Hidden Markov Models (Part 2)

BMI/CS 576
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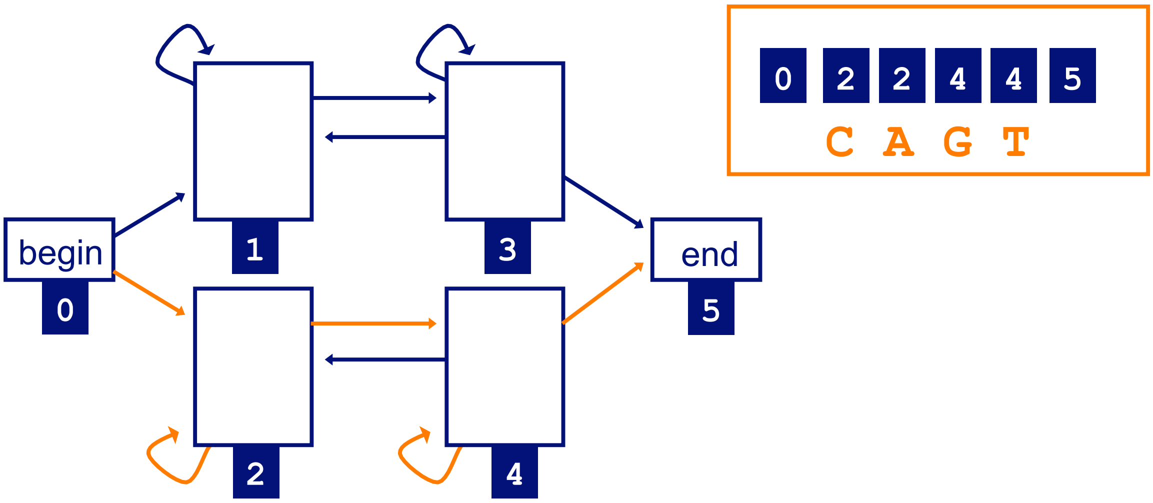
Three important questions

- How likely is a given sequence?
- What is the most probable "path" for generating a given sequence?
- How can we learn the HMM parameters given a set of sequences?

Learning without hidden information

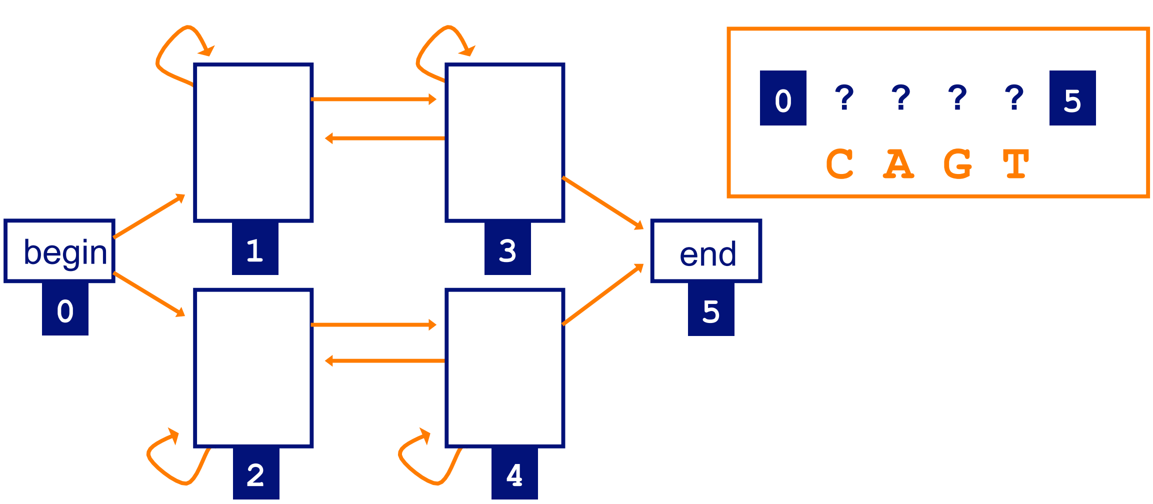
- learning is simple if we know the correct path for each sequence in our training set



- estimate parameters by counting the number of times each parameter is used across the training set

Learning with hidden information

- if we don't know the correct path for each sequence in our training set, consider all possible paths for the sequence



- estimate parameters through a procedure that counts the expected number of times each parameter is used across the training set

Learning parameters

- if we know the state path for each training sequence, learning the model parameters is simple
  - no hidden information during training
  - count how often each parameter is used
  - normalize/smooth to get probabilities
  - process is just like it was for Markov chain models

- if we don't know the path for each training sequence, how can we determine the counts?
  - key insight: estimate the counts by considering every path weighted by its probability

Learning parameters: the Baum-Welch algorithm

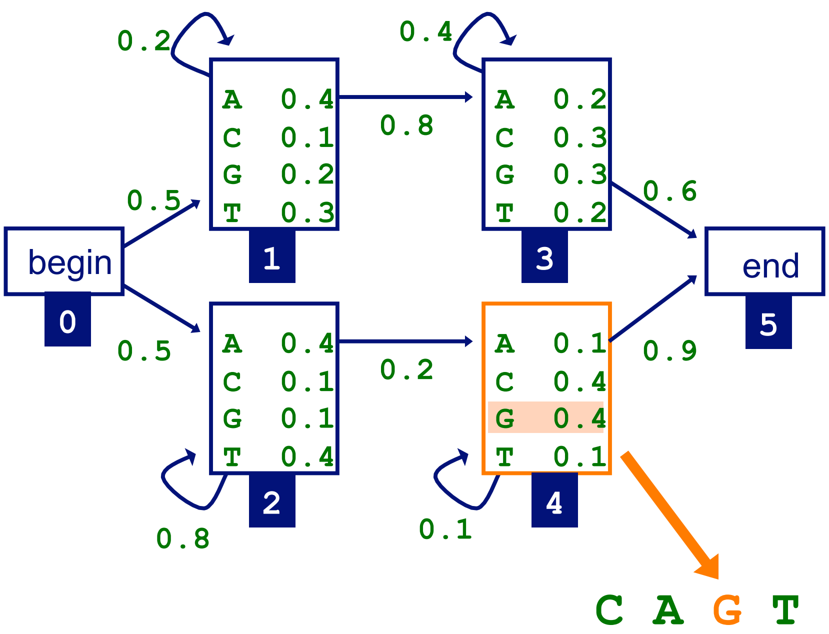
- *a.k.a* the Forward-Backward algorithm
- an *Expectation Maximization* (EM) algorithm
  - EM is a family of algorithms for learning probabilistic models in problems that involve hidden information
- in this context, the hidden information is the path that best explains each training sequence

Learning parameters: the Baum-Welch algorithm

- algorithm sketch:
  - initialize parameters of model
  - iterate until convergence
    - calculate the *expected* number of times each transition or emission is used
    - adjust the parameters to *maximize* the likelihood of these expected values

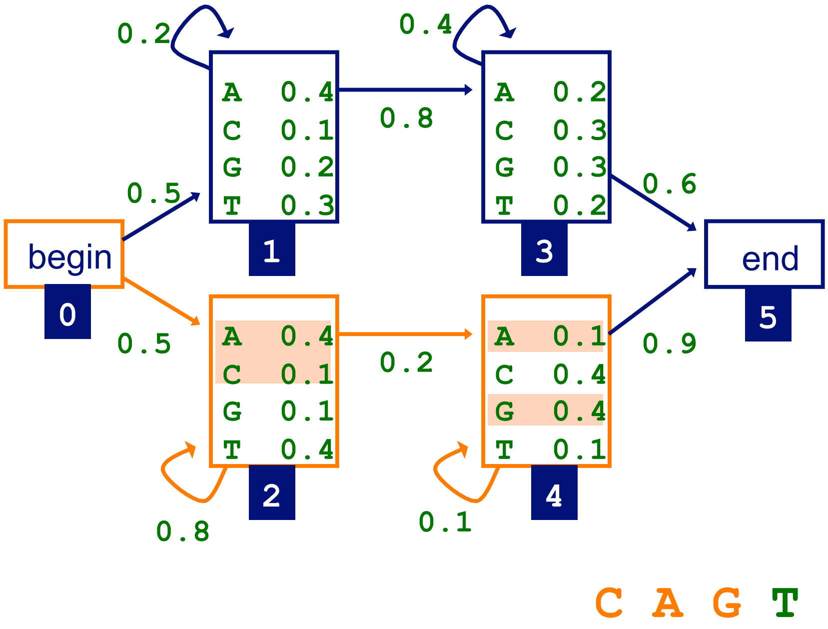
The expectation step

- we want to know the probability of generating sequence x with the i th symbol being produced by state k (for all x, i and k)



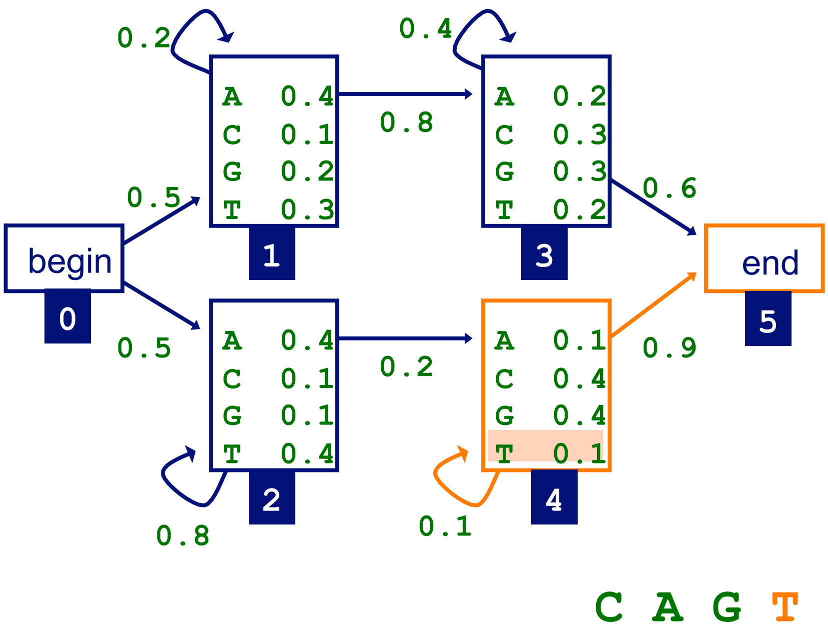
The expectation step

- the forward algorithm gives us $f_k(i)$, the probability of being in state k having observed the first i characters of x



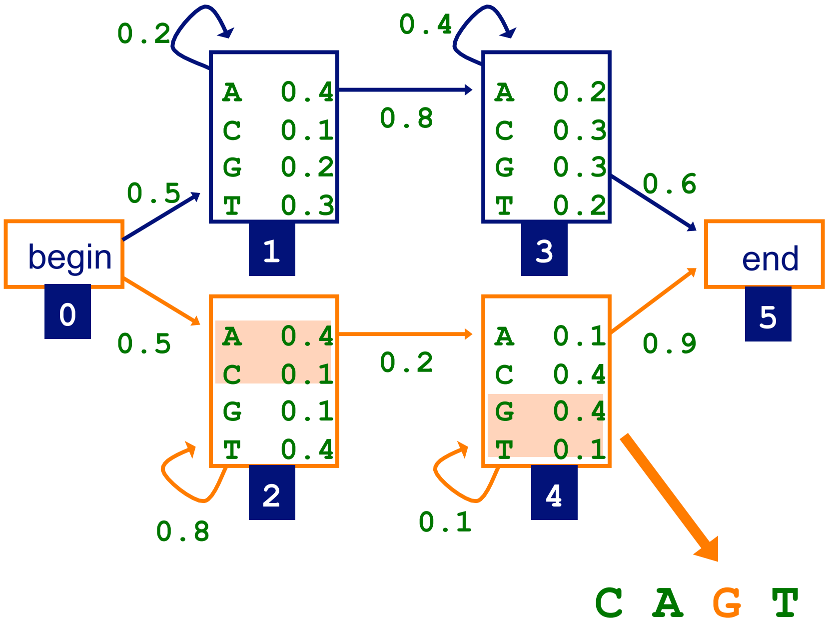
The expectation step

- the *backward algorithm* gives us $b_k(i)$, the probability of observing the rest of x, given that we're in state k after i characters

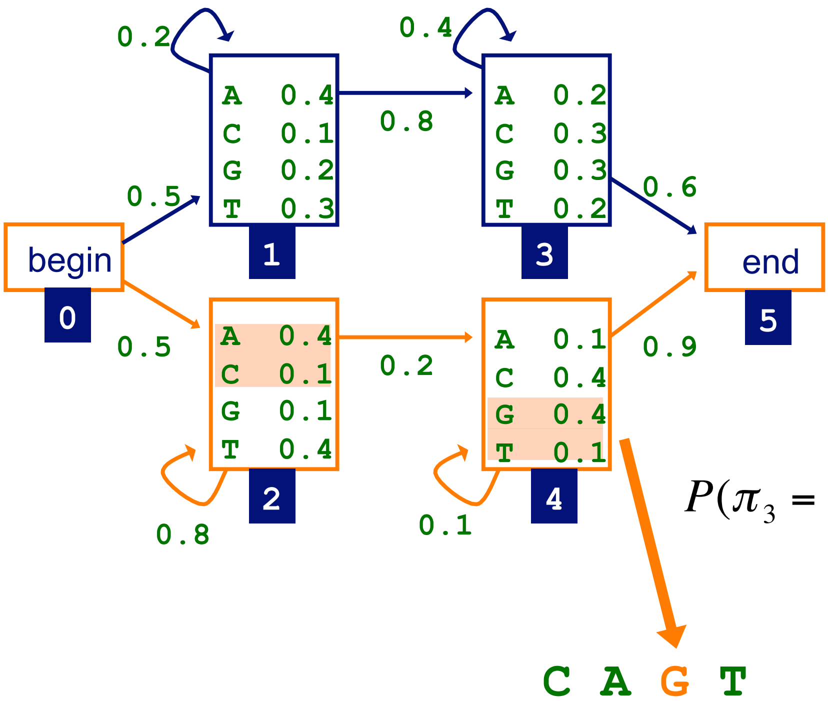


The expectation step

- putting forward and backward together, we can compute the probability of producing sequence x with the i th symbol being produced by state q



The expectation step



$$P(\pi_3 = 4 \mid x) = \frac{P(\pi_3 = 4, x)}{P(x)}$$

$$= \frac{f_4(3)b_4(3)}{f_5(4)}$$

The expectation step

- first, we need to know the probability of the i th symbol being produced by state k, given sequence x

$$P(\pi_i = k \mid x)$$

- given this we can compute our expected counts for state transitions, character emissions

The expectation step

- the probability of of producing x with the i th symbol being emitted by state k is

$$P(\pi_i = k, x) = P(x_1 \ldots x_i,\ \pi_i = k) \times$$
$$P(x_{i+1} \ldots x_L \mid \pi_i = k)$$

- the first term is $f_k(i)$, computed by the forward algorithm

- the second term is $b_k(i)$, computed by the backward algorithm

The backward algorithm

- initialization:

$$b_k(L) = a_{kN}$$

for states with a transition to *end* state

The backward algorithm

- recursion ($i = L \ldots 1$):

$$b_k(i) = \sum_l \begin{Bmatrix} a_{kl} b_l(i), & \text{if } l \text{ is silent state} \\ a_{kl} e_l(x_{i+1}) b_l(i+1), & \text{otherwise} \end{Bmatrix}$$

The backward algorithm

- termination:

$$P(x_1 \ldots x_L) = b_0(0) = \sum_l \begin{Bmatrix} a_{0l} b_l(0), & \text{if } l \text{ is silent state} \\ a_{0l} e_l(x_1) b_l(1), & \text{otherwise} \end{Bmatrix}$$

The expectation step

- now we can calculate the probability of the i th symbol being produced by state k, given x

$$P(\pi_i = k \mid x) = \frac{P(\pi_i = k, x)}{P(x)}$$

$$= \frac{f_k(i) b_k(i)}{P(x)}$$

$$\boxed{= \frac{f_k(i) b_k(i)}{f_N(L)}}$$

The expectation step

- now we can calculate the expected number of times letter c is emitted by state k
- here we've added the superscript j to refer to a specific sequence in the training set

$$n_{k,c} = \sum_{x^j} \left[\frac{1}{f_N^j(L)} \sum_{\{i \mid x_i^j = c\}} f_k^j(i) b_k^j(i) \right]$$

sum over sequences

sum over positions where c occurs in x

The expectation step

- and we can calculate the expected number of times that the transition from k to l is used

$$n_{k \to l} = \sum_{x^j} \frac{\sum_i f_k^j(i)\ a_{kl}\ e_l(x_{i+1}^j)\ b_l^j(i+1)}{f_N^j(L)}$$

- or if l is a silent state

$$n_{k \to l} = \sum_{x^j} \frac{\sum_i f_k^j(i)\ a_{kl}\ b_l^j(i)}{f_N^j(L)}$$

The maximization step

- Let $n_{k,c}$ be the expected number of emissions of c from state k for the training set
- estimate new emission parameters by:

$$e_k(c) = \frac{n_{k,c}}{\sum_{c'} n_{k,c'}}$$

- just like in the simple case
- but typically we'll do some "smoothing" (e.g. add pseudocounts)

The maximization step

- let $n_{k \to l}$ be the expected number of transitions from state k to state l for the training set
- estimate new transition parameters by:

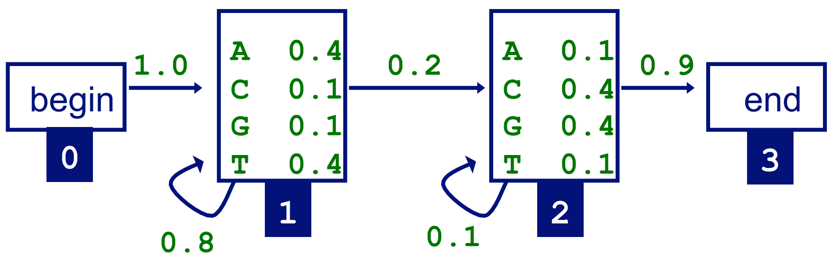
$$a_{kl} = \frac{n_{k \to l}}{\sum_{m} n_{k \to m}}$$

The Baum-Welch algorithm

- initialize the parameters of the HMM
- iterate until convergence
  - initialize $n_{k,c}$, $n_{k \to l}$ with pseudocounts
  - **E-step**: for each training set sequence $j = 1 \ldots n$
    - calculate $f_k(i)$ values for sequence j
    - calculate $b_k(i)$ values for sequence j
    - add the contribution of sequence j to $n_{k,c}$, $n_{k \to l}$
  - **M-step**: update the HMM parameters using $n_{k,c}$, $n_{k \to l}$

Baum-Welch algorithm example

- given
  - the HMM with the parameters initialized as shown
  - the training sequences **TAG, ACG**



- we'll work through one iteration of Baum-Welch

Baum-Welch example (cont)

- determining the forward values for TAG

$$
\begin{aligned}
& f_0(0) = 1 \\
& f_1(1) = e_1(T) \times a_{01} \times f_0(0) = 0.4 \times 1 = 0.4 \\
& f_1(2) = e_1(A) \times a_{11} \times f_1(1) = 0.4 \times 0.8 \times 0.4 = 0.128 \\
& f_2(2) = e_2(A) \times a_{12} \times f_1(1) = 0.1 \times 0.2 \times 0.4 = 0.008 \\
& f_2(3) = e_2(G) \times \left(a_{12} \times f_1(2) + a_{22} \times f_2(2)\right) = \\
& \qquad\qquad 0.4 \times (0.0008 + 0.0256) = 0.01056 \\
& f_3(3) = a_{23} \times f_2(3) = 0.9 \times 0.01056 = 0.009504
\end{aligned}
$$

- here we compute just the values that represent events with non-zero probability
- in a similar way, we also compute forward values for ACG

Baum-Welch example (cont)

- determining the backward values for TAG

$$
\begin{aligned}
& b_3(3) = 1 \\
& b_2(3) = a_{23} \times b_3(3) = 0.9 \times 1 = 0.9 \\
& b_2(2) = a_{22} \times e_2(G) \times b_2(3) = 0.1 \times 0.4 \times 0.9 = 0.036 \\
& b_1(2) = a_{12} \times e_2(G) \times b_2(3) = 0.2 \times 0.4 \times 0.9 = 0.072 \\
& b_1(1) = a_{11} \times e_1(A) \times b_1(2) + a_{12} \times e_2(A) \times b_2(2) = \\
& \qquad\qquad 0.8 \times 0.4 \times 0.072 + 0.2 \times 0.1 \times 0.036 = 0.02376 \\
& b_0(0) = a_{01} \times e_1(T) \times b_1(1) = 1.0 \times 0.4 \times 0.02376 = 0.009504
\end{aligned}
$$

- here we compute just the values that represent events with non-zero probability
- in a similar way, we also compute backward values for ACG

Baum-Welch example (cont)

- determining the expected emission counts for state 1

	contribution of TAG		contribution of ACG		pseudocount
$n_{1,A} =$	$\dfrac{f_1(2)b_1(2)}{f_3(3)}$	$+$	$\dfrac{f_1(1)b_1(1)}{f_3(3)}$	$+$	1
$n_{1,C} =$			$\dfrac{f_1(2)b_1(2)}{f_3(3)}$	$+$	1
$n_{1,G} =$					1
$n_{1,T} =$	$\dfrac{f_1(1)b_1(1)}{f_3(3)}$			$+$	1

*note that the forward/backward values in these two columns differ; in each column they are computed for the sequence associated with the column

Baum-Welch example (cont)

- determining the expected transition counts for state 1 (not using pseudocounts)

	contribution of TAG		contribution of ACG
$n_{1\to1} =$	$\dfrac{f_1(1)a_{11}e_1(A)b_1(2)}{f_3(3)}$	$+$	$\dfrac{f_1(1)a_{11}e_1(C)b_1(2)}{f_3(3)}$
$n_{1\to2} =$	$\dfrac{f_1(1)a_{12}e_2(A)b_2(2)+f_1(2)a_{12}e_2(G)b_2(3)}{f_3(3)}$	$+$	$\dfrac{f_1(1)a_{12}e_2(C)b_2(2)+f_1(2)a_{12}e_2(G)b_2(3)}{f_3(3)}$

- in a similar way, we also determine the expected emission/transition counts for state 2

Baum-Welch example (cont)

- determining probabilities for state 1

$$e_1(A) = \frac{n_{1,A}}{n_{1,A} + n_{1,C} + n_{1,G} + n_{1,T}}$$

$$e_1(C) = \frac{n_{1,C}}{n_{1,A} + n_{1,C} + n_{1,G} + n_{1,T}}$$

$$\vdots$$

$$a_{11} = \frac{n_{1\to 1}}{n_{1\to 1} + n_{1\to 2}}$$

$$a_{12} = \frac{n_{1\to 2}}{n_{1\to 1} + n_{1\to 2}}$$

Computational complexity of HMM algorithms

- given an HMM with S states and a sequence of length L, the complexity of the Forward, Backward and Viterbi algorithms is

$$O(S^2 L)$$

  – this assumes that the states are densely interconnected

- Given M sequences of length L, the complexity of Baum-Welch on <u>each iteration</u> is

$$O(MS^2 L)$$

Baum-Welch convergence

- some convergence criteria
  - likelihood of the training sequences changes little
  - fixed number of iterations reached
- usually converges in a small number of iterations
- will converge to a *local* maximum (in the likelihood of the data given the model)

$$\log P(\text{sequences} \mid \theta) = \sum_{x^j} \log P(x^j \mid \theta)$$

Learning and prediction tasks

- *learning*

  Given: a model, a set of training sequences

  Do: find model parameters that explain the training sequences with relatively high probability (goal is to find a model that *generalizes* well to sequences we haven't seen before)

- *classification*

  Given: a set of models representing different sequence classes, a test sequence

  Do: determine which model/class best explains the sequence

- *segmentation*

  Given: a model representing different sequence classes, a test sequence

  Do: segment the sequence into subsequences, predicting the class of each subsequence

Algorithms for learning and prediction tasks

- *learning*

  correct path known for each training sequence $\Rightarrow$ simple maximum-likelihood or Bayesian estimation

  correct path not known $\Rightarrow$ Forward-Backward algorithm + (ML or Bayesian estimation)

- *classification*

  simple Markov model $\Rightarrow$ calculate probability of sequence along single path for each model

  hidden Markov model $\Rightarrow$ Forward algorithm to calculate probability of sequence along all paths for each model

- *segmentation*

  hidden Markov model $\Rightarrow$ Viterbi algorithm to find most probable path for sequence