STA 4273H:
Statistical Machine Learning

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Lecture 11

Project Reminder

- Brief 5-minute presentations of projects will take place on Nov 19. You need to send me 6-7 slides in pdf formtat describing your project.

- **Deadline: Sunday Nov 17, 2012. Submit your slides by e-mail: rsalakhu@utstat.toronto.edu**

- You should have your name, and project title on the first slide.

- You will have 5-7 mins to briefly describe your project and what you would want to accomplish in this project.

- Brief presentations will be done in an alphabetical order.

Sequential Data

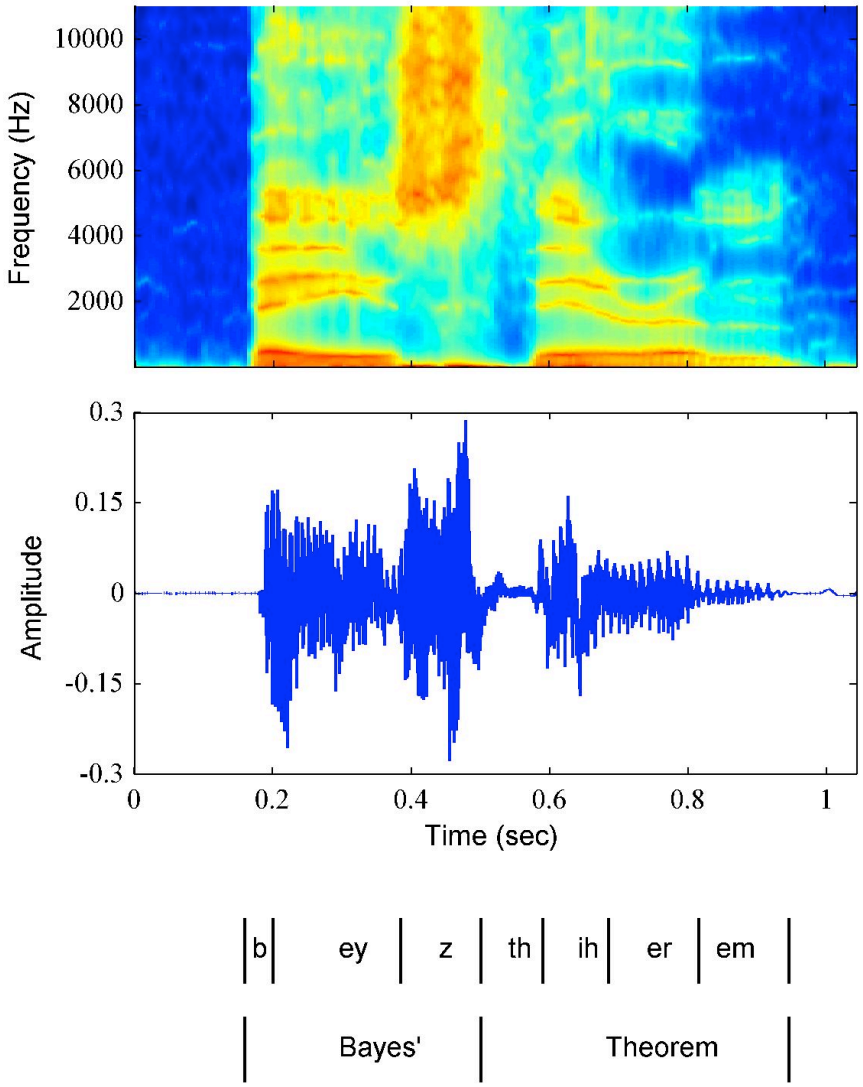
- So far we focused on problems that assumed that the data points were independent and identically distributed (i.i.d. assumption).
- Express the likelihood function as a product over all data points of the probability distribution evaluated at each data point.
- Poor assumption when working with sequential data.

- For many applications, e.g. financial forecasting, we want to predict the next value in a time series, given past values.

- Intuitively, the recent observations are likely to be more informative in predicting the future.

- Markov models: future predictions are independent of all but the most recent observations.

Example of a Spectrogram

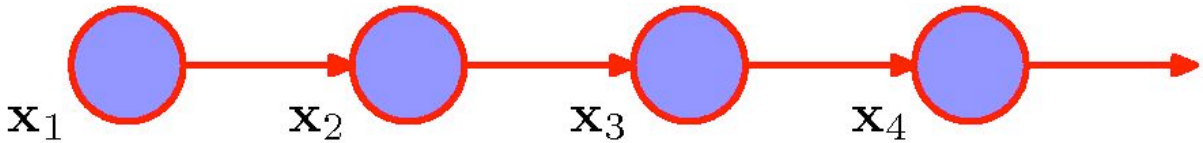


- Example of a spectrogram of a spoken word ‘Bayes theorem’:

- Successive observations are highly correlated.

Markov Models

- The simplest model is the first-order Markov chain:



- The joint distribution for a sequence of N observations under this model is:

$$p(\mathbf{x}_1, ..., \mathbf{x}_N) = p(\mathbf{x}_1) \prod_{n=2}^{N} p(\mathbf{x}_n | \mathbf{x}_{n-1}).$$

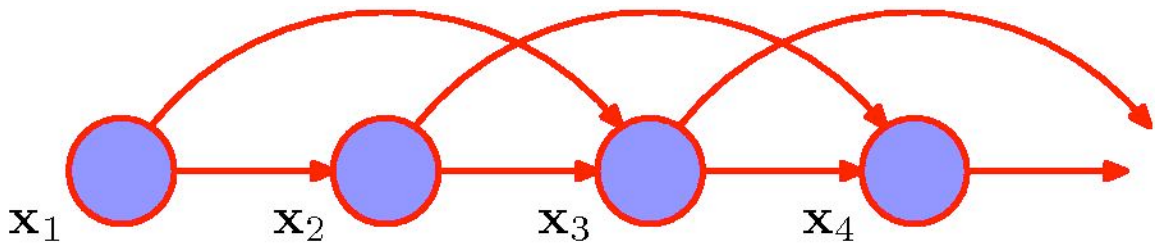
- From the d-separation property, the conditionals are given by:

$$p(\mathbf{x}_n | \mathbf{x}_1, ..., \mathbf{x}_{n-1}) = p(\mathbf{x}_n | \mathbf{x}_{n-1}).$$

- For many applications, these conditional distributions that define the model will be constrained to be equal.
- This corresponds to the assumption of a stationary time series.
- The model is known as homogenous Markov chain.

Second-Order Markov Models

- We can also consider a second-order Markov chain:



- The joint distribution for a sequence of N observations under this model is:

$$p(\mathbf{x}_1, ..., \mathbf{x}_N) = p(\mathbf{x}_1)p(\mathbf{x}_2|\mathbf{x}_1) \prod_{n=3}^{N} p(\mathbf{x}_n|\mathbf{x}_{n-1}, \mathbf{x}_{n-2}).$$

- We can similarly consider extensions to an Mth order Markov chain.
- Increased flexibility $\rightarrow$ Exponential growth in the number of parameters.
- Markov models need big orders to remember past “events”.

Learning Markov Models

- The ML parameter estimates for a simple Markov model are easy. Consider a Kth order model:

$$p(\mathbf{x}_N, ..., \mathbf{x}_{k+1} | \mathbf{x}_1, .., \mathbf{x}_k) = \prod_{n=k+1}^{N} p(\mathbf{x}_n | \mathbf{x}_{n-1}, \mathbf{x}_{n-2}, .., \mathbf{x}_{n-k}).$$

- Each window of k + 1 outputs is a training case for the model. $p(\mathbf{x}_n | \mathbf{x}_{n-1}, \mathbf{x}_{n-2}, .., \mathbf{x}_{n-k})$.

- Example: for discrete outputs (symbols) and a 2nd-order Markov model we can use the multinomial model:

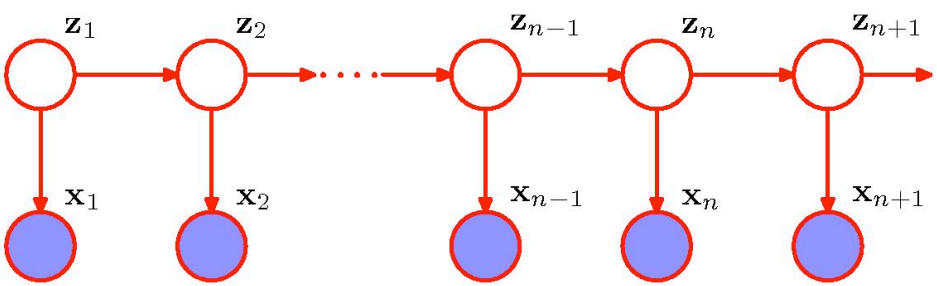
$$p(\mathbf{x}_n = m | \mathbf{x}_{n-1} = a, \mathbf{x}_{n-2} = b) = \alpha_{mab}.$$

- The maximum likelihood values for α are:

$$\alpha^*_{mab} = \frac{\text{num}[n,\ s.t.\ \mathbf{x}_n = m, \mathbf{x}_{n-1} = a, \mathbf{x}_{n-2} = b]}{\text{num}[n,\ s.t.\ \mathbf{x}_{n-1} = a, \mathbf{x}_{n-2} = b]}.$$

State Space Models

- How about the model that is not limited by the Markov assumption to any order.
- Solution: Introduce additional latent variables!



- Graphical structure known as the State Space Model.

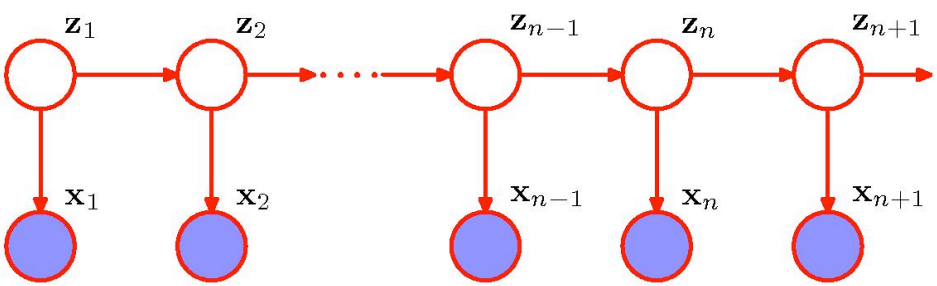
- For each observation x_n, we have a latent variable z_n. Assume that latent variables form a Markov chain.
- If the latent variables are discrete $\rightarrow$ Hidden Markov Models (HMMs). Observed variables can be discrete or continuous.

- If the latent and observed variables are Gaussian $\rightarrow$ Linear Dynamical System.

State Space Models

- The joint distribution is given by:

$$p(\mathbf{x}_1, ..., \mathbf{x}_N, \mathbf{z}_1, .., \mathbf{z}_N) = p(\mathbf{z}_1) \prod_{n=2}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1}) \prod_{n=1}^{N} p(\mathbf{x}_n|\mathbf{z}_n).$$



- Graphical structure known as the State Space Model.

- There is always a path connecting two observed variables x_n, x_m via latent variables.

- The predictive distribution:

$$p(\mathbf{x}_{n+1}|\mathbf{x}_1, ..., \mathbf{x}_N)$$

  does not exhibit any conditional independence properties! And so prediction depends on all previous observations.

- Even though hidden state sequence is first-order Markov, the output process is not Markov of any order!

Hidden Markov Model

- First order Markov chain generates hidden state sequence (known as transition probabilities):

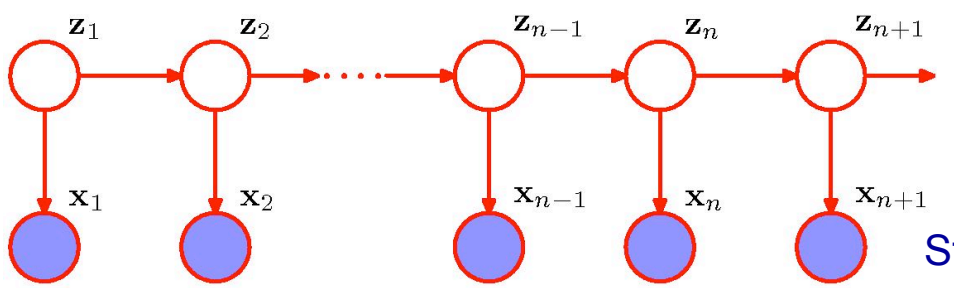
$$p(\mathbf{z}_n = k|\mathbf{z}_{n-1} = j) = A_{jk}, \qquad p(\mathbf{z}_1 = k) = \pi_k.$$

- A set of output probability distributions (**one per state**) converts state path into sequence of observable symbols/vectors (known as emission probabilities):

$$p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\phi}).$$

Gaussian, if **x** is continuous.

Conditional probability table if **x** is discrete.



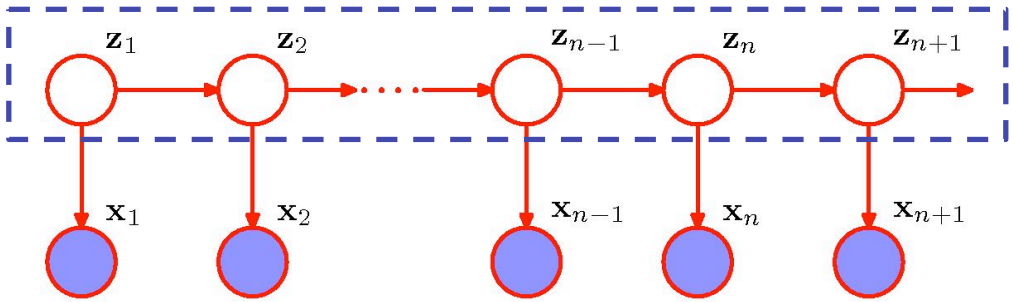
State transition

Observation model

$$p(\mathbf{x}_1, ..., \mathbf{x}_N, \mathbf{z}_1, .., \mathbf{z}_N) = p(\mathbf{z}_1) \prod_{n=2}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1}) \prod_{n=1}^{N} p(\mathbf{x}_n|\mathbf{z}_n).$$

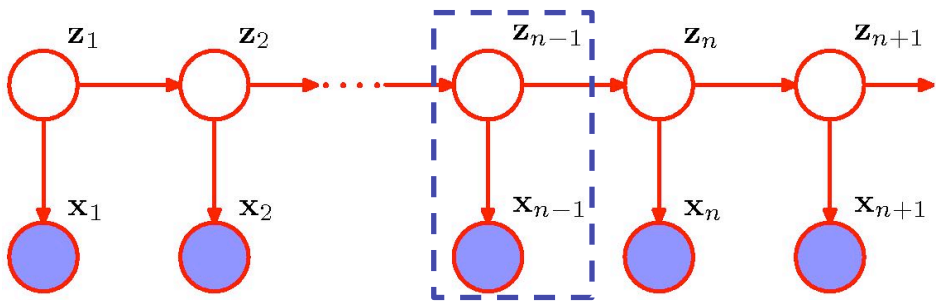
Links to Other Models

- You can view HMM as: A Markov chain with stochastic measurements.



- Or a mixture model with states coupled across time.

We will adopt this view, as we worked with mixture model before.



Transition Probabilities

- It will be convenient to use 1-of-K encoding for the latent variables.
- The matrix of transition probabilities takes form:

$$p(z_{nk} = 1 | z_{n-1,j} = 1) = A_{jk}, \sum_k A_{jk} = 1.$$

- The conditionals can be written as:

$$p(\mathbf{z}_n | \mathbf{z}_{n-1}, A) = \prod_{k=1}^{K} \prod_{j=1}^{K} A_{jk}^{z_{n-1,j} z_{nk}}, \quad p(\mathbf{z}_1 | \pi) = \prod_{k=1}^{K} \pi_k^{z_{1k}}.$$

- We will focus on homogenous models: all of the conditional distributions over latent variables share the same parameters **A**.

- Standard mixture model for i.i.d. data: special case in which all parameters A_{jk} are the same for all j.

- Or the conditional distribution $p(z_n|z_{n-1})$ is independent of z_{n-1}.

Emission Probabilities

- The emission probabilities take form:

$$p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\phi}) = \prod_{k=1}^{K} p(\mathbf{x}_n|\boldsymbol{\phi}_k)^{z_{nk}}.$$

- For example, for a continuous **x**, we have

$$p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\phi}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_{nk}}.$$

- For the discrete, multinomial observed variable **x**, using 1-of-K encoding, the conditional distribution takes form:

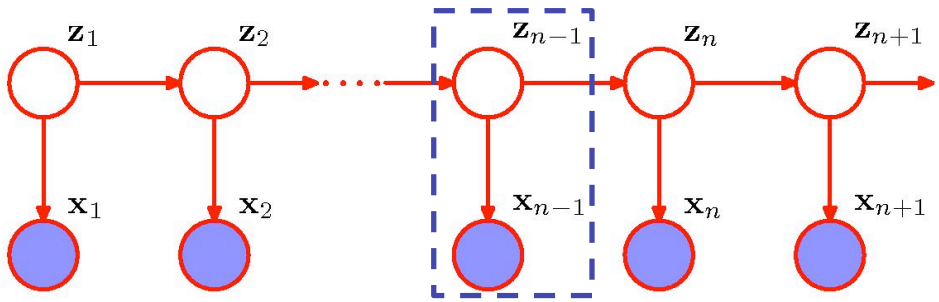
$$p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\phi}) = \prod_{i=1}^{D} \prod_{k=1}^{K} \mu_{ik}^{x_{ni} z_{nk}}.$$

HMM Model Equations

- The joint distribution over the observed and latent variables is given by:

$$p(\mathbf{X}, \mathbf{Z}|\theta) = p(\mathbf{z}_1|\boldsymbol{\pi}) \prod_{n=2}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1}, A) \prod_{n=1}^{N} p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\phi}),$$

where $\theta = \{\boldsymbol{\pi}, A, \boldsymbol{\phi}\}$ are the model parameters.

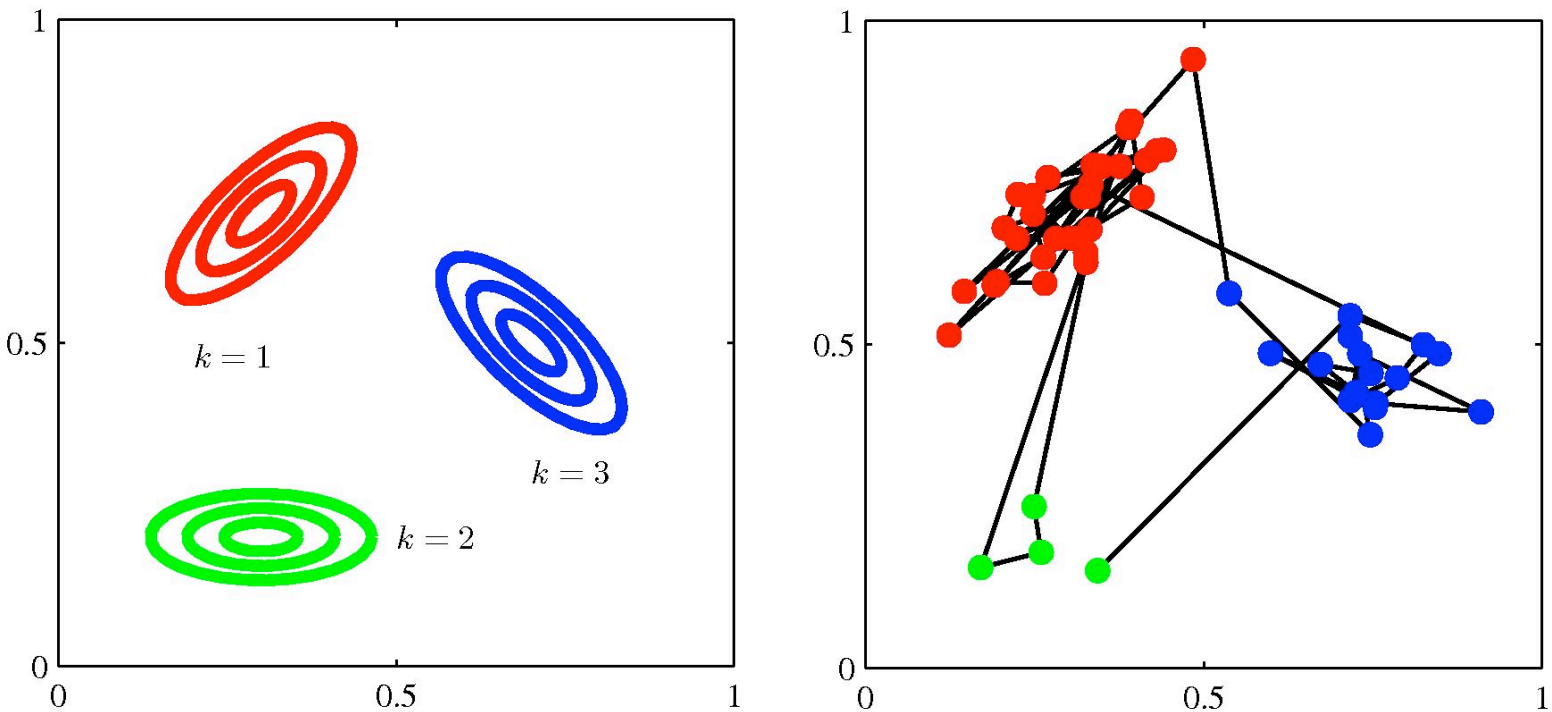


- Data are not i.i.d. Everything is coupled across time.

- Three problems: computing probabilities of observed sequences, inference of hidden state sequences, learning of parameters.

HMM as a Mixture Through Time

- Sampling from a 3-state HMM with a 2-d Gaussian emission model.



- The transition matrix is fixed: A_{kk}=0.9 and A_{jk} = 0.05.

Applications of HMMs

- Speech recognition.
- Language modeling
- Motion video analysis/tracking.
- Protein sequence and genetic sequence alignment and analysis.
- Financial time series prediction.

Maximum Likelihood for the HMM

- We observe a dataset **X** = $\{x_1,\ldots,x_N\}$.
- The goal is to determine model parameters $\theta = \{\boldsymbol{\pi}, A, \boldsymbol{\phi}\}$.
- The probability of observed sequence takes form:

$$p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta).$$

$$p(\text{observed sequence}) = \sum_{\text{all paths}} p(\text{observed outputs, state paths}).$$

- In contrast to mixture models, the joint distribution p(**X**,**Z** | θ) does not factorize over n.
- It looks hard: N variables, each of which has K states. Hence N^K total paths.
- Remember inference problem on a simple chain.

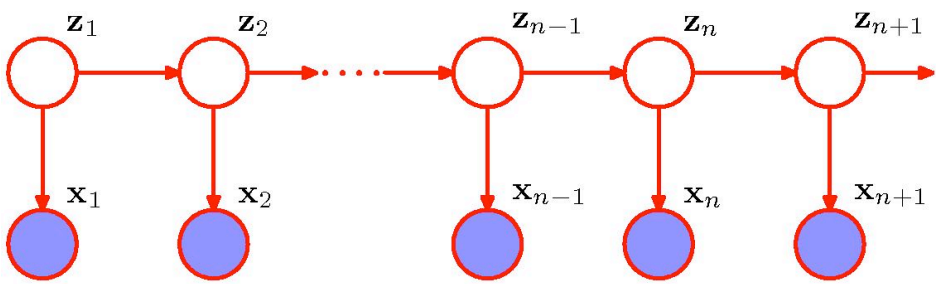
Probability of an Observed Sequence

- The joint distribution factorizes:

$$p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta) = \sum_{\mathbf{z}_1,\ldots,\mathbf{z}_n} p(\mathbf{z}_1, \mathbf{x}_1) \prod_{n=2}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1}) p(\mathbf{x}_n|\mathbf{z}_n)$$

$$= \sum_{\mathbf{z}_1} p(\mathbf{z}_1) p(\mathbf{x}_1|\mathbf{z}_1) \sum_{\mathbf{z}_2} p(\mathbf{z}_2|\mathbf{z}_1) p(\mathbf{x}_2|\mathbf{z}_2) \ldots$$

$$\sum_{\mathbf{z}_N} p(\mathbf{z}_N|\mathbf{z}_{N-1}) p(\mathbf{x}_N|\mathbf{z}_N).$$



- Dynamic Programming: By moving the summations inside, we can save a lot of work.

EM algorithm

- We cannot perform direct maximization (no closed form solution):

$$p(\mathbf{X}|\theta) = \sum_{\mathbf{Z}} p(\mathbf{X}, \mathbf{Z}|\theta).$$

- EM algorithm: we will derive efficient algorithm for maximizing the likelihood function in HMMs (and later for linear state-space models).

- E-step: Compute the posterior distribution over latent variables:

$$p(\mathbf{Z}|\mathbf{X}, \theta^{old}).$$

- M-step: Maximize the expected complete data log-likelihood:

$$Q(\theta, \theta^{old}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{old}) \log p(\mathbf{X}, \mathbf{Z}|\theta).$$

- If we knew the true state path, then ML parameter estimation would be trivial.

- We will first look at the E-step: Computing the true posterior distribution over the state paths.

Inference of Hidden States

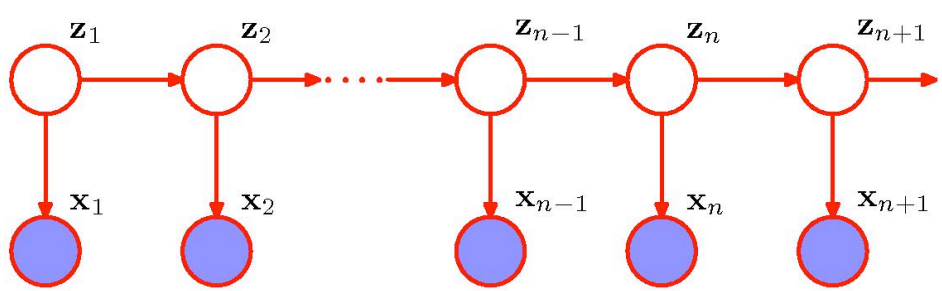
- We want to estimate the hidden states given observations. To start with, let us estimate a single hidden state:

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n|\mathbf{X}) = \frac{p(\mathbf{X}|\mathbf{z}_n)p(\mathbf{z}_n)}{p(\mathbf{X})}.$$

- Using conditional independence property, we obtain:

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

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



Inference of Hidden States

- Hence:

$$\gamma(\mathbf{z}_n) = \frac{p(\mathbf{x}_1, .., \mathbf{x}_n, \mathbf{z}_n)p(\mathbf{x}_{n+1}, ..., \mathbf{x}_N|\mathbf{z}_n)}{p(\mathbf{X})} = \frac{\alpha(\mathbf{z}_n)\beta(\mathbf{z}_n)}{p(\mathbf{X})}.$$

$$\alpha(\mathbf{z}_n) \equiv p(\mathbf{x}_1, .., \mathbf{x}_n, \mathbf{z}_n)$$

The joint probability of observing all of the data up to time n and z_n.

$$\beta(\mathbf{z}_n) \equiv p(\mathbf{x}_{n+1}, .., \mathbf{x}_N|\mathbf{z}_n).$$

The conditional probability of all future data from time n+1 to N.

- Each $\alpha(z_n)$ and $\beta(z_n)$ represent a set of K numbers, one for each of the possible settings of the 1-of-K binary vector z_n.

- We will derive efficient recursive algorithm, known as the alpha-beta recursion, or forward-backward algorithm.

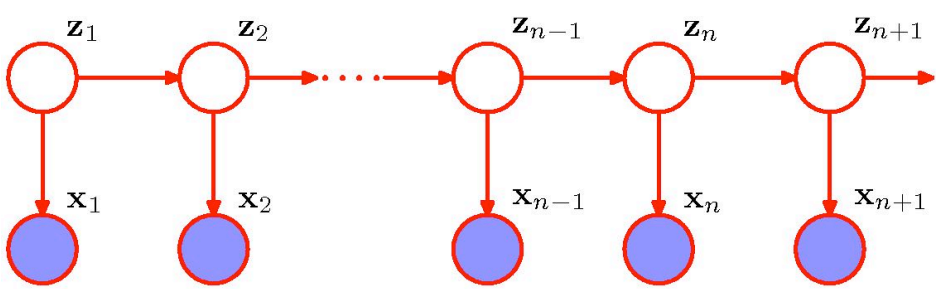
- Relates to the sum-product message passing algorithm for tree-structured graphical models.

The Forward (α) Recursion

- The forward recursion:

$$
\begin{aligned}
\alpha(\mathbf{z}_n) &= p(\mathbf{x}_1, .., \mathbf{x}_n, \mathbf{z}_n) \\
&= p(\mathbf{x}_n|\mathbf{z}_n)p(\mathbf{x}_1, .., \mathbf{x}_{n-1}, \mathbf{z}_n) \\
&= p(\mathbf{x}_n|\mathbf{z}_n) \sum_{\mathbf{z}_{n-1}} p(\mathbf{x}_1, .., \mathbf{x}_{n-1}, \mathbf{z}_{n-1}, \mathbf{z}_n) \\
&= p(\mathbf{x}_n|\mathbf{z}_n) \sum_{\mathbf{z}_{n-1}} p(\mathbf{x}_1, .., \mathbf{x}_{n-1}, \mathbf{z}_{n-1})p(\mathbf{z}_n|\mathbf{z}_{n-1}) \\
&= p(\mathbf{x}_n|\mathbf{z}_n) \sum_{\mathbf{z}_{n-1}} \alpha(\mathbf{z}_{n-1})p(\mathbf{z}_n|\mathbf{z}_{n-1})
\end{aligned}
$$

Computational cost scales like $O(K^2)$.



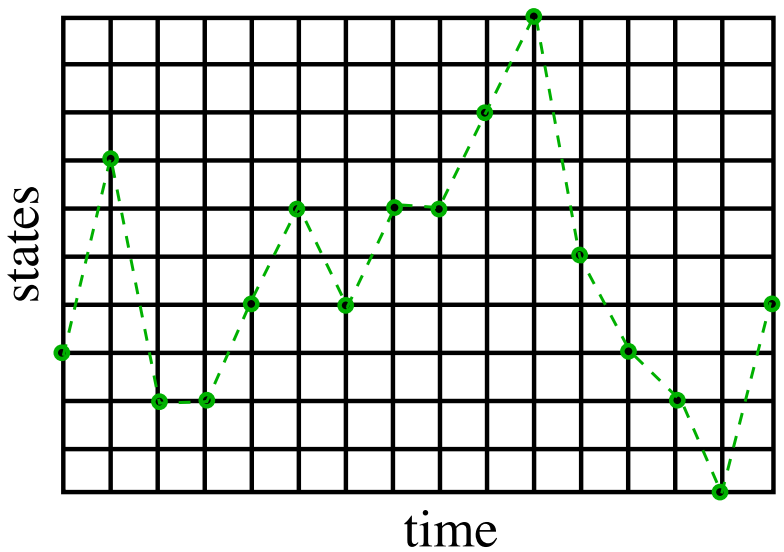
- Observe:

$$p(\mathbf{X}) = \sum_{\mathbf{z}_N} \alpha(\mathbf{z}_N).$$

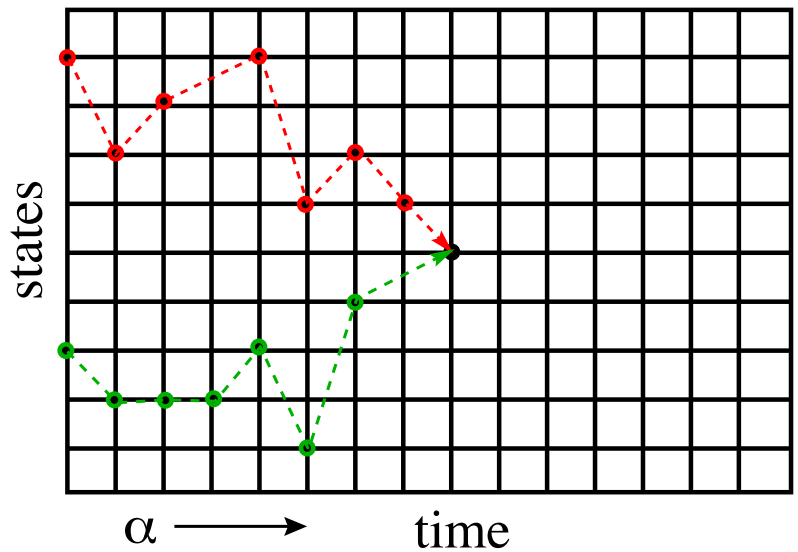
- This enables us to easily (cheaply) compute the desired likelihood.

The Forward (α) Recursion

- The forward recursion:



Exponentially many paths.

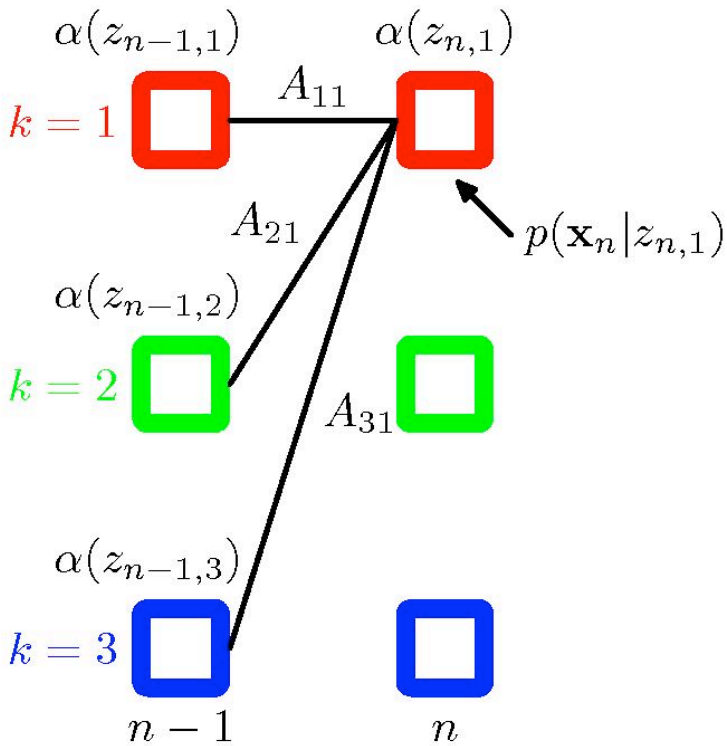


At each node, sum up the values of all incoming paths.

- This is exactly dynamic programming.

The Forward (α) Recursion

- Illustration of the forward recursion



Here $\alpha(z_{n,1})$ is obtained by

- Taking the elements $\alpha(z_{n-1},j)$
- Summing the up with weights A_{j1}, corresponding to $p(z_n \mid z_{n-1})$
- Multiplying by the data contribution $p(x_n \mid z_{n1})$.

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

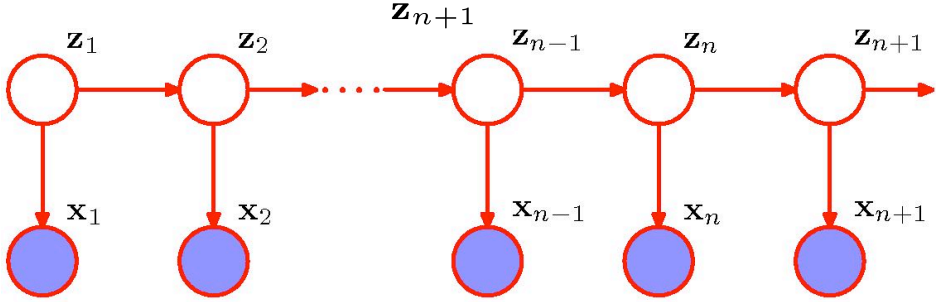
- The initial condition is given by:

$$\alpha(\mathbf{z}_1) = p(\mathbf{x}_1|\mathbf{z}_1)p(\mathbf{z}_1) = \prod_{k=1}^{K} \left[\pi_k p(\mathbf{x}_1|\boldsymbol{\phi}_k)\right]^{z_{1k}}.$$

The Backward (β) Recursion

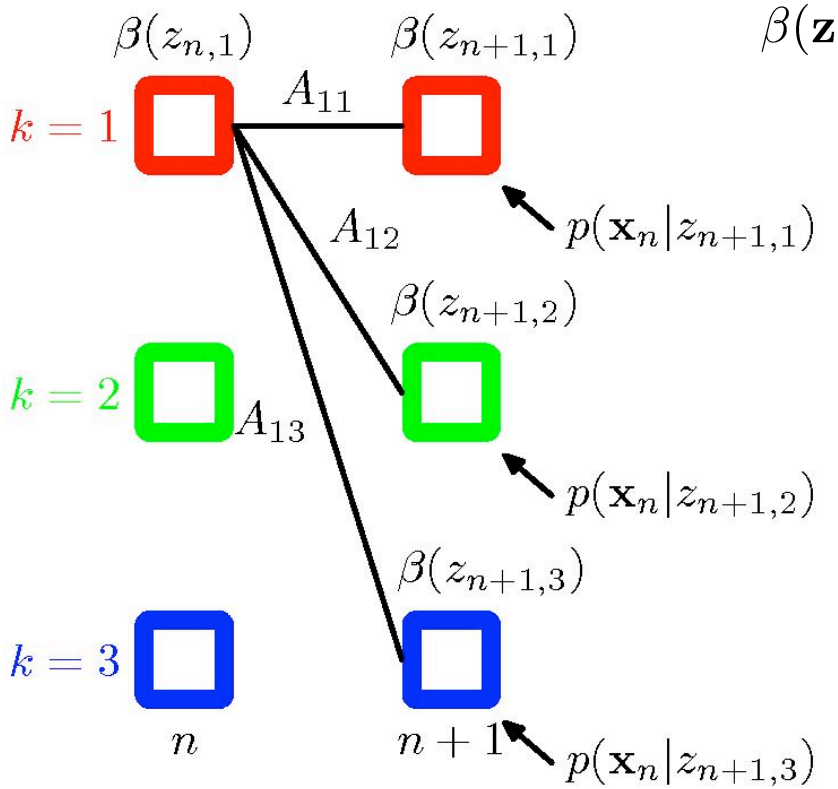
- There is also a simple recursion for $\beta(z_n)$:

$$
\begin{aligned}
\beta(\mathbf{z}_n) &= p(\mathbf{x}_{n+1}, .., \mathbf{x}_N | \mathbf{z}_n) \\
&= \sum_{\mathbf{z}_{n+1}} p(\mathbf{x}_{n+1}, ..., \mathbf{x}_N, \mathbf{z}_{n+1} | \mathbf{z}_n) \\
&= \sum_{\mathbf{z}_{n+1}} p(\mathbf{x}_{n+1}, ..., \mathbf{x}_N | \mathbf{z}_{n+1}, \mathbf{z}_n) p(\mathbf{z}_{n+1} | \mathbf{z}_n) \\
&= \sum_{\mathbf{z}_{n+1}} p(\mathbf{x}_{n+1}, ..., \mathbf{x}_N | \mathbf{z}_{n+1}) p(\mathbf{z}_{n+1} | \mathbf{z}_n) \\
&= \sum_{\mathbf{z}_{n+1}} p(\mathbf{x}_{n+2}, ..., \mathbf{x}_N | \mathbf{z}_{n+1}) p(\mathbf{x}_{n+1} | \mathbf{z}_{n+1}) p(\mathbf{z}_{n+1} | \mathbf{z}_n) \\
&= \sum_{\mathbf{z}_{n+1}} \beta(\mathbf{z}_{n+1}) p(\mathbf{x}_{n+1} | \mathbf{z}_{n+1}) p(\mathbf{z}_{n+1} | \mathbf{z}_n)
\end{aligned}
$$



The Backward (β) Recursion

- Illustration of the backward recursion



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

- Initial condition:

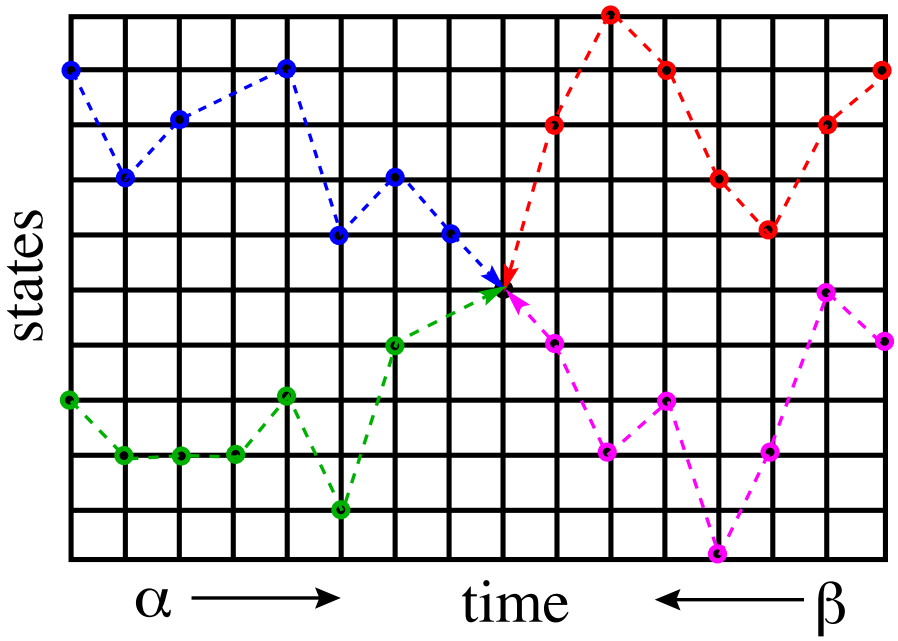
$$\begin{aligned} p(\mathbf{z}_N|\mathbf{X}) &= \frac{\alpha(\mathbf{z}_N)\beta(\mathbf{z}_N)}{p(\mathbf{X})} \\ &= \frac{p(\mathbf{X},\mathbf{z}_N)\beta(\mathbf{z}_N)}{p(\mathbf{X})}. \end{aligned}$$

- Hence:

$$\beta(\mathbf{z}_N) = 1.$$

The Backward (β) Recursion

- $\alpha(z_{nk})$ gives total inflow of probability to node (n,k).
- $\beta(z_{nk})$ gives total outflow of probability.



- In fact, we can do one forward pass to compute all the $\alpha(z_n)$ and one backward pass to compute all the $\beta(z_n)$ and then compute any $\gamma(z_n)$ we want. Total cost is $O(K^2N)$.

Computing Likelihood

- Note that

$$\sum_{\mathbf{z}_n} \gamma(\mathbf{z}_n) = \sum_{\mathbf{z}_n} p(\mathbf{z}_n|\mathbf{X}) = 1.$$

- We can compute the likelihood at any time using α - β recursion:

$$p(\mathbf{X}|\theta) = \sum_{\mathbf{z}_n} \alpha(\mathbf{z}_n)\beta(\mathbf{z}_n).$$

- In the forward calculation we proposed originally, we did this at the final time step n = N.

$$p(\mathbf{X}|\theta) = \sum_{\mathbf{z}_N} \alpha(\mathbf{z}_N).$$

Because $\beta(z_n)=1$.

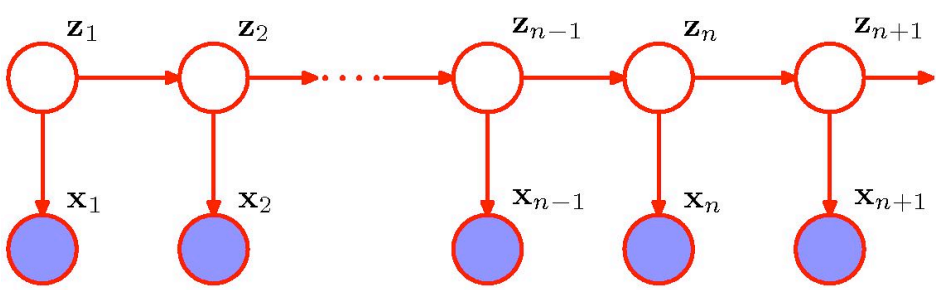
- This is a good way to check your code!

Two-Frame Inference

- We will also need the cross-time statistics for adjacent time steps:

$$
\begin{aligned}
\xi(\mathbf{z}_{n-1}, \mathbf{z}_n) &= p(\mathbf{z}_{n-1}, \mathbf{z}_n | \mathbf{X}) \\
&= \frac{p(\mathbf{X}|\mathbf{z}_{n-1}, \mathbf{z}_n) p(\mathbf{z}_{n-1}, \mathbf{z}_n)}{p(\mathbf{X})} \\
&= \frac{p(\mathbf{x}_1, .., \mathbf{x}_{n-1}|\mathbf{z}_{n-1}) p(\mathbf{x}_n|\mathbf{z}_n) p(\mathbf{x}_{n+1}, ..., \mathbf{x}_N|\mathbf{z}_n) p(\mathbf{z}_n|\mathbf{z}_{n-1}) p(\mathbf{z}_{n-1})}{p(\mathbf{X})} \\
&= \frac{\alpha(\mathbf{z}_{n-1}) p(\mathbf{x}_n|\mathbf{z}_n) p(\mathbf{z}_n|\mathbf{z}_{n-1}) \beta(\mathbf{z}_n)}{p(\mathbf{X})}.
\end{aligned}
$$

- This is a K $\times$ K matrix with elements ξ(i,j) representing the expected number of transitions from state i to state j that begin at time n-1, given all the observations.



- It can be computed with the same α and β recursions.

EM algorithm

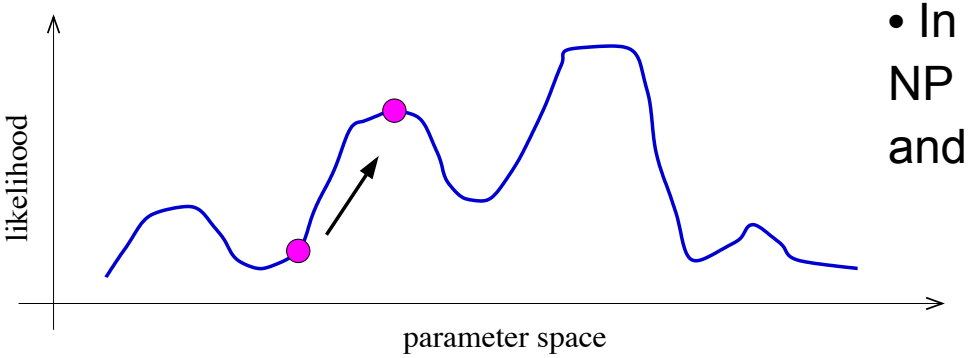
- Intuition: if only we knew the true state path then ML parameter estimation would be trivial.
- E-step: Compute the posterior distribution over the state path using α - β recursion (dynamic programming):

$$p(\mathbf{Z}|\mathbf{X}, \theta^{old}).$$

- M-step: Maximize the expected complete data log-likelihood (parameter re-estimation):

$$Q(\theta, \theta^{old}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{old}) \log p(\mathbf{X}, \mathbf{Z}|\theta).$$

- We then iterate. This is also known as a Baum-Welch algorithm (special case of EM).



- In general, finding the ML parameters is NP hard, so initial conditions matter a lot and convergence is hard to tell.

Complete Data Log-likelihood

- Complete data log-likelihood takes form:

$$\log p(\mathbf{X}, \mathbf{Z}|\theta) = \log \left[p(\mathbf{z}_1|\boldsymbol{\pi}) \prod_{n=2}^{N} p(\mathbf{z}_n|\mathbf{z}_{n-1}, A) \prod_{n=1}^{N} p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\phi}) \right]$$

$$= \log \left[\prod_{k=1}^{K} \pi_k^{z_{1k}} \prod_{n=2}^{N} \prod_{k=1}^{K} \prod_{j=1}^{K} A_{jk}^{z_{n-1,j}, z_{nk}} \prod_{n=1}^{N} \prod_{k=1}^{K} p(\mathbf{x}_n|\mathbf{z}_n)^{z_{nk}} \right]$$

$$= \sum_{k=1}^{K} z_{1k} \log \pi_k + \sum_{n=2}^{N} \sum_{k=1}^{K} \sum_{j=1}^{K} [z_{n-1,j} z_{nk}] \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} z_{nk} \log p(\mathbf{x}_n|\mathbf{z}_n).$$

transition model

observation model

- Statistics we need from the E-step are:

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n|\mathbf{X}).$$

$$\xi(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_{n-1}, \mathbf{z}_n|\mathbf{X}).$$

Expected Complete Data Log-likelihood

- The complete data log-likelihood takes form:

$$Q(\theta, \theta^{old}) = \sum_{\mathbf{Z}} p(\mathbf{Z}|\mathbf{X}, \theta^{old}) \log p(\mathbf{X}, \mathbf{Z}|\theta).$$

$$= \sum_{k=1}^{K} \gamma(z_{1k}) \log \pi_k + \sum_{n=2}^{N} \sum_{k=1}^{K} \sum_{j=1}^{K} \xi(z_{n-1,j} z_{nk}) \log A_{jk} + \sum_{n=1}^{N} \sum_{k=1}^{K} \gamma_{nk} \log p(\mathbf{x}_n|\mathbf{z}_n).$$

- Hence in the E-step we evaluate:

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n|\mathbf{X}).$$

$$\xi(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_{n-1}, \mathbf{z}_n|\mathbf{X}).$$

- In the M-step we optimize Q with respect to parameters: $\theta = \{\boldsymbol{\pi}, A, \boldsymbol{\phi}\}$.

Parameter Estimation

- Initial state distribution: expected number of times in state k at time 1:

$$\pi_k^{new} = \frac{\gamma(z_{1k})}{\sum_{j=1}^{K} \gamma(z_{1j})}.$$

- Expected # of transitions from state j to k which begin at time n-1:

$$\xi(\mathbf{z}_{n-1,j}, \mathbf{z}_{n,k}) = p(\mathbf{z}_{n-1,j}, \mathbf{z}_{n,k} | \mathbf{X}),$$

so the estimated transition probabilities are:

$$A_{jk}^{new} = \frac{\sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nk})}{\sum_{l=1}^{K} \sum_{n=2}^{N} \xi(z_{n-1,j}, z_{nl})}.$$

- The EM algorithm must be initialized by choosing starting values for π and **A**.

- Note that any elements of π or **A** that initially are set to zero will remain zero in subsequent EM updates.

Parameter Estimation: Emission Model

- For the case of discrete multinomial observed variables, the observation model takes form:

$$p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\phi}) = \prod_{i=1}^{D}\prod_{k=1}^{K} \mu_{ik}^{x_{ni}z_{nk}}.$$

Same as fitting Bernoulli mixture model.

- And the corresponding M-step update: $\mu_{ik}^{new} = \frac{\sum_{n=1}^{N}\gamma(z_{nk})x_{ni}}{\sum_{n=1}^{N}\gamma(z_{nk})}.$

- For the case of the Gaussian emission model:

$$p(\mathbf{x}_n|\mathbf{z}_n, \boldsymbol{\phi}) = \prod_{k=1}^{K} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)^{z_{nk}}.$$

Remember:

$$\gamma(\mathbf{z}_n) = p(\mathbf{z}_n|\mathbf{X}).$$

- And the corresponding M-step updates:

$$\boldsymbol{\mu}_k^{new} = \frac{1}{N_k}\sum_n \gamma(z_{nk})\mathbf{x}_n, \quad N_k = \sum_n \gamma(z_{nk}),$$

$$\boldsymbol{\Sigma}_k^{new} = \frac{1}{N_k}\sum_{n=1}^{N} \gamma(y_{nk})(\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T,$$

Same as fitting a Gaussian mixture model.

Viterbi Decoding

- The numbers $\gamma(z_n)$ above gave the probability distribution over all states at any time.

- By choosing the state $\gamma^*(z_n)$ with the largest probability at each time, we can make an "average" state path. This is the path with the maximum expected number of correct states.

- To find the single best path, we do Viterbi decoding which is Bellman's dynamic programming algorithm applied to this problem.

- The recursions look the same, except with max instead of $\sum$.

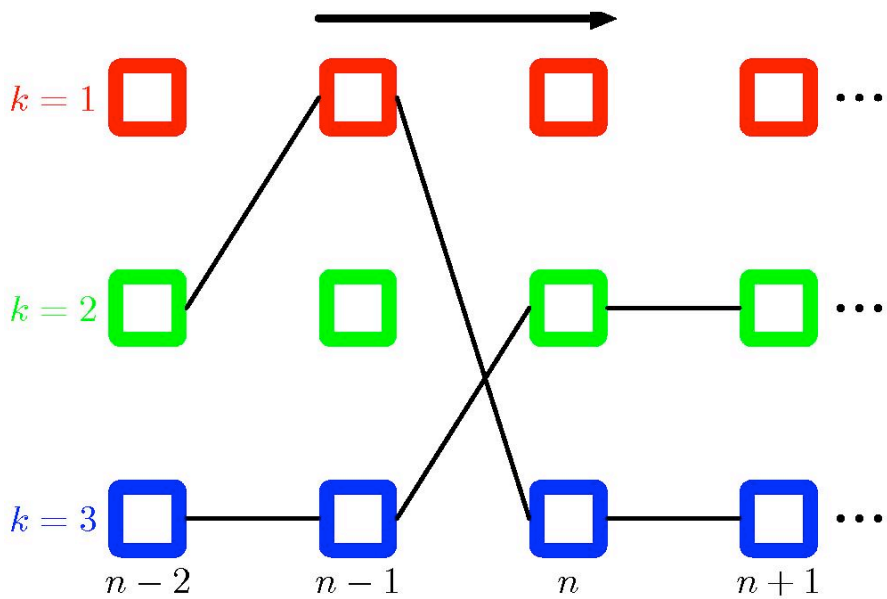
- Same dynamic programming trick: instead of summing, we keep the term with the highest value at each node.

- There is also a modified EM (Baum-Welch) training based on the Viterbi decoding. Like K-means instead of mixtures of Gaussians.

- Relates to the max-sum algorithm for tree structured graphical models.

Viterbi Decoding

• A fragment of the HMM lattice showing two possible paths:

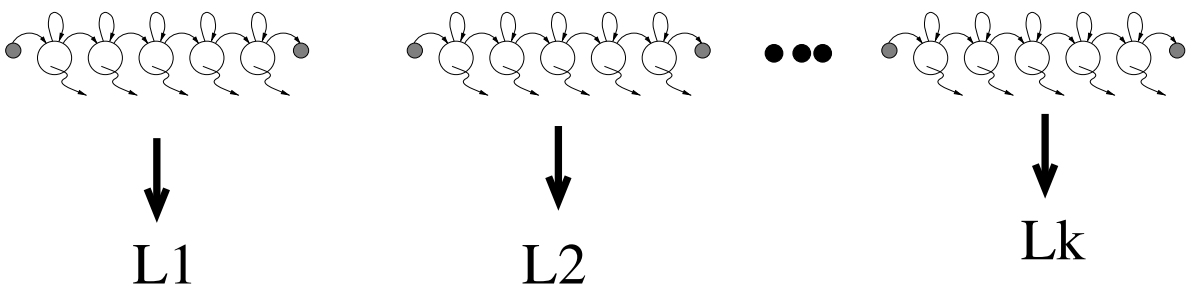


• Viterbi decoding efficiently determines the most probable path from the exponentially many possibilities.

• The probability of each path is given by the product of the elements of the transition matrix A_{jk}, along with the emission probabilities associated with each node in the path.

Using HMMs for Recognition

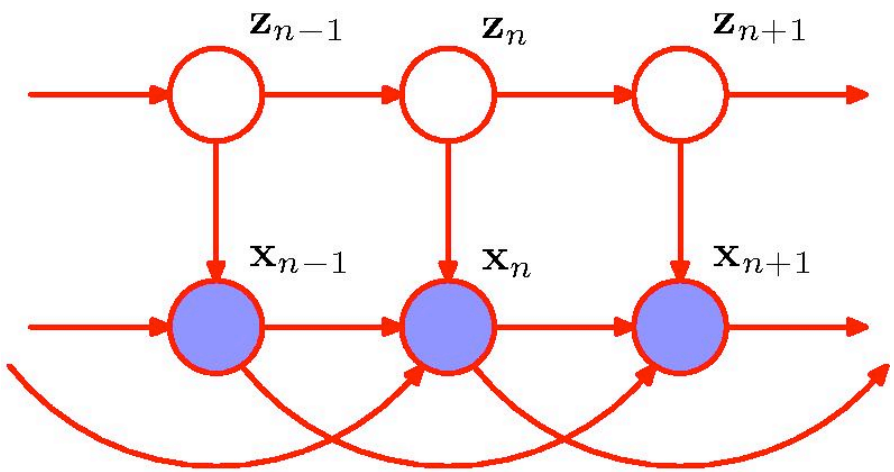
- We can use HMMs for recognition by:
  - training one HMM for each class (requires labeled training data)
  - evaluating probability of an unknown sequence under each HMM
  - classifying unknown sequence by choosing an HMM with highest likelihood



- This requires the solution of two problems:
  - Given model, evaluate probability of a sequence. (We can do this exactly and efficiently.)
  - Given some training sequences, estimate model parameters. (We can find the local maximum using EM.)

Autoregressive HMMs

• One limitation of the standard HMM is that it is poor at capturing long-range correlations between observations, as these have to be mediated via the first order Markov chain of hidden states.



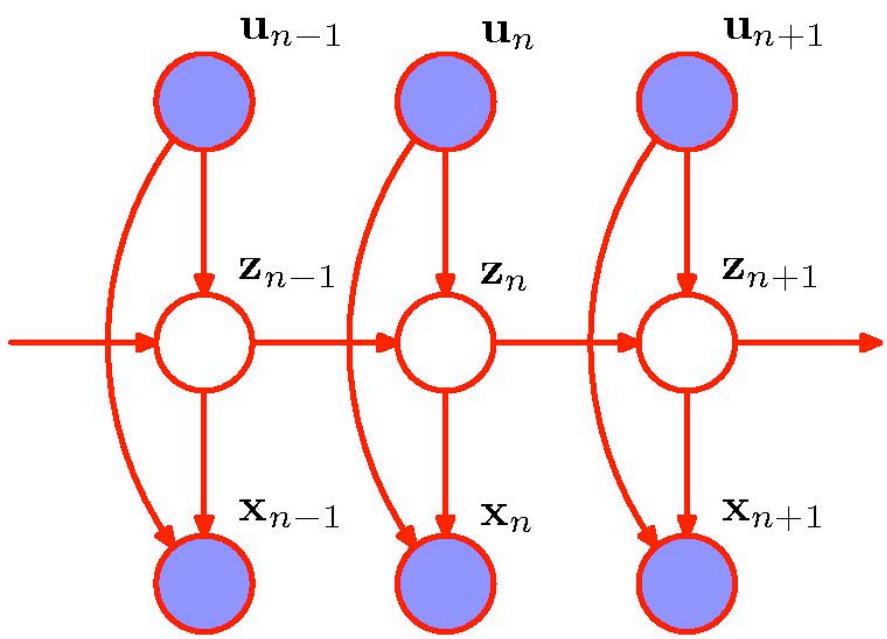
• Autoregressive HMM: The distribution over x_n depends depends on a subset of previous observations.

• The number of additional links must be limited to avoid an excessive number of free parameters.

• The graphical model framework motivates a number of different models based on HMMs.

Input-Output HMMs

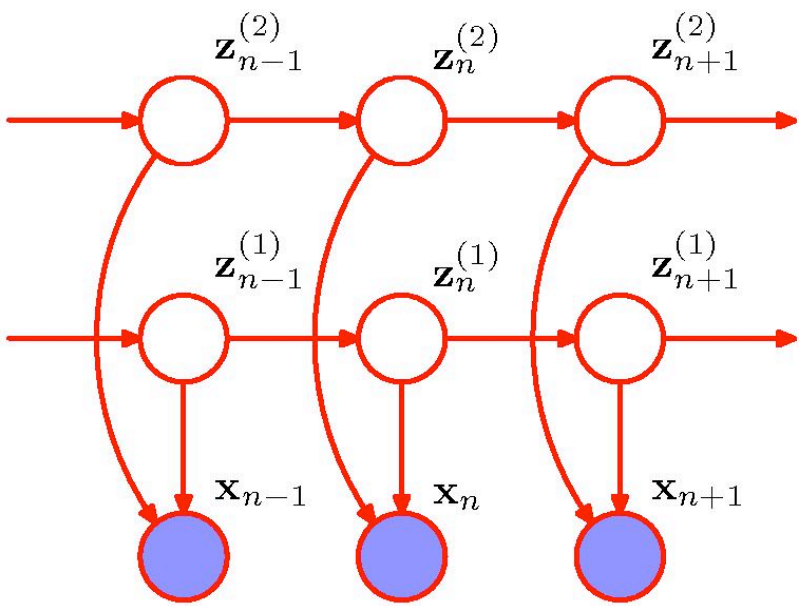
• Both the emission probabilities and the transition probabilities depend on the values of a sequence of observations $u_1,\ldots,u_N$.



• Model parameters can be efficiently fit using EM, in which the E-step involves forward-backward recursion.

Factorial HMMs

• Example of Factorial HMM comprising of two Markov chains of latent variables:



• Motivation: In order to represent 10 bits of information at a given time step, a standard HMM would need $K=2^{10}=1024$ states.

• Factorial HMMs would use 10 binary chains.

• Much more powerful model.

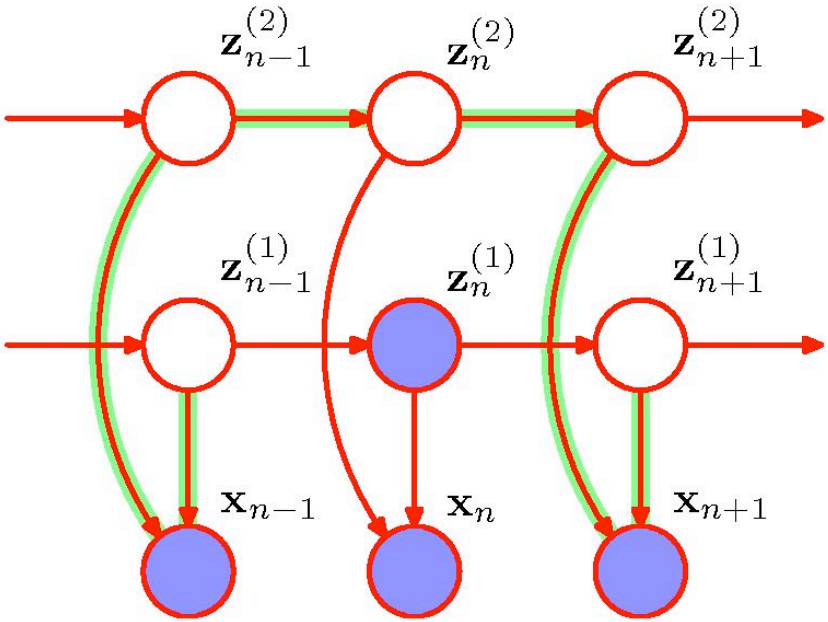
• The key disadvantage: Exact inference is intractable.

• Observing the **x** variables introduces dependencies between latent chains.

• Hence E-step for this model **does not** correspond to running forward-backward along the M latent chain independently.

Factorial HMMs

• The conditional independence property: $z_{n+1} \perp z_{n-1} \mid z_n$ does not hold for the individual latent chains.



• There is no efficient exact E-step for this model.

• One solution would be to use MCMC techniques to obtain approximate sample from the posterior.

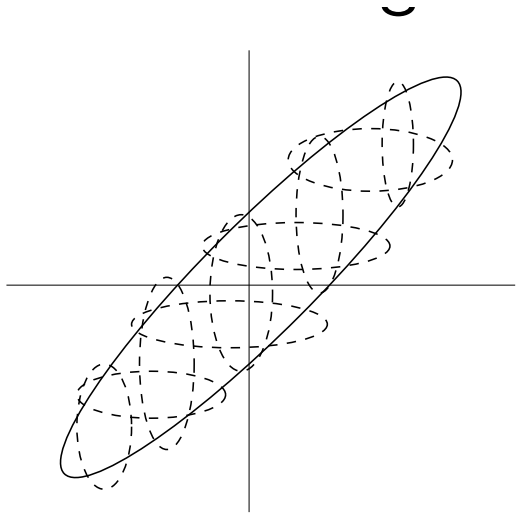
• Another alternative is to resort to variational inference.

• The variational distribution can be described by M separate Markov chains corresponding to the latent chains in the original model (structured mean-field approximation).

Regularizing HMMs

- There are two problems:
  - for high dimensional outputs, lots of parameters in the emission model
  - with many states, transition matrix has many (squared) elements

- First problem: full covariance matrices in high dimensions or discrete symbol models with many symbols have lots of parameters. To estimate these accurately requires a lot of training data.



- We can use mixtures of diagonal covariance Gaussians.

- For discrete data, we can use mixtures of base rates.

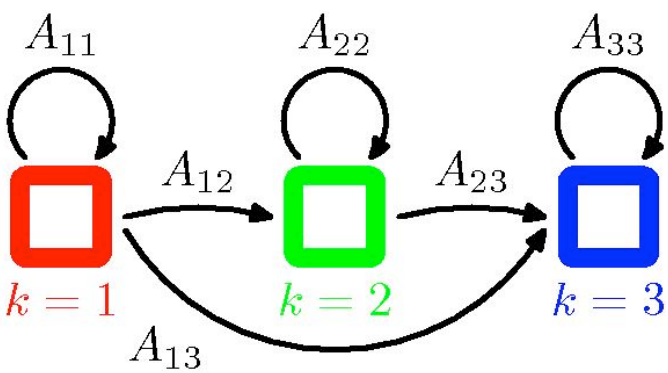
- We can also tie parameters across states.

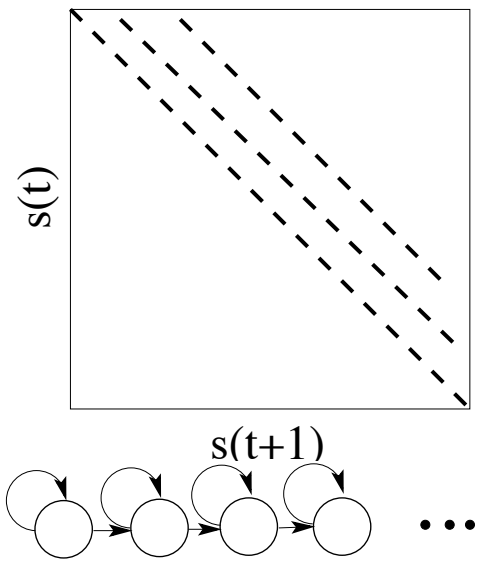
Regularizing Transition Matrices

• One way to regularize large transition matrices is to constrain them to be sparse: instead of being allowed to transition to any other state, each state has only a few possible successor states.

• A very effective way to constrain the transitions is to order the states in the HMM and allow transitions only to states that come later in the ordering.

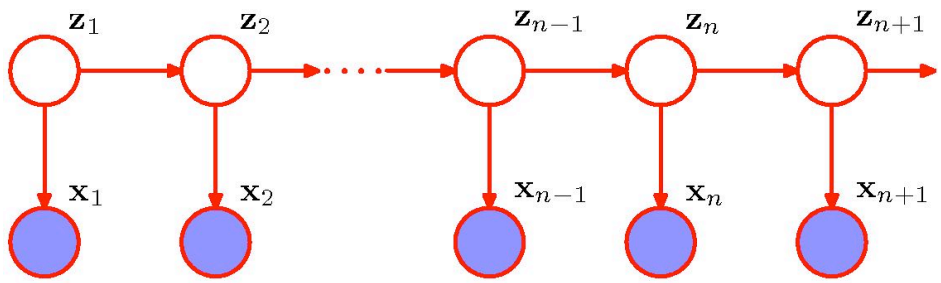
• Such models are known as "linear HMMs", "chain HMMs" or "left- to-right HMMs". Transition matrix is upper- diagonal (usually only has a few bands).





Linear Dynamical Systems

• In HMMs, latent variables are discrete but with arbitrary emission probability distributions.



• We now consider a linear-Gaussian state-space model, so that latent variables and observed variables are multivariate Gaussian distributions.

• An HMM can be viewed as an extension of the mixture models to allow for sequential correlations in the data

• Similarly, the linear dynamical system (LDS) can be viewed as a generalization of the continuous latent variable models, such as probabilistic PCA.

Linear Dynamical Systems

- The model is represented by a tree-structured directed graph, so inference can be solved efficiently using the sum-product algorithm.

- The forward recursions, analogous to the α-messages of HMMs are known as the Kalman filter equations.

- The backward recursions, analogous to the β-messages, are known as the Kalman smoother equations.

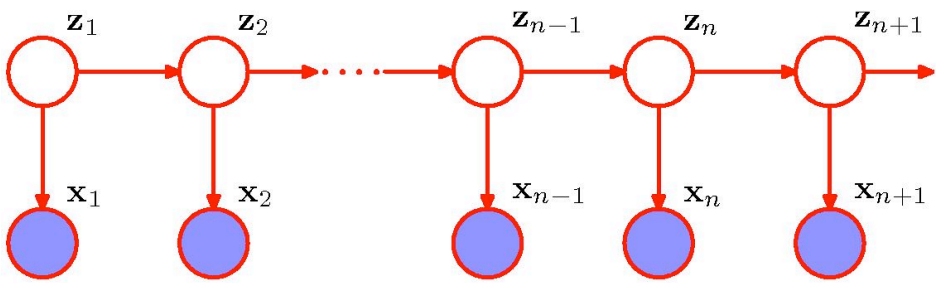
- The Kalman filter is used in many real-time tracking applications.

- Because the LDS is a linear-Gaussian model, the joint distribution over all variables, as well as marginals and conditionals, will be Gaussian.

- This leads to tractable inference and learning.

The Model

- We can write the transition and emission distributions in the general form:



$$p(\mathbf{z}_n|\mathbf{z}_{n-1}) = \mathcal{N}(\mathbf{z}_n|\mathbf{A}\mathbf{z}_{n-1}, \mathbf{\Gamma}),$$

$$p(\mathbf{x}_n|\mathbf{z}_n) = \mathcal{N}(\mathbf{x}_n|\mathbf{C}\mathbf{z}_n, \mathbf{\Sigma}),$$

$$p(\mathbf{z}_1) = \mathcal{N}(\mathbf{z}_1|\boldsymbol{\mu}_0, \mathbf{V}_0).$$

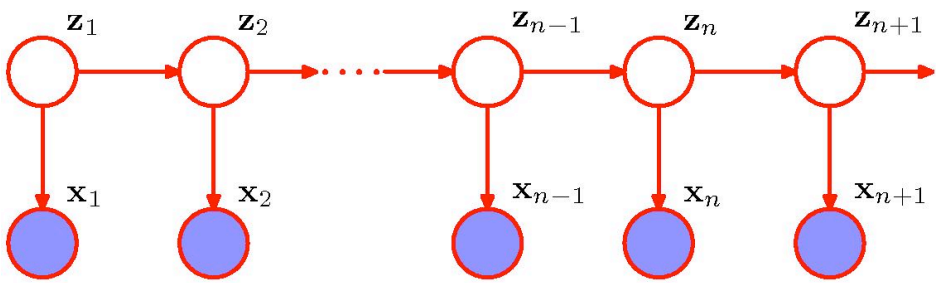
- These can be expressed in terms of noisy linear equations:

$$\begin{aligned} \mathbf{z}_n &= \mathbf{A}\mathbf{z}_{n-1} + \mathbf{w}_n, & \mathbf{w} &\sim \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{\Gamma}), \\ \mathbf{x}_n &= \mathbf{C}\mathbf{z}_n + \mathbf{v}_n, & \mathbf{v} &\sim \mathcal{N}(\mathbf{v}|\mathbf{0}, \mathbf{\Sigma}), \\ \mathbf{z}_1 &= \boldsymbol{\mu}_0 + \mathbf{u}, & \mathbf{u} &\sim \mathcal{N}(\mathbf{u}|\mathbf{0}, \mathbf{V}_0). \end{aligned}$$

- Model parameters $\theta = \{\mathbf{A}, \mathbf{\Gamma}, \mathbf{C}, \mathbf{\Sigma}, \boldsymbol{\mu}_0, \mathbf{V}_0\}$ can be learned using EM algorithm (similar to standard HMM case).

Inference in LDS

- Consider forward equations. The initial message is Gaussian, and since each of the factors is Gaussian, all subsequent messages will also be Gaussians.



$$\begin{aligned} \mathbf{z}_n &= \mathbf{A}\mathbf{z}_{n-1} + \mathbf{w}_n, & \mathbf{w} &\sim \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{\Gamma}), \\ \mathbf{x}_n &= \mathbf{C}\mathbf{z}_n + \mathbf{v}_n, & \mathbf{v} &\sim \mathcal{N}(\mathbf{v}|\mathbf{0}, \mathbf{\Sigma}), \\ \mathbf{z}_1 &= \boldsymbol{\mu}_0 + \mathbf{u}, & \mathbf{u} &\sim \mathcal{N}(\mathbf{u}|\mathbf{0}, \mathbf{V}_0). \end{aligned}$$

- Similar to HMMs, let us define the normalized version of $\alpha(z_n)$:

$$\hat{\alpha}(\mathbf{z}_n) = p(\mathbf{z}_n|\mathbf{x}_1, ..., \mathbf{x}_n) = \frac{\alpha(\mathbf{z}_n)}{p(\mathbf{x}_1, ..., \mathbf{x}_n)} = \mathcal{N}(\mathbf{z}_n|\boldsymbol{\mu}_n, \mathbf{V}_n).$$

Remember: for HMMs

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

- Using forward recursion, we get:

$$\begin{aligned} c_n \hat{\alpha}(\mathbf{z}_n) &= p(\mathbf{x}_n|\mathbf{z}_n) \int \hat{\alpha}(\mathbf{z}_{n-1}) p(\mathbf{z}_n|\mathbf{z}_{n-1}) d\mathbf{z}_{n-1} \\ &= \mathcal{N}(\mathbf{x}_n|\mathbf{C}\mathbf{z}_n, \mathbf{\Sigma}) \int \mathcal{N}(\mathbf{z}_{n-1}|\boldsymbol{\mu}_{n-1}, \mathbf{V}_{n-1}) \mathcal{N}(\mathbf{z}_n|\mathbf{A}\mathbf{z}_{n-1}, \mathbf{\Gamma}) d\mathbf{z}_{n-1}. \end{aligned}$$

Inference in LDS

- Hence we obtain:

$$
\begin{aligned}
c_n \hat{\alpha}(\mathbf{z}_n) &= p(\mathbf{x}_n|\mathbf{z}_n) \int \hat{\alpha}(\mathbf{z}_{n-1}) p(\mathbf{z}_n|\mathbf{z}_{n-1}) d\mathbf{z}_{n-1} \\
&= \mathcal{N}(\mathbf{x}_n|\mathbf{C}\mathbf{z}_n, \boldsymbol{\Sigma}) \int \mathcal{N}(\mathbf{z}_{n-1}|\boldsymbol{\mu}_{n-1}, \mathbf{V}_{n-1}) \mathcal{N}(\mathbf{z}_n|\mathbf{A}\mathbf{z}_{n-1}, \boldsymbol{\Gamma}) d\mathbf{z}_{n-1}.
\end{aligned}
$$

in which case $\alpha(z_n)$ is Gaussian:

$$
c_n \hat{\alpha}(\mathbf{z}_n) = \mathcal{N}(\mathbf{z}_n|\boldsymbol{\mu}_n, \mathbf{V}_n).
$$

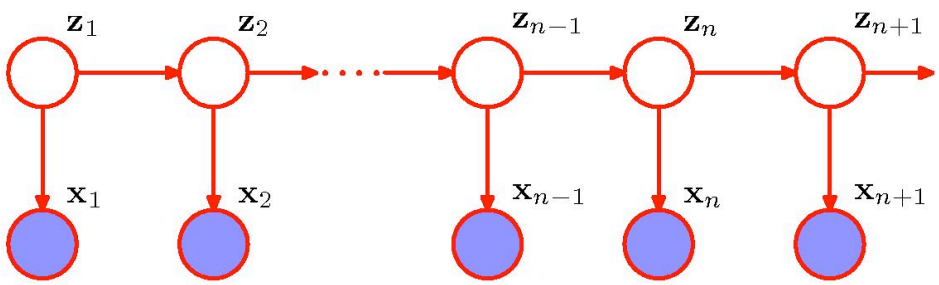
$$
\begin{aligned}
\boldsymbol{\mu}_n &= \mathbf{A}\boldsymbol{\mu}_{n-1} + \mathbf{K}_n(\mathbf{x}_n - \mathbf{C}\mathbf{A}\boldsymbol{\mu}_{n-1}) \\
\mathbf{V}_n &= (\mathbf{I} - \mathbf{K}_n\mathbf{C})\mathbf{P}_{n-1} \\
\mathbf{P}_{n-1} &= \mathbf{A}\mathbf{V}_{n-1}\mathbf{A}^T + \boldsymbol{\Gamma}.
\end{aligned}
$$

and we have also defined the Kalman gain matrix:

$$
\mathbf{K}_n = \mathbf{P}_{n-1}\mathbf{C}^T \left(\mathbf{C}\mathbf{P}_{n-1}\mathbf{C}^T + \boldsymbol{\Sigma}\right)^{-1}.
$$

Kalman Filter

- Let us examine the evolution of the mean:



$$\begin{aligned} \mathbf{z}_n &= \mathbf{A}\mathbf{z}_{n-1} + \mathbf{w}_n, & \mathbf{w} &\sim \mathcal{N}(\mathbf{w}|\mathbf{0}, \mathbf{\Gamma}), \\ \mathbf{x}_n &= \mathbf{C}\mathbf{z}_n + \mathbf{v}_n, & \mathbf{v} &\sim \mathcal{N}(\mathbf{v}|\mathbf{0}, \mathbf{\Sigma}), \\ \mathbf{z}_1 &= \boldsymbol{\mu}_0 + \mathbf{u}, & \mathbf{u} &\sim \mathcal{N}(\mathbf{u}|\mathbf{0}, \mathbf{V}_0). \end{aligned}$$

Prediction of the mean over z_n.

Predicted observation for x_n.

$$\boldsymbol{\mu}_n = \mathbf{A}\boldsymbol{\mu}_{n-1} + \mathbf{K}_n(\mathbf{x}_n - \mathbf{C}\mathbf{A}\boldsymbol{\mu}_{n-1}).$$

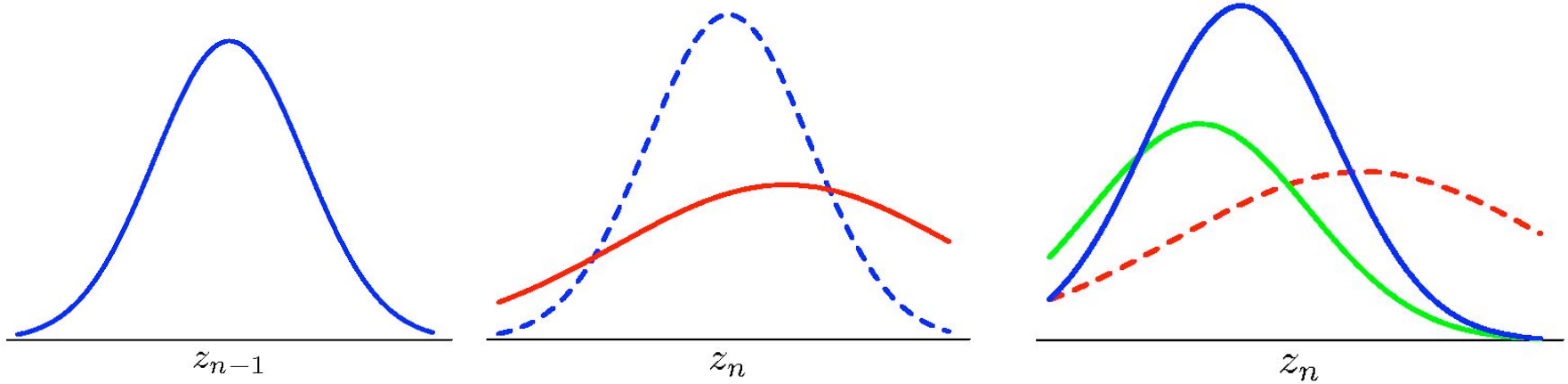
Predicted mean plus the correction term controlled by the Kalman gain matrix.

Error between the predicted observation x_n and the actual observation x_n.

- We can view the Kalman filter as a process of making subsequent predictions and then correcting these predictions in the light of the new observations.

Kalman Filter

- Example:



$p(\mathbf{z}_{n-1}|\mathbf{x}_1, ..., \mathbf{x}_{n-1})$

blue curve

$p(\mathbf{z}_n|\mathbf{x}_1, ..., \mathbf{x}_{n-1})$

red curve

incorporate transition model

$p(\mathbf{z}_n|\mathbf{x}_1, ..., \mathbf{x}_n)$

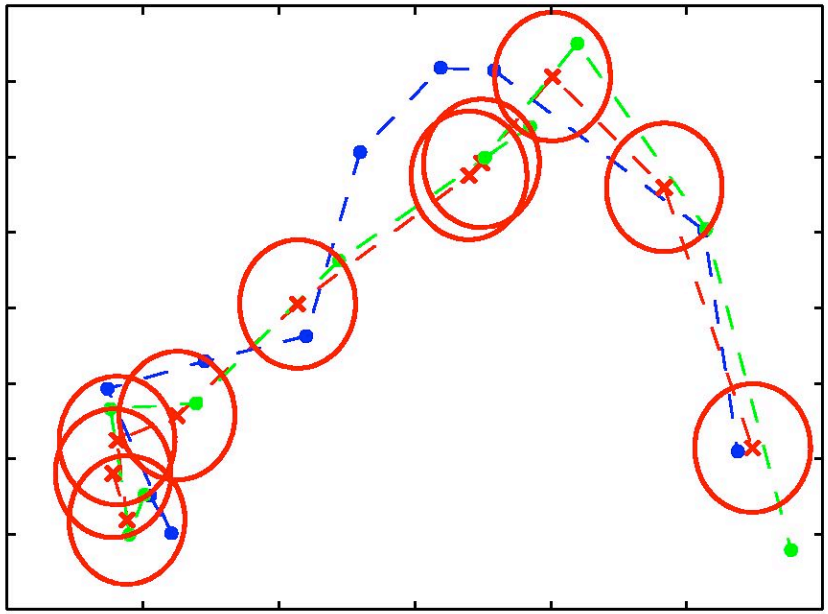
blue curve

incorporate new observation (density of the new point is given by the green curve)

- The new observation has shifted and narrowed the distribution compared to (see red curve) $p(\mathbf{z}_n|\mathbf{x}_1, ..., \mathbf{x}_{n-1})$.

Tracking Example

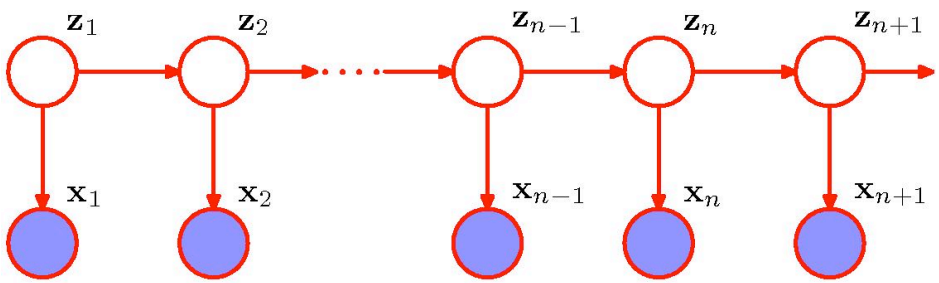
- LDS that is being used to track a moving object in 2-D space:



- Blue points indicate the true position of the object.
- Green points denote the noisy measurements.
- Red crosses indicate the means of the inferred posterior distribution of the positions inferred by the Kalman filter.

Particle Filters

- For dynamical systems that are non-Gaussian (e.g. emission densities are non-Gaussian), we can use sampling methods to find a tractable solution to the inference problem.
- Consider a class of distributions represented by the graphical model:



- Suppose we observed $X_n = \{x_1,\ldots,x_n\}$, and we wish to approximate:

$$
\begin{aligned}
\mathbb{E}[f(\mathbf{z}_n)] &= \int f(\mathbf{z}_n)p(\mathbf{z}_n|\mathbf{X}_n)d\mathbf{z}_n \\
&= \int f(\mathbf{z}_n)p(\mathbf{z}_n|\mathbf{x}_n,\mathbf{X}_{n-1})d\mathbf{z}_n \\
&= \frac{\int f(\mathbf{z}_n)p(\mathbf{x}_n|\mathbf{z}_n)p(\mathbf{z}_n|\mathbf{X}_{n-1})d\mathbf{z}_n}{\int p(\mathbf{x}_n|\mathbf{z}_n)p(\mathbf{z}_n|\mathbf{X}_{n-1})d\mathbf{z}_n} \approx \sum_{l=1}^{L} w_n^{(l)} f(\mathbf{z}_n^{(l)}),
\end{aligned}
$$

Particle Filters

- Hence

$$\mathbb{E}[f(\mathbf{z}_n)] = \int f(\mathbf{z}_n)p(\mathbf{z}_n|\mathbf{X}_n)d\mathbf{z}_n \approx \sum_{l=1}^{L} w_n^{(l)} f(\mathbf{z}_n^{(l)}), \quad \mathbf{z}_n^{(l)} \sim p(\mathbf{z}_n|\mathbf{X}_{n-1}),$$

with importance weights:

$$w_n^{(l)} = \frac{p(\mathbf{x}_n|\mathbf{z}_n^{(l)})}{\sum_{m=1}^{L} p(\mathbf{x}_n|\mathbf{z}_n^{(m)})}.$$

- Hence the posterior $p(z_n \mid X_n)$ is represented by the set of L samples together with the corresponding importance weights.

- We would like to define a sequential algorithm.
- Suppose that a set of samples and weights have been obtained at time step n.
- We wish to find the set of new samples and weights at time step n+1.

Particle Filters

- From our previous result, let $f(\mathbf{z}_n) = p(\mathbf{z}_{n+1}|\mathbf{z}_n)$,

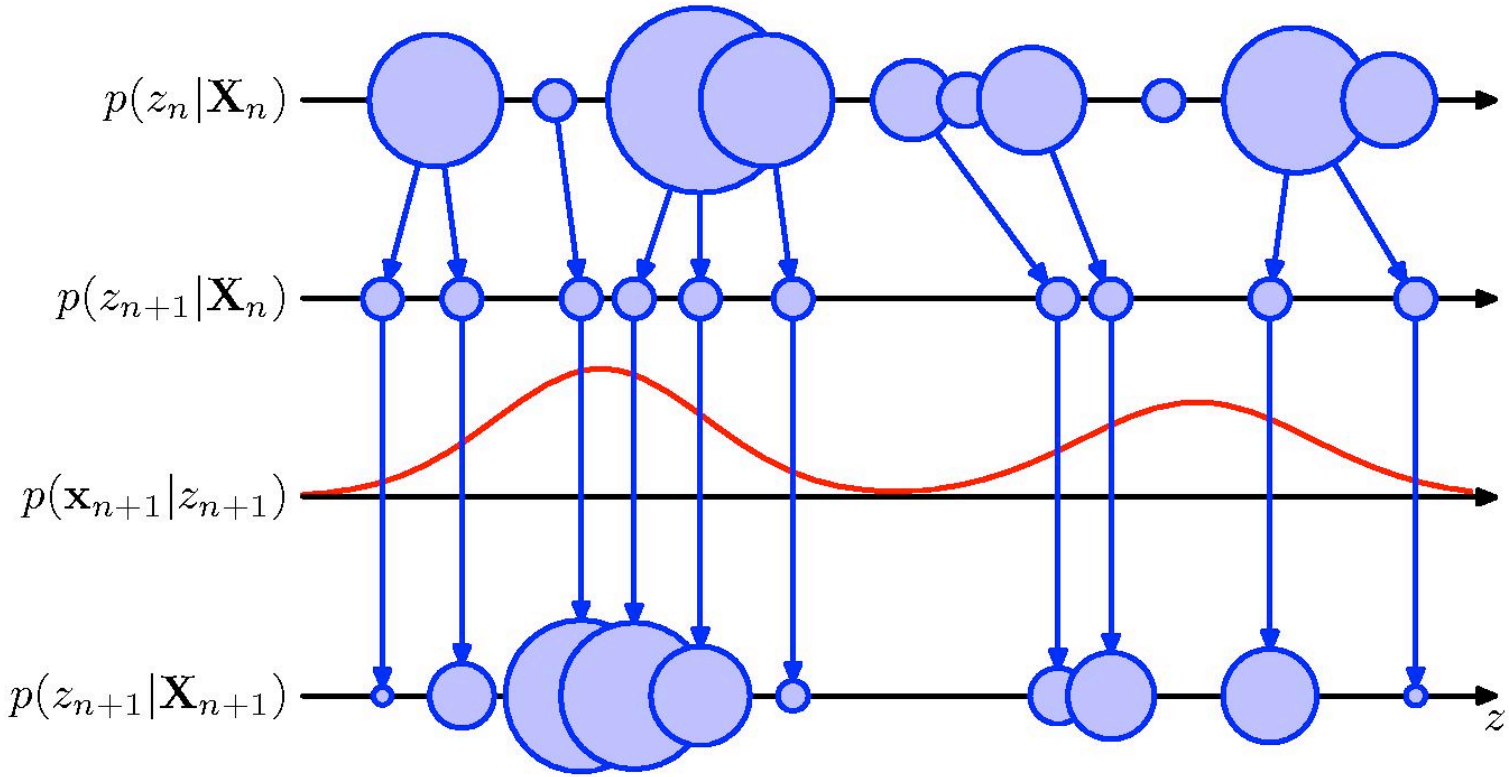
$$
\begin{aligned}
p(\mathbf{z}_{n+1}|\mathbf{X}_n) &= \int p(\mathbf{z}_{n+1}|\mathbf{z}_n) p(\mathbf{z}_n|\mathbf{X}_n) d\mathbf{z}_n \\
&\approx \sum_{l=1}^{L} w_n^{(l)} p(\mathbf{z}_{n+1}|\mathbf{z}_n^{(l)}), \quad \mathbf{z}_n^{(l)} \sim p(\mathbf{z}_n|\mathbf{X}_{n-1}),
\end{aligned}
$$

$$
w_n^{(l)} = \frac{p(\mathbf{x}_n|\mathbf{z}_n^{(l)})}{\sum_{m=1}^{L} p(\mathbf{x}_n|\mathbf{z}_n^{(m)})}.
$$

- Summary of the particle filter algorithm:
  - At time n, we have a sample representation of the posterior distribution $p(z_n \mid X_n)$ expressed as L samples with corresponding weights.
  - We next draw L samples from the mixture distribution (above).
  - For each sample, we then use the new observation to re-evaluate the weights:

$$
w_{n+1}^{(l)} = \frac{p(\mathbf{x}_{n+1}|\mathbf{z}_{n+1}^{(l)})}{\sum_{m=1}^{L} p(\mathbf{x}_{n+1}|\mathbf{z}_{n+1}^{(m)})}.
$$

Example



- At time n, the posterior $p(z_n \mid X_n)$ is represented as a mixture distribution.
- We draw a set of L samples from this distribution (incorporating the transition model).
- The new weights evaluated by incorporating the new observation x_{n+1}.