A gentle introduction to Hidden Markov Models

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Outline

What is sequence labeling?

Markov models

Hidden Markov models

Finding the most likely state sequence

Estimating HMMs

Conclusion

Sequence labeling

- Input: a sequence $\boldsymbol{x} = (x_1, \ldots, x_n)$ (usually n may vary)
- Output: a *sequence* $\boldsymbol{y} = (x_1, \ldots, y_n)$, where *$y_i$ is a label for x_i*

Part of speech (POS) tagging:

$$\begin{array}{llllllll} \boldsymbol{y}: & \text{DT} & \text{JJ} & \text{NN} & \text{VBD} & \text{NNP} & . \\ \boldsymbol{x}: & \text{the} & \text{big} & \text{cat} & \text{bit} & \text{Sam} & . \end{array}$$

Noun-phrase chunking:

$$\begin{array}{lllllll} \boldsymbol{y}: & [\text{NP} & \text{NP} & \text{NP}] & \_ & [\text{NP}] & . \\ \boldsymbol{x}: & \text{the} & \text{big} & \text{cat} & \text{bit} & \text{Sam} & . \end{array}$$

Named entity detection:

$$\begin{array}{llllllll} \boldsymbol{y}: & [\text{CO} & \text{CO}] & \_ & [\text{LOC}] & \_ & [\text{PER}] & \_ \\ \boldsymbol{x}: & \text{XYZ} & \text{Corp.} & \text{of} & \text{Boston} & \text{announced} & \text{Spade's} & \text{resignation} \end{array}$$

Speech recognition: The $\boldsymbol{x}$ are 100 msec. time slices of acoustic input, and the $\boldsymbol{y}$ are the corresponding phonemes (i.e., y_i is the phoneme being uttered in time slice x_i)

Sequence labeling with probabilistic models

- General idea: develop a probabilistic model $\mathrm{P}(\boldsymbol{y}, \boldsymbol{x})$
  - use this to compute $\mathrm{P}(\boldsymbol{y}|\boldsymbol{x})$ and $\hat{\boldsymbol{y}}(\boldsymbol{x}) = \mathrm{argmax}_{\boldsymbol{y}}\, \mathrm{P}(\boldsymbol{y}|\boldsymbol{x})$
- A *Hidden Markov Model* (HMM) factors:

$$\mathrm{P}(\boldsymbol{y}, \boldsymbol{x}) \;\; = \;\; \mathrm{P}(\boldsymbol{y})\, \mathrm{P}(\boldsymbol{x}|\boldsymbol{y})$$

- $\mathrm{P}(\boldsymbol{y})$ is the probability of sequence $\boldsymbol{y}$
  - In an HMM, $\mathrm{P}(\boldsymbol{y})$ is a *Markov chain*
    - in applications, $\boldsymbol{y}$ is usually "hidden"
  - $\mathrm{P}(\boldsymbol{x}|\boldsymbol{y})$ is the *emission model*.

Outline

Markov models of sequences

- Let $\boldsymbol{y} = (y_1, \ldots, y_n)$, where $y_i \in \mathcal{Y}$ and n is fixed

$$\begin{aligned} \mathrm{P}(\boldsymbol{y}) &= \mathrm{P}(y_1)\,\mathrm{P}(y_2|y_1)\,\mathrm{P}(y_3|y_1, y_2)\,\ldots\,\mathrm{P}(y_n|y_1, \ldots, y_{n-1}) \\ &= \mathrm{P}(y_1) \prod_{i=2}^{n} \mathrm{P}(y_i|y_{1:i-1}) \end{aligned}$$

  where $y_{i:j}$ is the subsequence $(y_i, \ldots, y_j)$ of $\boldsymbol{y}$
- In a (first-order) *Markov chain*:

$$\mathrm{P}(y_i|y_{1:i-1}) = \mathrm{P}(y_i|y_{i-1}) \text{ for } i > 1$$

- In a *homogenous* Markov chain, $\mathrm{P}(y_i|y_{i-1})$ does not depend on i, so probability of a sequence is completely determined by:

$$\begin{aligned} \mathrm{P}(y_1) &= \iota(y_1) && \textit{(start probabilities)} \\ \mathrm{P}(y_i|y_{i-1}) &= \sigma(y_{i-1}, y_i) && \textit{(transition probabilities)}, \text{ so:} \\ \mathrm{P}(\boldsymbol{y}) &= \iota(y_1) \prod_{i=2}^{n} \sigma(y_{i-1}, y_i) \end{aligned}$$

Markov models of varying-length sequences

- To define a model of sequences $\boldsymbol{y} = (y_1, \ldots, y_n)$ of varying lengths n, need to define $\mathrm{P}(n)$
- An easy way to do this:
  - add a new *end marker* symbol '$\triangleleft$' to $\mathcal{Y}$
  - pad all sequences with this end-marker

$$\boldsymbol{y} \quad = \quad y_1, y_2, \ldots, y_n, \triangleleft, \triangleleft, \ldots$$

  - set $\sigma(\triangleleft, \triangleleft) = 1$, i.e., $\triangleleft$ is a *sink state*
  - so $\sigma(y, \triangleleft)$ is probability of sequence ending after state y
- We can also incorporate the start probabilities $\boldsymbol{\iota}$ into $\boldsymbol{\sigma}$ by introducing a new *begin marker* $y_0 = \triangleright$

$$\begin{aligned}\boldsymbol{y} \quad &= \quad \triangleright, y_1, y_2, \ldots, y_n, \triangleleft, \triangleleft, \ldots, \text{ so:} \\ \mathrm{P}(\boldsymbol{y}) \quad &= \quad \prod_{i=1}^{\infty} \sigma(y_{i-1}, y_i) \quad \text{(only compute to } i = n+1\text{)}\end{aligned}$$

Outline

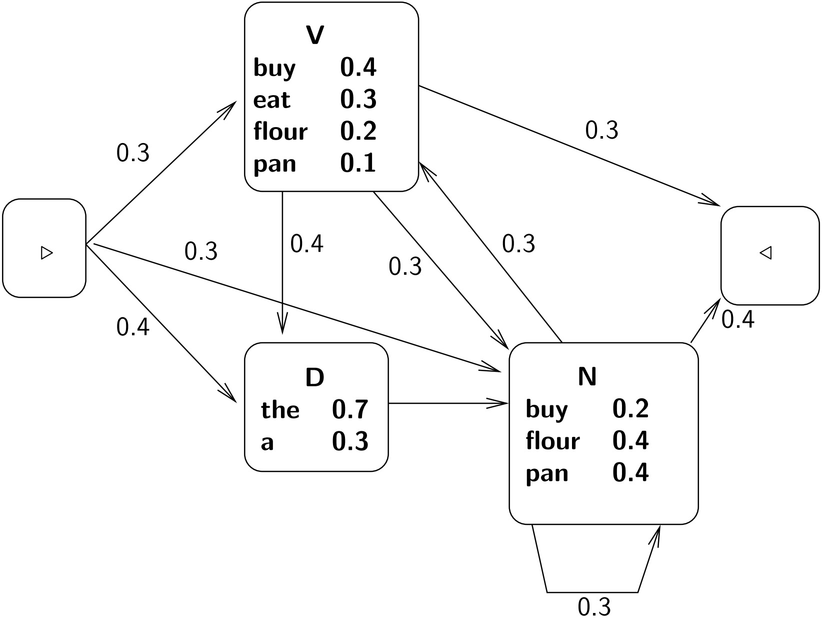
Hidden Markov models

- An HMM is specified by:
  - A *state-to-state transition matrix* $\boldsymbol{\sigma}$, where $\sigma(y, y')$ is the probability of moving from state y to state y'
  - A *state-to-observation emission matrix* $\boldsymbol{\tau}$, where $\tau(y, x)$ is the probability of emitting x in state y

$$
\begin{aligned}
\mathrm{P}(\boldsymbol{y}, \boldsymbol{x}) &= \mathrm{P}(\boldsymbol{y})\,\mathrm{P}(\boldsymbol{x}|\boldsymbol{y}) \\
\mathrm{P}(\boldsymbol{y}) &= \prod_{i=1}^{n+1} \mathrm{P}(y_i|y_{i-1}) \;=\; \prod_{i=1}^{n+1} \sigma(y_{i-1}, y_i) \\
\mathrm{P}(\boldsymbol{x}|\boldsymbol{y}) &= \prod_{i=1}^{n} \mathrm{P}(x_i|y_i) \;=\; \prod_{i=1}^{n} \tau(y_i, x_i)
\end{aligned}
$$

- I.e., each x_i is generated conditioned on y_i with probability $\tau(y_i, x_i)$

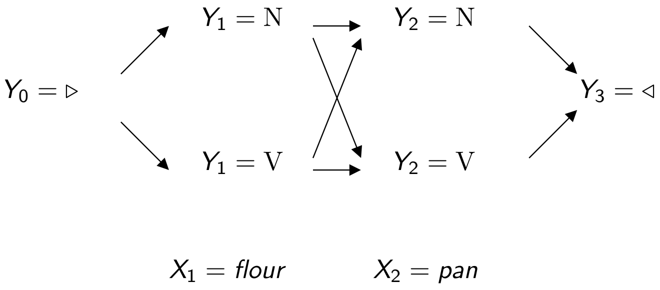
HMMs as stochastic automata



Bayes net representation of an HMM

$$\begin{tikzcd}
Y_0 = \triangleleft \arrow[r] & Y_1 = \mathrm{V} \arrow[r] \arrow[d] & Y_2 = \mathrm{D} \arrow[r] \arrow[d] & Y_3 = \mathrm{N} \arrow[r] \arrow[d] & Y_4 = \triangleleft \\
 & X_1 = \text{flour} & X_2 = \text{the} & X_3 = \text{pan} &
\end{tikzcd}$$

Trellis representation of HMM



- The trellis representation represents the possible state sequences $\boldsymbol{y}$ for *a single observation sequence* $\boldsymbol{x}$
- A trellis is a DAG with *nodes* (i, y), where $i \in 0, \ldots, n+1$ and $y \in \mathcal{Y}$ and *edges* from $(i-1, y')$ to (i, y)
- It plays a crucial role in *dynamic programming algorithms* for HMMs

Outline

Two important inference problems

- Given an HMM $\boldsymbol{\sigma}, \boldsymbol{\tau}$ and an observation sequence $\boldsymbol{x}$:
  - what is *the most likely state sequence* $\hat{\boldsymbol{y}} = \mathrm{argmax}_{\boldsymbol{y}} \mathrm{P}(\boldsymbol{x}, \boldsymbol{y})$?
  - what is the *probability of a sequence* $\mathrm{P}(\boldsymbol{x}) = \sum_{\boldsymbol{y}} \mathrm{P}(\boldsymbol{x}, \boldsymbol{y})$?
- If the sequences are short enough, can be solved by exhaustively enumerating $\boldsymbol{y}$
- Given a sequence of length n and an HMM with m states, can be solved using dynamic programming in $O(n\, m^2)$ time

Key observation: $\mathrm{P}(\boldsymbol{x}, \boldsymbol{y})$ factorizes!

$$\begin{aligned}
\mathrm{P}(\boldsymbol{x}, \boldsymbol{y}) &= \left(\prod_{i=1}^{n} \sigma(y_{i-1}, y_i)\, \tau(y_i, x_i)\right) \sigma(y_n, \triangleleft), \text{ so:} \\
-\log \mathrm{P}(\boldsymbol{x}, \boldsymbol{y}) &= \left(\sum_{i=1}^{n} -\log(\sigma(y_{i-1}, y_i)\, \tau(y_i, x_i))\right) - \log \sigma(y_n, \triangleleft)
\end{aligned}$$

- Given observation sequence $\boldsymbol{x}$, define a trellis with *edge weights*

$$\begin{aligned}
w((i-1, y'), (i, y)) &= -\log(\sigma(y_{i-1}, y_i)\, \tau(y_i, x_i)) \\
w((n, y), (n+1, \triangleleft)) &= -\log(\sigma(y, \triangleleft))
\end{aligned}$$

- Then the $-\log$ probability of any state sequence $\boldsymbol{y}$ is the sum of the weights of the corresponding path in the trellis

Finding the most likely state sequence $\hat{\boldsymbol{y}}$

- Goal: find $\hat{\boldsymbol{y}} = \operatorname{argmax}_{\boldsymbol{y}} \mathrm{P}(\boldsymbol{x}, \boldsymbol{y})$
- Algorithm:
  - Construct a trellis with edge weights

$$
\begin{aligned}
w((i-1, y'), (i, y)) &= -\log(\sigma(y_{i-1}, y_i)\,\tau(y_i, x_i)) \\
w((n, y), (n+1, \triangleleft)) &= -\log(\sigma(y, \triangleleft))
\end{aligned}
$$

  - Run a *shortest path algorithm* on this trellis, which returns a state sequence with lowest $-\log$ probability

The Viterbi algorithm for finding $\hat{\boldsymbol{y}}$

- Idea: given $\boldsymbol{x} = (x_1, \ldots, x_n)$, let $\mu(k, u)$ be the maximum probability of any state sequence $y_1, \ldots, y_k$ ending in $y_k = u \in \mathcal{Y}$.

$$\mu(k, u) \quad = \quad \max_{\boldsymbol{y}_{1:k} \,:\, y_k = u} \mathrm{P}(\boldsymbol{x}_{1:k}, \boldsymbol{y}_{1:k})$$

  - Base case: $\mu(0, \triangleright) = 1$
  - Recursive case:

$$\mu(k, u) \quad = \quad \max_{u'} \mu(k-1, u')\, \sigma(u', u)\, \tau(u, x_k)$$

  - Final case: $\mu(n+1, \triangleleft) \;=\; \max_{u'} \mu(n, u')\, \sigma(u', \triangleleft)$
- To find $\hat{\boldsymbol{y}}$, for each trellis node (k, u) keep a *back-pointer* to *most likely predecessor*

$$\rho(k, u) \quad = \quad \operatorname*{argmax}_{u' \in \mathcal{Y}} \mu(k-1, u')\, \sigma(u', u)\, \tau(u, x_k)$$

Why does the Viterbi algorithm work?

$$
\begin{aligned}
\mu(k,u) &= \max_{\boldsymbol{y}_{1:k}\,:\,y_k=u} \mathrm{P}(\boldsymbol{x}_{1:k},\boldsymbol{y}_{1:k}) \\
&= \max_{\boldsymbol{y}_{1:k}\,:\,y_k=u} \prod_{i=1}^{k} \sigma(y_{i-1},y_i)\,\tau(y_i,x_i) \\
&= \max_{\boldsymbol{y}_{1:k-1}} \left(\prod_{i=1}^{k-1} \sigma(y_{i-1},y_i)\,\tau(y_i,x_i) \right) \sigma(y_{k-1},u)\,\tau(u,x_k) \\
&= \max_{u'} \left(\max_{\boldsymbol{y}_{1:k-1}\,:\,y_{k-1}=u'} \prod_{i=1}^{k-1} \sigma(y_{i-1},y_i)\,\tau(y_i,x_i) \right) \sigma(u',u)\,\tau(u,x_k) \\
&= \max_{u'} \mu(k-1,u')\,\sigma(u',u)\,\tau(u,x_k)
\end{aligned}
$$

The sum-product algorithm for computing $\mathrm{P}(\boldsymbol{x})$

- Goal: compute $\mathrm{P}(\boldsymbol{x}) = \sum_{\boldsymbol{y} \in \mathcal{Y}^n} \mathrm{P}(\boldsymbol{x}, \boldsymbol{y})$
- Idea: given $\boldsymbol{x} = (x_1, \ldots, x_n)$, let $\alpha(k, u)$ be the *sum of the probabilities* of $x_1, \ldots, x_k$ and all state sequences $y_1, \ldots, y_k$ ending in $y_k = u$.

$$\alpha(k, u) \;=\; \sum_{y_{1:k} \,:\, y_k = u} \mathrm{P}(\boldsymbol{x}_{1:k}, \boldsymbol{y}_{1:k})$$

  - Base case: $\alpha(0, \triangleright) = 1$
  - Recursive case: for $k = 1, \ldots, n$:

$$\alpha(k, u) \;=\; \sum_{u'} \alpha(k-1, u')\, \sigma(u', u)\, \tau(u, x_i)$$

  - Final case: $\alpha(n+1, \triangleleft) \;=\; \sum_{u'} \alpha(n, u')\, \sigma(u', \triangleleft)$
- The $\boldsymbol{\alpha}$ are called *forward probabilities*

Outline

Estimating HMMs from *visible data*

- Training data: $D = ((\boldsymbol{x}_1, \boldsymbol{y}_1), \ldots, (\boldsymbol{x}_n, \boldsymbol{y}_n))$, where the $\boldsymbol{x}_i$ and $\boldsymbol{y}_i$ are *sequences*
  - for conceptual simplicity, assume that the data comes as two long sequences $D = (\boldsymbol{x}, \boldsymbol{y})$
- Then the MLE is:

$$
\begin{aligned}
\hat{\sigma}(y', y) &= \frac{c(y', y)}{\sum_{y \in \mathcal{Y}} c(y', y)} \\
\hat{\tau}(y, x) &= \frac{c(y, x)}{\sum_{x \in \mathcal{X}} c(y, x)}, \text{ where:} \\
c(y', y) &= \text{the number of times state } y' \text{ precedes state } y \text{ in } \boldsymbol{y} \\
c(y, x) &= \text{the number of times state } y \text{ emits } x \text{ in } (\boldsymbol{x}, \boldsymbol{y})
\end{aligned}
$$

Estimating HMMs from *hidden data* using EM

- EM iteration at time t:

$$\sigma(y', y)^{(t)} = \frac{\mathrm{E}[c(y', y)]}{\sum_{y \in \mathcal{Y}} \mathrm{E}[c(y', y)]}$$

$$\tau(y, x)^{(t)} = \frac{\mathrm{E}[c(y, x)]}{\sum_{x \in \mathcal{X}} \mathrm{E}[c(y, x)]}, \text{ where:}$$

$$\mathrm{E}[c(y', y)] = \sum_{\boldsymbol{y} \in \mathcal{Y}^n} c(y', y) \, \mathrm{P}(\boldsymbol{y} | \boldsymbol{x}, \boldsymbol{\sigma}^{(t-1)}, \boldsymbol{\tau}^{(t-1)})$$

$$\mathrm{E}[c(y, x)] = \sum_{\boldsymbol{y} \in \mathcal{Y}^n} c(y, x) \, \mathrm{P}(\boldsymbol{y} | \boldsymbol{x}, \boldsymbol{\sigma}^{(t-1)}, \boldsymbol{\tau}^{(t-1)})$$

- Key computational problem: *computing these expectations efficiently*
- Dynamic programming to the rescue!

Expectations require marginal probabilities

- Suppose we could efficiently compute the *marginal probabilities*:

$$\mathrm{P}(Y_i = y' | \boldsymbol{x}) \;\;=\;\; \frac{\sum_{\boldsymbol{y} \in \mathcal{Y}^n \,:\, y_i = y'} \mathrm{P}(\boldsymbol{y}, \boldsymbol{x})}{\mathrm{P}(\boldsymbol{x})}$$

- Then we could efficiently compute:

$$\mathrm{E}[c(y', x')] \;\;=\;\; \sum_{i \,:\, x_i = x'} \mathrm{P}(Y_i = y' | \boldsymbol{x})$$

- Efficiently computing $\mathrm{E}[c(y', y)]$ requires computation of a different marginal probability

Backward probabilities

- Idea: given $\boldsymbol{x} = (x_1, \ldots, x_n)$, let $\beta(k, v)$ be the *sum of the probabilities* of $x_{k+1}, \ldots, x_n$ and all state sequences $y_{k+1}, \ldots, y_n$ conditioned on $y_k = v$.

$$\beta(k, v) \quad = \quad \sum_{y_{k:n} \,:\, y_k = v} \mathrm{P}(\boldsymbol{x}_{k+1:n}, \boldsymbol{y}_{k+1:n} | Y_k = v)$$

  - Base case: $\beta(n, v) = \sigma(v, \triangleleft)$ for each $v \in \mathcal{Y}$
  - Recursive case: for $k = n-1, \ldots, 0$:

$$\beta(k, v) \quad = \quad \sum_{v'} \sigma(v, v')\, \tau(v', x_{k+1})\, \beta(k+1, v')$$

- The $\boldsymbol{\beta}$ are called *backward probabilities*

Computing marginals from forward and backward probabilities

$$
\begin{aligned}
\mathrm{P}(Y_i = u|\boldsymbol{x}) &= \frac{1}{\mathrm{P}(\boldsymbol{x})} \sum_{\boldsymbol{y}\in\mathcal{Y}^n \,:\, y_i=u} \mathrm{P}(\boldsymbol{y},\boldsymbol{x}) \\
&= \frac{1}{\mathrm{P}(\boldsymbol{x})} \sum_{y_{1:k} \,:\, y_i=u} \; \sum_{y_{i:n} \,:\, y_i=u} \mathrm{P}(\boldsymbol{x}_{1:i},\boldsymbol{y}_{1:i})\mathrm{P}(\boldsymbol{x}_{i+1:n},\boldsymbol{y}_{i:n}) \\
&= \frac{1}{\mathrm{P}(\boldsymbol{x})} \left(\sum_{y_{1:k} \,:\, y_i=u} \mathrm{P}(\boldsymbol{x}_{1:i},\boldsymbol{y}_{1:i}) \right) \left(\sum_{y_{k:n} \,:\, y_i=u} \mathrm{P}(\boldsymbol{x}_{i+1:n},\boldsymbol{y}_{i:n}) \right) \\
&= \frac{1}{\mathrm{P}(\boldsymbol{x})} \, \alpha(i,u)\, \beta(i,u)
\end{aligned}
$$

- So the marginal $\mathrm{P}(Y_i|\boldsymbol{x})$ can be efficiently computed from $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$

Outline

Conclusion

- Hidden Markov Models (HMMs) can be used to label a sequence of observations
- There are efficient dynamic programming algorithms to find the most likely label sequence and the marginal probability of a label
- The expectation-maximization algorithm can be used to learn an HMM from unlabeled data
- The expected values required for EM can be efficiently computed