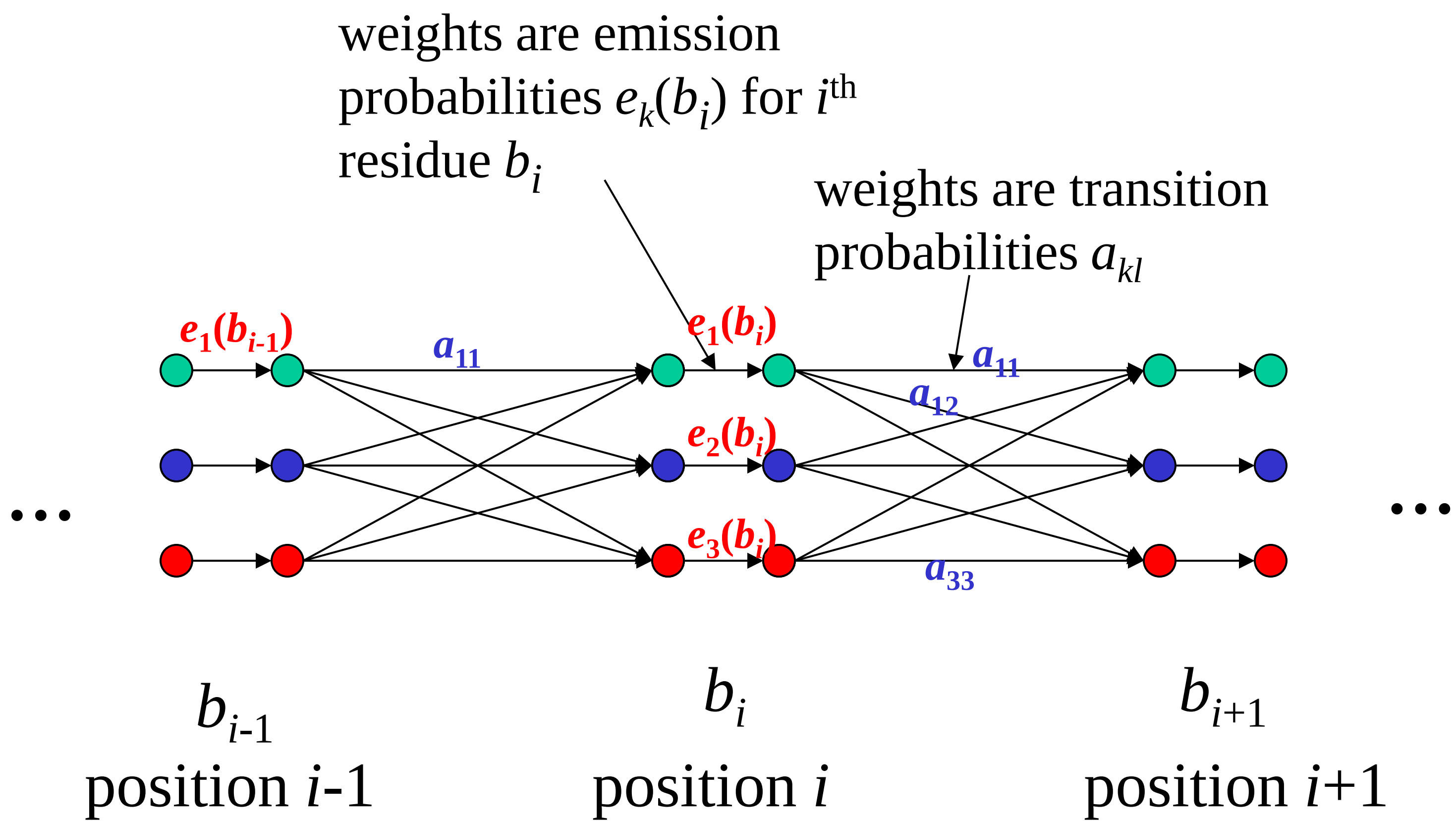
Today's Lecture

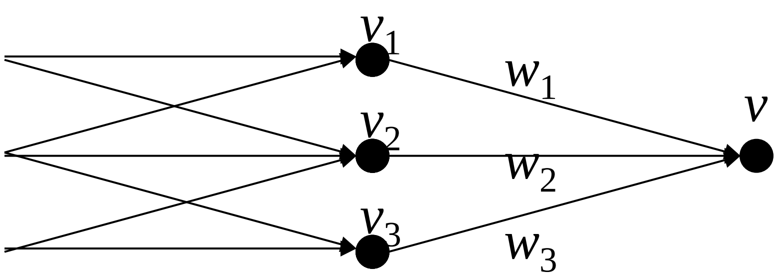
- Forward/Backward algorithm
- Baum-Welch training

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



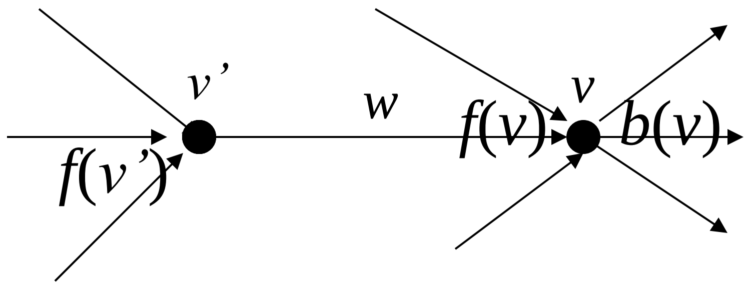
For each vertex v, let $f(v) = \sum_{\text{paths } p \text{ ending at } v} \text{weight}(p)$, where weight($p$) = *product* of edge weights in p. Only consider paths starting at ‘begin’ node.

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

Forward/backward algorithm

- Work through graph in forward direction:
  - compute and store $f(v)$
- Then work through graph in backward direction:
  - compute $b(v)$
  - compute $f(v)\ b(v)$ and $f(v)wb(v)$ as above, store in appropriate cumulative sums
  - only need to store $b(v)$ until have computed b's at next position
- Posterior probability of being in state s at position i is $f(v)\ b(v)$ / *total sequence prob*
  - where v is the corresponding graph node

Baum-Welch training

- Special case of EM (‘expectation-maximization’) algorithm
- like Viterbi training, but
  - uses *all* paths, each weighted by its probability

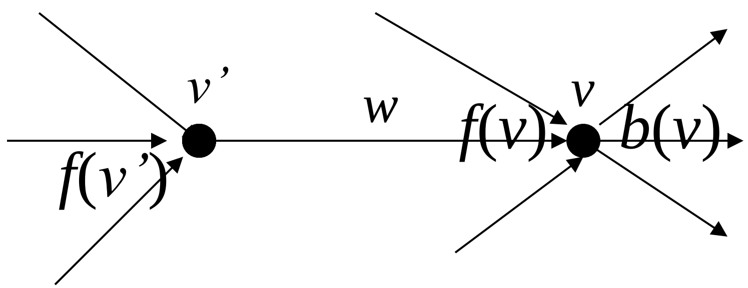
    rather than just highest probability path.
- sometimes give significantly better results than Viterbi
  - e.g. for PFAM

Implementing Baum-Welch

- An edge in the WDAG contributes *fractional* (or *weighted*) *counts* given by its posterior probability:

- (*): $\left(\sum_{\text{all paths } p \text{ through edge } e} \text{weight}(p)\right) / \left(\sum_{\text{all paths } p} \text{weight}(p)\right)$

(Fractional counts are computed using forward-backward algorithm)



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– Compute new param estimates

- $e_k(b)$^ = (frac. # times symbol *b* emitted by state *k*) / (frac. # times state *k* occurs)
- a_{kl} ^ = (frac. # times state *k* followed by state *l*) / (frac. # times state *k* occurs)
  - (In denom,, omit frac counts at last position of sequence)

where "frac. # times" is given by (*) for appropriate edge type (emission or transition)

– New Baum-Welch parameter estimates have higher likelihood
    - general property of EM algorithm
    - not true in general for Viterbi training

– Iterate: get series of estimates converging to a *local* maximum on likelihood surface

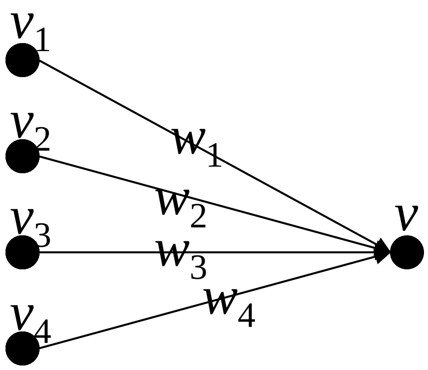
Search of parameter space

- ML estimates correspond by definition to *global* maximum;
- but there may be many *local* maxima, and EM or Viterbi search can get “trapped” in one
- remedies:
  - Consider multiple starts (multiple choices for starting parameters)
  - use “reasonable values” to start search (e.g. unlikely transitions should be given small initial probabilities)

- Allow search to “jump” out of local maxima:
  - Add “noise” to counts at each iteration; gradually reduce the amount of noise
  - Use Viterbi-like training, but
    - sample paths probabilistically
      - (in retracing Viterbi path, choose edge at random according to its prob, rather than taking highest prob parent);
    - use “temperature” T to adjust probabilities;
      - initially with large T making all probs approximately equal;
      - then gradually reduce T
    - similar to Gibbs sampler

Probabilistic Viterbi Backtracking

reset all weights w to $w^{1/T}$. For large T (>> 1), this makes distinct w's relatively close; for small T (<< 1), relatively far apart



choose parent v_i with probability $w_i\, f(v_i) \,/\, f(v)$. For large T, all parents almost equally likely to be chosen; for small T, strongly favor largest (max) $w_i\, f(v_i)$

given choice of paths, re-estimate weights; iterate