Time Series Clustering

Machine Learning for Behavioral Data

May 9, 2022

Today's Topic

Week	Lecture/Lab
9	Spring Break
10	Guest Lecture: Neuroscience
11	Unsupervised Learning
12	**Unsupervised Learning**
13	Ethical Machine Learning
14	Ethical Machine Learning
15	Project Presentations

- **K-Means, Spectral Clustering**
- **Choosing the optimal K***
- **Clustering time-series data**

Getting ready for today’s lecture…

- **If not done yet**: clone the repository containing the Jupyter notebook and data for today’s lecture into your Noto workspace
- SpeakUp room for today’s lecture:

https://go.epfl.ch/mlbd-lecture

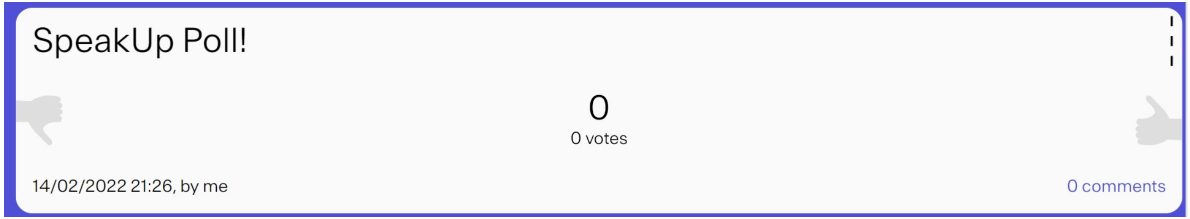
Short quiz about the past…

In K-Means, which of the following parameters affect the goodness of the solution?

a) Number of iterations

b) Initial positioning of cluster centers

c) Choice of k



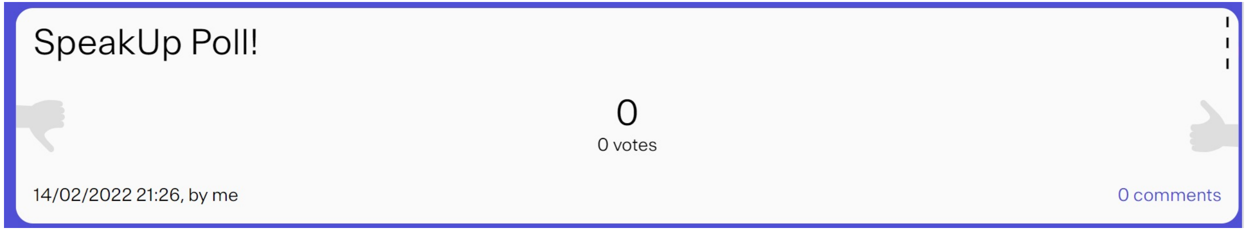
https://go.epfl.ch/mlbd-lecture

Short quiz about the past…

K-Means is useful when dealing with non-convex clusters:

a) True

b) False



https://go.epfl.ch/mlbd-lecture

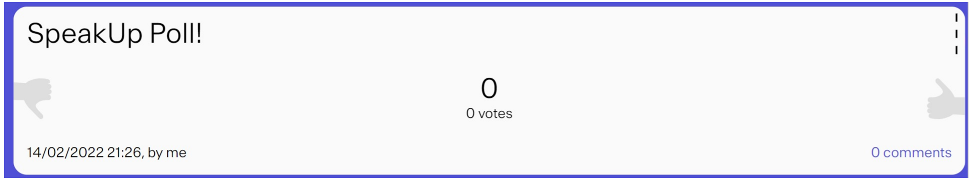
Short quiz about the past…

In a binary classification problem, it is appropriate to use the following activation function for the output layer:

a) Linear

b) Tanh

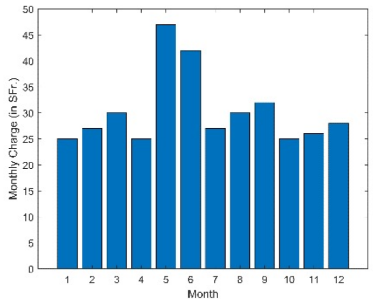
c) Sigmoid



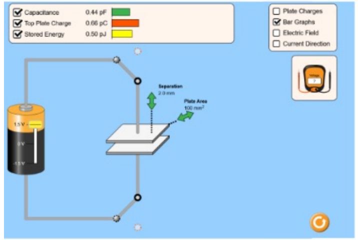
https://go.epfl.ch/mlbd-lecture

Today – Clustering Time Series Data

1. Aggregating features over time
2. Defining fixed time intervals (weeks, levels in a game, etc.)
3. Dynamic Time Warping



4. String Metrics
5. Markov Models



Action Sequences

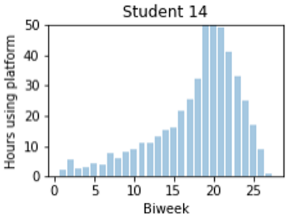
Learning Objectives

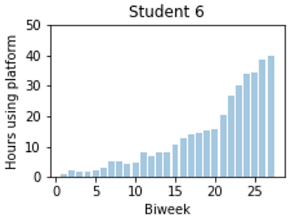
You should be able to:

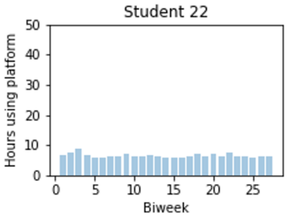
- Explain the different approaches to time series clustering
- Describe their advantages and disadvantages and when it is appropriate to use them
- Implement these approaches (lecture/lab session)
- Apply them to real-world data (lab session)

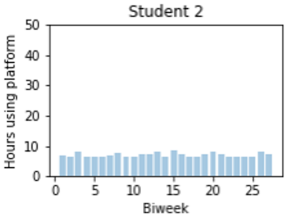
Today’s Use Case

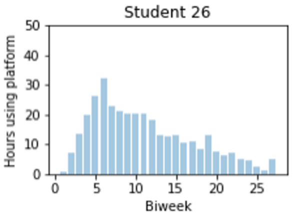
- Synthetic data of 30 high school students
- Time spent on an e-learning platform over one year (computed per biweek)
- Three clusters: 1) precrastinators, 2) regular, 3) procrastinators

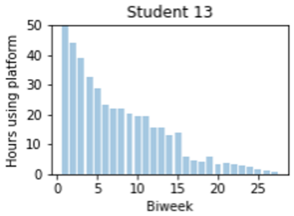












Agenda

- **Aggregating features over time**
- Defining fixed time intervals (weeks, levels in a game, etc.)
- Dynamic Time Warping
- String Metrics
- Markov Models
- Additional Practice (if time permits)

Aggregating features over time

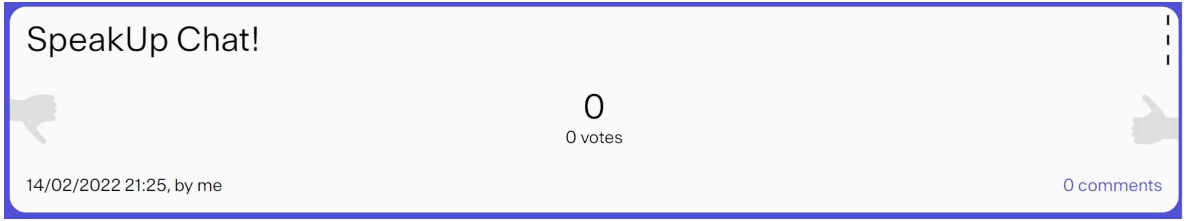
- We compute the value of the feature over the whole time series (average, maximum, range, standard deviation)
- We do not explicitly represent changes in features over time

➡ We can use standard distance/similarity measures

Your Turn – Aggregated Data

Run spectral clustering on the average number of hours:

- Can we interpret the different clusters?
- Are we able to retrieve the procrastination patterns? If not, why not?



Agenda

- Aggregating features over time
- **Defining fixed time intervals (weeks, levels in a game, etc.)**
- Dynamic Time Warping
- String Metrics
- Markov Models
- Additional Practice

Using fixed time intervals

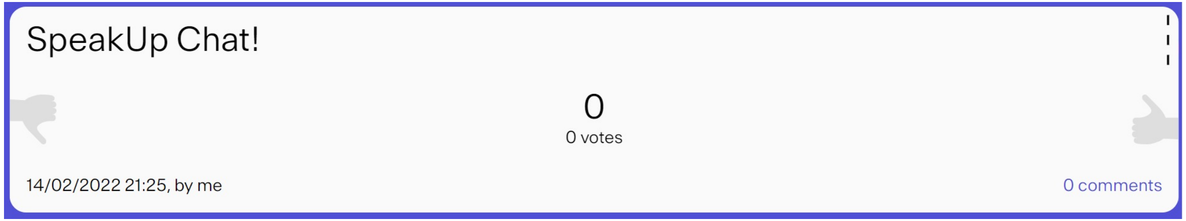
- Compute the feature value at fixed points in time (e.g., weeks, level in a game)
- We obtain feature vectors with the same length for every student

➡ We can use standard distance measures

Your Turn – Fixed Time Intervals

Run spectral clustering on the vectors of biweeks (dimension = 27) using Euclidean distance:

- What is the optimal number of clusters?
- How do the results differ from the aggregated feature results?



Agenda

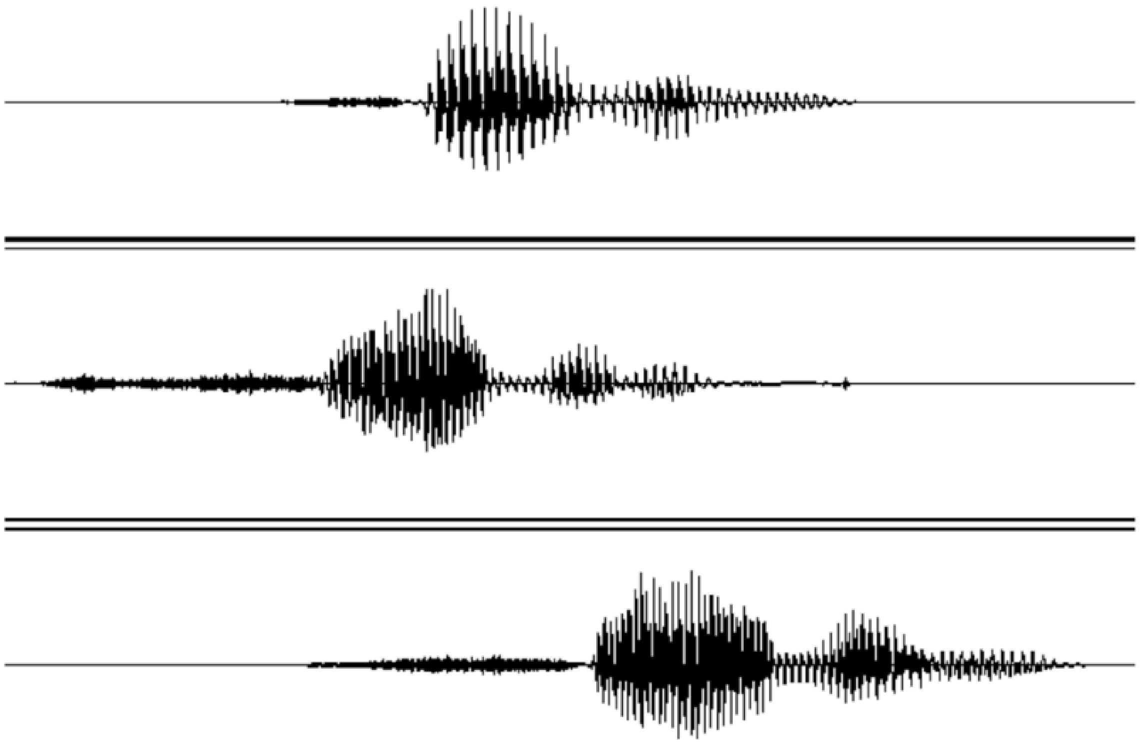
- Aggregating features over time
- Defining fixed time intervals (weeks, levels in a game, etc.)
- **Dynamic Time Warping**
- String Metrics
- Markov Models
- Additional Practice (if time permits)

Dynamic Time Warping

- Compute distance between two time series, which may vary in speed
- Time series can have different lengths

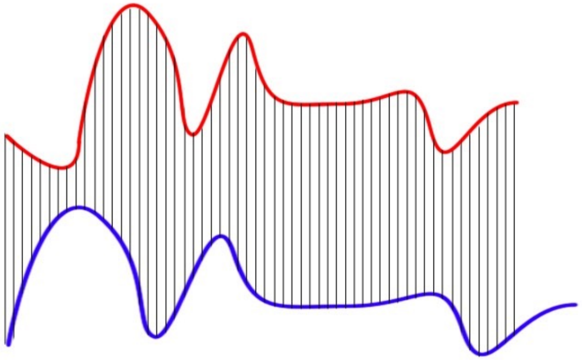
➡ Develop a **one-to-many** match, i.e. find an *optimal alignment* between two time series

Example: Spoken Digits

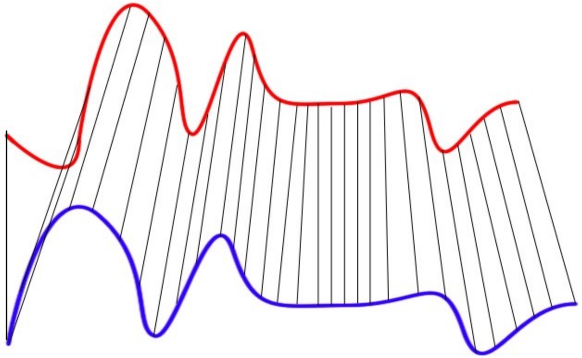


[*Image Credit: CS 498, Signals AI, University of Illinois*]

Dynamic Time Warping vs. Euclidean Distance



Euclidean Distance



Dynamic Time Warping

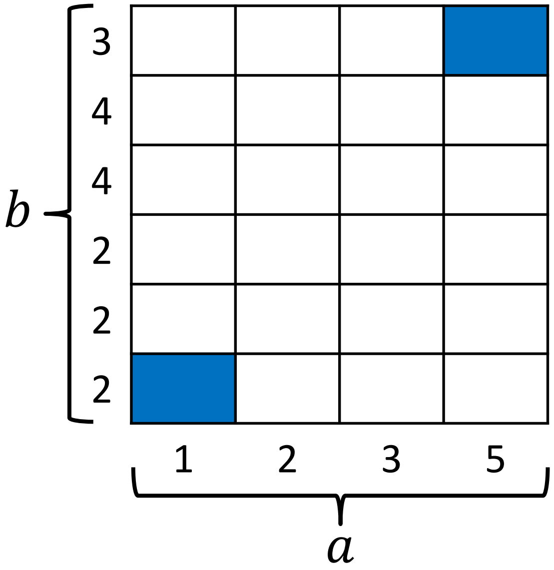
[*Image Credit: https://towardsdatascience.com/dynamic-time-warping-3933f25fcdd*]

Dynamic Time Warping: Rules

- **Goal**: minimize $D(a, b) = \min_{\emptyset} \sum_k d(a_{\emptyset(k)}, b_{\emptyset(k)})$
- **Rules** (given two sequences $\boldsymbol{a}$ and $\boldsymbol{b}$):
  - Every index of $\boldsymbol{a}$ must be matched with one or more indices from $\boldsymbol{b}$, and vice versa
  - The first index from $\boldsymbol{a}$ must be matched with the first index from $\boldsymbol{b}$ (but it does not have to be its only match)
  - The last index from $\boldsymbol{a}$ must be matched with the last index from $\boldsymbol{b}$ (but it does not have to be its only match)
  - The mapping of the indices from $\boldsymbol{a}$ to indices from $\boldsymbol{b}$ must be monotonically increasing, and vice versa, i.e. if $j > i$ are indices from $\boldsymbol{a}$, then there must not be two indices $m > n$ in $\boldsymbol{b}$, such that index i is matched with index m and index j is matched with index n, and vice versa

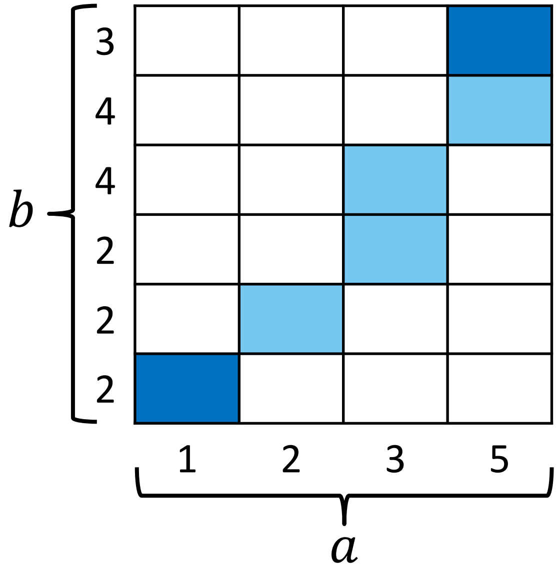
Dynamic Time Warping: Example

$$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$$



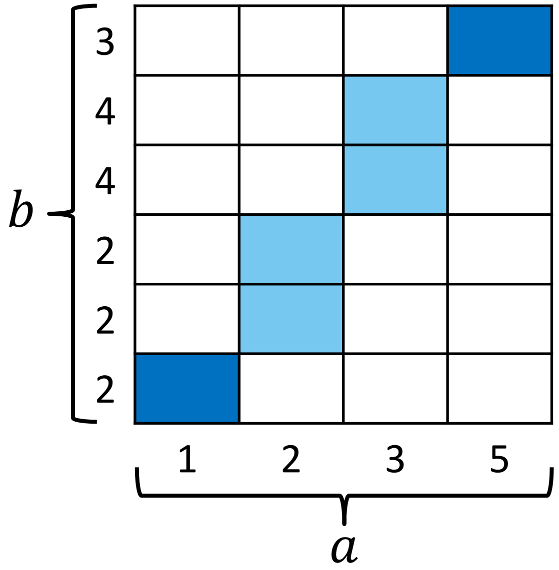
Dynamic Time Warping: Example

$$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$$



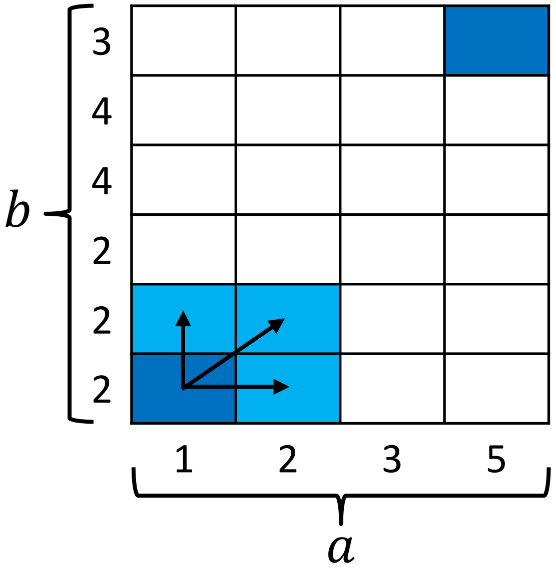
Dynamic Time Warping: Example

$a = [1,2,3,5]$ $\quad$ $b = [2,2,2,4,4,3]$



Dynamic Time Warping: Possible Paths

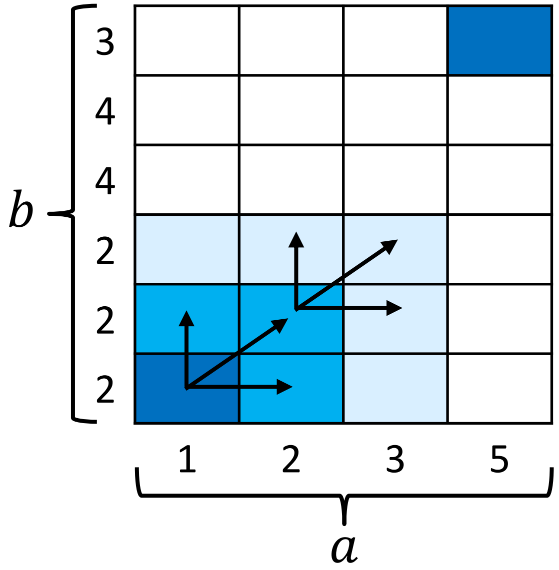
$$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$$



- Three possible paths from each square

Dynamic Time Warping: Possible Paths

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

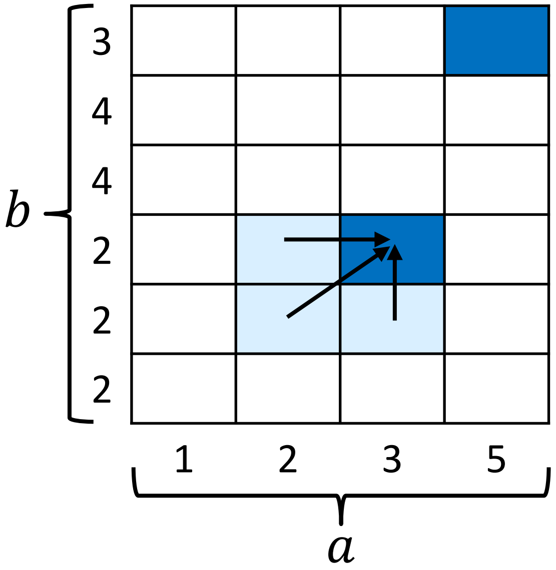


- Three possible paths from each square
- Every choice leads to three more possible paths

➡ $\approx 3^{4 \cdot 6}$ options

Dynamic Time Warping: Minimum Path

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$



- For any cell C (matching indices i, j): three possible precursor cells
- Minimum cost (distance) for getting to C

$$d(i,j) + \min(D(i-1,j), D(i-1,j-1), D(i,j-1))$$

Dynamic Time Warping: Example

$$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
a	1	2	3	5

1. Compute pairwise distances

b				
3				
4				
4				
2				
2				
2				
a	1	2	3	5

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \quad b = [2,2,2,4,4,3]$

b \ a	1	2	3	5
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3

1. Compute pairwise distances

b \ a	1	2	3	5
3				
4				
4				
2				
2				
2	1			

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5]$ $\quad$ $b = [2,2,2,4,4,3]$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
	1	2	3	5
	a			

1. Compute pairwise distances

b				
3	11			
4	9			
4	6			
2	3			
2	2			
2	1			
	1	2	3	5
	a			

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
a	1	2	3	5

1. Compute pairwise distances

b				
3	11			
4	9			
4	6			
2	3			
2	2			
2	1	1	2	5
a	1	2	3	5

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
	1	2	3	5
		a		

1. Compute pairwise distances

b				
3	11			
4	9			
4	6			
2	3			
2	2	?		
2	1	1	2	5
	1	2	3	5
		a		

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

b \ a	1	2	3	5
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3

1. Compute pairwise distances

b \ a	1	2	3	5
3	11			
4	9			
4	6			
2	3			
2	2	1		
2	1	1	2	5

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \quad b = [2,2,2,4,4,3]$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
a	1	2	3	5

1. Compute pairwise distances

b				
3	11			
4	9			
4	6			
2	3			
2	2	1	?	
2	1	1	2	5
a	1	2	3	5

2. Compute minimum distance path

Dynamic Time Warping: Example

$$\boxed{a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]}$$

b

3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
	1	2	3	5

a

1. Compute pairwise distances

b

3	11			
4	9			
4	6			
2	3			
2	2	1	2	
2	1	1	2	5
	1	2	3	5

a

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
	1	2	3	5
	a			

1. Compute pairwise distances

b				
3	11			
4	9			
4	6			
2	3			
2	2	1	2	?
2	1	1	2	5
	1	2	3	5
	a			

2. Compute minimum distance path

Dynamic Time Warping: Example

$$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
a	1	2	3	5

1. Compute pairwise distances

b				
3	11			
4	9			
4	6			
2	3			
2	2	1	2	5
2	1	1	2	5
a	1	2	3	5

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

b \ a	1	2	3	5
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3

1. Compute pairwise distances

Goal

b \ a	1	2	3	5
3	11	6	3	5
4	9	5	3	3
4	6	3	2	3
2	3	1	2	5
2	2	1	2	5
2	1	1	2	5

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

Goal

b				
3	11	6	3	5
4	9	5	3	3
4	6	3	2	3
2	3	1	2	5
2	2	1	2	5
2	1	1	2	5
	1	2	3	5
	a			

2. Compute minimum distance path

Dynamic Time Warping: Example

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

Goal

b \ a	1	2	3	5
3	11	6	3	5
4	9	5	3	3
4	6	3	2	3
2	3	1	2	5
2	2	1	2	5
2	1	1	2	5

2. Compute minimum distance path

Dynamic Time Warping: Example

$$\boxed{a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]}$$

$$a = [1,2,3,5]$$

$$b = [2,2,2,4,4,3]$$

Goal

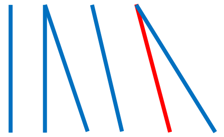
b \ a	1	2	3	5
3	11	6	3	5
4	9	5	3	3
4	6	3	2	3
2	3	1	2	5
2	2	1	2	5
2	1	1	2	5

2. Compute minimum distance path

Dynamic Time Warping: Example

$$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$$

$a = [1,2,3,5]$



$b = [2,2,2,4,4,3]$

Goal

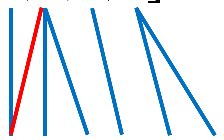
b				
3	11	6	3	5
4	9	5	3	3
4	6	3	2	3
2	3	1	2	5
2	2	1	2	5
2	1	1	2	5
	1	2	3	5
	a			

2. Compute minimum distance path

Dynamic Time Warping: Example

$$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$$

$$a = [1,2,3,5]$$



$$b = [2,2,2,4,4,3]$$

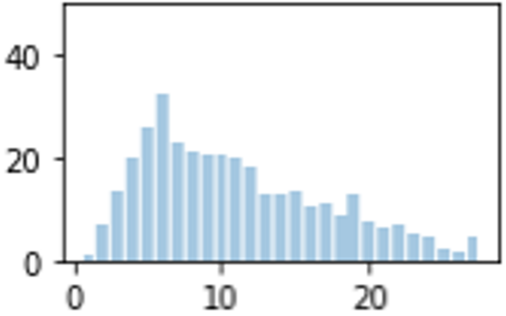
Goal

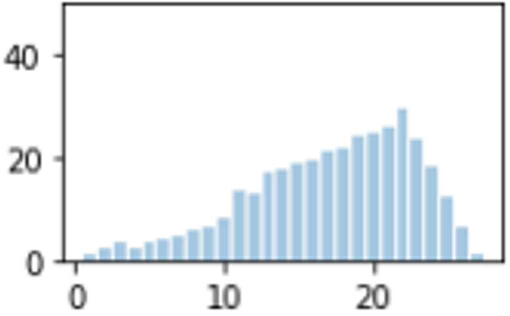
b \ a	1	2	3	5
3	11	6	3	5
4	9	5	3	3
4	6	3	2	3
2	3	1	2	5
2	2	1	2	5
2	1	1	2	5

2. Compute minimum distance path

Dynamic Time Warping: Window

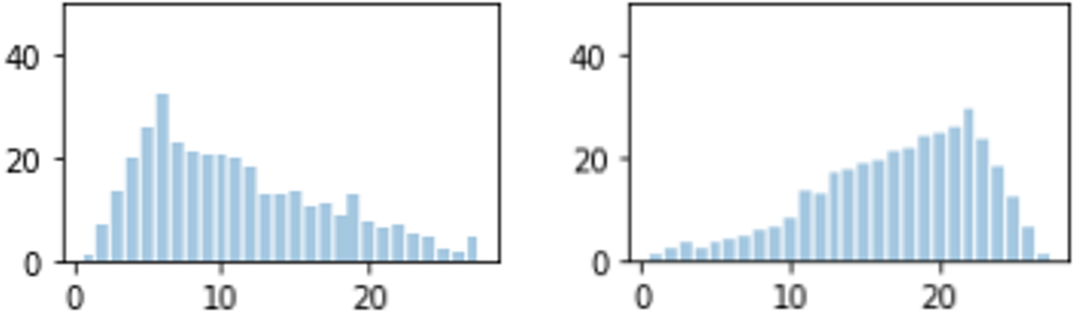
- Sometimes, we might want to constrain the mapping





Dynamic Time Warping: Window

- Sometimes, we might want to constrain the mapping



- We introduce an window size w: an element in sequence $\boldsymbol{a}$ at index i can only be mapped to elements at index $i - w, \ldots, i + w$ in sequence $\boldsymbol{b}$

Dynamic Time Warping: $w = 2$

$a = [1,2,3,5] \quad b = [2,2,2,4,4,3]$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
a	1	2	3	5

1. Compute pairwise distances

b				
3				
4				
4				
2				
2				
2				
a	1	2	3	5

2. Compute minimum distance path

Dynamic Time Warping: $w = 2$

$a = [1,2,3,5] \quad b = [2,2,2,4,4,3]$

3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
b / a	1	2	3	5

1. Compute pairwise distances

3	-			
4	-			
4	-			
2	3			
2	2			
2	1			
b / a	1	2	3	5

2. Compute minimum distance path

Dynamic Time Warping: $w = 2$

$a = [1,2,3,5]$ $b = [2,2,2,4,4,3]$

b \ a	1	2	3	5
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3

1. Compute pairwise distances

b \ a	1	2	3	5
3	-	-		
4	-	-		
4	-	3		
2	-	1		
2	2	1		
2	1	1		

2. Compute minimum distance path

Dynamic Time Warping: $w = 2$

$a = [1,2,3,5] \qquad b = [2,2,2,4,4,3]$

b				
3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
	1	2	3	5
	a			

1. Compute pairwise distances

b				
3	-	-	-	
4	-	-	3	
4	-	-	2	
2	-	1	2	
2	2	1	2	
2	1	1	2	
	1	2	3	5
	a			

2. Compute minimum distance path

Dynamic Time Warping: $w = 2$

$a = [1,2,3,5]$ $\quad$ $b = [2,2,2,4,4,3]$

3	2	1	0	2
4	3	2	1	1
4	3	2	1	1
2	1	0	1	3
2	1	0	1	3
2	1	0	1	3
	1	2	3	5

1. Compute pairwise distances

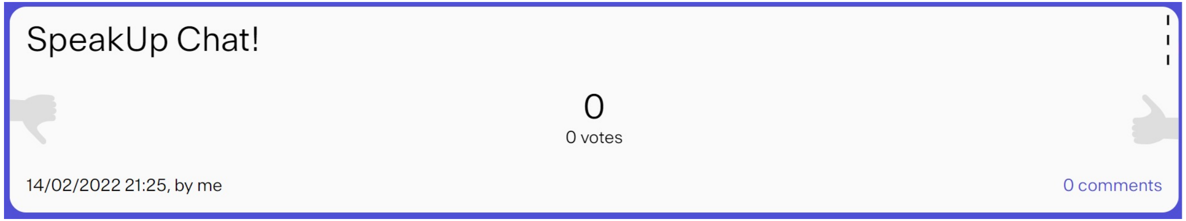
3	-	-	-	5
4	-	-	-	3
4	-	-	2	3
2	-	1	2	5
2	2	1	2	5
2	1	1	2	-
	1	2	3	5

2. Compute minimum distance path

Your Turn – Dynamic Time Warping

Run spectral clustering using DTW with a window size of $w = 3$:

- How do the results differ from previous results?
- What happens if you set $w = 0$?
- And if you set $w = 27$?



Agenda

- Aggregating features over time
- Defining fixed time intervals (weeks, levels in a game, etc.)
- Dynamic Time Warping
- **String Metrics**
- Markov Models
- Additional Practice (if time permits)

Example from Research: String Metrics

$$C1 \rightarrow C2 \rightarrow C3 \rightarrow C4 \rightarrow R4 \rightarrow P \rightarrow C5 \rightarrow R5 \rightarrow P$$

$$C4 \rightarrow R4 \rightarrow P \rightarrow C5 \rightarrow R5 \rightarrow P$$

[*Visualization and Confirmatory Clustering of Sequence Data from a Simulation-Based Assessment Task*, Berger et al., EDM 2014]

Example from Research: String Metrics

- Levensthein distance: minimal number of single character edits (insertion, deletion, substitution) to change one string into the other
- Longest common subsequence (LCS): string similarity measure, find the longest common subsequence between two sequences

[*Visualization and Confirmatory Clustering of Sequence Data from a Simulation-Based Assessment Task*, Berger et al., EDM 2014]

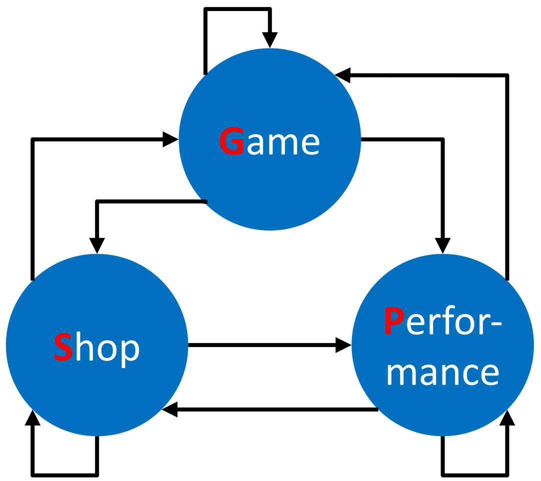
Agenda

- Aggregating features over time
- Defining fixed time intervals (weeks, levels in a game, etc.)
- Dynamic Time Warping
- String Metrics
- **Markov Models**
- Additional Practice (if time permits)

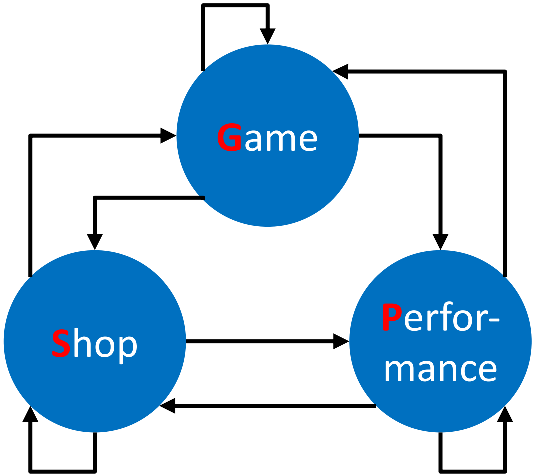
Markov Models

- Detailed action sequences provide rich temporal information
- Might contain a considerable amount of noise
- We might be interested not in the detailed sequence, but in patterns (which actions tend to follow each other)

Markov Models



Markov Models



$$G \to S \to G \to S \to G \to P \to S \to G$$

$$G \to G \to G \to G \to P \to G \to G$$

$$G \to P \to S \to G \to P \to S$$

Parameters: Maximum Likelihood Estimation

$$G \rightarrow S \rightarrow G \rightarrow S \rightarrow G \rightarrow P \rightarrow S \rightarrow G \rightarrow S \rightarrow S \rightarrow G \rightarrow G \rightarrow S \rightarrow G \rightarrow P \rightarrow G \rightarrow$$
$$P \rightarrow S \rightarrow G \rightarrow S \rightarrow \mathrm{G} \rightarrow S \rightarrow S \rightarrow G \rightarrow S \rightarrow \mathrm{G} \rightarrow G \rightarrow S \rightarrow \mathrm{G} \rightarrow S \rightarrow S \rightarrow G \rightarrow S$$

$$p(S|G) = \frac{10}{15} = 0.67$$

$$p(G|G) = \frac{2}{15} = 0.13$$

$$p(P|G) = \frac{3}{15} = 0.20$$

$$\begin{array}{cc} & \begin{array}{ccc} \boldsymbol{G} & \boldsymbol{S} & \boldsymbol{P} \end{array} \\ \begin{array}{c} \boldsymbol{G} \\ \boldsymbol{S} \\ \boldsymbol{P} \end{array} & \begin{pmatrix} 0.13 & 0.67 & 0.20 \\ 0.79 & 0.11 & 0 \\ 0.33 & 0.67 & 0 \end{pmatrix} \end{array}$$

Stationary Distribution

$$G \to S \to G \to S \to G \to P \to S \to G \to S \to S \to G \to G \to S \to G \to P \to G \to$$
$$P \to S \to G \to S \to \mathrm{G} \to S \to S \to G \to S \to \mathrm{G} \to G \to S \to \mathrm{G} \to S \to S \to G \to S$$

$$\begin{array}{cc} & \begin{array}{ccc} \boldsymbol{G} & \boldsymbol{S} & \boldsymbol{P} \end{array} \\ \begin{array}{c} \boldsymbol{G} \\ \boldsymbol{S} \\ \boldsymbol{P} \end{array} & \begin{pmatrix} 0.13 & 0.67 & 0.20 \\ 0.89 & 0.11 & 0 \\ 0.33 & 0.67 & 0 \end{pmatrix} \end{array}$$

$$\boxed{\pi \mathrm{T} = \pi}$$

Stationary Distribution

$$G \to S \to G \to S \to G \to P \to S \to G \to S \to S \to G \to G \to S \to G \to P \to G \to P \to S \to G \to S \to \mathrm{G} \to S \to S \to G \to S \to \mathrm{G} \to G \to S \to \mathrm{G} \to S \to S \to G \to S$$

$$\begin{array}{cc} & \begin{array}{ccc} \boldsymbol{G} & \boldsymbol{S} & \boldsymbol{P} \end{array} \\ \begin{array}{c} \boldsymbol{G} \\ \boldsymbol{S} \\ \boldsymbol{P} \end{array} & \begin{pmatrix} 0.13 & 0.67 & 0.20 \\ 0.89 & 0.11 & 0 \\ 0.33 & 0.67 & 0 \end{pmatrix} \end{array}$$

$$\boxed{\pi \mathrm{T} = \pi}$$

$$\pi = [0.48 \quad 0.43 \quad 0.09]$$

Expected Frequencies

- When sequences get very long (n gets large), how often do we expect to observe the transitions?

$$
\begin{array}{cc}
 & \begin{array}{ccc} \boldsymbol{G} & \boldsymbol{S} & \boldsymbol{P} \end{array} \\
\begin{array}{c} \boldsymbol{G} \\ \boldsymbol{S} \\ \boldsymbol{P} \end{array} & \begin{pmatrix} 0.06 & 0.32 & 0.10 \\ 0.38 & 0.05 & 0 \\ 0.03 & 0.06 & 0 \end{pmatrix}
\end{array}
$$

Distance Metrics

- Based on Frobenius Norm: equivalent to Euclidean distance over vectors

$$D_2(A,B) = \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{m}\left(a_{ij} - b_{ij}\right)^2}$$

Distance Metrics

- Kullback-Leibler Divergence: measures difference between two probability distributions

$$D_{KL}(P||Q) = \sum_{x \in X} P(x) \cdot \log(\frac{P(x)}{Q(x)})$$

- Jensen-Shannon Divergence: measures difference between two probability distributions

$$D_{JS}(P||Q) = \frac{1}{2} D_{KL}(P||M) + \frac{1}{2} D_{KL}(M||Q) \qquad M = \frac{1}{2}(P + Q)$$

Distance Metrics

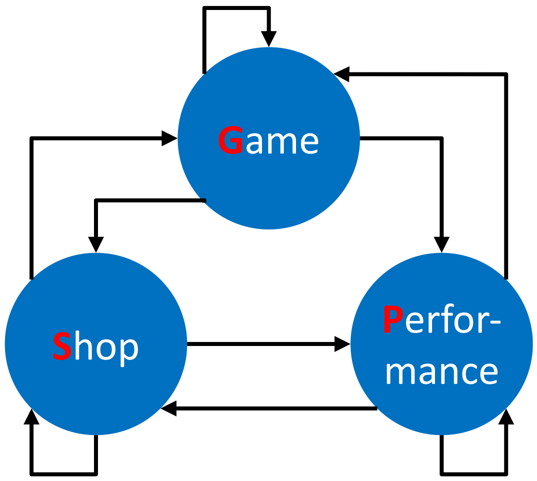
- Hellinger Distance: measures difference between two probability distributions

$$D_H(P||Q) = \frac{1}{\sqrt{2}}\sqrt{\sum_{i=1}^{n}(\sqrt{p_i} - \sqrt{q_i})^2}$$

Distance between samples: Options

- Compute distance between stationary distributions: use Hellinger Distance (or Jensen-Shannon Divergence)
- Compute distance between transition matrices: use Frobenius Distance
- Compute distance between expected frequencies: use Hellinger Distance (or Jensen-Shannon Divergence)

Example from Research: Spelling Learning



Three clusters:

- Focused on the task
- Children, who frequently check performance/shop in-between tasks
- Spend long amounts of time off-task

Agenda

- Aggregating features over time
- Defining fixed time intervals (weeks, levels in a game, etc.)
- Dynamic Time Warping
- String Metrics
- Markov Models
- **Additional Practice (if time permits)**

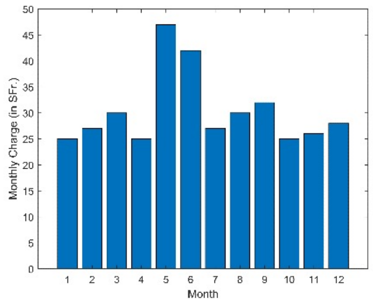
Your Turn – Flipped Classroom

Cluster the students of the flipped classroom course based on their consistency:

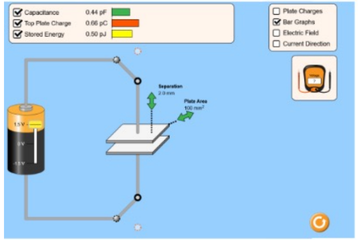
- Cluster the students using DTW and spectral clustering and visualize the heuristics for selecting the optimal number of clusters as well as timelines of the students for each cluster.
- Discuss your results: what is the optimal number of clusters? Can you interpret the obtained clusters?

Summary - Handling Time Series Data

1. Aggregating features over time
2. Defining fixed time intervals (weeks, levels in a game, etc.)
3. Dynamic Time Warping



4. String Measures
5. Markov Models



Action Sequences