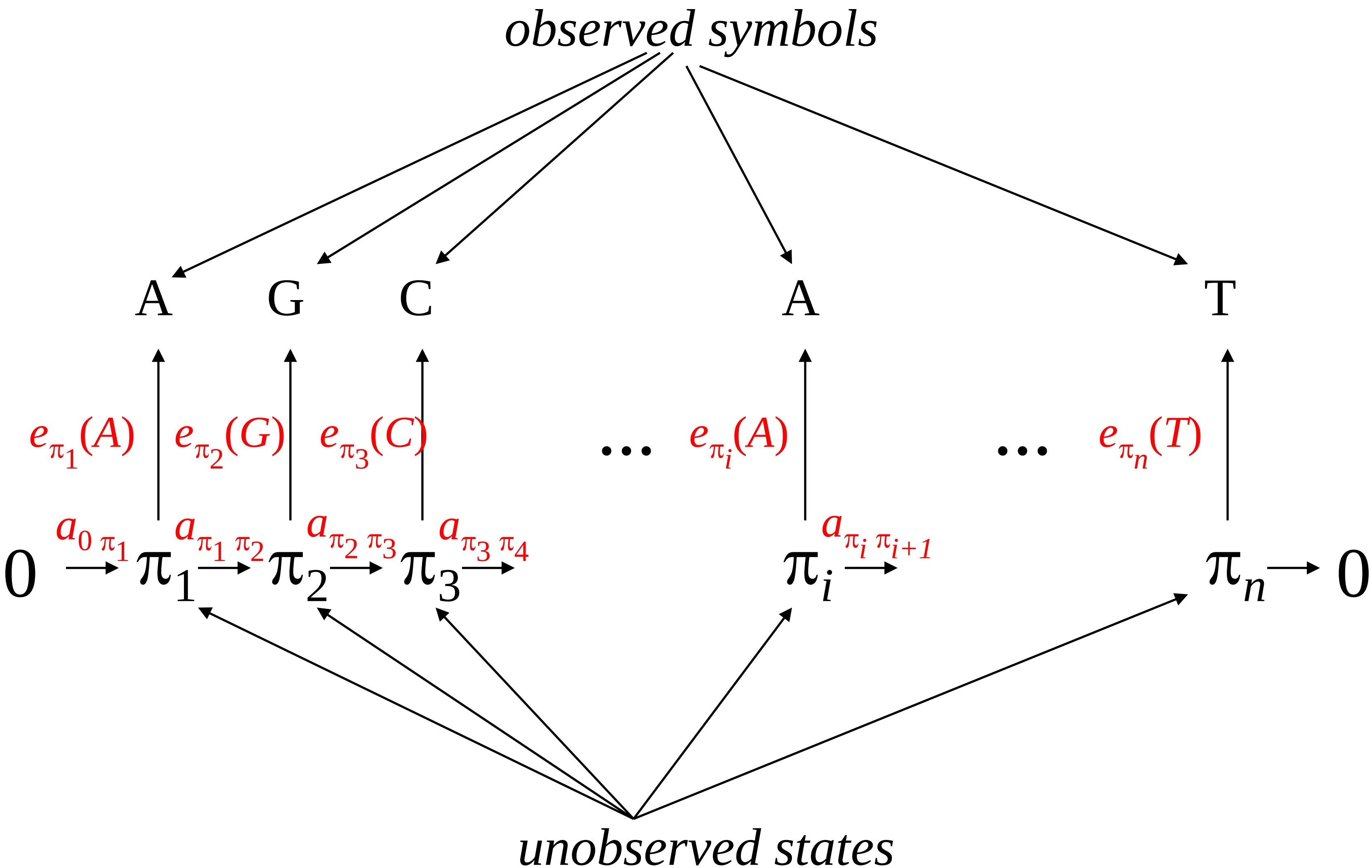
Today's Lecture -- HMMs

- Probability calculations
  - WDAG
  - Viterbi algorithm
- Parameter estimation
  - Viterbi training
- Forward algorithm

Hidden Markov Model



HMM Probabilities of Sequences

- Prob of sequence of states $\pi_1\pi_2\pi_3 \ldots \pi_n$ is
  $a_{0\pi_1} a_{\pi_1\pi_2} a_{\pi_2\pi_3} a_{\pi_3\pi_4} \ldots a_{\pi_{n-1}\pi_n}$.
- Prob of seq of observed symbols $b_1b_2b_3 \ldots b_n$,
  conditional on state sequence is
  $e_{\pi_1}(b_1)e_{\pi_2}(b_2)\, e_{\pi_3}(b_3) \ldots e_{\pi_n}(b_n)$
- Joint probability $= a_{0\pi_1}\prod^{n}_{i=1} a_{\pi_i\pi_{i+1}}\, e_{\pi_i}(b_i)$
  (define $a_{\pi_n\pi_{n+1}}$ to be 1)
- (Unconditional) prob of observed sequence
  = sum (of joint probs) over all possible state paths
  - not practical to compute directly, by 'brute force'! We will use dynamic programming.

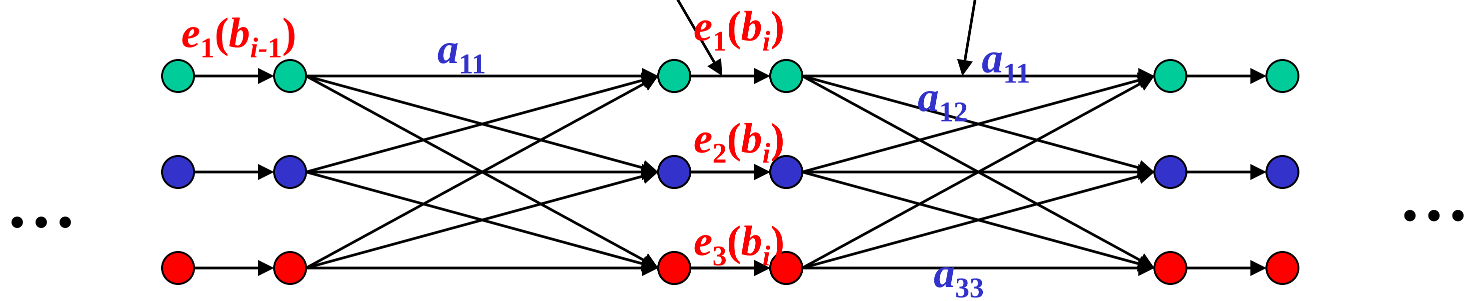
Computing HMM Probabilities

- WDAG structure for sequence HMMs:
  - for i^{th} position in seq (i = 1, ... n), have 2 nodes for each state:
    - total # nodes = $2ns + 1$, where n = seq length, s = # states
  - Pair of nodes for a given state at i^{th} position is connected by an *emission* edge
    - Weight is the emission prob for i^{th} observed residue.
    - Can omit node pair if emission prob = 0.
  - Have *transition* edges connecting (right-hand) state nodes at position i with (left-hand) state nodes at position i+1
    - Weights are transition probs
    - Can omit edges with transition prob = 0.

WDAG for 3-state HMM, length *n* sequence

weights are emission probabilities $e_k(b_i)$ for i^{th} residue b_i

weights are transition probabilities a_{kl}

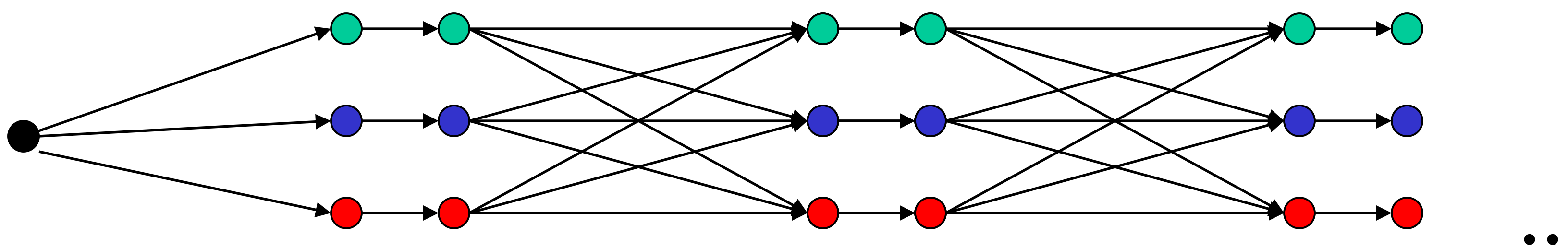


b_{i-1} position i-1

b_i position i

b_{i+1} position i+1

Beginning of Graph



begin state

b_1
position 1

b_2
position 2

b_3
position 3

- ***Paths*** through graph from begin node to end node correspond to ***sequences of states***
- ***Product weight*** along path

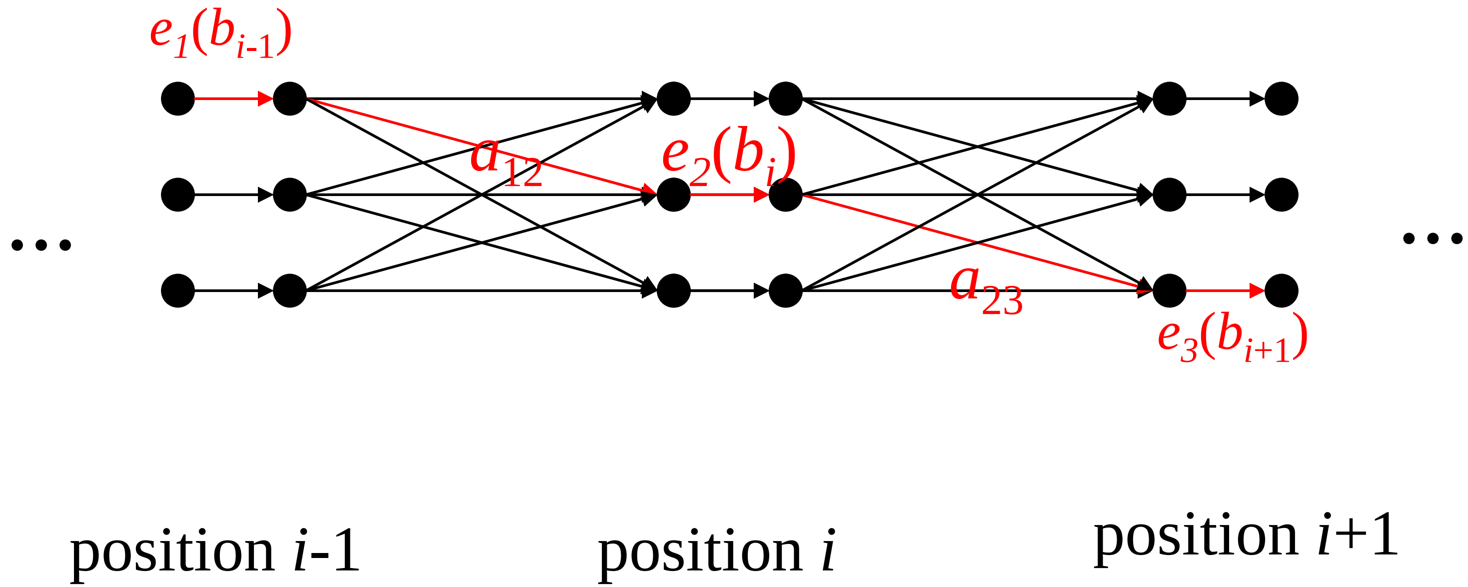
  = ***joint probability*** of state sequence & observed symbol sequence
- ***Highest-weight path*** = ***highest probability state sequence***
- ***Sum*** *of (product) path weights*, ***over all paths***,

  = ***probability of observed sequence***
- ***Sum*** *of (product) path weights* ***over***
  - all paths *going through a particular node*, or
  - all paths *that include a particular edge*,

  divided by prob of observed sequence,

  = ***posterior probability*** of that edge or node

Path Weights



- By general results on WDAGs, can use dynamic programming to find highest weight path:

  = “Viterbi algorithm” to find highest probability path (most probable “parse”)

  – in this case can use log probabilities & sum weights

  – (N.B. paths are constrained to begin at the begin node!)

The Viterbi path is

the *most probable parse*!

Complexity

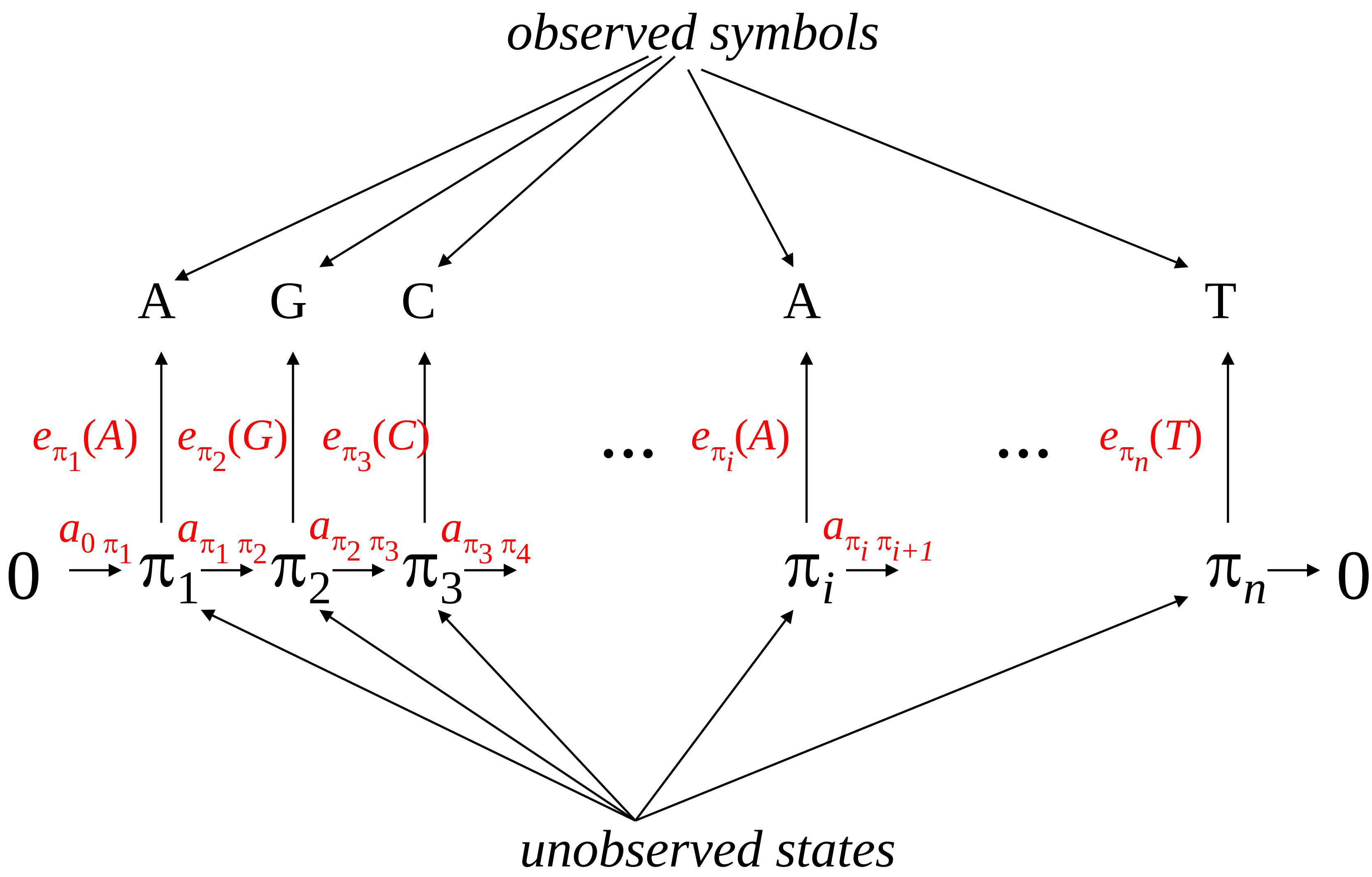
- $= O(|V|+|E|)$, i.e. total # nodes and edges.
- # nodes = $2ns + 2$
  - where n = sequence length,
  - s = # states.
- # edges = $(n - 1)s^2 + ns + 2s$

- So overall complexity is $O(ns^2)$
  - (actually s^2 can be reduced to # ‘allowed’ transitions between states – depends on model topology).

HMM Parameter Estimation

- Suppose parameter values (transition & emission probs) unknown
- Need to estimate from set of training sequences
- *Maximum likelihood* (ML) estimation (= choice of param vals to maximize prob of data) is preferred
  - optimality properties of ML estimates discussed in Ewens & Grant

Hidden Markov Model



Parameter estimation when state sequence is *known*

- When underlying state sequence for each training sequence is *known*,
  - e.g.: site model

then ML estimates are given by:

  - emission probabilities:

    $e_k(b)$^ = (# times symbol b emitted by state k) / (# times state k occurs) .

  - transition probabilities:

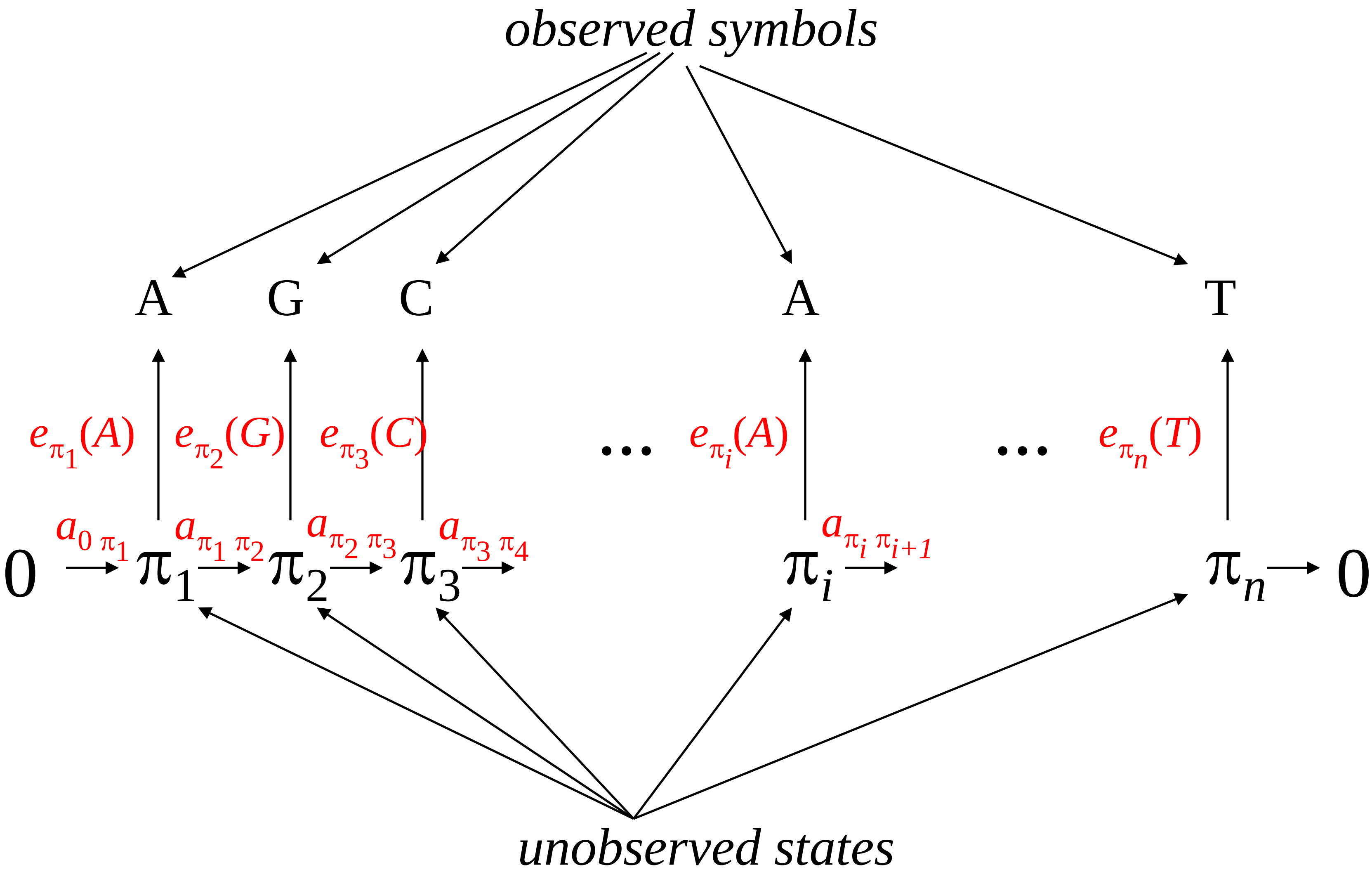
    a_{kl} ^ = (# times state k followed by state l) / (# times state k occurs)

  - in denominator above, *omit occurrence at last position of sequence* (for transition probabilities)
    - But include it for emission probs
  - can include pseudocounts, to incorporate prior expectations/avoid small sample overfitting (Bayesian justification)

Parameter estimation when state sequence *unknown*

- *Viterbi training*
  1. choose starting parameter values
  2. find highest weight paths (Viterbi) for each sequence
  3. estimate new emission and transition probs as above, *assuming* Viterbi state sequence is true
  4. iterate steps 2 and 3 until convergence
     - not guaranteed to occur – but nearly always does
  5. does *not* necessarily give ML estimates, but often are reasonably good

Hidden Markov Model



More algorithms

- Can also use dynamic programming to find
  - sum of all product path weights
    - = "forward algorithm" for probability of observed sequence
  - sum of all product path weights through particular node or particular edge
    - = "forward/backward algorithm" to find posterior probabilities
- Now must use product weights and non-log-transformed probabilities
  - because need to *add* probabilities

- In each case, compute successively for each node (by increasing depth: left to right)
  - the sum of the weights of all paths ending at that node
  - N.B. paths are constrained to begin at the begin node!
- In forward/backward algorithm,
  - work through all nodes a second time, in opposite direction
    - i.e. in reverse graph – constraining paths to start in rightmost column of nodes

WDAG for 3-state HMM, length *n* sequence

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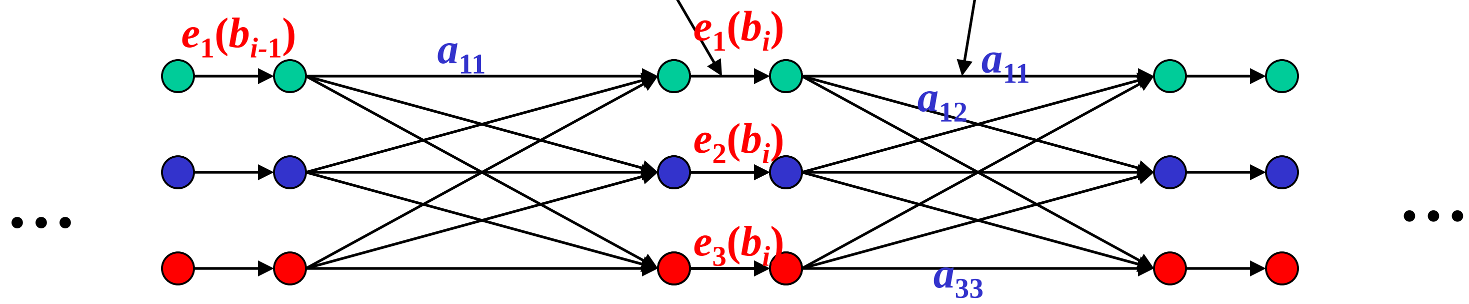


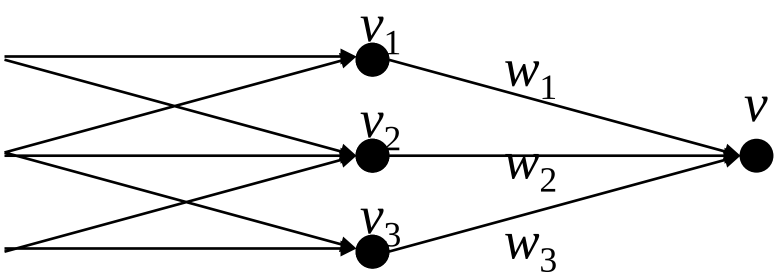
b_{i-1} position i-1

b_i position i

b_{i+1} position i+1

For each vertex v, let $f(v) = \sum_{\text{paths } p \text{ ending at } v} \text{weight}(p)$, where weight($p$) = *product* of edge weights in p. Only consider paths starting at 'begin' node.

Compute $f(v)$ by dynam. prog: $f(v) = \sum_i w_i\, f(v_i)$, where
v_i ranges over the parents of v, and
w_i = weight of the edge from v_i to v.



Similarly for $b(v) = \sum_{p \text{ beginning at } v} \text{weight}(p)$

The paths *beginning* at v are the ones *ending* at v in the *reverse (or inverted) graph*