The forward-backward algorithm

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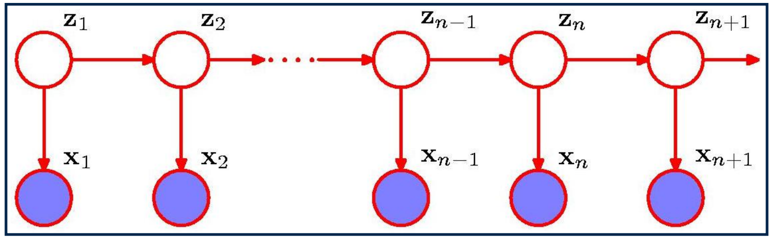
HMM Topics

1. What is an HMM?
2. State-space Representation
3. HMM Parameters
4. Generative View of HMM
5. Determining HMM Parameters Using EM
6. Forward-Backward or α–β algorithm
7. HMM Implementation Issues:
    a) Length of Sequence
    b) Predictive Distribution
    c) Sum-Product Algorithm
    d) Scaling Factors
    e) Viterbi Algorithm

Forward-Backward Algorithm

- E step: efficient procedure to evaluate $\gamma(z_n)$ and $\xi(z_{n\text{-}1}, z_n)$
- Graph of HMM, a tree→



  - Implies that posterior distribution of latent variables can be obtained efficiently using message passing algorithm
- In HMM it is called *forward-backward* algorithm or *Baum-Welch Algorithm*
- Several variants lead to exact marginals
  - Method called *alpha-beta* discussed here

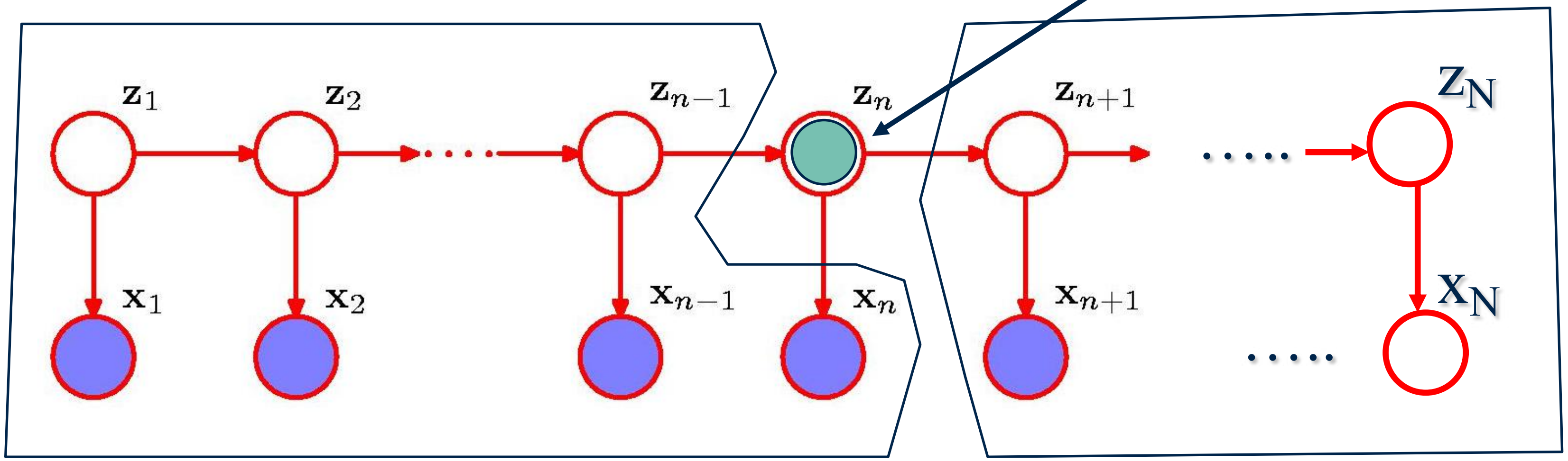
Derivation of Forward-Backward

- Several conditional-independences (A-H) hold

A. $$\boxed{p(\mathrm{X}|\mathrm{z}_n) = p(\mathrm{x}_1,..\mathrm{x}_n|\mathrm{z}_n)\ p(\mathrm{x}_{n+1},..\mathrm{x}_N|\mathrm{z}_n)}$$

- Proved using d-separation:

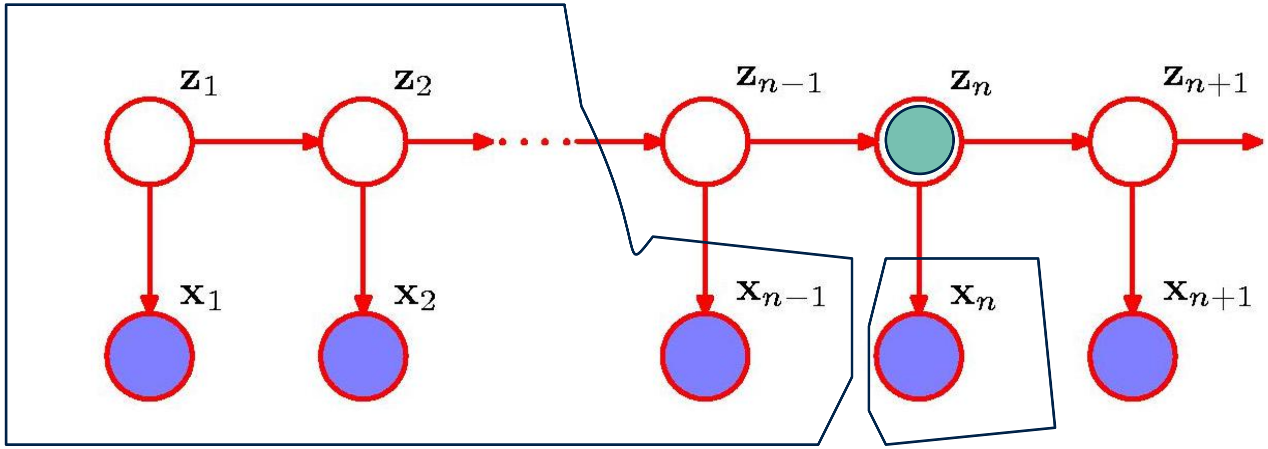
Path from x_1 to x_{n-1} passes through z_n which is observed.
Path is head-to-tail. Thus $(\mathrm{x}_1,..\mathrm{x}_{n-1}) \perp\!\!\!\perp \mathrm{x}_n \mid \mathrm{z}_n$
Similarly $(\mathrm{x}_1,..\mathrm{x}_{n-1},\mathrm{x}_n) \perp\!\!\!\perp \mathrm{x}_{n+1},..x_N \mid \mathrm{z}_n$



Conditional independence B

- Since $(x_1,..x_{n-1}) \perp\!\!\!\perp x_n \mid z_n$ we have

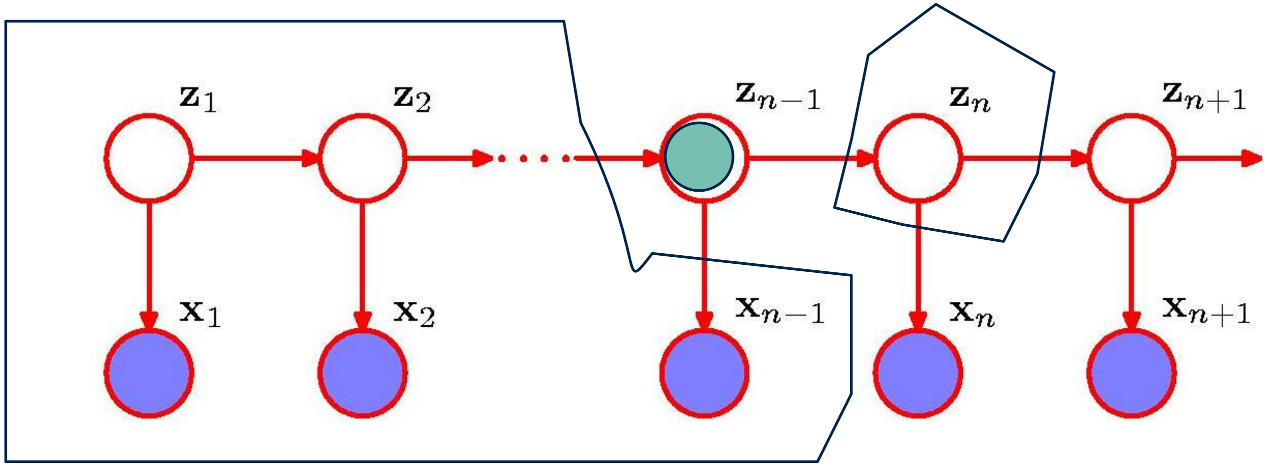
B. $\boxed{p(x_1,..x_{n-1}|x_n,z_n) = p(x_1,..x_{n-1}|z_n)}$



Conditional independence C

- Since $(x_1,..x_{n-1}) \perp\!\!\!\perp z_n \mid z_{n-1}$

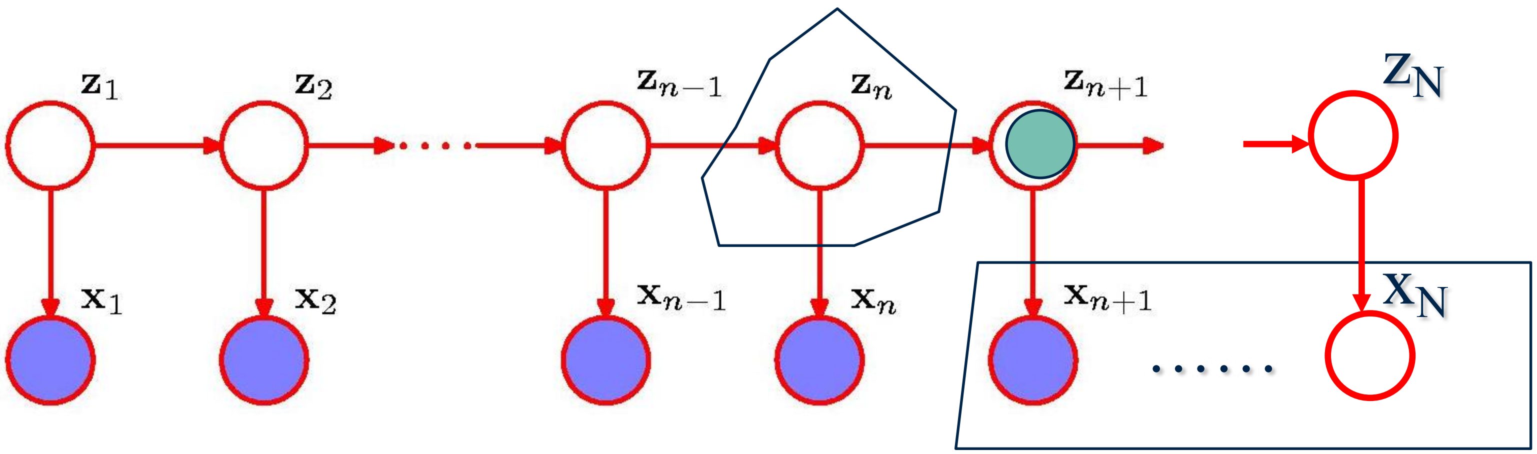
C. $\boxed{p(x_1,..x_{n-1}|z_{n-1},z_n) = p\,(\,x_1,..x_{n-1}|z_{n-1}\,)}$



Conditional independence D

- Since $$(x_{n+1},..x_N) \perp\!\!\!\perp z_n \mid z_{n+1}$$

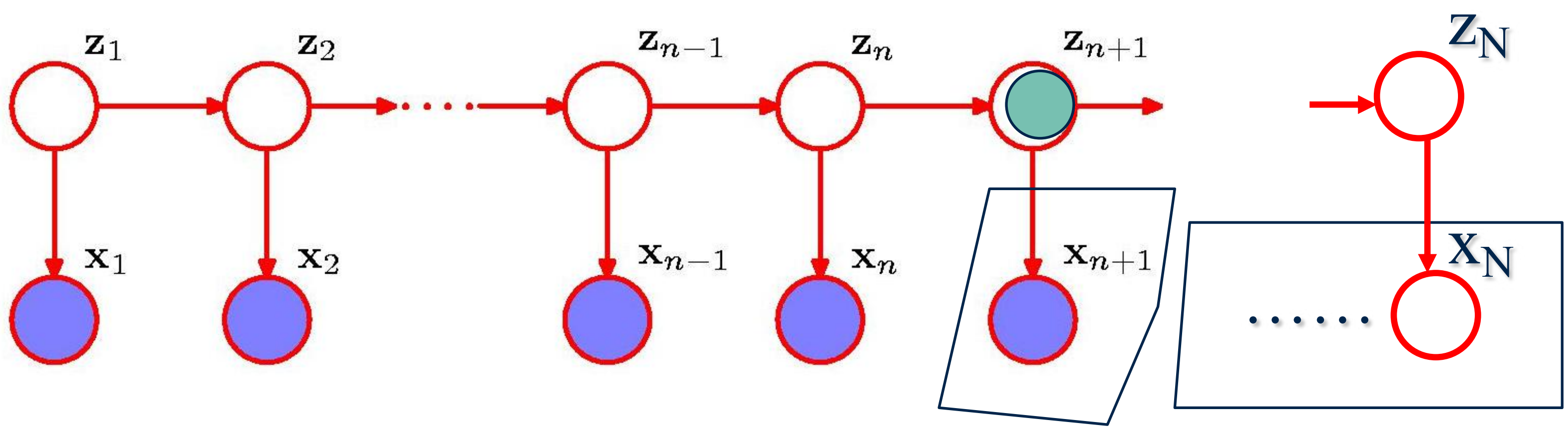
D. $p(x_{n+1},..x_N|z_n,z_{n+1}) = p\,(\,x_1,..x_N|z_{n+1}\,)$



Conditional independence E

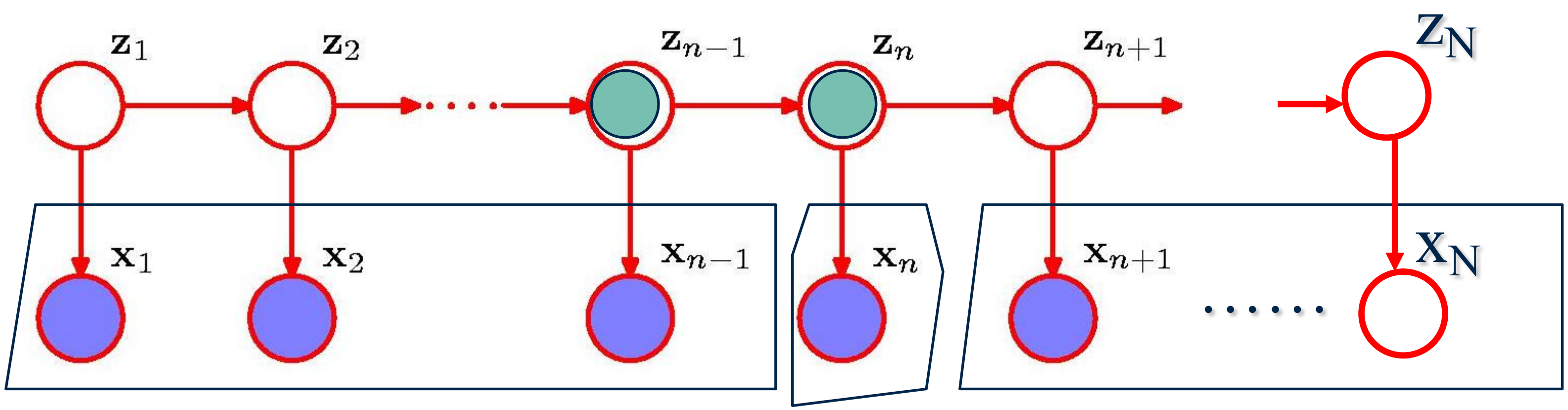
- Since $(\mathbf{x}_{n+2},..\mathbf{x}_N) \perp\!\!\!\perp \mathbf{z}_n \mid \mathbf{z}_{n+1}$

E. $p(\mathbf{x}_{n+2},..\mathbf{x}_N|\mathbf{z}_{n+1},\mathbf{x}_{n+1}) = p\,(\,\mathbf{x}_{n+2},..\mathbf{x}_N|\mathbf{z}_{n+1}\,)$



Conditional independence F

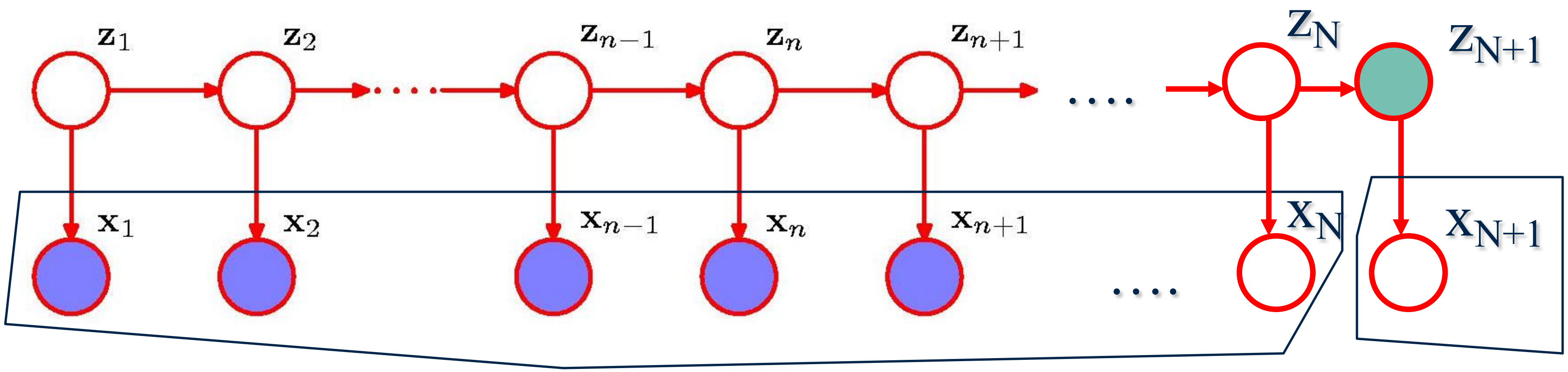
F. $p(X|z_{n-1},z_n) = p(x_1,..x_{n-1}|z_{n-1})p(x_n|z_n)$
$p(x_{n+1},..x_N|z_n)$



Conditional independence G

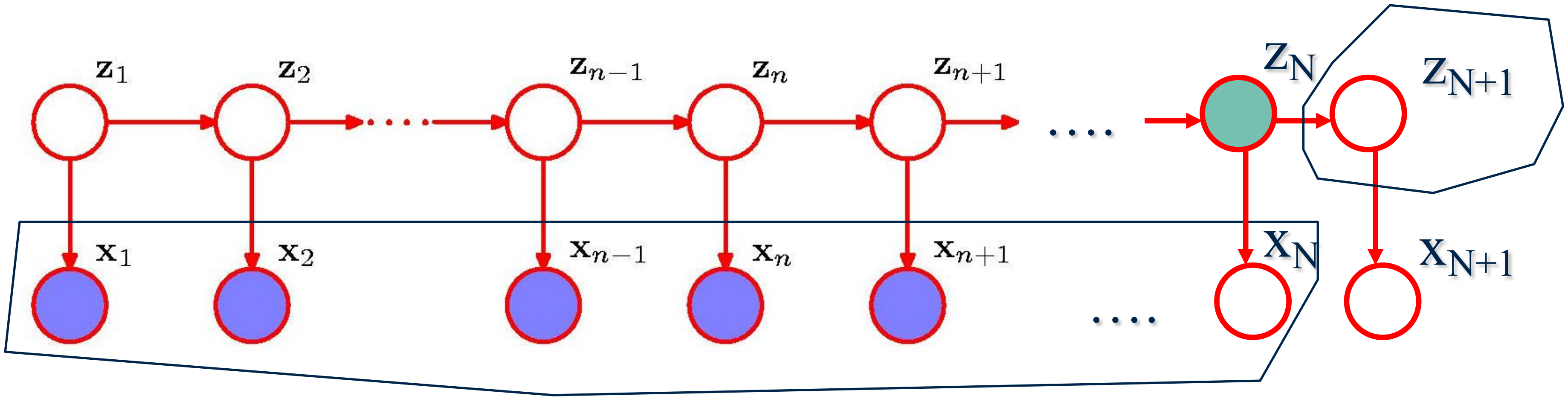
Since $(x_1,..x_N) \perp\!\!\!\perp x_{N+1} \mid z_{N+1}$

G. $\boxed{p(x_{N+1}|X,z_{N+1}) = p(x_{N+1}|z_{N+1})}$



Conditional independence H

H. $$\boxed{p(z_{N+1} | z_N , X) = p(z_{N+1} | z_N)}$$



Evaluation of $\gamma(z_n)$

- Recall that this is to efficiently compute the E step of estimating parameters of HMM

  $\gamma(z_n) = p(z_n|X,\theta^{old})$: Marginal posterior distribution of latent variable z_n

- We are interested in finding posterior distribution $p(z_n|x_1,..x_N)$
- This is a vector of length K whose entries correspond to expected values of z_{nk}

Introducing alpha and beta

- Using Bayes theorem $\gamma(\mathrm{z}_n) = p(z_n \mid \mathrm{X}) = \dfrac{p(\mathrm{X} \mid z_n)p(z_n)}{p(\mathrm{X})}$
- Using conditional independence A

$$\gamma(\mathrm{z}_n) = \frac{p(\mathrm{x}_1,..\mathrm{x}_n \mid \mathrm{z}_n)p(\mathrm{x}_{n+1},..\mathrm{x}_N \mid \mathrm{z}_n)p(\mathrm{z}_n)}{p(\mathrm{X})}$$

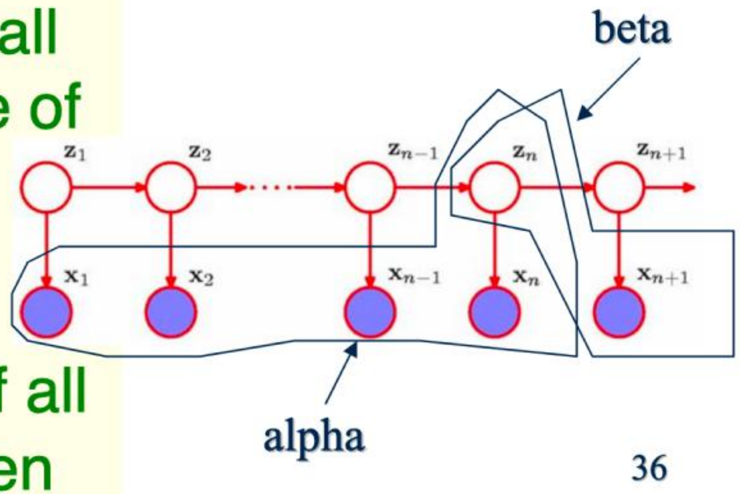
$$= \frac{p(\mathrm{x}_1,..\mathrm{x}_n, \mathrm{z}_n)p(\mathrm{x}_{n+1},..\mathrm{x}_N \mid \mathrm{z}_n)}{p(\mathrm{X})} = \boxed{\frac{\alpha(\mathrm{z}_n)\beta(\mathrm{z}_n)}{p(\mathrm{X})}}$$

- where $\boxed{\alpha(\mathrm{z}_n) \equiv p(\mathrm{x}_1,..,\mathrm{x}_n,\mathrm{z}_n)}$

  which is the probability of observing all given data up to time n and the value of z_n

$$\boxed{\beta(\mathrm{z}_n) \equiv p(\mathrm{x}_{n+1},..,\mathrm{x}_N \mid \mathrm{z}_n)}$$

  which is the conditional probability of all future data from time $n+1$ up to N given the value of z_n



Recursion relation for alpha

$$
\begin{aligned}
\alpha(\mathrm{z}_n) &= p(\mathrm{x}_1,..,\mathrm{x}_n,\mathrm{z}_n) \\
&= \underline{p(\mathrm{x}_1,..,\mathrm{x}_n \mid \mathrm{z}_n)}p(\mathrm{z}_n) \text{ by Bayes rule} \\
&= \underline{p(\mathrm{x}_n \mid \mathrm{z}_n)p(\mathrm{x}_1,..,\mathrm{x}_{n-1} \mid \mathrm{z}_n)}p(\mathrm{z}_n) \text{ by conditional independence B} \\
&= p(\mathrm{x}_n \mid \mathrm{z}_n)p(\mathrm{x}_1,..,\mathrm{x}_{n-1},\mathrm{z}_n) \text{ by Bayes rule} \\
&= p(\mathrm{x}_n \mid \mathrm{z}_n)\sum_{\mathrm{z}_{n-1}} p(\mathrm{x}_1,..,\mathrm{x}_{n-1},\mathrm{z}_{n-1},\mathrm{z}_n) \text{ by Sum Rule} \\
&= p(\mathrm{x}_n \mid \mathrm{z}_n)\sum_{\mathrm{z}_{n-1}} p(\mathrm{x}_1,..,\mathrm{x}_{n-1},\mathrm{z}_n \mid \mathrm{z}_{n-1})p(\mathrm{z}_{n-1}) \text{ by Bayes rule} \\
&= p(\mathrm{x}_n \mid \mathrm{z}_n)\sum_{\mathrm{z}_{n-1}} p(\mathrm{x}_1,..,\mathrm{x}_{n-1} \mid \mathrm{z}_{n-1})p(\mathrm{z}_n \mid \mathrm{z}_{n-1})p(\mathrm{z}_{n-1}) \text{ by cond. ind. C} \\
&= p(\mathrm{x}_n \mid \mathrm{z}_n)\sum_{\mathrm{z}_{n-1}} p(\mathrm{x}_1,..,\mathrm{x}_{n-1},\mathrm{z}_{n-1})p(\mathrm{z}_n \mid \mathrm{z}_{n-1}) \text{ by Bayes rule} \\
&= p(\mathrm{x}_n \mid \mathrm{z}_n)\sum_{\mathrm{z}_{n-1}} \alpha(\mathrm{z}_{n-1})p(\mathrm{z}_n \mid \mathrm{z}_{n-1}) \text{ by definition of } \alpha
\end{aligned}
$$

Forward recursion for alpha evaluation

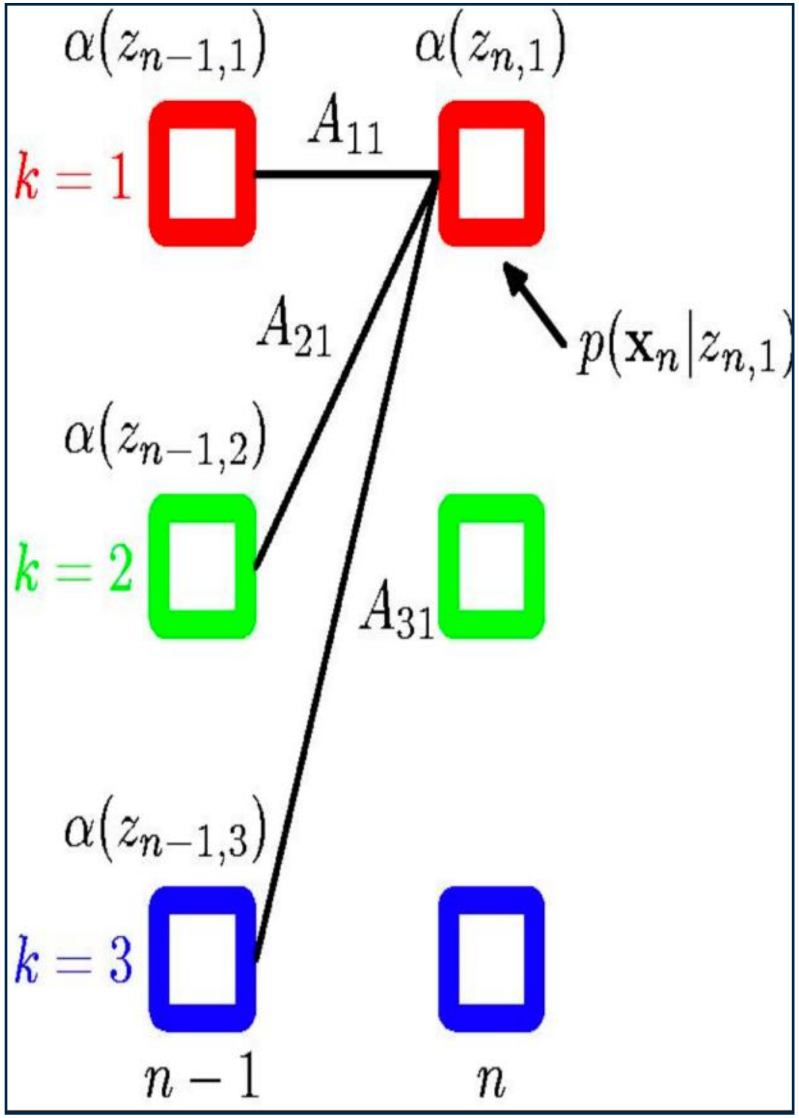
- Recursion Relation is

$$\alpha(\mathbf{z}_n) = p(\mathbf{x}_n \mid \mathbf{z}_n) \sum_{z_{n-1}} \alpha(\mathbf{z}_{n-1}) p(\mathbf{z}_n \mid \mathbf{z}_{n-1})$$

- There are K terms in the summation
  - Has to be evaluated for each of K values of z_n
  - Each step of recursion is $O(K^2)$
- Initial condition is

$$\alpha(\mathbf{z}_1) = p(\mathbf{x}_1, \mathbf{z}_1) = p(\mathbf{z}_1) p(\mathbf{x}_1 \mid \mathbf{z}_1) = \prod_{k=1}^{K} \{\pi_k p(\mathbf{x}_1 \mid \phi_k)\}^{z_{1k}}$$

- Overall cost for the chain in $O(K^2N)$



Recursion relation for beta

$$\beta(\mathrm{z}_n) = p(\mathrm{x}_{n+1},..,\mathrm{x}_N \mid \mathrm{z}_n)$$

$$= \sum_{z_{n+1}} p(\mathrm{x}_{n+1},..,\mathrm{x}_N, \mathrm{z}_{n+1} \mid \mathrm{z}_n) \text{ by Sum Rule}$$

$$= \sum_{z_{n+1}} p(\mathrm{x}_{n+1},..,\mathrm{x}_N \mid \mathrm{z}_n, \mathrm{z}_{n+1}) p(\mathrm{z}_{n+1}|\mathrm{z}_n) \text{ by Bayes rule}$$

$$= \sum_{z_{n+1}} p(\mathrm{x}_{n+1},..,\mathrm{x}_N \mid \mathrm{z}_{n+1}) p(\mathrm{z}_{n+1}|\mathrm{z}_n) \text{ by Cond ind. D}$$

$$= \sum_{z_{n+1}} p(\mathrm{x}_{n+2},..,\mathrm{x}_N \mid \mathrm{z}_{n+1}) p(\mathrm{x}_{n+1}|\mathrm{z}_{n+1}) p(\mathrm{z}_{n+1}|\mathrm{z}_n) \text{ by Cond. ind E}$$

$$= \sum_{z_{n+1}} \beta(\mathrm{z}_{n+1}) p(\mathrm{x}_{n+1}|\mathrm{z}_{n+1}) p(\mathrm{z}_{n+1}|\mathrm{z}_n) \text{ by definition of } \beta$$

Backward recursion for beta

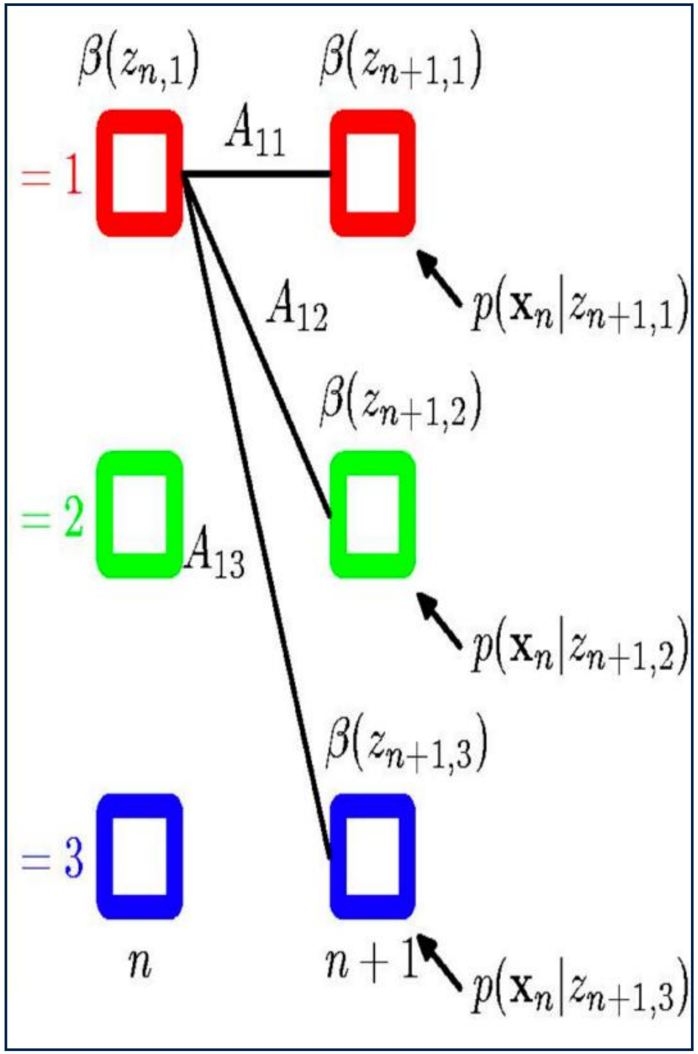
- Backward message passing

$$\beta(\mathbf{z}_n) = \sum_{z_{n+1}} \beta(\mathbf{z}_{n+1}) p(\mathbf{x}_{n+1}|\mathbf{z}_n) p(\mathbf{z}_{n+1}|\mathbf{z}_n)$$

- Evaluates $\beta(\mathbf{z}_n)$ in terms of $\beta(\mathbf{z}_{n+1})$
- Starting condition for recursion is

$$p(\mathbf{z}_N \mid \mathbf{X}) = \frac{p(\mathbf{X}, \mathbf{z}_N)\beta(\mathbf{z}_N)}{p(\mathbf{X})}$$

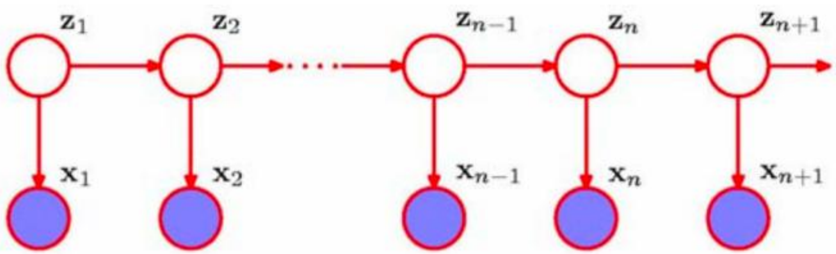
- Is correct provided we set $\beta(\mathbf{z}_N) = 1$ for all settings of $\mathbf{z}_N$
  - This is the initial condition for backward computation



M-step Equations

- In the M-step equations $p(\mathbf{x})$ will cancel out

$$\boxed{\mu_k = \frac{\sum_{n=1}^{N} \gamma(z_{nk})\mathbf{x}_n}{\sum_{n=1}^{N} \gamma(z_{nk})}}$$



$$p(\mathrm{X}) = \sum_{z_n} \alpha(z_n)\beta(z_n)$$

Evaluation of Quantities $\xi(z_{n-1},z_n)$

- They correspond to the values of the conditional probabilities $p(z_{n-1},z_n|X)$ for each of the K x K settings for (z_{n-1},z_n)

$$\xi(z_{n-1},z_n) = p(z_{n-1},z_n \mid X) \text{ by definition}$$

$$= \frac{p(X|z_{n-1},z_n)p(z_{n-1},z_n)}{p(X)} \text{ by Bayes Rule}$$

$$= \frac{p(x_1,..x_{n-1}|z_{n-1})p(x_n \mid z_n)p(x_{n+1},..,x_N \mid z_n)p(z_n \mid z_{n-1})p(z_{n-1})}{p(X)} \text{ by cond ind F}$$

$$= \frac{\alpha(z_{n-1})p(x_n \mid z_n)p(z_n \mid z_{n-1})\beta(z_n)}{p(X)}$$

- Thus we calculate $\xi(z_{n-1},z_n)$ directly by using results of the α and β recursions

Summary of EM to train HMM

Step 1: Initialization

- Make an initial selection of parameters θ^{old} where $\theta = (\pi, A, \phi)$
  1. π is a vector of K probabilities of the states for latent variable z_1
  2. A is a K x K matrix of transition probabilities A_{ij}
  3. ϕ are parameters of conditional distribution $p(x_k|z_k)$
- A and π parameters are often initialized uniformly
- Initialization of ϕ depends on form of distribution
  - For Gaussian:
    - parameters μ_k initialized by applying K-means to the data, Σ_k corresponds to covariance matrix of cluster

Summary of EM to train HMM

Step 2: E Step

- Run both forward α recursion and backward β recursion
- Use results to evaluate $\gamma(z_n)$ and $\xi(z_{n-1},z_n)$ and the likelihood function

Step 3: M Step

- Use results of E step to find revised set of parameters θ^{new} using M-step equations

Alternate between E and M

until convergence of likelihood function

Values for $p(\mathrm{x}_n|\mathrm{z}_n)$

- In recursion relations, observations enter through conditional distributions $p(\mathrm{x_n}|\mathrm{z_n})$
- Recursions are independent of
  - Dimensionality of observed variables
  - Form of conditional distribution
    - So long as it can be computed for each of K possible states of z_n
- Since observed variables $\{\mathrm{x}_n\}$ are fixed they can be pre-computed at the start of the EM algorithm

Length of Sequence

- HMM can be trained effectively if length of sequence is sufficiently long
  - True of all maximum likelihood approaches
- Alternatively we can use multiple short sequences
  - Requires straightforward modification of HMM-EM algorithm
- Particularly important in left-to-right models
  - In given observation sequence, a given state transition for a non-diagonal element of A occurs only once

Predictive Distribution

- Observed data is $X=\{x_1,..,x_N\}$
- Wish to predict x_{N+1}
- Application in financial forecasting

$$p(\mathbf{x}_{N+1}\mid X)=\sum_{z_{N+1}} p(\mathbf{x}_{N+1},\mathbf{z}_{N+1}\mid X)$$

$$=\sum_{z_{N+1}} p(\mathbf{x}_{N+1}|\mathbf{z}_{N+1}\mid X)p(\mathbf{z}_{N+1}\mid X) \text{ by Product Rule}$$

$$=\sum_{z_{N+1}} p(\mathbf{x}_{N+1}|\mathbf{z}_{N+1})\sum_{z_N} p(\mathbf{z}_{N+1},z_N\mid X) \text{ by Sum Rule}$$

$$=\sum_{z_{N+1}} p(\mathbf{x}_{N+1}|\mathbf{z}_{N+1})\sum_{z_N} p(\mathbf{z}_{N+1}\mid z_N)p(z_N\mid X) \text{ by conditional ind H}$$

$$=\sum_{z_{N+1}} p(\mathbf{x}_{N+1}|\mathbf{z}_{N+1})\sum_{z_N} p(\mathbf{z}_{N+1}\mid z_N)\frac{p(z_N,X)}{p(X)} \text{ by Bayes rule}$$

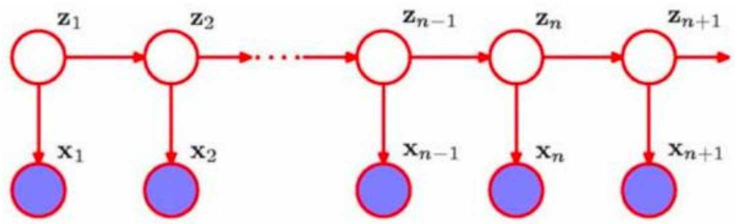
$$=\frac{1}{p(X)}\sum_{z_{N+1}} p(\mathbf{x}_{N+1}|\mathbf{z}_{N+1})\sum_{z_N} p(\mathbf{z}_{N+1}\mid z_N)\alpha(z_N) \text{ by definition of } \alpha$$

- Can be evaluated by first running forward α recursion and summing over z_N and z_{N+1}
- Can be extended to subsequent predictions of x_{N+2}, after x_{N+1} is observed, using a fixed amount of storage

Sum-Product and HMM

- HMM graph is a tree and hence *sum-product* algorithm can be used to find local marginals for hidden variables
  - Equivalent to forward-backward algorithm
  - Sum-product provides a simple way to derive alpha-beta recursion formulae
- Transform directed graph to factor graph
  - Each variable has a node, small squares represent factors, undirected links connect factor nodes to variables used

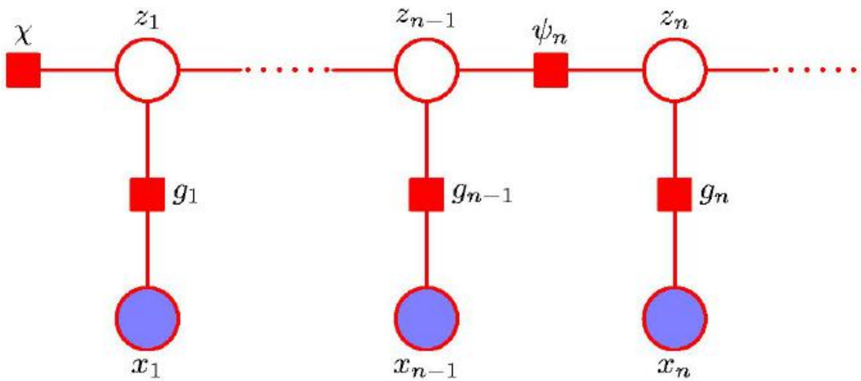
HMM Graph



Joint distribution

$$p(x_1,..x_N,z_1,..z_n)=p(z_1)\left[\prod_{n=2}^{N}p(z_n\mid z_{n-1})\right]\prod_{n=1}^{N}p(x_n\mid z_n)$$

Fragment of Factor Graph



Deriving alpha-beta from Sum-product

- Begin with simplified form of factor graph
- Factors are given by

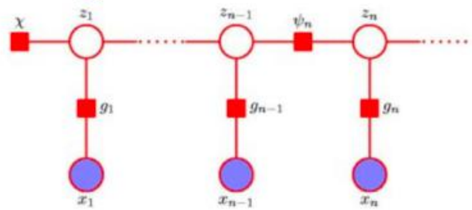
$$h(z_1) = p(z_1)p(x_1 \mid z_1)$$
$$f_n(z_{n-1}, z_n) = p(z_n \mid z_{n-1})p(x_n \mid z_n)$$

- Messages propagated are

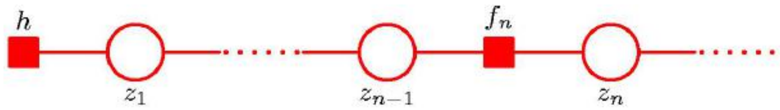
$$\mu_{\mathrm{z}_{n-1}\to f_n}(\mathrm{z}_{n-1}) = \mu_{f_{n-1}\to \mathrm{z}_{n-1}}(\mathrm{z}_{n-1})$$
$$\mu_{f_n\to \mathrm{z}_n}(\mathrm{z}_n) = \sum_{\mathrm{z}_{n-1}} f_n(\mathrm{z}_{n-1}, \mathrm{z}_n)\mu_{\mathrm{z}_{n-1}\to f_n}(\mathrm{z}_{n-1})$$

- Can show that α recursion is computed
- Similarly starting with the root node β recursion is computed
- So also γ and ξ are derived

Fragment of Factor Graph



Simplified by absorbing emission probabilities into transition probability factors



Final Results

$$\alpha(\mathrm{z}_n) = p(\mathrm{x}_n \mid \mathrm{z}_n)\sum_{z_{n-1}} \alpha(\mathrm{z}_{n-1})p(\mathrm{z}_n \mid \mathrm{z}_{n-1})$$

$$\beta(\mathrm{z}_n) = \sum_{z_{n+1}} \beta(z_{n+1})p(\mathrm{x}_{n+1} \mid \mathrm{z}_n)p(z_{n+1} \mid \mathrm{z}_n)$$

$$\gamma(\mathrm{z}_n) = \frac{\alpha(\mathrm{z}_n)\beta(\mathrm{z}_n)}{p(\mathrm{X})}$$

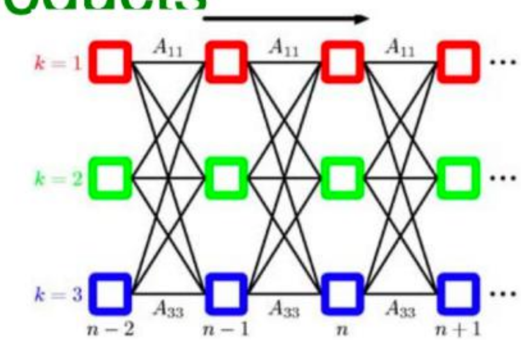
$$\xi(\mathrm{z}_{n-1}, \mathrm{z}_n) = \frac{\alpha(\mathrm{z}_{n-1})p(\mathrm{x}_n \mid \mathrm{z}_n)p(\mathrm{z}_n \mid \mathrm{z}_{n-1})\beta(\mathrm{z}_n)}{p(X)}$$

Scaling Factors

- Implementation issue for small probabilities
- At each step of recursion

$$\alpha(\mathrm{z}_n) = p(\mathrm{x}_n \mid \mathrm{z}_n) \sum_{z_{n-1}} \alpha(\mathrm{z}_{n-1}) p(\mathrm{z}_n \mid \mathrm{z}_{n-1})$$

  - To obtain new value of $\alpha(z_n)$ from previous value $\alpha(z_{n-1})$ we multiply $p(z_n|z_{n-1})$ and $p(x_n|z_n)$
  - These probabilities are small and products will underflow
  - Logs don't help since we have sums of products



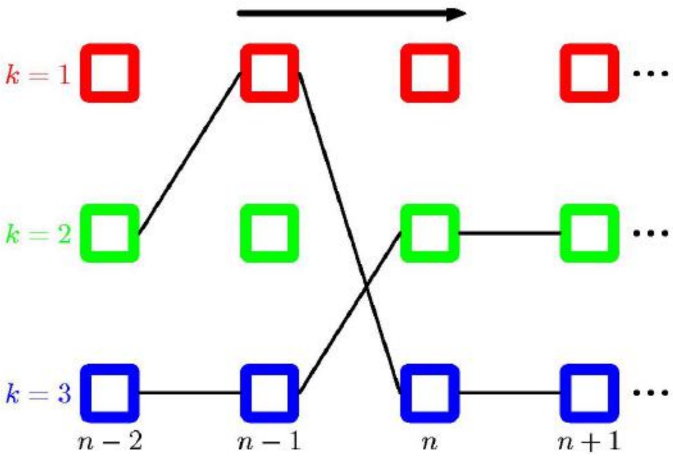
- Solution is rescaling
  - of $\alpha(z_n)$ and $\beta(z_n)$ whose values remain close to unity

The Viterbi Algorithm

- Finding most probable sequence of hidden states for a given sequence of observables
- In speech recognition: finding most probable phoneme sequence for a given series of acoustic observations
- Since graphical model of HMM is a tree, can be solved exactly using *max-sum* algorithm
  - Known as Viterbi algorithm in the context of HMM
  - Since max-sum works with log probabilities no need to work with re-scaled varaibles as with forward-backward

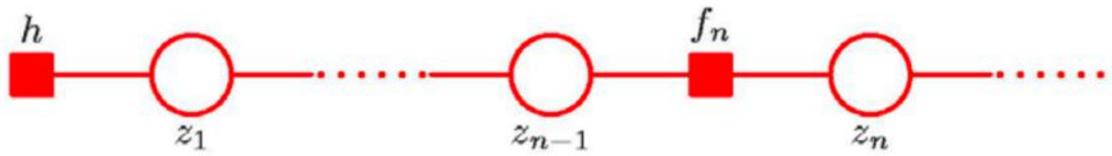
Viterbi Algorithm for HMM

- Fragment of HMM lattice showing two paths
- Number of possible paths grows exponentially with length of chain
- Viterbi searches space of paths efficiently
  - Finds most probable path with computational cost linear with length of chain



Deriving Viterbi from Max Sum

- Start with simplified factor graph



- Treat variable z_N as root node, passing messages to root from leaf nodes
- Messages passed are

$$\mu_{z_n \to f_{n+1}}(z_n) = \mu_{f_n \to z_n}(z_n)$$

$$\mu_{f_{n+1} \to z_{n+1}}(z_{n+1}) = \max_{z_n} \left\{ \ln f_{n+1}(z_n, z_{n+1}) + \mu_{z_n \to f_{n+1}}(z_n) \right\}$$