

CSCI567 Machine Learning (Fall 2025)

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Administration

Reminder: HW3 is due on Nov 5th.

Outline

- 1 Principal Component Analysis (PCA)
- 2 Markov models
- 3 Hidden Markov Model

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Dimensionality reduction

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There are many approaches, we focus on a linear method:

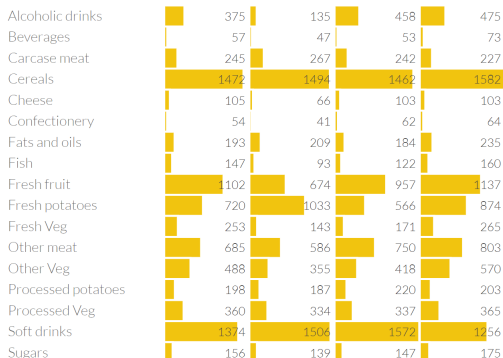
Principal Component Analysis (PCA)

Example

picture from here

Consider the following dataset:

- 17 features, each represents the average consumption of some food

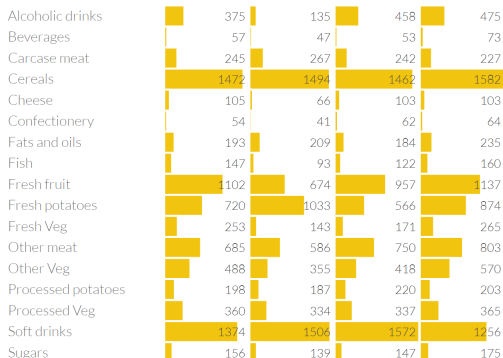


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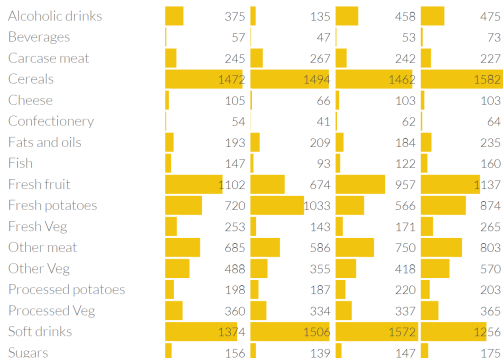


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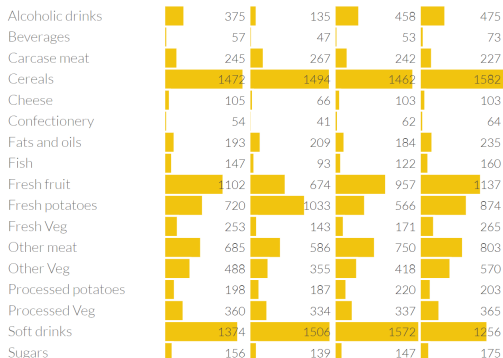
What can you tell?

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What can you tell?

Hard to say anything looking at all these 17 features.

Example

[picture from here](#)

PCA can help us!

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PCA can help us! The **first principal component** of this dataset:



i.e. we **reduce the dimensionality from 17 to just 1.**

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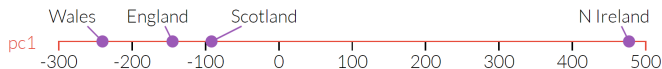
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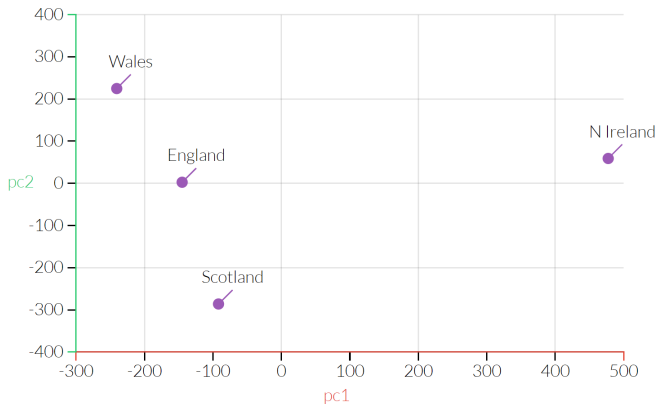
Now one data point is clearly different from the rest!

That turns out to be data from **Northern Ireland**, *the only country not on the island of Great Britain out of the 4 samples.*

Example

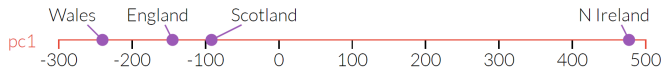
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PCA can find the **second (and more) principal component** of the data too:



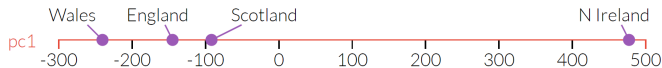
High level idea

How does PCA find these principal components (PC)?



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The first PC is in fact **the direction with the most variance**, i.e. the direction where the data is most spread out.

Finding the first PC

More formally, we want to find a direction $\boldsymbol{v} \in \mathbb{R}^D$ with $\|\boldsymbol{v}\|_2 = 1$, so that the **projection of the dataset on this direction has the most variance**,

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- we will simply assume $\{\mathbf{x}_n\}$ is centered (to avoid notation $\mathbf{x}'_n$)

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where the columns of $\mathbf{U}^T$ are unit **eigenvectors** $\mathbf{u}_1, \dots, \mathbf{u}_D$ of $\mathbf{X}^T \mathbf{X}$ with corresponding **eigenvalues** $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_D \geq 0$.

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Conclusion: the first PC is the top eigenvector of the covariance matrix!

Finding the other PCs

If v_1 is the first PC, then the **second PC** is found via

$$\max_{\mathbf{v}_2: \|\mathbf{v}_2\|_2=1, \mathbf{v}_1^T \mathbf{v}_2=0} \mathbf{v}_2^T (\mathbf{X}^T \mathbf{X}) \mathbf{v}_2$$

i.e. the direction that maximizes the variance among all other dimensions

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Conclusion: the d -th principal component is the d -th eigenvector (sorted by the eigenvalue from largest to smallest).

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(Optional) Step 4 “Reconstruct” original dataset as $\mathbf{XV}\mathbf{V}^T \in \mathbb{R}^{N \times D}$

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For **visualization**, also often pick $p = 1$ or $p = 2$.

Another visualization example

A famous study of **genetic map**

- dataset: **genomes of 1,387 Europeans**

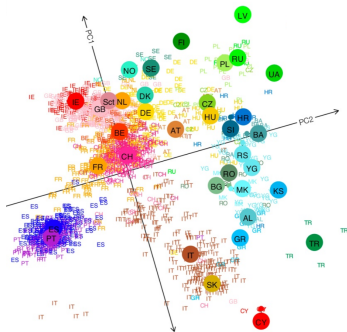
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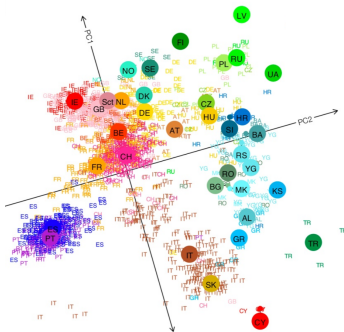
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Genetic variation is highly structured by geography; top PCs correspond to geographic factors.

Compression Example

Dataset: 256×256 ($\approx 65K$ pixels)
dimensional images of about 2500
faces, all framed similarly
($N = 2500$, $D \approx 65,000$)

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The principal components (called
eigenfaces $\in \mathbb{R}^D$) are themselves
interpretable too!



Figure 2. Seven of the eigenfaces calculated from the input images of Figure 1.

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PCA finds the subspace (out of the
space of all 256×256 images) where
faces lie



Figure 2. Seven of the eigenfaces calculated from the input images of Figure 1.

Word embedding via PCA

Create **meaningful vector representation** of words; see project.



Outline

- 1 Principal Component Analysis (PCA)
- 2 Markov models
 - Markov chain
 - Learning Markov models
- 3 Hidden Markov Model

Sequential data and Markov models

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- text or speech data
- stock market data
- gene data

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Markov models are powerful probabilistic tools to analyze them:

Sequential data and Markov models

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- text or speech data
- stock market data
- gene data

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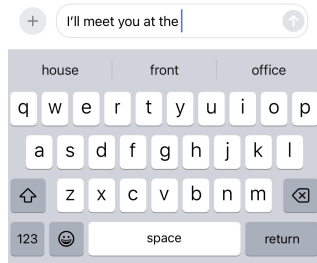
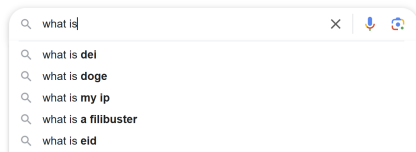
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Markov models are powerful probabilistic tools to analyze them:

- not the state-of-the-art for e.g. Natural Language Processing (NLP)
- but still extremely useful in many areas (in particular, it is the foundation of *reinforcement learning*)

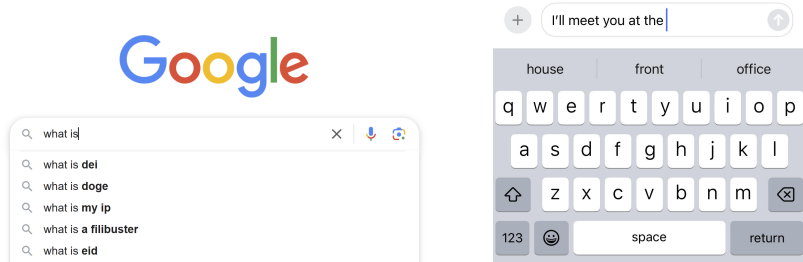
A motivating example

Next word prediction



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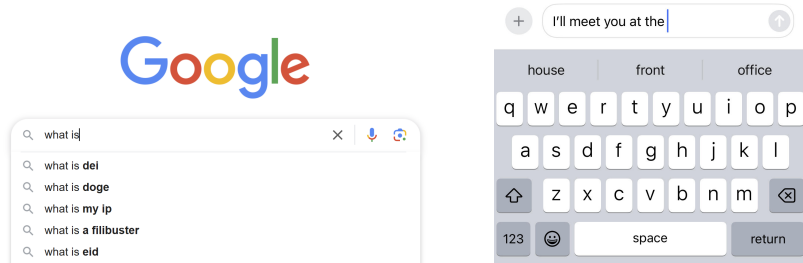


Can be formulated as predicting the probability of the next word/state:

$$P(Z_{t+1} \mid Z_1, \dots, Z_t)?$$

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abbreviated as $P(Z_{t+1} \mid \mathbf{Z}_{1:t})$ (i.e., $\mathbf{Z}_{1:t}$ denotes the sequence $Z_1, \dots, Z_t$).

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- $P(Z_1 = s) = \pi_s$
- $(\{\pi_s\}, \{a_{s,s'}\}) = (\boldsymbol{\pi}, \mathbf{A})$ are **parameters of the model**

Examples

- Example 1 (**Language model**)

States $[S]$ represent a dictionary of words,

$$a_{\text{ice,cream}} = P(Z_{t+1} = \text{cream} \mid Z_t = \text{ice})$$

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- Example 2 (**Weather**)

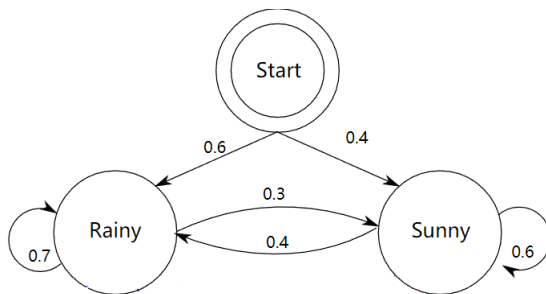
States $[S]$ represent weather at each day

$$a_{\text{sunny,rainy}} = P(Z_{t+1} = \text{rainy} \mid Z_t = \text{sunny})$$

Graph representation

picture from Wikipedia

It is intuitive to represent a Markov model as a **graph**



High-order Markov chain

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High-order Markov chain

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$$\begin{aligned} P(Z_{t+1} = \text{office} \mid Z_{1:t} = \text{I'll meet you at the}) \\ = P(Z_{t+1} = \text{office} \mid Z_t = \text{the}) \quad (\text{bigram, unreasonable}) \end{aligned}$$

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Higher-order Markov chains make it more reasonable, e.g.

$$P(Z_{t+1} \mid Z_{1:t}) = P(Z_{t+1} \mid Z_t, Z_{t-1}) \quad (\text{second-order Markov})$$

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i.e. the current word only depends on the last two words (the **trigram** model).

n -gram model

$$\begin{aligned} &P(Z_{t+1} = \text{office} \mid Z_{1:t} = \text{l'll meet you at the}) \\ &= P(Z_{t+1} = \text{office} \mid Z_{t-1:t} = \text{at the}) \end{aligned} \quad (\text{trigram})$$

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For simplicity, we will only consider standard Markov chains.

Learning from examples

Now suppose we have observed N sequences of examples:

- $z_{1,1}, \dots, z_{1,T}$
- $\dots$
- $z_{n,1}, \dots, z_{n,T}$
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From these observations how do we *learn the model parameters* $(\pi, \mathbf{A})$?

Finding the MLE

Same story, find the **MLE**.

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$$= \sum_s \mathbb{I}[z_1 = s] \ln \pi_s + \sum_{s, s'} \left(\sum_{t=2}^T \mathbb{I}[z_{t-1} = s, z_t = s'] \right) \ln a_{s, s'}$$

Finding the MLE

Summing over all N sequences, we obtain the joint log-likelihood:

$$L(\boldsymbol{\pi}, \mathbf{A}) = \sum_s (\text{\#initial states with value } s) \ln \pi_s \\ + \sum_{s,s'} (\text{\#transitions from } s \text{ to } s') \ln a_{s,s'}$$

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The MLE $\operatorname{argmax}_{\boldsymbol{\pi}, \mathbf{A}} L(\boldsymbol{\pi}, \mathbf{A})$ is:

$$\pi_s \propto \text{\#initial states with value } s \\ a_{s,s'} \propto \text{\#transitions from } s \text{ to } s'$$

Example

Suppose we observed the following 2 sequences of length 5

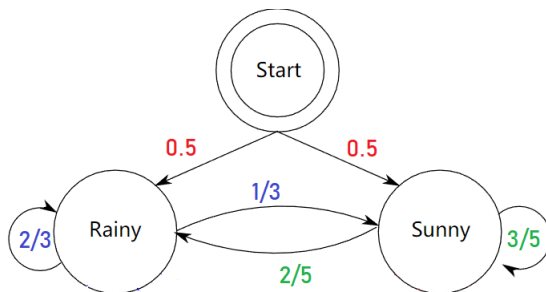
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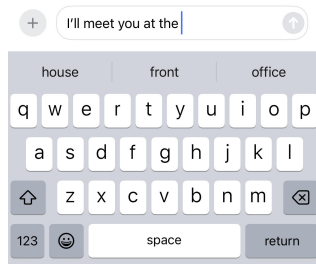
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MLE is the following model



n -gram example

Recall: I'll meet you at the _____.

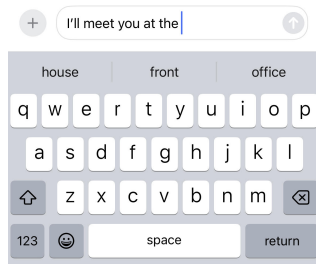


n -gram example

Recall: I'll meet you at the _____.

Suppose

- we use a 5-gram model

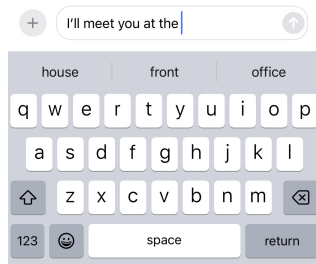


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Recall: I'll meet you at the _____.

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- we use a 5-gram model
- “meet you at the” appears 1000 times in the training set:
 - “meet you at the house” appears 500 times
 - “meet you at the front” appears 300 times
 - “meet you at the office” appears 200 times



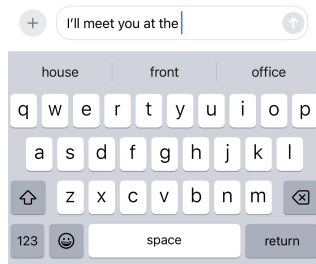
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Then the model predicts the next word as “house” with prob. 0.5, “front” with prob. 0.3, and “office” with prob. 0.2.



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adapted from Stanford CS224n

After learning the model, can also **generate texts** by repeatedly sampling conditioning on what have been generated:

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Surprisingly grammatical! but *incoherent*...

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Outline

- 1 Principal Component Analysis (PCA)
- 2 Markov models
- 3 Hidden Markov Model
 - Inferring HMMs
 - Learning HMMs

Markov model with outcomes/observations

Now suppose each state Z_t also “emits” some **outcome/observation** $X_t \in [O]$ based on the following model

$$P(X_t = o \mid Z_t = s) = b_{s,o} \quad (\text{emission probability})$$

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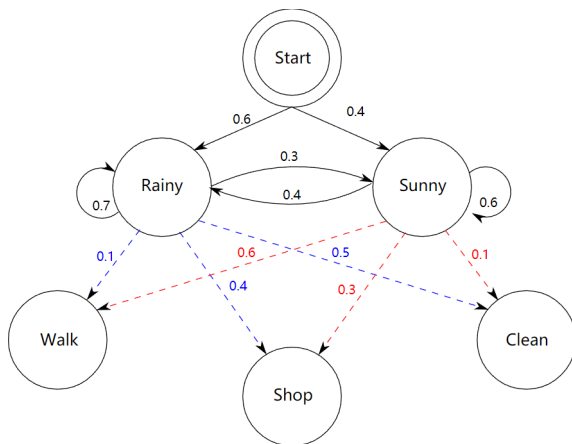
independent of anything else.

The model parameters are $(\{\pi_s\}, \{a_{s,s'}\}, \{b_{s,o}\}) = (\boldsymbol{\pi}, \boldsymbol{A}, \boldsymbol{B})$.

Another (toy) running example

picture from Wikipedia

On each day, we also observe **Bob's activity: walk, shop, or clean**, which only depends on the weather of that day.



Joint likelihood

The joint log-likelihood of a **state-outcome sequence** $z_1, x_1, \dots, z_T, x_T$ is

$$\ln P(Z_{1:T} = z_{1:T}, X_{1:T} = x_{1:T})$$

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 &= \ln \pi_{z_1} + \sum_{t=2}^T \ln a_{z_{t-1}, z_t} + \sum_{t=1}^T \ln b_{z_t, x_t}
 \end{aligned}$$

Learning the model

If we observe N state-outcome sequences: $z_{n,1}, x_{n,1}, \dots, z_{n,T}, x_{n,T}$ for $n = 1, \dots, N$, the MLE is again very simple (verify yourself):

$$\pi_s \propto \text{\textcolor{blue}{\#initial states with value } } s$$

$$a_{s,s'} \propto \text{\textcolor{blue}{\#transitions from } } s \text{ to } s'$$

$$b_{s,o} \propto \text{\textcolor{blue}{\#state-outcome pairs } } (s, o)$$

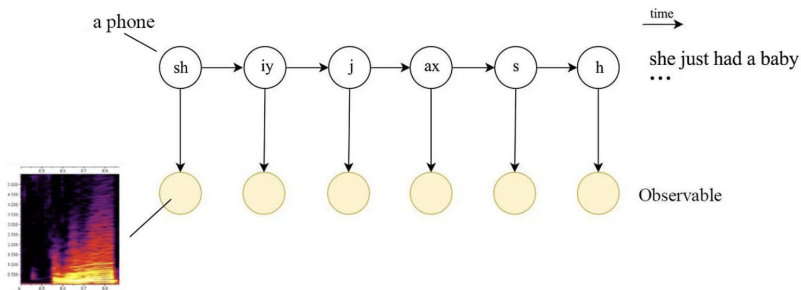
Hidden Markov models

However, *most often we do not observe the states!* Hence the name
Hidden Markov Model (HMM)

Hidden Markov models

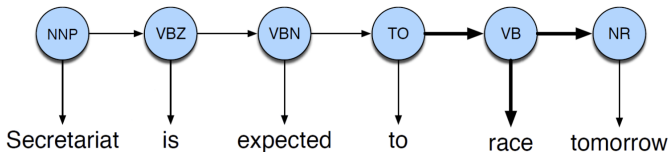
However, *most often we do not observe the states!* Hence the name **Hidden Markov Model (HMM)**

- **speech recognition**: observe the speech $X_{1:T}$ but not the underlying words/phones $Z_{1:T}$



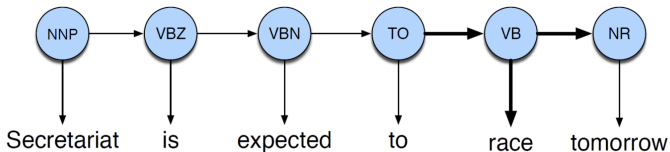
Hidden Markov models (cont.)

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See programming project!

Learning HMMs

How to learn HMMs?

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- then discuss how to **learn** the model (key: **EM**)

What can we infer about an HMM?

Knowing the parameter of an HMM, we can infer

- **most likely hidden states path, given an observation sequence**

$$\operatorname{argmax}_{z_{1:T}} P(Z_{1:T} = z_{1:T} \mid X_{1:T} = x_{1:T})$$

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- **the probability of observing some sequence**

$$P(X_{1:T} = x_{1:T})$$

e.g. prob. of observing Bob's activities "walk, walk, shop, clean, walk, shop, shop" for one week

What can we infer for a known HMM?

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- **the state at some point, given an observation sequence**

$$P(Z_t = s \mid X_{1:T} = x_{1:T})$$

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e.g. given Bob's activities for one week, how was the weather like on Wed and Thu?

Forward and backward messages

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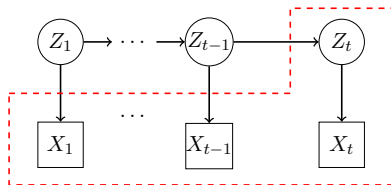
- **backward messages**: for each s and t

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Computing forward messages

Key: *establish recursion*

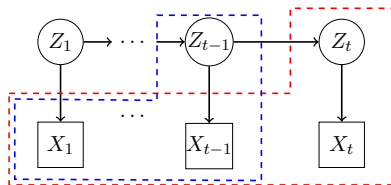
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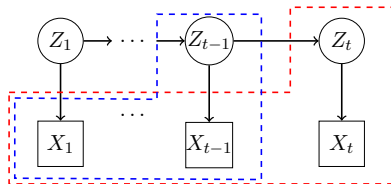
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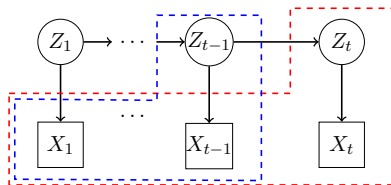
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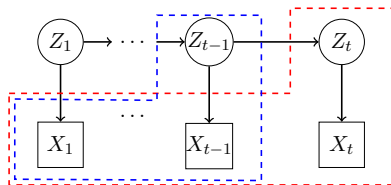
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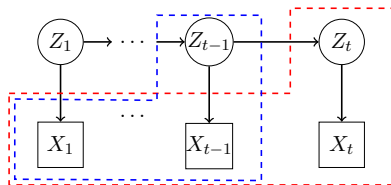
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Base case: $\alpha_s(1) = P(Z_1 = s, X_1 = x_1) = \pi_s b_{s,x_1}$

Forward procedure

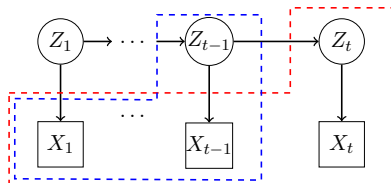
Forward procedure

For all $s \in [S]$, compute $\alpha_s(1) = \pi_s b_{s,x_1}$.

For $t = 2, \dots, T$

- for each $s \in [S]$, compute

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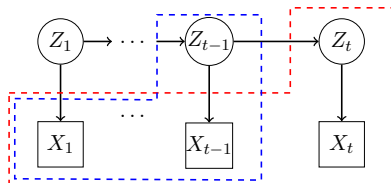
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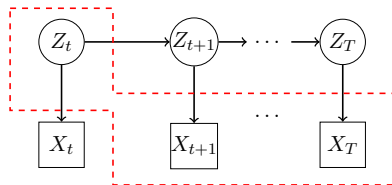
- $O(S^2T)$ time
- $O(ST)$ space



Computing backward messages

Again, establish a recursion

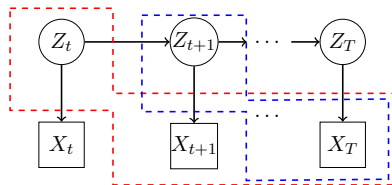
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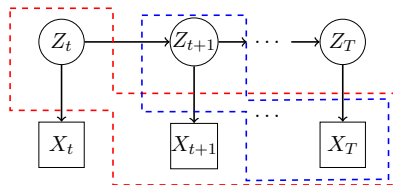
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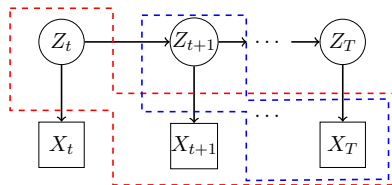
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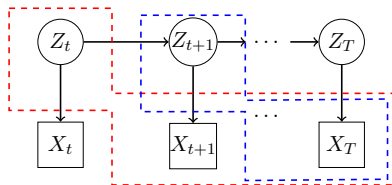
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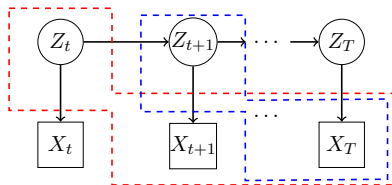
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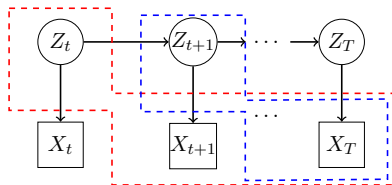
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Base case: $\beta_s(T) = 1$

Backward procedure

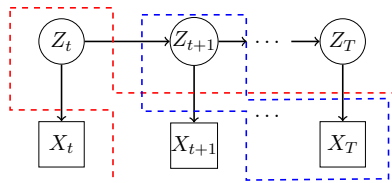
Backward procedure

For all $s \in [S]$, set $\beta_s(T) = 1$.

For $t = T - 1, \dots, 1$

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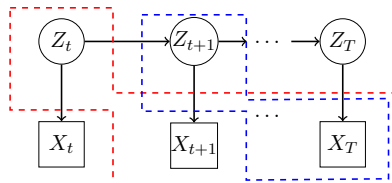
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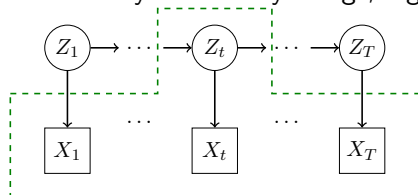
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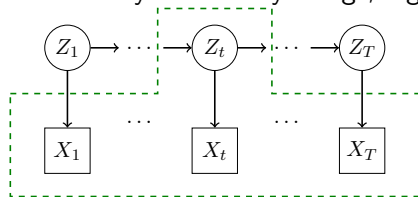
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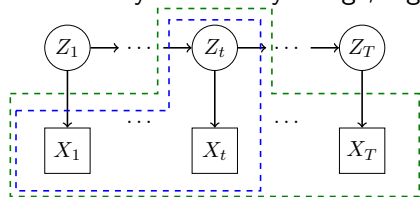
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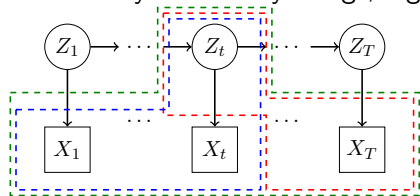
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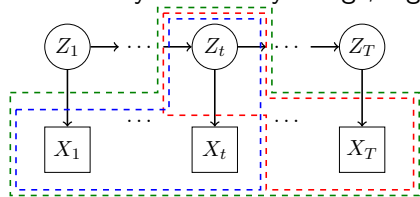
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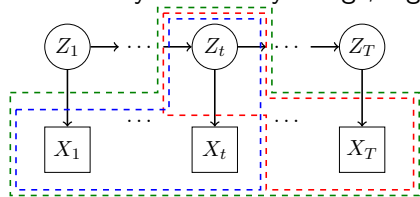


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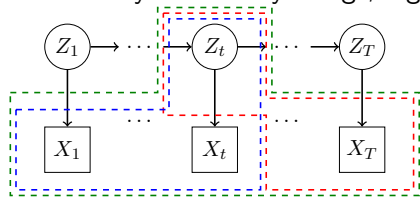
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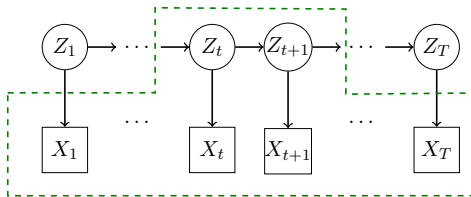
the probability of observing the sequence $x_{1:T}$.

This is true for any t ; a good way to check correctness of your code.

Using forward and backward messages

Another example: the conditional probability of transition s to s' at time t

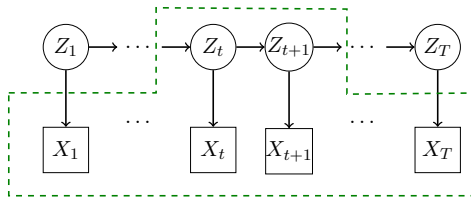
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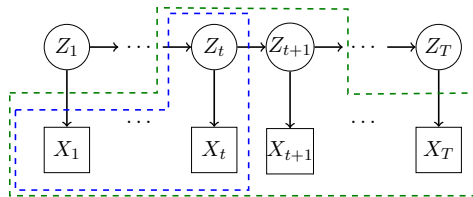
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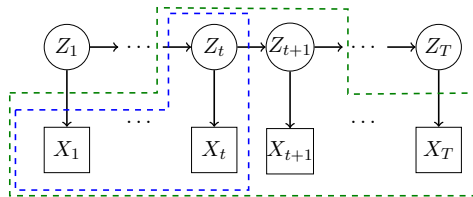
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$$= \alpha_s(t) P(Z_{t+1} = s' \mid Z_t = s) P(X_{t+1:T} = x_{t+1:T} \mid Z_{t+1} = s')$$



Using forward and backward messages

Another example: the conditional probability of transition s to s' at time t

$$\xi_{s,s'}(t)$$

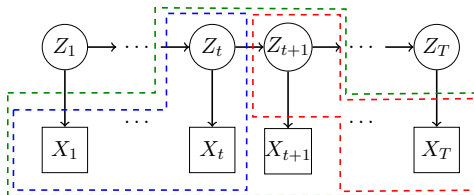
$$= P(Z_t = s, Z_{t+1} = s' \mid X_{1:T} = x_{1:T})$$

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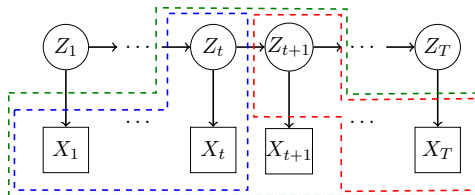
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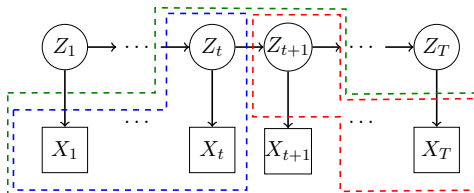
$$= \alpha_s(t)a_{s,s'}b_{s',x_{t+1}}\beta_{s'}(t+1)$$



Using forward and backward messages

Another example: the conditional probability of transition s to s' at time t

$$\begin{aligned}
 & \xi_{s,s'}(t) \\
 &= P(Z_t = s, Z_{t+1} = s' \mid X_{1:T} = x_{1:T}) \\
 &\propto P(Z_t = s, Z_{t+1} = s', X_{1:T} = x_{1:T}) \\
 &= P(Z_t = s, X_{1:t} = x_{1:t}) P(Z_{t+1} = s', X_{t+1:T} = x_{t+1:T} \mid Z_t = s, X_{1:t} = x_{1:t}) \\
 &= \alpha_s(t) P(Z_{t+1} = s' \mid Z_t = s) P(X_{t+1:T} = x_{t+1:T} \mid Z_{t+1} = s') \\
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 &= \alpha_s(t) a_{s,s'} b_{s',x_{t+1}} \beta_{s'}(t+1)
 \end{aligned}$$



The normalization constant is in fact again $P(X_{1:T} = x_{1:T})$

Finding the most likely path

Can't use forward and backward messages directly to find the most likely path, but it is **very similar to the forward procedure**.

Finding the most likely path

Can't use forward and backward messages directly to find the most likely path, but it is **very similar to the forward procedure**. Key: compute

$$\delta_s(t) = \max_{z_{1:t-1}} P(Z_t = s, Z_{1:t-1} = z_{1:t-1}, X_{1:t} = x_{1:t})$$

the probability of the most likely path for time $1 : t$ ending at state s

Computing $\delta_s(t)$

Observe

$$\delta_s(t) = \max_{z_{1:t-1}} P(Z_t = s, Z_{1:t-1} = z_{1:t-1}, X_{1:t} = x_{1:t})$$

Computing $\delta_s(t)$

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$$\begin{aligned}\delta_s(t) &= \max_{z_{1:t-1}} P(Z_t = s, Z_{1:t-1} = z_{1:t-1}, X_{1:t} = x_{1:t}) \\ &= \max_{s'} \max_{z_{1:t-2}} P(Z_t = s, Z_{t-1} = s', Z_{1:t-2} = z_{1:t-2}, X_{1:t} = x_{1:t})\end{aligned}$$

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 &= b_{s,x_t} \max_{s'} a_{s',s} \delta_{s'}(t-1) \quad (\text{recursion!})
 \end{aligned}$$

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Base case: $\delta_s(1) = P(Z_1 = s, X_1 = x_1) = \pi_s b_{s,x_1}$

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Base case: $\delta_s(1) = P(Z_1 = s, X_1 = x_1) = \pi_s b_{s,x_1}$

Exactly the same as forward messages except replacing “sum” by “max”!

Viterbi Algorithm (!)

Viterbi Algorithm

For each $s \in [S]$, compute $\delta_s(1) = \pi_s b_{s,x_1}$.

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Example: $x_{1:4} = \text{clean, shop, walk, walk}$

Viterbi Algorithm

For each $s \in [S]$, compute $\delta_s(1) = \pi_s b_{s,x_1}$.

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For each $s \in [S]$, compute $\delta_s(1) = \pi_s b_{s,x_1}$.

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$$\delta_{\text{sunny}}(1) = \pi_{\text{sunny}} b_{\text{sunny}, \text{clean}}$$

Example: $x_{1:4} = \text{clean, shop, walk, walk}$

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...

$$\delta_{\text{sunny}}(1) = \pi_{\text{sunny}} b_{\text{sunny}, \text{clean}}$$

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Example: $x_{1:4} = \text{clean, shop, walk, walk}$

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$$\delta_{\text{sunny}}(1) = \pi_{\text{sunny}} b_{\text{sunny}, \text{clean}}$$

$$\delta_{\text{rainy}}(1) = \pi_{\text{rainy}} b_{\text{rainy}, \text{clean}}$$

$$\delta_{\text{sunny}}(1) = 0.25$$

$$\delta_{\text{rainy}}(1) = 0.4$$

(numbers are made up here)

Example: $x_{1:4} = \text{clean, shop, walk, walk}$

Viterbi Algorithm

...

For each $t = 2, \dots, T$ and each $s \in [S]$, compute

$$\delta_s(t) = b_{s,x_t} \max_{s'} a_{s',s} \delta_{s'}(t-1), \quad \Delta_s(t) = \operatorname{argmax}_{s'} a_{s',s} \delta_{s'}(t-1).$$

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$$\delta_{\text{sunny}}(2) = b_{\text{sunny},\text{shop}} \max_{s' \in \{\text{sunny}, \text{rainy}\}} a_{s',\text{sunny}} \delta_{s'}(1)$$

$$\delta_{\text{sunny}}(1) = 0.25$$

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Viterbi Algorithm

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Example: $x_{1:4} = \text{clean, shop, walk, walk}$

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$$\delta_{\text{sunny}}(1) = 0.25$$

$$\delta_{\text{sunny}}(2) = 0.1$$

$$\delta_{\text{rainy}}(1) = 0.4$$

$$\delta_{\text{rainy}}(2) = 0.19$$

Example: $x_{1:4} = \text{clean, shop, walk, walk}$

Viterbi Algorithm

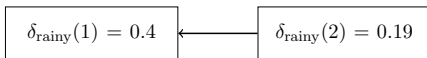
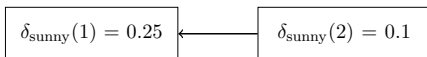
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Arrows represent the “**argmax**”, i.e. $\Delta_s(t)$.

Example: $x_{1:4} = \text{clean, shop, walk, walk}$

Viterbi Algorithm

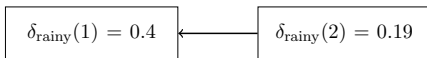
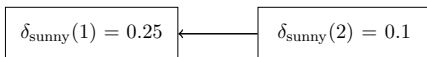
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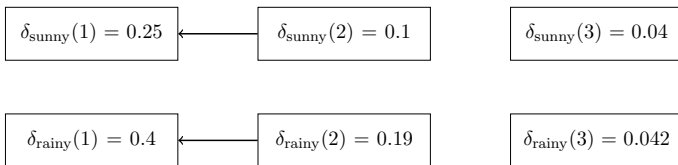
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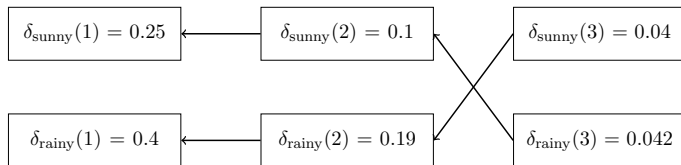
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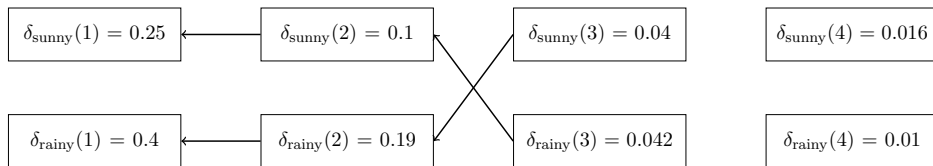
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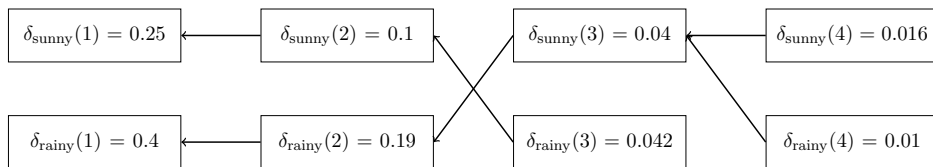
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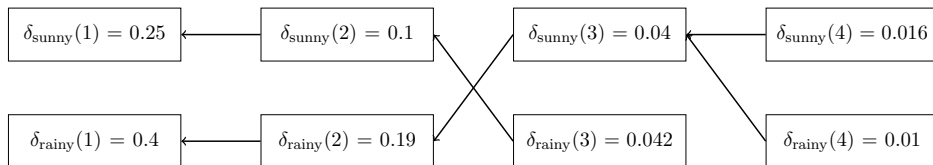
Viterbi Algorithm

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Backtracking: let $z_T^* = \operatorname{argmax}_s \delta_s(T)$.

For each $t = T, \dots, 2$: set $z_{t-1}^* = \Delta_{z_t^*}(t)$.

Output the most likely path $z_1^*, \dots, z_T^*$.



The most likely path is “

”

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Viterbi Algorithm

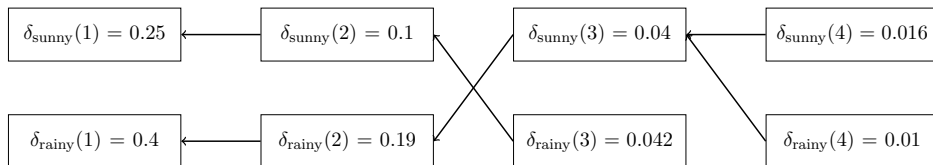
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$$z_4^* = \operatorname{argmax}_{s \in \{\text{sunny, rainy}\}} \delta_s(4)$$



The most likely path is “

”

Example: $x_{1:4} = \text{clean, shop, walk, walk}$

Viterbi Algorithm

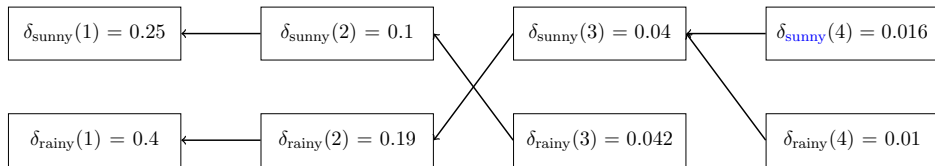
...

Backtracking: let $z_T^* = \operatorname{argmax}_s \delta_s(T)$.

For each $t = T, \dots, 2$: set $z_{t-1}^* = \Delta_{z_t^*}(t)$.

Output the most likely path $z_1^*, \dots, z_T^*$.

$$z_4^* = \operatorname{argmax}_{s \in \{\text{sunny}, \text{rainy}\}} \delta_s(4) = \text{sunny},$$



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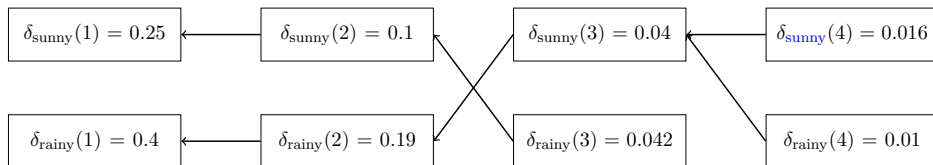
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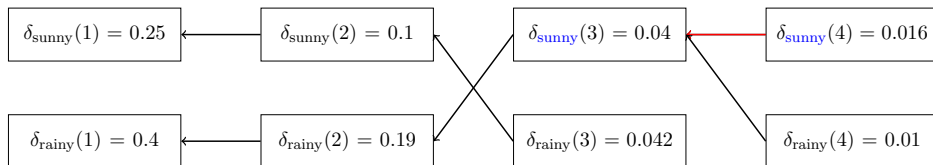
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(just follow the arrow!)

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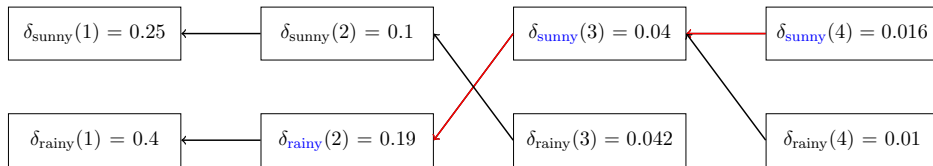
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The most likely path is “ **rainy, sunny, sunny** ”

Example: $x_{1:4} = \text{clean, shop, walk, walk}$

Viterbi Algorithm

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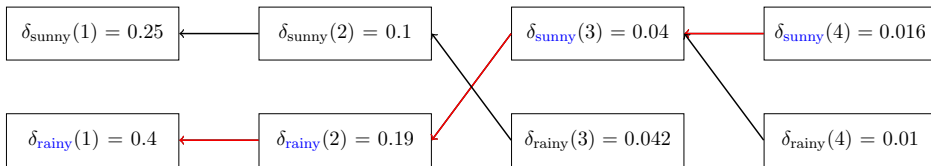
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Need to apply **EM** again! Known as the **Baum–Welch algorithm**.

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We have discussed how to compute

$$\begin{aligned} \gamma_s(t) &= P(Z_t = s \mid X_{1:T} = x_{1:T}) \\ \xi_{s, s'}(t) &= P(Z_t = s, Z_{t+1} = s' \mid X_{1:T} = x_{1:T}) \end{aligned}$$

Applying EM: M-Step

The maximizer of complete log-likelihood is simply doing **weighted counting** (compared to the unweighted counting on Slide 36):

$$\pi_s \propto \sum_n \gamma_s^{(n)}(1) = \mathbb{E}_q [\text{\textcolor{blue}{\#initial states with value } } s]$$

$$a_{s,s'} \propto \sum_n \sum_{t=1}^{T-1} \xi_{s,s'}^{(n)}(t) = \mathbb{E}_q [\text{\textcolor{blue}{\#transitions from } } s \text{ to } s']$$

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(Recall how EM for GMM updates parameters using weighted averages.)

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Step 3 Return to Step 1 if not converged

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Several algorithms:

- forward and backward procedures
- inferring HMMs based on forward and backward messages
- Viterbi algorithm and variants (see today's discussion)
- Baum–Welch algorithm