log p(x,z;\theta)]$$

$$\lim_{z \in \mathbb{Z}} f(E[x])$$

$$Evidence: \log p(x;\theta)$$

- **Evidence lower bound (ELBO)**:  $\mathcal{L}(q, \theta)$
- q: chosen to be a family of tractable distributions
- ldea: maximize the ELBO instead of log  $p(x; \theta)$

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- KL divergence: measures "distance" between two distributions (not symmetric!) KL(P(19)  $\neq$  KL(9(1P) KL( $q \parallel p$ )  $\geq$  0 with equality iff  $q(z) = p(z \mid x)$ .
- $ELBO = evidence KL \leq evidence$

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Justification for maximizing ELBO



Let  $\theta^*$ ,  $q^*$  be the global optimzer of  $\mathcal{L}(q, \theta)$ , then  $\theta^*$  is the global optimizer of log  $p(x; \theta)$ . (Proof: exercise)

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#### Summary

**Latent variable models**: clustering, latent structure, missing lables etc. Parameter estimation: maximum marginal log-likelihood Challenge: directly maximize the **evidence**  $\log p(x; \theta)$  is hard Solution: maximize the **evidence lower bound**:

$$\mathsf{ELBO} = \mathcal{L}(q, \theta) = -\mathsf{KL}(q(z) \| p(z \mid x; \theta)) + \log p(x; \theta)$$

Why does it work?

$$egin{aligned} q^*(z) &= p(z \mid x; heta) \quad orall heta \in \Theta \ \mathcal{L}(q^*, heta^*) &= \max_{ heta} \log p(x; heta) \end{aligned}$$

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# EM algorithm

# Coordinate ascent on $\mathcal{L}(q, \theta)$

- 1. Random initialization:  $\theta^{\text{old}} \leftarrow \theta_0$
- 2. Repeat until convergence

(i) 
$$q(z) \leftarrow \arg \max_q \mathcal{L}(q, \theta^{\mathsf{old}})$$

**Expectation** (the E-step):  $q^*(z) = p(z \mid x; \theta^{\text{old}})$  $EUB_{0} = L(q^{*}, \theta) = J(\theta) = \sum_{z \in \mathcal{Z}} q^{*}(z) \log \frac{p(x, z; \theta)}{q^{*}(z)}$ (ii)  $\theta^{\mathsf{new}} \leftarrow \arg \max_{\theta} \mathcal{L}(q^*, \theta)$ Max Minimization (the M-step):  $\theta^{\text{new}} \leftarrow \arg \max J(\theta)$ max expected complete dore  $\theta$  trkelihood. EM puts no constraint on q in the E-step and assumes the M-step is easy. In general, both steps can be hard.

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Exercise: prove that EM increases the marginal likelihood monotonically

$$\log p(x; \theta^{\mathsf{new}}) \geq \log p(x; \theta^{\mathsf{old}}) .$$

Does EM converge to a global maximum?

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# EM for multinomial naive Bayes Setting: $x = (x_1, ..., x_m) \in \mathcal{V}^m, z \in \{1, ..., K\}, \mathcal{D} = \{x^{(i)}\}_{i=1}^N$

E-step:

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# EM for multinomial naive Bayes

M-step has closed-form solution:

$$\theta_{z} = \frac{\sum_{x \in \mathcal{D}} q_{x}^{*}(z)}{\sum_{z \in \mathcal{Z}} \sum_{x \in \mathcal{D}} \underbrace{q_{x}^{*}(z)}_{\text{soft label count}}}$$
$$\theta_{w|z} = \frac{\sum_{x \in \mathcal{D}} q_{x}^{*}(z) \text{count}(w \mid x)}{\sum_{w \in \mathcal{V}} \sum_{x \in \mathcal{D}} \underbrace{q_{x}^{*}(z) \text{count}(w \mid x)}_{\text{soft word count}}}$$

Similar to the MLE solution except that we're using soft counts.

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M-step for multinomial naive Bayes

$$\begin{split} & \max_{\theta} \sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \left( \sum_{w \in \mathcal{V}} \log \theta_{w|z}^{\operatorname{count}(w|x)} + \log \theta_z \right) \\ & \text{s.t.} \quad \sum_{w \in \mathcal{V}} \theta_{w|z} = 1 \quad \forall w \in \mathcal{V}, \quad \sum_{z \in \mathcal{Z}} \theta_z = 1 \end{split}$$

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## Summary

**Expectation minimization (EM)** algorithm: maximizing ELBO  $\mathcal{L}(q, \theta)$  by coordinate ascent

**E-step**: Compute the expected complete data log-likelihood  $J(\theta)$  using  $q^*(z) = p(z \mid x; \theta^{\text{old}})$ 

**M-step**: Maximize  $J(\theta)$  to obtain  $\theta^{\text{new}}$ 

Assumptions: E-step and M-step are easy to compute

Properties: Monotonically improve the likelihood and converge to a stationary point

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### HMM recap

Setting:

- etting: Hidden states  $z_i \in \mathcal{Y}$  (e.g. POS tags) Observations  $x_i \in \mathcal{X}$  (e.g. words)  $\mathcal{Y}(\mathcal{X}(\mathcal{Y}))$
- Observations  $x_i \in \mathcal{X}$  (e.g. words)

$$p(x_{1:m}, y_{1:m}) = \prod_{i=1}^{m} \underbrace{p(x_i \mid y_i)}_{\text{emission probability}} \prod_{i=1}^{m} \underbrace{p(y_i \mid y_{i-1})}_{\text{transition probability}}$$

Parameters:

- ► Transition probabilities:  $p(y_i = t | y_{i-1} = t') = \theta_{t|t'}$
- Emission probabilities:  $p(x_i = w \mid y_i = t) = \gamma_{w \mid t}$

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$$y_0 = *, y_m = \text{STOP}$$

Task: estimate parameters given incomplete observations

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# E-step for HMM

E-step:

$$q^{*}(z) = p(z \mid x; \theta, \gamma)$$

$$\mathcal{L}(q^{*}, \theta, \gamma) = \sum_{x \in \mathcal{D}} \sum_{\substack{z \in \mathcal{Z} \\ expected \text{ complete log-likelihood}}} \sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_{x}^{*}(z) \log \prod_{i=1}^{m} p(x_{i} \mid z_{i})p(z_{i} \mid z_{i-1})$$

$$= \sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_{x}^{*}(z) \sum_{i=1}^{m} \left( \log \underbrace{p(x_{i} \mid z_{i}; \gamma)}_{\gamma_{x_{i}|z_{i}}} + \log \underbrace{p(z_{i} \mid z_{i-1}; \theta)}_{\theta_{z_{i}|z_{i-1}}} \right)$$

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# M-step for HMM

M-step (similar to the NB solution):

$$\max_{\theta,\gamma} \mathcal{L}(q^*,\theta,\gamma) = \sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \sum_{i=1}^m \left( \log \gamma_{x_i|z_i} + \log \theta_{z_i|z_{i-1}} \right)$$

Emission probabilities:

$$\gamma_{w|t} = \frac{\sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \operatorname{count}(w, t \mid x, z)}{\sum_{w' \in \mathcal{X}} \sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \operatorname{count}(w', t \mid x, z)}$$
  
$$\operatorname{count}(w, t \mid x, z) \stackrel{\text{def}}{=} \# \text{ word-tag pairs } (w, t) \text{ in } (x, z)$$

Transition probabilities:

$$\theta_{t|t'} = \frac{\sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \operatorname{count}(t' \to t \mid z)}{\sum_{a \in \mathcal{Y}} \sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \operatorname{count}(t' \to a \mid z)}$$
$$\operatorname{count}(t' \to t \mid z) \stackrel{\text{def}}{=} \# \text{ tag bigrams } (t', t) \text{ in } z$$

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Group sequences where  $z_i = t$ :

$$\sum_{z \in \mathcal{Y}^m} q_x^*(z) \operatorname{count}(w, t \mid x, z) = \sum_{i=1}^m \mu_x(z_i = t) \mathbb{I}[x_i = w]$$
$$\mu_x(z_i = t) = \sum_{\{z \in \mathcal{Y}^m \mid z_i = t\}} q_x^*(z)$$



$$\sum_{z \in \mathcal{Y}^m} q_x^*(z) \operatorname{count}(t' \to t \mid z) = \sum_{i=1}^m \mu_x(z_i = t, z_{i-1} = t')$$
$$\mu_x(z_i = t) = \sum_{\{z \in \mathcal{Y}^m \mid z_i = t, z_{i-1} = t\}} q_x^*(z)$$

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#### Compute tag marginals

 $\mu_{x}(z_{i} = t): \text{ probability of the } i\text{-th tag being } t \text{ given observed words } x$   $\mu_{x}(z_{i} = t) = \sum_{z:z_{i} = t}^{p} q_{x}^{*}(z) \propto \sum_{z:z_{i} = t}^{m} \prod_{j=1}^{m} \underbrace{q(x_{i} \mid z_{i})q(z_{i} \mid z_{i-1})}_{\psi(z_{i}, z_{i-1})} \underbrace{q(x_{i} \mid z_{i-1})}_{\psi(x_{i}, z_{i-1})} \underbrace$  $=\sum_{z:z_{i}=t}\prod_{j=1}^{t}\psi(z_{j},z_{j-1})\prod_{j=i}^{t}\psi(z_{j},z_{j-1})$  $=\sum_{t'}\sum_{z:z_{i}=t,z_{i-1}=t'}\prod_{j=1}^{i-1}\psi(z_{j},z_{j-1})\prod_{j=i}^{m}\psi(z_{j},z_{j-1})$   $=\sum_{t'}\left(\sum_{\substack{z_{1:i-1}\\z_{i-1}=t'}}\prod_{j=1}^{i-1}\psi(z_{j},z_{j-1})\right)\psi(t,t')\left(\sum_{\substack{z_{i+1:m}\\z_{j}=t}}\prod_{j=i+1}^{m}\psi(z_{j},z_{j-1})\right)\psi(t,t')\left(\sum_{\substack{z_{i+1:m}\\z_{j}=t}}\prod_{j=i+1}^{m}\psi(z_{j},z_{j-1})\right)\psi(t,t')\left(\sum_{\substack{z_{i+1:m}\\z_{j}=t}}\prod_{j=i+1}^{m}\psi(z_{j},z_{j-1})\right)\psi(t,t')\left(\sum_{\substack{z_{i+1:m}\\z_{j}=t}}\prod_{j=i+1}^{m}\psi(z_{j},z_{j-1})\right)\psi(t,t')\right)$  $=\sum_{t'} \alpha[i-1,t]\psi(t,t')\beta[i,t] = \alpha[i,t]\beta[i,t]$ SQ Q

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#### Compute tag marginals

**Forward probabilities**: probability of tag sequence prefix ending at  $z_i = t$ .

$$\alpha[i,t] \stackrel{\text{def}}{=} q(x_1,\ldots,x_i,z_i=t)$$
  
$$\alpha[i,t] = \sum_{t' \in \mathcal{Y}} \alpha[i-1,t']\psi(t',t)$$
  
$$\psi(t' \to t)$$

**Backward probabilities**: probability of tag sequence suffix starting from  $z_{i+1}$  give  $z_i = t$ .

$$\beta[i,t] \stackrel{\text{def}}{=} q(x_{i+1},\ldots,x_m \mid z_i = t)$$
  
$$\beta[i,t] = \sum_{t' \in \mathcal{Y}} \beta[i+1,t']\psi(t,t')$$
  
$$\psi(t \rightarrow t')$$

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#### Compute tag marginals

1. Compute forward and backward probabilities

$$\begin{aligned} \alpha[i,t] & \forall i \in \{1,\ldots,m\}, t \in \mathcal{Y} \cup \{\texttt{STOP}\} \\ \beta[i,t] & \forall i \in \{m,\ldots,1\}, t \in \mathcal{Y} \cup \{*\} \end{aligned}$$

2. Comptute the tag unigram and bigram marginals

$$\mu_{x}(z_{i} = t) \stackrel{\text{def}}{=} q(z_{i} = t \mid x) \qquad \begin{array}{l} q(z_{i}, x) \\ = \frac{\alpha[i, t]\beta[i, t]}{q(x)} = \frac{\alpha[i, t]\beta[i, t]}{\alpha[m, \text{STOP}]} \\ \mu_{x}(z_{i-1} = t', z_{i} = t) \stackrel{\text{def}}{=} q(z_{i-1} = t', z_{i} = t \mid x) \\ = \frac{\alpha[i-1, t']\psi(t', t)\beta[i, t]}{q(x)} \end{array}$$

In practice, compute in the log space.

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#### Updated parameters

Emission probabilities:

$$\gamma_{w|t} = \frac{\sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \text{count}(w, t \mid x, z)}{\sum_{w' \in \mathcal{X}} \sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \text{count}(w', t \mid x, z)}$$
$$= \frac{\sum_{x \in \mathcal{D}} \sum_{i=1}^m \mu_x(z_i = t) \mathbb{I}[x_i = w]}{\sum_{w' \in \mathcal{X}} \sum_{x \in \mathcal{D}} \sum_{i=1}^m \mu_x(z_i = t) \mathbb{I}[x_i = w']}$$

Transition probabilities:

$$\theta_{t|t'} = \frac{\sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \operatorname{count}(t' \to t \mid z)}{\sum_{a \in \mathcal{Y}} \sum_{x \in \mathcal{D}} \sum_{z \in \mathcal{Z}} q_x^*(z) \operatorname{count}(t' \to a \mid z)}$$
$$= \frac{\sum_{x \in \mathcal{D}} \sum_{i=1}^m \mu_x(z_{i-1} = t', z_i = t)}{\sum_{a \in \mathcal{Y}} \sum_{x \in \mathcal{D}} \sum_{i=1}^m \mu_x(z_{i-1} = t', z_i = a)}$$

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# Summary

EM for HMM:

- 1. Randomly initialize the emission and transition probabilities
- 2. Repeat until convergence
  - (i) Compute forward and backward probabilities
  - (ii) Update the emission and transition probabilities using expected counts
  - If the solution is bad, re-run EM with a different random seed.

General EM:

- One example of variational methods (use a tractable q to approximate p)
- May need approximation in both the E-step and the M-step
- Useful in probabilistic models and Bayesian methods

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