Statistical Machine Learning

Christian Walder

Machine Learning Research Group
CSIRO Data61

and

College of Engineering and Computer Science
The Australian National University

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(Many figures from C. M. Bishop, "Pattern Recognition and Machine Learning")

Outlines

Part XXI

Sequential Data 1

Sequential Data

- Often data is not *i.i.d.*, *e.g.*
  - time series (finance, daily rainfall, speech, . . .),
  - DNA sequences,
  - Natural language text (English, Chinese, . . .).
- Current data may not be independent of previous data.
- The distribution of the observed data may change as the sequence progresses.
- Note: Use ‘past’ and ‘future’ to describe an order on the observations, but the concept of sequence is not restricted to temporal sequences.

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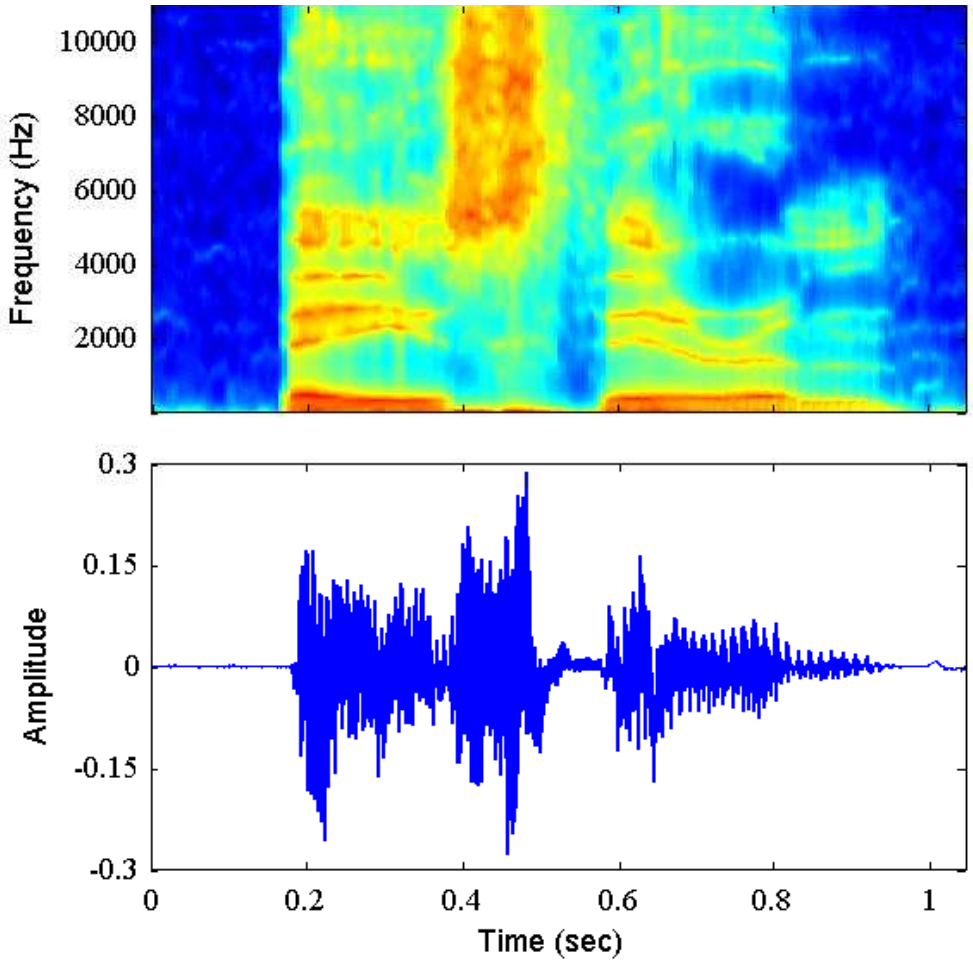
Sequential Data Example



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Stationary vs. Nonstationary Sequential Distributions

- Stationary:
  Data evolves in time, but the distribution from which it is drawn stays the same.
- Nonstationary:
  The generative distribution changes itself with time.

We will focus on the stationary case.

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Sequence Modelling Challenges

- Goal:
  Predict the next value in a sequence.
- Assumption:
  Not all previous data equally influence the next value.
- Technical problem:
  How to store an ever growing history of observations?)
- Assume that recent observations are more likely to be informative for the prediction of the next value than less recent observations.
- Is this always a good assumption?

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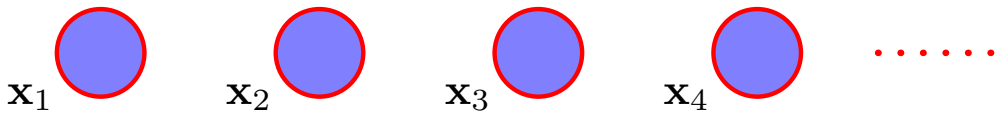
Limitations of Modelling a Sequence as i.i.d.

- Example:
  Binary variable recording whether it rained or not on a day.
- Only information from such a model: frequency of rainfall.
- Can only use the frequency to predict whether it rains tomorrow or not. (Maybe not so bad for Canberra ;-)
- Usually:
  Observing whether it rained today helps to predict the weather for tomorrow.
- Need to relax the *i.i.d.* assumption to grasp this idea.



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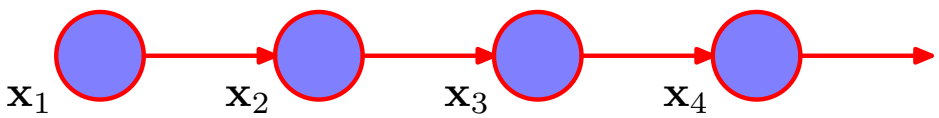
The Markov Model

- One of the simplest ways to relax the i.i.d. assumption.
- Use the product rule to exactly express the joint distribution

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

- Assume that each of the conditional expressions depends only on the most recent.
- First-order Markov chain

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



Markov Model: Forecasting

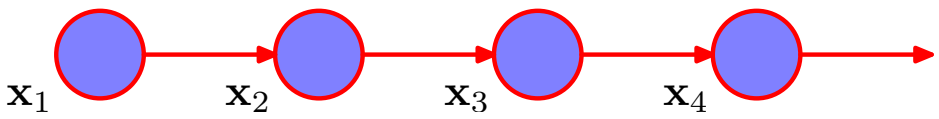
- Given the factorisation of the first-order Markov chain

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

- What is the conditional distribution for observation $\mathbf{x}_n$ given the previous observations?

$$\begin{aligned} p(\mathbf{x}_n \mid \mathbf{x}_1, \ldots, \mathbf{x}_{n-1}) &= \frac{p(\mathbf{x}_1, \ldots, \mathbf{x}_n)}{p(\mathbf{x}_1, \ldots, \mathbf{x}_{n-1})} \\ &= \frac{p(\mathbf{x}_1) \prod_{i=2}^{n} p(\mathbf{x}_i \mid \mathbf{x}_{i-1})}{p(\mathbf{x}_1) \prod_{j=2}^{n-1} p(\mathbf{x}_j \mid \mathbf{x}_{j-1})} \\ &= p(\mathbf{x}_n \mid \mathbf{x}_{n-1}) \end{aligned}$$

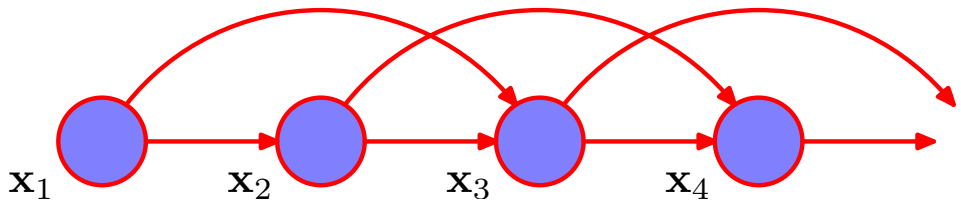
Also clear from the graphical D-separation:



Second-order Markov Chain

- Assume that, say, the trend in the previous observations provides important information in predicting the next value.
- For a trend, we need at least two previous observations.

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



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M^{th}-order Markov Chain

- Extend this idea to an M^{th}-order Markov chain in which the probability of each observation depends on the previous M observations

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_N) = p(\mathbf{x}_1)\, p(\mathbf{x}_2 \mid \mathbf{x}_1) \ldots p(\mathbf{x}_M \mid \mathbf{x}_1, \ldots \mathbf{x}_{M-1}) \times \prod_{n=M+1}^{N} p(\mathbf{x}_n \mid \mathbf{x}_{n-1}, \mathbf{x}_{n-2} \ldots \mathbf{x}_{n-M})$$

- What is a reasonable M?

M^{th}-order Markov Chain

Assuming K states for each variable, how many parameters does a M^{th}-order Markov chain have?

- $M = 0$: no Markov parameter, *i.i.d.* data
- $M = 1$: First-order Markov chain, $K - 1$ parameters for each of the K states of the previous observation. Number of parameters: $K(K-1)$.
- M : M^{th}-order Markov Chain, $K - 1$ parameters for each of the K states of the previous M obervation. Number of parameters: $K^M(K-1)$.
- Number of parameters grows exponentially with the order of the Markov chain. Impractical for larger M.

(Neglects the special case of the first few observations)

Extending the Model

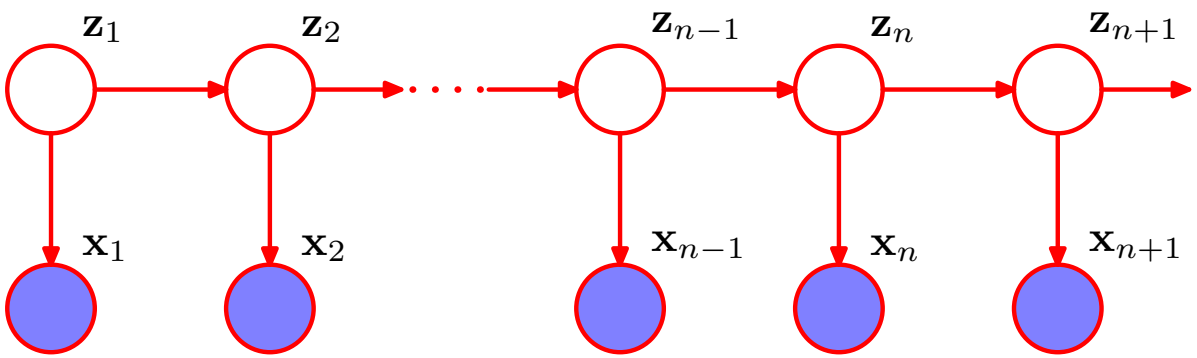
- Goal: We want a model which is NOT restricted to the Markov assumption to any order. BUT can be specified by a limited number of free parameters.
- Use the idea of latent variables to construct a rich class of models out of simple components.
- (Remember mixture of Gaussians.)

State Space Model

- For each observation $\mathbf{x}_n$, a latent variable $\mathbf{z}_n$ is added.
- The type and dimensionality of $\mathbf{z}_n$ can differ from $\mathbf{x}_n$.
- Assume Markovian latent variables, *i.e.*

$$\mathbf{z}_{n+1} \perp\!\!\!\perp \mathbf{z}_{n-1} \,|\, \mathbf{z}_n$$

- As a directed graphical model:



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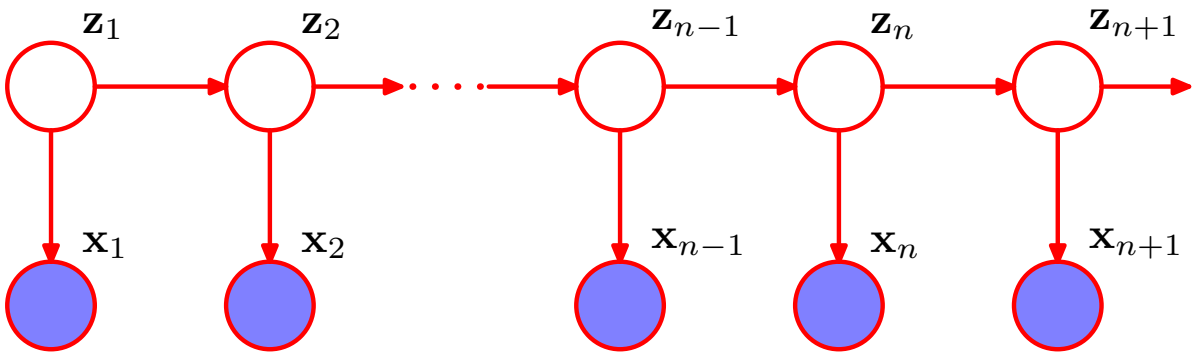
State Space Model - Basic Properties

- Joint distribution:

$$p(\mathbf{x}_1, \ldots, \mathbf{x}_N, \mathbf{z}_1, \ldots, \mathbf{z}_N) = p(\mathbf{z}_1) \left[\prod_{n=2}^{N} p(\mathbf{z}_n \mid \mathbf{z}_{n-1}) \right] \prod_{n=1}^{N} p(\mathbf{x}_n \mid \mathbf{z}_n)$$

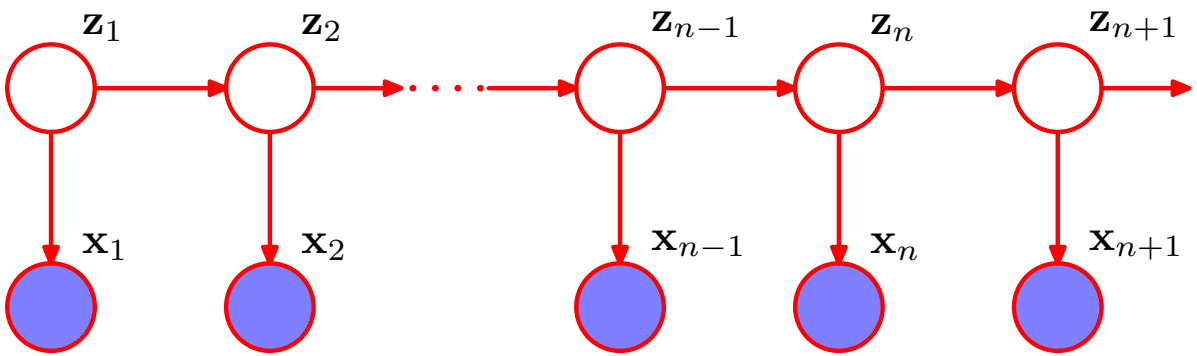
- D-separation:
  - all pairs of $\mathbf{x}_i$ and $\mathbf{x}_j$ are not D-separated.
  - Forecast $p(\mathbf{x}_{n+1} \mid \mathbf{x}_1, \ldots, \mathbf{x}_n)$ depends on the entire history.
  - The $\mathbf{x}_n$ are not (fixed order) Markovian.



State Space Model - Two Important Varieties

Two important models described by this graphical model.

- Hidden Markov Model or HMM:
  - Latent $\mathbf{z}_n$ are discrete.
  - Observed $\mathbf{x}_n$ may be discrete or continuous.
- Linear Dynamical System:
  - Latent and observed variables are continuous.
  - In particular, latent and observed variables are Gaussian with a linear-Gaussian dependence of the conditional distribution on their parents.



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Hidden Markov Model

- State space model with discrete latent variables.

$$p(\mathbf{x}_1,\ldots,\mathbf{x}_N,\mathbf{z}_1,\ldots,\mathbf{z}_N) = p(\mathbf{z}_1)\left[\prod_{n=2}^{N} p(\mathbf{z}_n \mid \mathbf{z}_{n-1})\right]\prod_{n=1}^{N} p(\mathbf{x}_n \mid \mathbf{z}_n)$$

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

- Each step can be viewed as an extension of the mixture distribution model where each of the component densities is $p(\mathbf{x} \mid \mathbf{z})$. Choice of mixture component depends now on the previous state and is represented by $p(\mathbf{z}_n \mid \mathbf{z}_{n-1})$.
- Latent variables are discrete multinomial variables $\mathbf{z}_n$ describing which component of the mixture is responsible for generating the corresponding observable $\mathbf{x}_n$.

Hidden Markov Model: Latent Dynamics

- Assume 1-in-K coding scheme.
- Each latent variable $\mathbf{z}_n$ has K different states.
- Initial latent node $\mathbf{z}_1$ has no parent, therefore the marginal distribution is given by a vector of probabilities $\boldsymbol{\pi}$ with $\pi_k = p(z_{1k} = 1)$ so that

$$p(\mathbf{z}_1 \mid \boldsymbol{\pi}) = \prod_{k=1}^{K} \pi_k^{z_{1k}} \qquad \sum_k \pi_k = 1$$

- The conditional distribution $p(\mathbf{z}_n \mid \mathbf{z}_{n-1})$ is a table (matrix) with $K \times K$ entries, denoted by $\mathbf{A} \in [0,1]^{K \times K}$.
- The elements of $\mathbf{A}$ are called transition probabilities

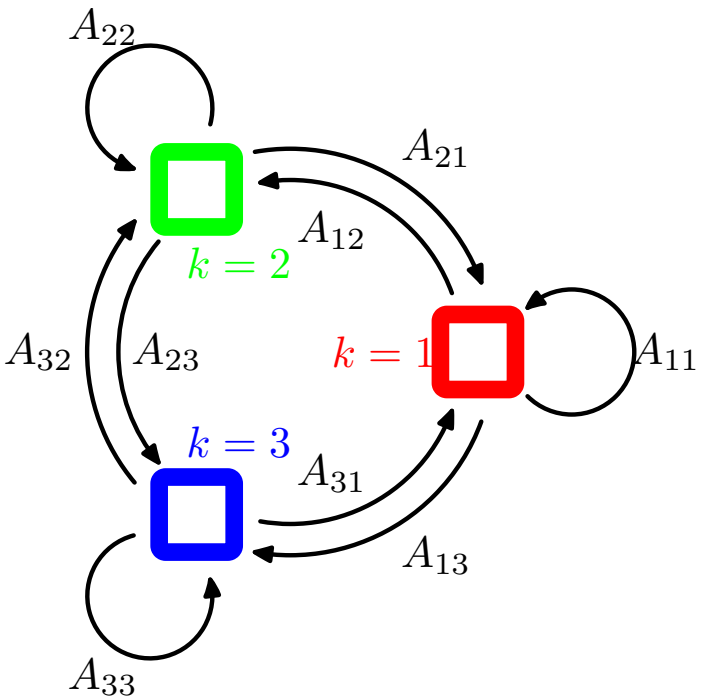
$$A_{jk} = p(z_{n,k} = 1 \mid z_{n-1,j} = 1).$$

satisfying $0 \leq A_{jk} \leq 1$ and $\sum_{k=1}^{K} A_{jk} = 1$.

Hidden Markov Model - Transition Diagram

- Given the state $\mathbf{z}_{n-1}$ at step $n-1$, now what is the next state $\mathbf{z}_n$?

$$p(\mathbf{z}_n \mid \mathbf{z}_{n-1}, \mathbf{A}) = \prod_{k=1}^{K} \prod_{j=1}^{K} A_{jk}^{z_{n-1,j}\, z_{nk}}$$



Transition Diagram for a model with three possible states. Black lines denote the elements of the transition matrix A_{jk}.

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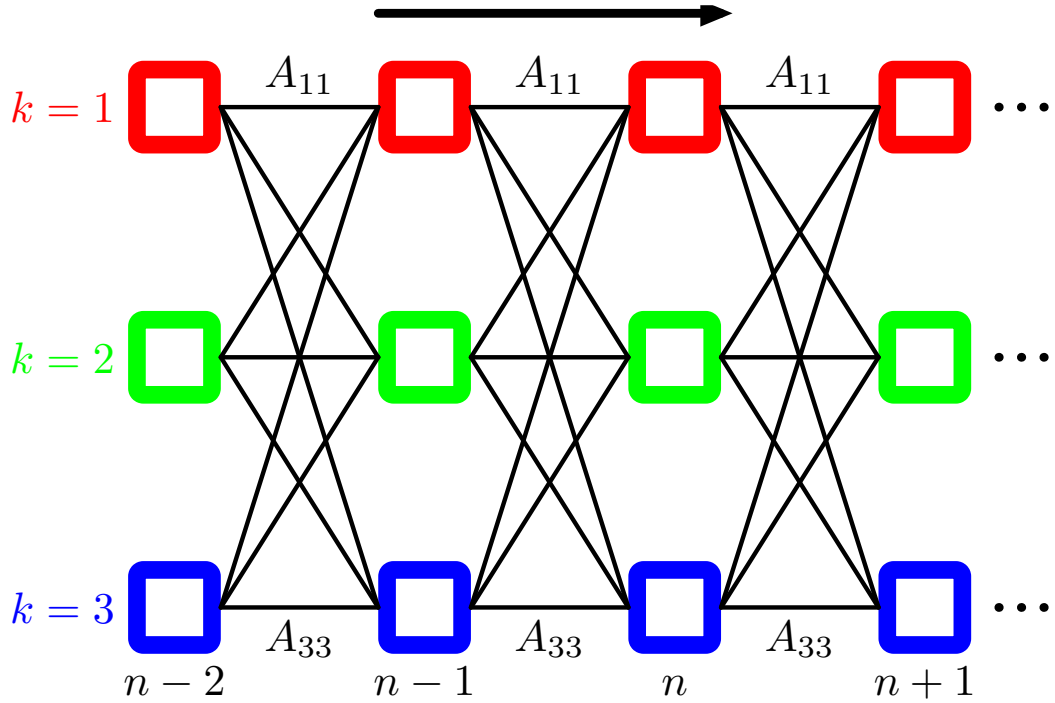
HMM - Unfolded Transition Diagram

- Unfold the transition diagram over the steps to get a lattice, or trellis. (Note, the transitions $\mathbf{A}$ in each step can be different.)



Unfolded Transition Diagram for a model with 3 possible states. Each column corresponds to one latent variable $\mathbf{z}_n$.

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Hidden Markov Model - Emission Probabilities

- Complete the HMM by defining the emission probabilities $p(\mathbf{x}_n \mid \mathbf{z}_n, \phi)$ where ϕ is a set of parameters governing the conditional distributions.
- As $\mathbf{x}_n$ is observed, and ϕ is given, $p(\mathbf{x}_n \mid \mathbf{z}_n, \phi)$ is a K-dimensional vector corresponding to the K possible states of the binary vector $\mathbf{z}_n$.
- Emission probabilities can be represented as

$$p(\mathbf{x}_n \mid \mathbf{z}_n, \phi) = \prod_{k=1}^{K} p(\mathbf{x}_n \mid \phi_k)^{z_{nk}}$$

Hidden Markov Model - Homogeneous

- Remember: Transition probability in a Markov chain $T(\mathbf{z}_{n-1}, \mathbf{z}_n) = p(\mathbf{z}_n \mid \mathbf{z}_{n-1})$.
- A Hidden Markov Model is called homogeneous if the transition probabilities are the same for all steps n

$$p(\mathbf{z}_n \mid \mathbf{z}_{n-1}) = p(\mathbf{z}_{n-1} \mid \mathbf{z}_{n-2}) \qquad \forall\, n = 3, \ldots, N$$

- Assume a homogeneous HMM in the following.

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Homogeneous Hidden Markov Model

- Joint probability distribution over both latent and observed variables

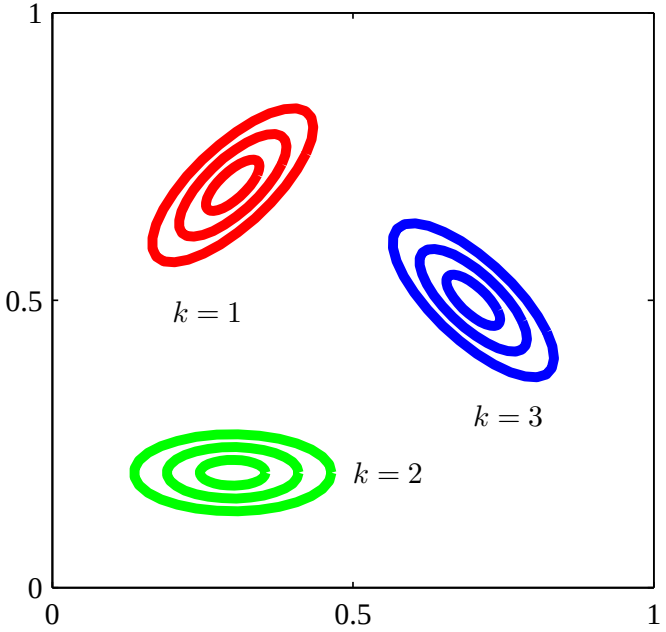
$$p(\mathbf{X}, \mathbf{Z} \mid \boldsymbol{\theta}) = p(\mathbf{z}_1 \mid \boldsymbol{\pi}) \left[\prod_{n=2}^{N} p(\mathbf{z}_n \mid \mathbf{z}_{n-1}, \mathbf{A}) \right] \prod_{m=1}^{N} p(\mathbf{x}_m \mid \mathbf{z}_m, \phi)$$

  where $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$, $\mathbf{Z} = (\mathbf{z}_1, \ldots, \mathbf{z}_N)$, and $\boldsymbol{\theta} = \{\boldsymbol{\pi}, \mathbf{A}, \phi\}$.

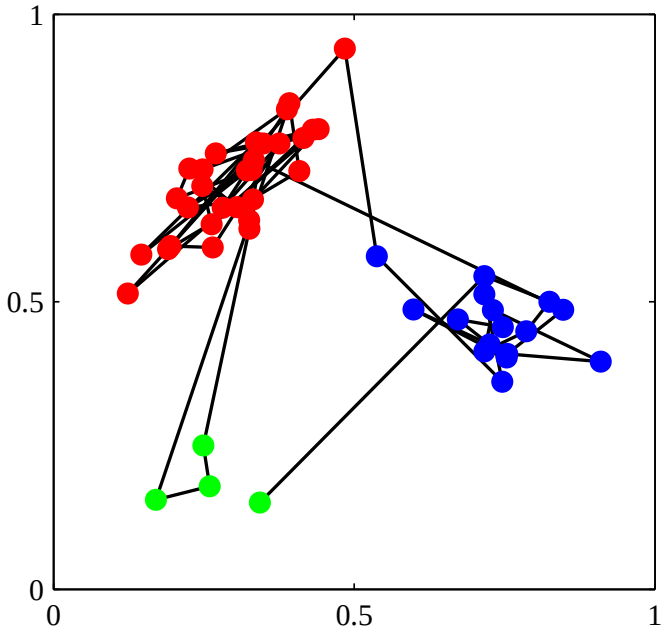
- Most of the discussion will be independent of the particular choice of emission probabilities (e.g. discrete tables, Gaussians, mixture of Gaussians).

Homogeneous HMM - Generative View

- Sampling from a hidden Markov model having a 3-state latent variable $\mathbf{z}$ and a Gaussian emission model $p(\mathbf{x} \mid \mathbf{z})$ where $\mathbf{x} \in \mathbb{R}^2$.



Contours of constant probability for the emission probabilities.



Sampling with 5% probability of change to each of the other states.

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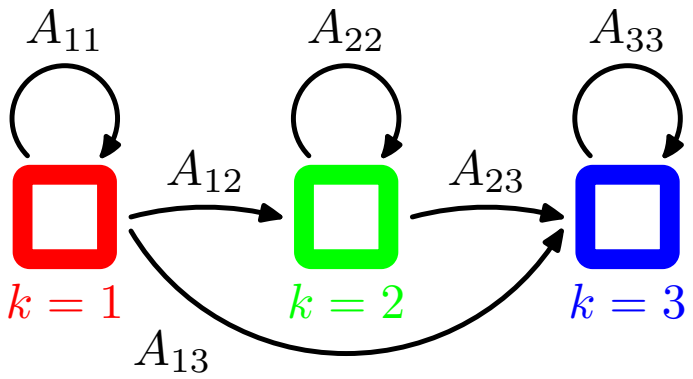
Hidden Markov Model - Variants

- Create variants of HMM by imposing constraints on the transition matrix $\mathbf{A}$.
- Left-to-right HMM : set all elements of $\mathbf{A}$ above the diagonal to zero, $A_{jk} = 0$ for $k < j$.
- Set the initial state probability $p(z_{11}) = 1$ and $p(z_{1j}) = 0$ for $j \neq 1$.
- Then, every sequence is constrained to start in state $k = 1$ and every state left can not be revisited again.



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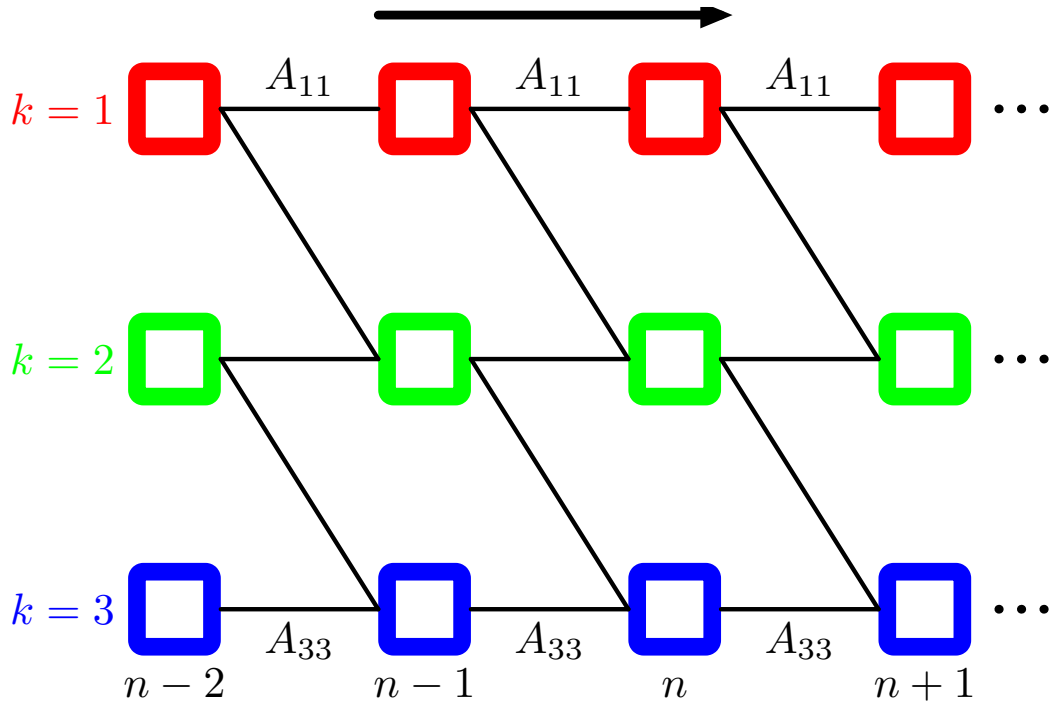
Hidden Markov Model - Variants

- Further restrict the transition matrix $\mathbf{A}$ to ensure that no large changes in the state space occur $A_{jk} = 0$ for $k > j + \Delta$ where Δ is the maximal change of state in one step.



Example of a HMM with $\Delta = 1$.

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Hidden Markov Model - Handwritten Digits

- Digitize the trajectory online.
- $\mathbf{x}_i$ represent fixed width line segments at 16 different angles.
- Coincidentally also $K = 16$ states.
- $\Rightarrow$ 16 $\times$ 16 transition and emission parameter matrices.
- Trained with 45 examples of the digit '2'.
- Left-to-right transmission probability with $\Delta = 1$.
- Upper row: training samples lower row: model samples.