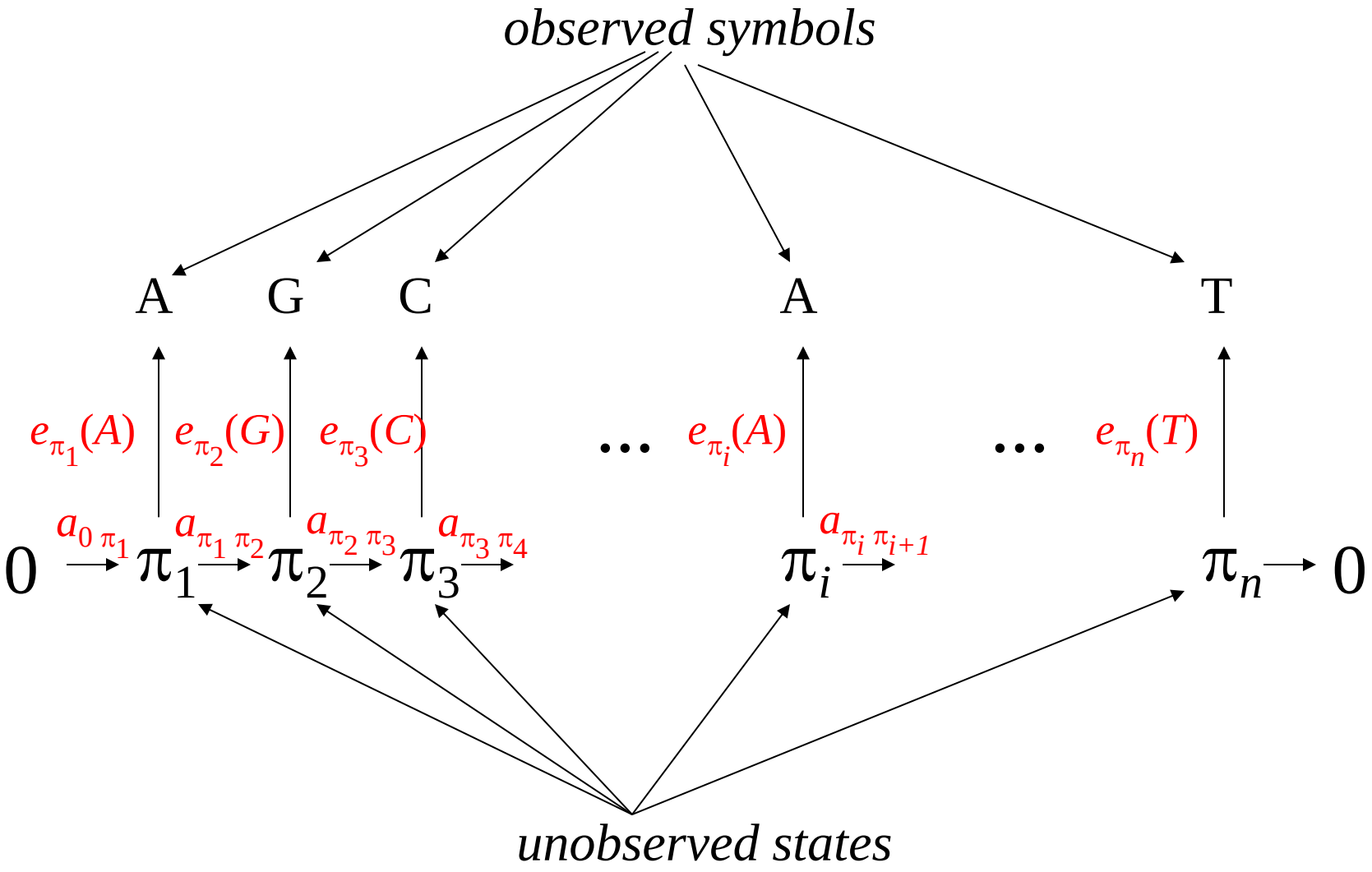
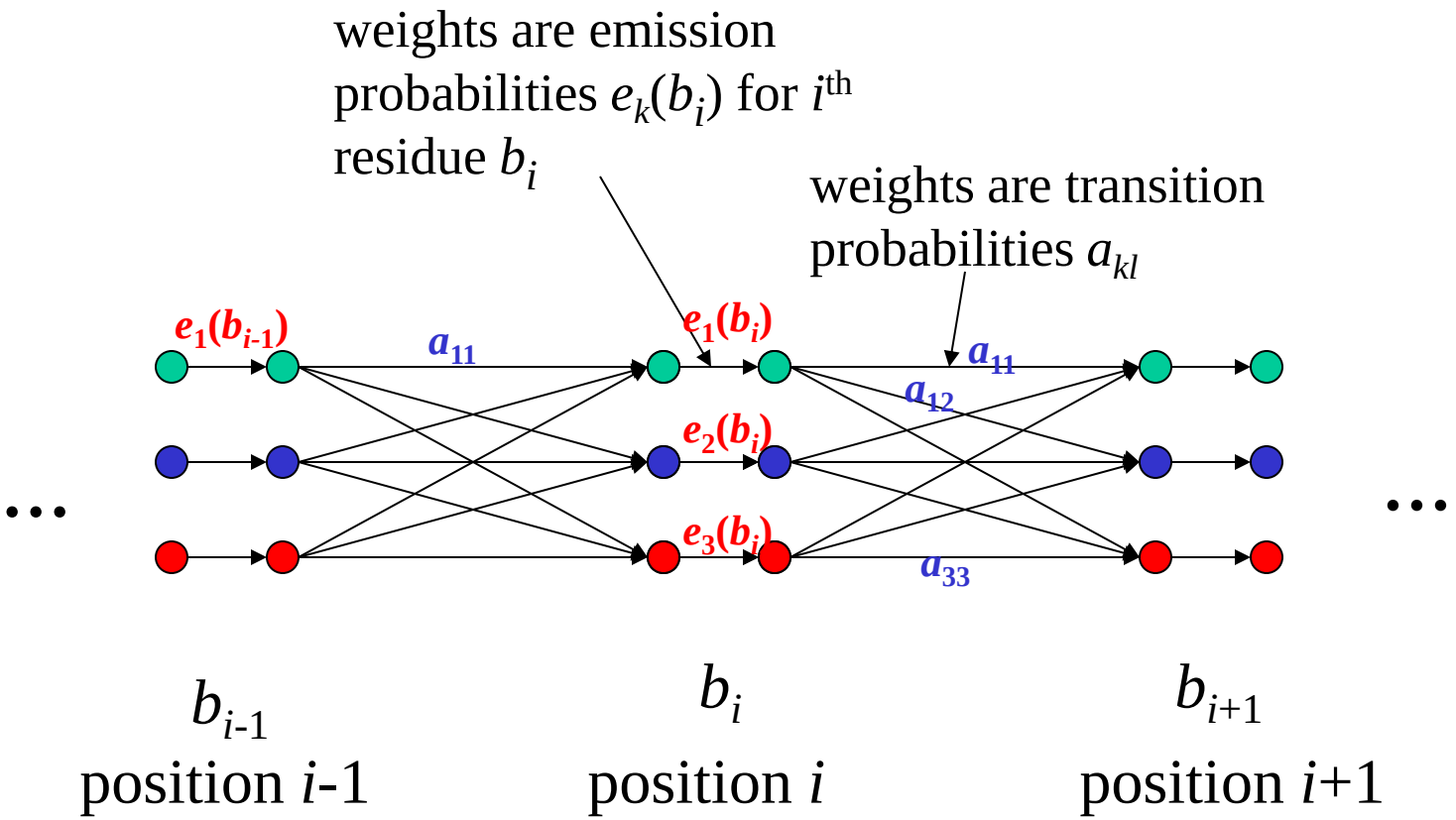
Today's Lecture

- Parameter estimation
  - Viterbi training
- Forward & forward/backward algorithms

Hidden Markov Model



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



- ***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

Complexity

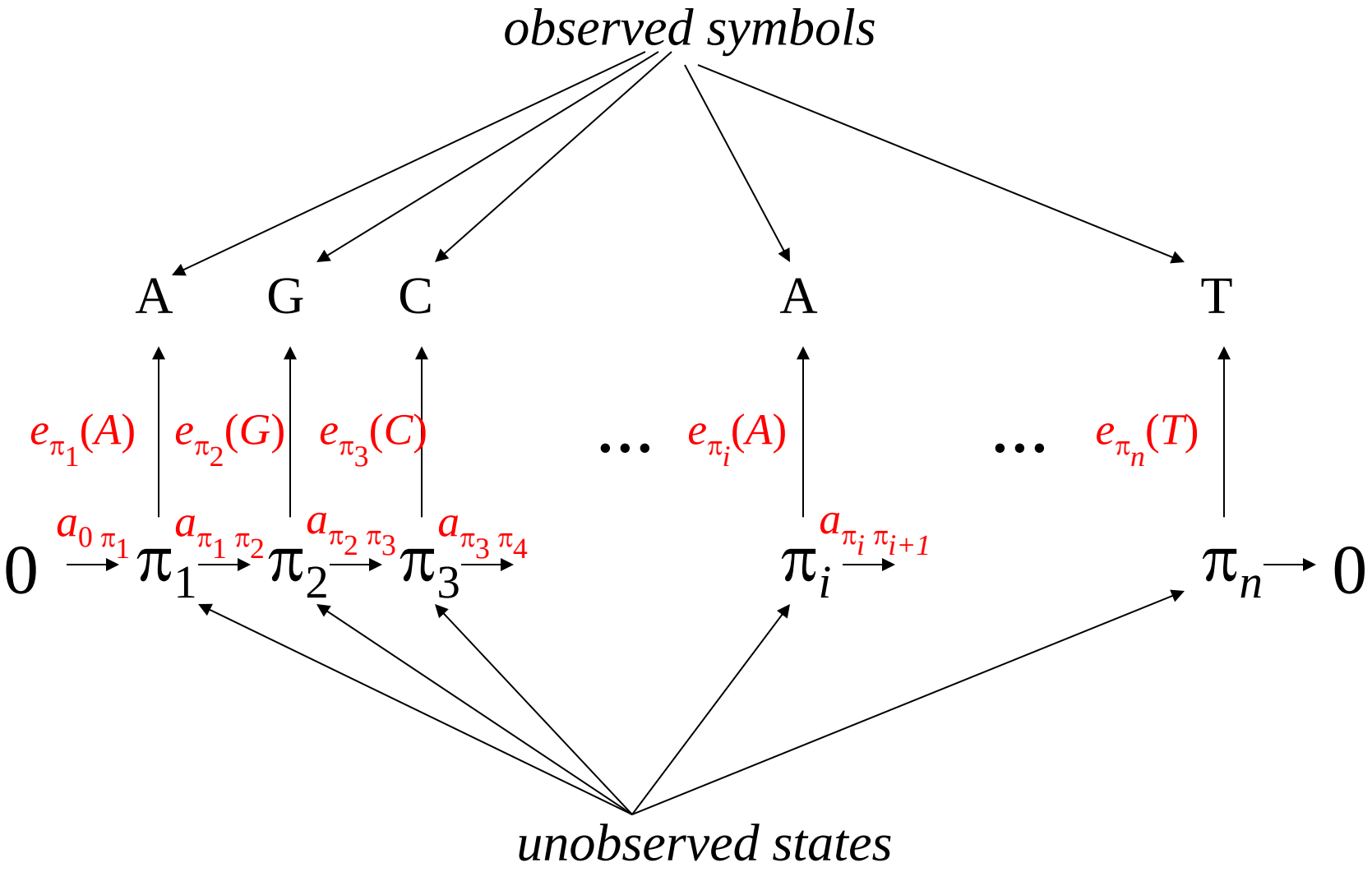
- = $O(|V|+|E|)$, i.e. total # nodes and edges.
- # nodes = $2ns + 2$
  - where n = sequence length,
  - s = # states.
- # edges = $(n-1)s^2 + ns + 2s$

- 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:

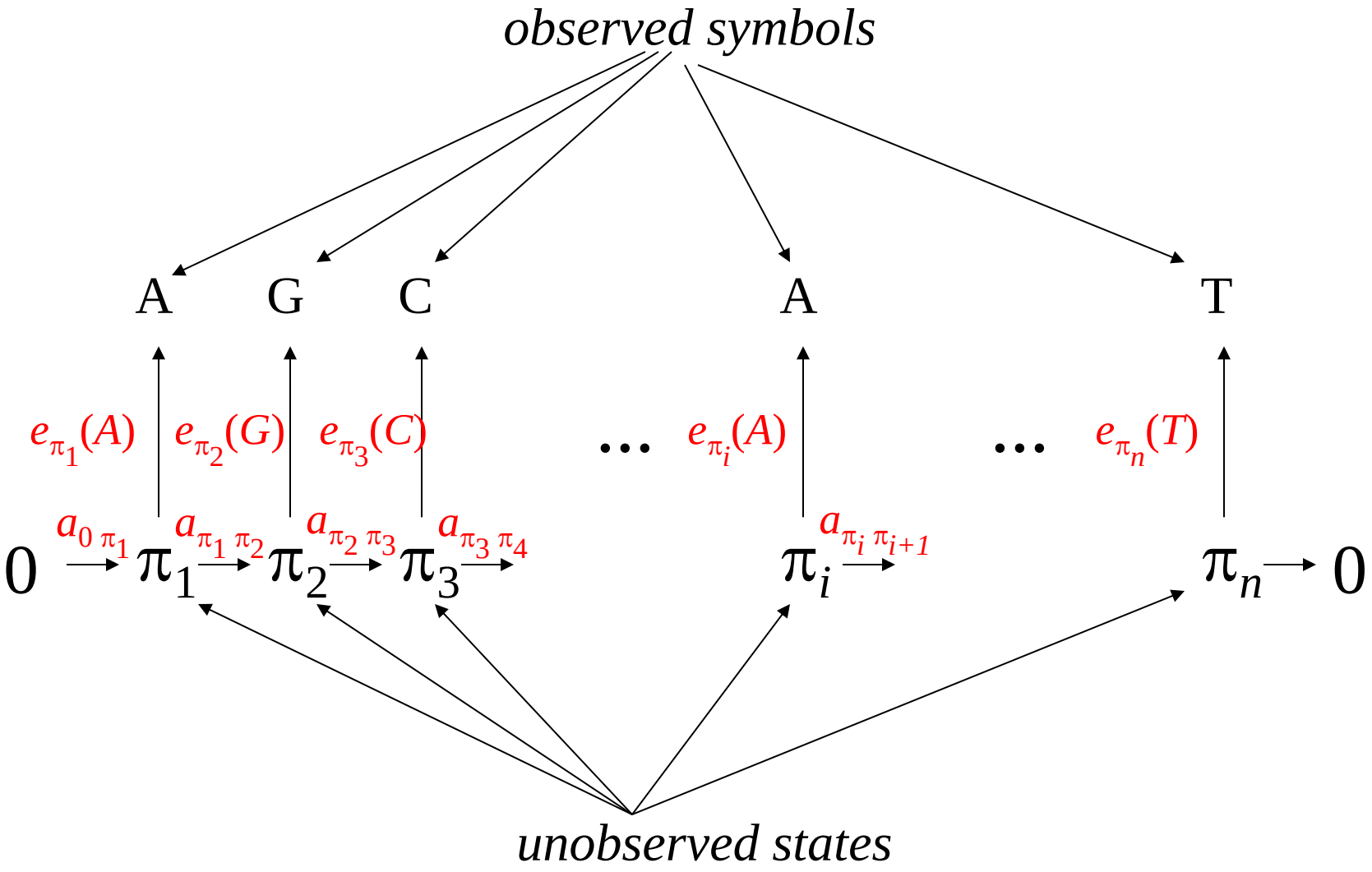
    a_{kl} ^ = (# times state k followed by state l) / (# times state k occurs)
  - in denominator above, *omit occurrence at last position of sequence* (for transition probabilities)
    - But include it for emission probs
  - can include pseudocounts, to incorporate prior expectations/avoid small sample 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

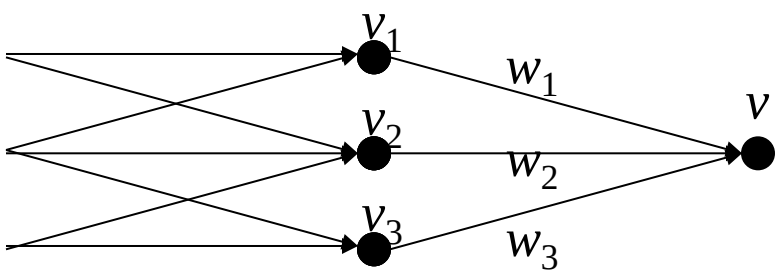
    = "forward algorithm" for probability of observed sequence
  - sum of all product path weights through particular node or particular edge

    = "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

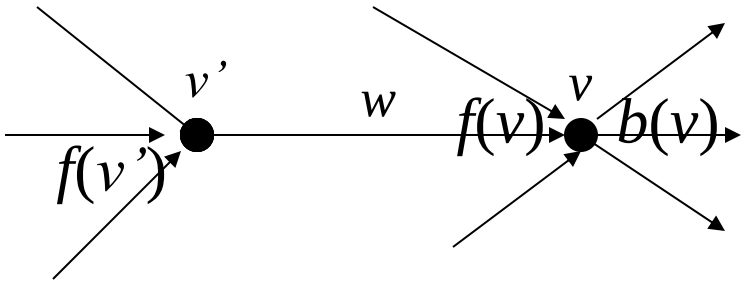
For each vertex v, let $f(v) = \sum_{\text{paths } p \text{ ending at } v} \text{weight}(p)$, where weight($p$) = *product* of edge weights in p. Only consider paths starting at 'begin' node.

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*



$f(v)b(v)$ = sum of the path weights of all paths *through v*.

$f(v')wb(v)$ = sum of the path weights of all paths *through the edge (v',v)*

- Numerical issues: multiplying many small values can cause underflow. Remedies:
  - *Scale* weights to be close to 1 (affects all paths by same constant factor – which can be multiplied back later); or
  - (where possible) use log weights, so can add instead of multiplying.
  - see Rabiner & Tobias Mann links on web page
    - & will discuss further in discussion section