Introduction to Hidden Markov models

Mark Johnson

Macquarie University

September 17, 2014



Outline

Sequence labelling

- Hidden Markov Models
- Finding the most probable label sequence
- Higher-order HMMs
- Summary



What is sequence labelling?

- A sequence labelling problem is one where:
 - the input consists of a sequence $\mathbf{X} = (X_1, \dots, X_n)$, and
 - the output consists of a sequence $\mathbf{Y} = (Y_1, \dots, Y_n)$ of labels, where:
 - Y_i is the label for element X_i
- Example: Part-of-speech tagging

$$\left(\begin{array}{c} \textbf{Y} \\ \textbf{X} \end{array}\right) \ = \ \left(\begin{array}{cc} \mathrm{Verb}, & \mathrm{Determiner}, & \mathrm{Noun} \\ \mathrm{spread}, & \mathrm{the}, & \mathrm{butter} \end{array}\right)$$

• Example: Spelling correction

$$\left(\begin{array}{c} \boldsymbol{Y} \\ \boldsymbol{X} \end{array}\right) \ = \ \left(\begin{array}{cc} \mathrm{write,} & \mathrm{a,} & \mathrm{book} \\ \mathrm{rite,} & \mathrm{a,} & \mathrm{buk} \end{array}\right)$$



Named entity extraction with IOB labels

- Named entity recognition and classification (NER) involves finding the named entities in a text and identifying what type of entity they are (e.g., person, location, corporation, dates, etc.)
- NER can be formulated as a sequence labelling problem
- Inside-Outside-Begin (IOB) labelling scheme indicates the beginning and span of each named entity

B-ORG I-ORG 0 0 0 B-LOC I-I OC I-I OC \cap Macquarie University is located in New South Wales

• The IOB labelling scheme lets us identify adjacent named entities

I-LOC B-LOC 1-1 OC I-LOC B-LOC 0 B-LOC 0 New South Wales Northern Territory and Queensland are . . . This technology can extract information from:

- news stories
- financial reports
- classified ads



Other applications of sequence labelling

- Speech transcription as a sequence labelling task
 - ► The input X = (X₁,...,X_n) is a sequence of *acoustic frames* X_i, where X_i is a set of features extracted from a 50msec window of the speech signal
 - ▶ The output **Y** is a sequence of words (the transcript of the speech signal)
- Financial applications of sequence labelling
 - identifying trends in price movements
- Biological applications of sequence labelling
 - gene-finding in DNA or RNA sequences



A first (bad) approach to sequence labelling

- Idea: train a supervised classifier to predict entire label sequence at once B-ORG I-ORG O O O B-LOC I-LOC I-LOC O Macquarie University is located in New South Wales .
- Problem: the number of possible label sequences grows exponentially with the length of the sequence
 - ▶ with *binary labels*, there are 2ⁿ different label sequences of a sequence of length n (2³² = 4 billion)
- \Rightarrow most labels won't be observed even in very large training data sets
 - This approach fails because it has massive *sparse data problems*



A better approach to sequence labelling

- Idea: train a supervised classifier to *predict the label of one word at a time*
 - B-LOCI-LOCOOOOB-LOCOWesternAustraliaisthelargeststateinAustralia.
- Avoids sparse data problems in label space
- As well as current word, classifiers can use *previous and following words as features*
- But this approach can produce inconsistent label sequences

0	B-LOC	I-ORG	I-ORG	0	0	0	0
The	New	York	Times	is	а	newspaper	

- ⇒ Track dependencies between adjacent labels
 - "chicken-and-egg" problem that Hidden Markov Models solve!



Outline

Sequence labelling

Hidden Markov Models

Finding the most probable label sequence

Higher-order HMMs

Summary



The big picture

- Optimal classifier: $\widehat{\textbf{y}}(\textbf{x}) = \text{argmax}_{\textbf{y}} \operatorname{P}(\textbf{Y}{=}\textbf{y} \mid \textbf{X}{=}\textbf{x})$
- How can we avoid *sparse data* problems when estimating $P(\mathbf{Y} \mid \mathbf{X})$
- \Rightarrow Decompose $\mathrm{P}(\textbf{Y} \mid \textbf{X})$ into a product of distributions that don't have sparse data problems
 - How can we compute the argmax over all possible label sequences y?
- ⇒ Use the Viterbi algorithm (dynamic programming over a trellis) to search over an exponential number of sequences **y** in linear time



Introduction to Hidden Markov models

- Hidden Markov models (HMMs) are a simple sequence labelling model
- HMMs are noisy channel models generating

$$P(\mathbf{X}, \mathbf{Y}) = P(\mathbf{X} | \mathbf{Y})P(\mathbf{Y})$$

 the source model P(Y) is a Markov model (e.g., a bigram language model)

$$\mathbf{P}(\mathbf{Y}) = \prod_{i=1}^{n+1} \mathbf{P}(Y_i \mid Y_{i-1})$$

• the channel model P(X | Y) generates each X_i independently, i.e.,

$$P(\mathbf{X} | \mathbf{Y}) = \prod_{i=1}^{n} P(X_i | Y_i)$$

• At testing time we only know X, so Y is unobserved or hidden



Terminology in Hidden Markov Models

- Hidden Markov models (HMMs) generate pairs of sequences (x, y)
- The sequence **x** is called:
 - the input sequence, or
 - the observations, or
 - the visible data

because \mathbf{x} is given when an HMM is used for sequence labelling

- The sequence **y** is called:
 - the label sequence, or
 - the tag sequence, or
 - the hidden data

because \mathbf{y} is unknown when an HMM is used for sequence labelling

- A $y \in \mathcal{Y}$ is sometimes called a *hidden state* because an HMM can be viewed as a *stochastic automaton*
 - each different $y \in \mathcal{Y}$ is a state in the automaton
 - the x are emissions from the automaton



Review: Naive Bayes models

• The naive Bayes model:

 $P(Y, X_1, \dots, X_m) = P(Y) P(X_1 | Y) \dots P(X_m | Y)$

- In a Naive Bayes classifier, the X_i are *features* and Y is the class label we want to predict
 - $P(X_i | Y)$ can be Bernoulli, multinomial, Gaussian etc.



Review: Markov models and *n*-gram language models

• An bigram language model is a *first-order Markov model* that *factorises* the distribution over a sequence **y** into a product of conditional distributions:

$$\mathbf{P}(\mathbf{y}) = \prod_{i=1}^{m} \mathbf{P}(y_i \mid y_{i-n}, \dots, y_{i-1})$$

- ▶ pad **y** with end markers, i.e., $\mathbf{y} = (\$, y_1, y_2, \dots, y_m, \$)$
- In a bigram language model, \mathbf{y} is a sentence and the y_i are words.
- First-order Markov model as a Bayes net:

$$\$ \longrightarrow Y_1 \longrightarrow Y_2 \longrightarrow Y_3 \longrightarrow Y_4 \longrightarrow \$$$



Hidden Markov models

• A Hidden Markov Model (\mathbf{s}, \mathbf{t}) defines a probability distribution over an item sequence $\mathbf{X} = (X_1, \dots, X_n)$, where each $X_i \in \mathcal{X}$, and a label sequence $\mathbf{Y} = (Y_1, \dots, Y_n)$, where each $Y_i \in \mathcal{Y}$, as:

$$P(\mathbf{X}, \mathbf{Y}) = P(\mathbf{X} | \mathbf{Y}) P(\mathbf{Y})$$

$$P(\mathbf{Y}=(\$, y_1, ..., y_n, \$)) = \prod_{i=1}^{n+1} P(Y_i = y_i | Y_{i-1} = y_{i-1})$$

$$= \prod_{i=1}^{n+1} s_{y_i, y_{i-1}} \quad (i.e., P(Y_i = y | Y_{i-1} = y') = s_{y, y'})$$

$$P(\mathbf{X}=(x_1, ..., x_n) | \mathbf{Y}=(\$, y_1, ..., y_n, \$))$$

$$= \prod_{i=1}^{n} P(X_i = x_i | Y_i = y_i)$$

$$= \prod_{i=1}^{n} t_{x_i, y_i} \quad (i.e., P(X_i = x | Y_i = y) = t_{x, y})$$



Hidden Markov models as Bayes nets

- A Hidden Markov Model (HMM) defines a joint distribution P(X, Y) over:
 - *item sequences* $\mathbf{X} = (X_1, \dots, X_n)$ and
 - label sequences $\mathbf{Y} = (Y_0 = \$, Y_1, \dots, Y_n, Y_{n+1} = \$)$:

$$\mathbf{P}(\mathbf{X}, \mathbf{Y}) = \left(\prod_{i=1}^{n} \mathbf{P}(Y_i \mid Y_{i-1}) \mathbf{P}(X_i \mid Y_i)\right) \mathbf{P}(Y_{n+1} \mid Y_n)$$

• HMMs can be expressed as Bayes nets, and standard message-passing inference algorithms work well with HMMs





The parameters of an HMM

- An HMM is specified by two matrices:
 - ► a matrix s, where s_{y,y'} = P(Y_i=y | Y_{i-1}=y') is the probability of a label y following the label y'
 - this is the same as in a bigram language model
 - remember to pad ${\boldsymbol y}$ with begin/end of sentence markers $\$
 - ► a matrix t, where t_{x,y} = P(X_i=x | Y_i = y) is the probability of an item x given the label y
 - similiar to the feature-class probability $P(F_j \mid Y)$ in naive Bayes
- If the set of labels is $\mathcal Y$ and the vocabulary is $\mathcal X$, then
 - **s** is an $m \times m$ matrix, where $m = |\mathcal{Y}|$.
 - **t** is a $v \times m$ matrix, where $v = |\mathcal{X}|$.



HMM estimate of a labelled sequence's probability

		$y_i \setminus y_{i-1}$	\$	Verb	Det	Noun		\mathbf{x}	Vorb	Det	Noun
		\$	0	0.3	0.1	0.3		$x_i \setminus y_i$	verb	Del	Noun
		¥ 		0.0	0.1	0.0		spread	0.5	0.1	0.4
s =	=	Verb	Verb 0.4	0.4 0.1	0.1	0.3	t =		01	<u> </u>	01
		Det	04	04	01	02		the	0.1	0.0	0.1
	Det	0.1	0.1	0.1	0.2		butter	0.4	0.1	0.5	
	Noun	0.2	0.2	0.7	0.2		20000	0.1	0.1	0.0	

P(X = (spread, the, butter), Y = (Verb, Det, Noun))

- $= s_{\text{S,Verb}} \cdot s_{\text{Det,Verb}} \cdot s_{\text{Noun,Det}} \cdot s_{\text{S,Noun}}$
 - $\cdot t_{
 m spread,Verb} \cdot t_{
 m the,Det} \cdot t_{
 m butter,Noun}$
- $= 0.4 \cdot 0.4 \cdot 0.7 \cdot 0.3 \cdot 0.5 \cdot 0.8 \cdot 0.5$
- \cong 0.009



A HMM as a stochastic automaton

State to state transition probabilities

$y_i \setminus y_{i-1}$	\$	Verb	Det	Noun
\$	0	0.3	0.1	0.3
Verb	0.4	0.1	0.1	0.3
Det	0.4	0.4	0.1	0.2
Noun	0.2	0.2	0.7	0.2



$x_i \setminus y_i$	Verb	Det	Noun
spread	0.5	0.1	0.4
the	0.1	0.8	0.1
butter	0.4	0.1	0.5



P (X=(spread, the, butter), Y=(Verb, Det, Noun))

$$= s_{\rm S,Verb} \cdot s_{\rm Det,Verb} \cdot s_{\rm Noun,Det} \cdot s_{\rm S,Noun}$$

 $\cdot t_{
m spread,Verb} \cdot t_{
m the,Det} \cdot t_{
m butter,Noun}$

 $= 0.4 \cdot 0.4 \cdot 0.7 \cdot 0.3 \cdot 0.5 \cdot 0.8 \cdot 0.5$

Estimating an HMM from labelled data

- Training data consists of labelled sequences of data items
- Estimate s_{y,y'} = P(Y_i=y | Y_{i-1}=y') from label sequences y (just as for language models)
 - If n_{y,y'} is the number of times y follows y' in training label sequences and n_{y'} is the number of times y' is followed by anything, then:

$$\hat{\hat{s}}_{y,y'} = rac{n_{y,y'}+1}{n_{y'}+|\mathcal{Y}|}$$

- Be sure to count the end-markers \$
- Estimate t_{x,y} = P(X_i = x | Y_i = y) from pairs of item sequences x and their corresponding label sequence y
 - ► If r_{x,y} is the number of times a data item x is labelled y, and r_y is the number of times y appears in a label sequence, then:

$$\hat{t}_{x,y} = \frac{r_{x,y}+1}{r_y+|\mathcal{X}|}$$



Estimating an HMM example

D	=	Verl spread	b 1 ad b	Noun outter), (Verb	er	De th	et Nour e sprea				
		$y_i \setminus y_{i-1}$	\$	Verb	Det	Noun			$y_i \setminus y_{i-1}$	\$	Verb	Det	Noun
n	=	\$	0	0	0	2		$\hat{\mathbf{s}} =$	\$	1/6	1/6	1/5	3/6
		Verb	2	0	0	0	ŝ		Verb	3/6	1/6	1/5	1/6
		Det	0	1	0	0			Det	1/6	2/6	1/5	1/6
		Noun	0	1	1	0			Noun	1/6	2/6	2/5	1/6
		$x_i \setminus y_i$	Verb	Det	Noui	n			$x_i \setminus y_i \mid N$	/erb	Det N	loun	
r	_	spread	1	0	1	_	÷ _	. –	spread 2	2/5	1/4 2	2/5	
	_	the	0	1	0		ι —		the	L/5	2/4 :	L/5	
		butter	1	0	1				butter 2	2/5	1/4 2	2/5	



Outline

Sequence labelling

Hidden Markov Models

Finding the most probable label sequence

Higher-order HMMs

Summary



Why is finding the most probable label sequence hard

• When we use an HMM, we're given data items **x** and want to return *the most probable label sequence*:

$$\widehat{\mathbf{y}}(\mathbf{x}) = \operatorname{argmax}_{\mathbf{y} \in \mathcal{Y}^n} P(\mathbf{X}{=}\mathbf{x} \mid \mathbf{Y}{=}\mathbf{y}) P(\mathbf{Y}{=}\mathbf{y})$$

- If x has n elements and each item has $m = |\mathcal{Y}|$ possible labels, the number of possible label sequences is m^n
 - the number of possible label sequences grows *exponentially* with the length of the string
 - ⇒ exhaustive search for the optimal label sequence become impossible once n is large
- But the Viterbi algorithm finds the most probable label sequence $\hat{\mathbf{y}}(\mathbf{x})$ in O(n) (linear) time using dynamic programming over a trellis
 - the Viterbi algorithm is actually just the *shortest path* algorithm on the *trellis*



The trellis

• Given input **x** of length *n*, the *trellis* is a *directed acyclic graph* where:

- ► the nodes are all pairs (i, y) for y ∈ Y and i ∈ 1,..., n, plus a starting node and a final node
- ▶ there are edges from the starting node to all nodes (1, y) for each $y \in \mathcal{Y}$
- For each y', y ∈ 𝔅 and each i ∈ 2,..., n there is an edge from (i − 1, y') to (i, y)
- ▶ for each $y \in \mathcal{Y}$ there is an edge from (n, y) to the final node
- Every possible **y** is a path through the trellis

$$(1, \operatorname{Verb}) \xrightarrow{(2, \operatorname{Verb})} (3, \operatorname{Verb}) \xrightarrow{(3, \operatorname{Verb})} (3, \operatorname{Verb}) \xrightarrow{(3, \operatorname{Verb})} (3, \operatorname{Det}) \xrightarrow{(1, \operatorname{Det})} (2, \operatorname{Det}) \xrightarrow{(3, \operatorname{Det})} (3, \operatorname{Noun}) \xrightarrow{(1, \operatorname{Noun})} (2, \operatorname{Noun}) \xrightarrow{(3, \operatorname{Noun})} (3, \operatorname{Noun})$$



Using a trellis to find the most probable label sequence ${\boldsymbol{y}}$

- One-to-one correspondence between *paths from start to finish in the trellis* and *label sequences* **y**
- High level description of algorithm:
 - associate each edge in the trellis with a weight (a number)
 - the product of the weights along a path from start to finish will be

$$P(\textbf{X}{=}\textbf{x},\textbf{Y}{=}\textbf{y})$$

- use dynamic programming to find highest scoring path from start to finish
- return the corresponding label sequence $\widehat{\mathbf{y}}(\mathbf{x})$
- Conditioned on the input **X**, the distribution $P(\mathbf{Y} | \mathbf{X})$ is an *inhomogenous (i.e., time-varying) Markov chain*
 - the transition probabilities $P(Y_i | Y_{i-1}, X_i)$ depend on X_i and hence i



Rearranging the terms in the HMM formula

• Rearrange terms so all terms associated with a time *i* are together

$$P(\mathbf{X}, \mathbf{Y}) = P(\mathbf{Y}) P(\mathbf{X} | \mathbf{Y}) = s_{y_1, \$} \cdot s_{y_2, y_1} \cdot \ldots \cdot s_{y_n, y_{n-1}} \cdot s_{\$, y_n} \cdot t_{x_1, y_1} \cdot t_{x_2, y_2} \cdot \ldots \cdot t_{x_n, y_n} = s_{y_1, \$} \cdot t_{x_1, y_1} \cdot s_{y_2, y_1} \cdot t_{x_2, y_2} \cdot \ldots \cdot s_{y_n, y_{n-1}} \cdot t_{x_n, y_n} \cdot s_{\$, y_n} = \left(\prod_{i=1}^n s_{y_i, y_{i-1}} \cdot t_{x_i, y_i}\right) \cdot s_{\$, y_n}$$

- Trellis edge weights:
 - weight on edge from start node to node (1, y) is $w_{1,y,\$} = s_{y,\$} \cdot t_{x_1,y}$
 - weight on edge from node (i 1, y') to node (i, y) is $w_{i,y,y'} = s_{y,y'} \cdot t_{x_i,y}$
 - weight on edge from node (n, y) to final node is $w_{n+1,\$,y} = s_{\$,y}$

 \Rightarrow product of weights on edges of path **y** in trellis is P(X=x, Y=y)



Trellis for *spread the butter*





s

Finding the highest-scoring path



- The score of a path is the product of the weights of the edges along that path
- Key insight: the highest-scoring path to a node (i, y) must begin with a highest-scoring path to some node (i - 1, y')
- Let MaxScore(*i*, *y*) be the score of the highest scoring path to node (*i*, *y*). Then:

• To find the highest scoring path, compute MaxScore(*i*, *y*) for *i* = 1, 2, ..., *n* + 1 in turn



Finding the highest-scoring path example (1)



$$\mathbf{w}_1 = \frac{\underbrace{y_1 \setminus y_0}_{Verb} \quad \begin{array}{c} \$ \\ \hline Verb \\ Det \\ Noun \\ 0.08 \end{array}$$

- MaxScore(1, Verb) = 0.2
 - MaxScore(1, Det) = 0.04
- MaxScore(1, Noun) = 0.08



Finding the highest-scoring path example (2)



- Verb Det Noun $y_2 \setminus y_1$ MaxScore(1, Verb) 0.2 = Verb 0.01 0.01 0.03 MaxScore(1, Det) = 0.04 W₂ 0.32 Det 0.08 0.16 MaxScore(1, Noun) = 0.08 Noun 0.02 0.07 0.02
 - MaxScore(2, Verb) = 0.0024 via Noun MaxScore(2, Det) = 0.064 via Verb MaxScore(2, Noun) = 0.004 via Noun



Finding the highest-scoring path example (3)



MaxScoro(2 Vorb)	_	0.0024		_	$y_3 \setminus y_2$	Verb	Det	Noun
MaxScore(2, Verb)	_	0.0024		_	Verb	0.04	0.04	0.12
MaxScore(2, Det)	_	0.004	W 3 —	-	Det	0.04	0.01	0.02
maxScore(2, Noun)	= 0	0.004			Noun	0.1	0.35	0.1



Finding the highest-scoring path example (4)



 $\begin{array}{rcl} \mathrm{MaxScore}(3,\mathrm{Det}) &=& 0.00064 \\ \mathrm{MaxScore}(3,\mathrm{Noun}) &=& 0.0224 \end{array} \qquad \mathbf{w}_4 &=& \frac{\mathbf{v}_4 \mathbf{v}_3}{\mathbf{s}} \quad \frac{\mathbf{v}_{CD}}{\mathbf{s}} \quad \frac{\mathbf{v}_{CD}}{\mathbf{s$

MaxScore(4, \$) = 0.00672 via Noun



Forward-backward algorithms

- This dynamic programming algorithm is an instance of a general family of algorithms known as *forward-backward algorithms*
- The *forward pass* computes a probability of a *prefix* of the input
- The backward pass computes a probability of a suffix of the input
- With these it is possible compute:
 - the marginal probability of any state given the input $P(Y_i = y | \mathbf{X} = x)$
 - ▶ the marginal probability of any adjacent pair of states P(Y_{i−1}=y, Y_i=y' | X = x)
 - ▶ the expected number of times any pair of states is seen in the input $E[n_{y,y'} \mid \mathbf{x}]$
- These are required for estimating HMMs from unlabelled data using the *Expectation-Maximisation Algorithm*



Outline

- Sequence labelling
- Hidden Markov Models
- Finding the most probable label sequence
- Higher-order HMMs
- Summary



The "order" of an HMM

- The order of an HMM is the number of previous labels used to predict the current label Y_i
- A *first-order HMM* uses the previous label Y_{i-1} to predict Y_i :

$$\mathbf{P}(\mathbf{Y}) = \prod_{i=1}^{n+1} \mathbf{P}(Y_i \mid Y_{i-1})$$

(the HMMs we've seen so far are all first-order HMMs)

• A second-order HMM uses the previous two labels Y_{i-2} and Y_{i-1} to predict Y_i :

$$P(\mathbf{Y}) = \prod_{i=1}^{n+1} P(Y_i | Y_{i-1}, Y_{i-2})$$

- the parameters used in a second-order HMM are more complex
- **s** is a three-dimensional array of size $m \times m \times m$, where $m = |\mathcal{Y}|$

$$P(Y_i = y | Y_{i-1} = y', Y_{i-2} = y'') = s_{y,y',y''}$$



Bayes net representation of a 2nd-order HMM





The trellis in higher-order HMMs

- The nodes in the trellis encode the information required from "the past" in order to predict the next label *Y_i*
 - ► a first-order HMM tracks one past label \Rightarrow trellis states are pairs (i, y'), where $Y_{i-1} = y'$
 - ► a second-order HMM tracks two past labels \Rightarrow trellis states are triples (i, y', y''), where $Y_{i-1} = y'$ and $Y_{i-2} = y''$
 - ▶ in a k-th order HMM, trellis states consist of a position index i and k Y-values for Y_{i-1}, Y_{i-2},..., Y_{i-k}
- This means that for a sequence X of length n and where the number of states |𝔅| = m, a k-th order HMM has O(n ⋅ m^k) nodes in the trellis
- Since every edge is visited a constant number of times, the computational complexity of the Viterbi algorithm is also O(n · m^{k+1}).



Outline

- Sequence labelling
- Hidden Markov Models
- Finding the most probable label sequence
- Higher-order HMMs
- Summary



Summary

- Sequence labelling is an important kind of structured prediction problem
- Hidden Markov Models (HMMs) can be viewed as a generalisation of Naive Bayes models where the label Y is generated by a Markov model
 - HMMs can also be viewed as stochastic automata with a hidden state
- *Forward-backward algorithms* are dynamic programming algorithms that can compute:
 - ▶ the Viterbi (i.e., most likely) label sequence for a string
 - the expected number of times each state-output or state-state transition is used in the analysis of a string
- HMMs make the same independence assumptions as Naive Bayes
 - Conditional Random Fields (CRFs) are a generalisation of HMMs that relax these independence assumptions
 - CRFs are the sequence labelling generalisation of logistic regression

