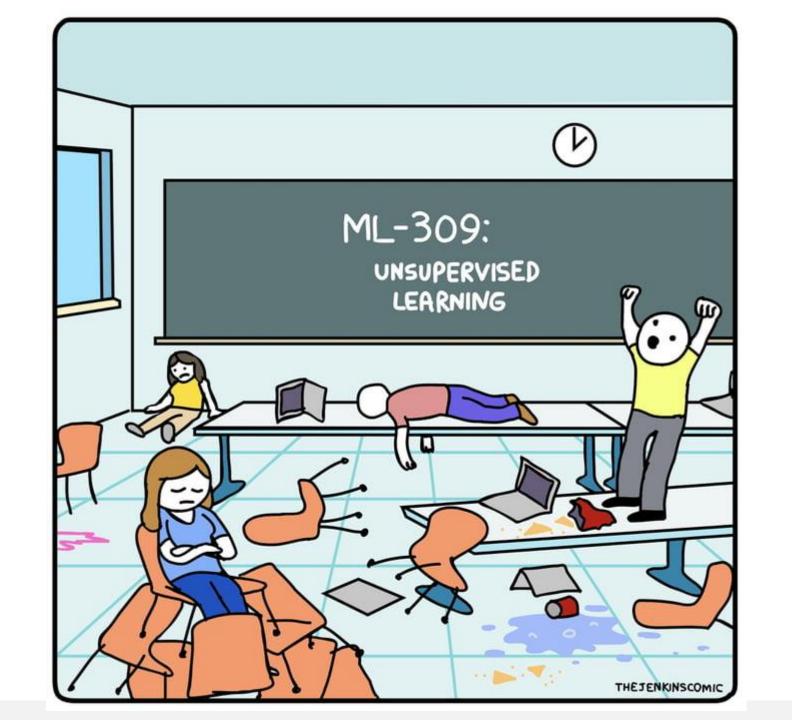
Unsupervised Learning

Vishal Patel

Spring 2024



SUPERVISED LEARNING

$$X = \begin{pmatrix} x_{11} & x_{12} & x_{13} & \dots & x_{1j} \\ x_{21} & x_{22} & x_{23} & \dots & x_{2j} \\ x_{31} & x_{32} & x_{33} & \dots & x_{3j} \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & x_{n3} & \dots & x_{nj} \end{pmatrix} \qquad y = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{pmatrix}$$

The goal is to fit **a model that relates the target to the features**, with the aim of accurately predicting the response

for future observations.

UNSUPERVISED LEARNING

The goal is to understand the relationships between the observations or between the features.

Clustering

Partition observations[†] into groups based on similarity.

E.g., Customer Segmentation.

A Few More Examples

- 1. A **cancer researcher** might assay gene expression levels in 100 patients with breast cancer. The researcher might then **look for subgroups** among the breast cancer samples, or among the genes, in order to obtain a better understanding of the disease.
- 2. An **online shopping site** might try to **identify groups of shoppers** with similar browsing and purchase histories, as well as items that are of particular interest to the shoppers within each group. Then an individual shopper can be preferentially shown the items in which the shopper is particularly likely to be interested, based on the purchase histories of similar shoppers.
- 3. A **search engine** might choose what search results to display to a particular individual based on the click histories of **other individuals with similar search patterns**.

Clustering Methods

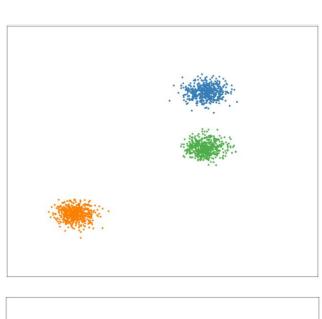
1

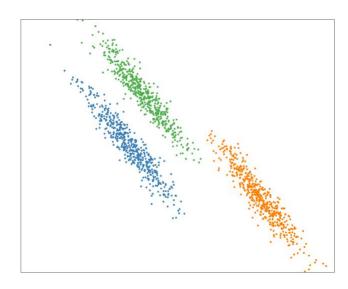
Distance-Based

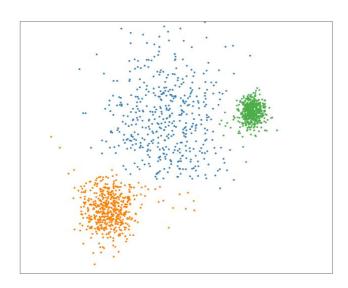
2

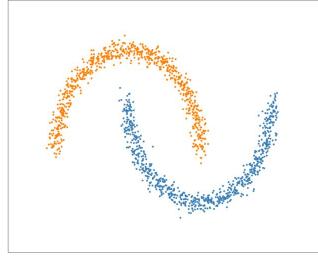
Density-Based

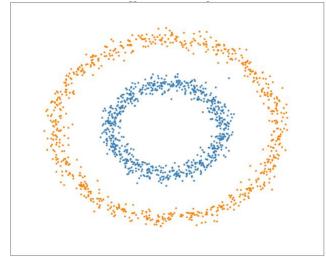
The Geometry of Clusters

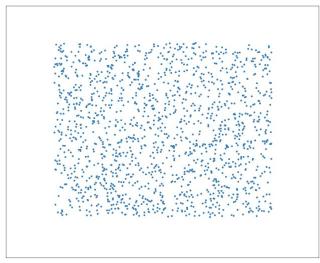






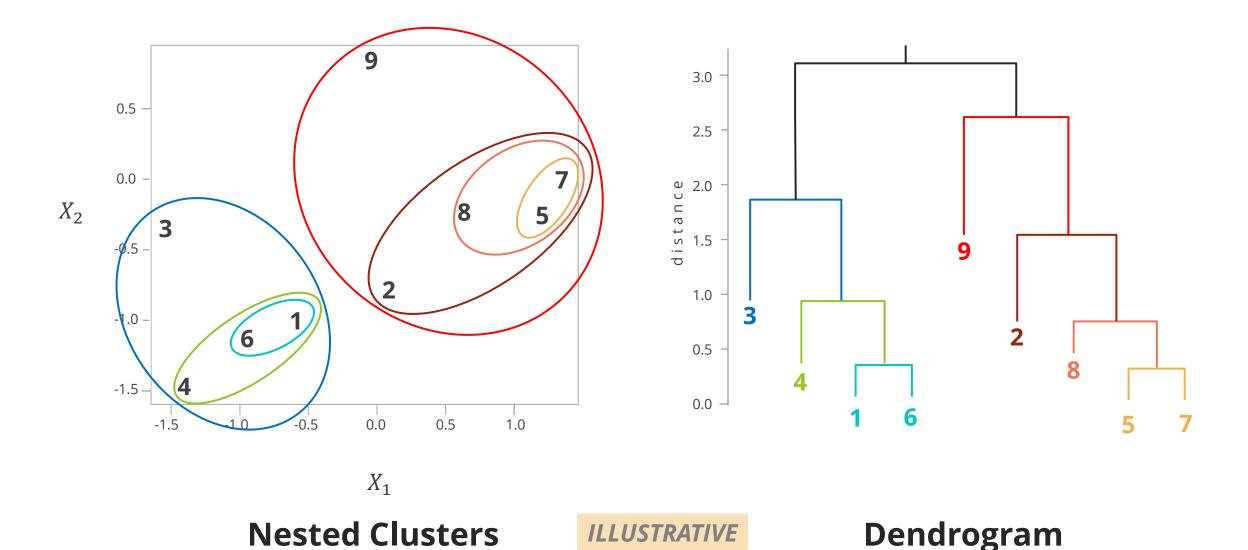






Hierarchical Clustering

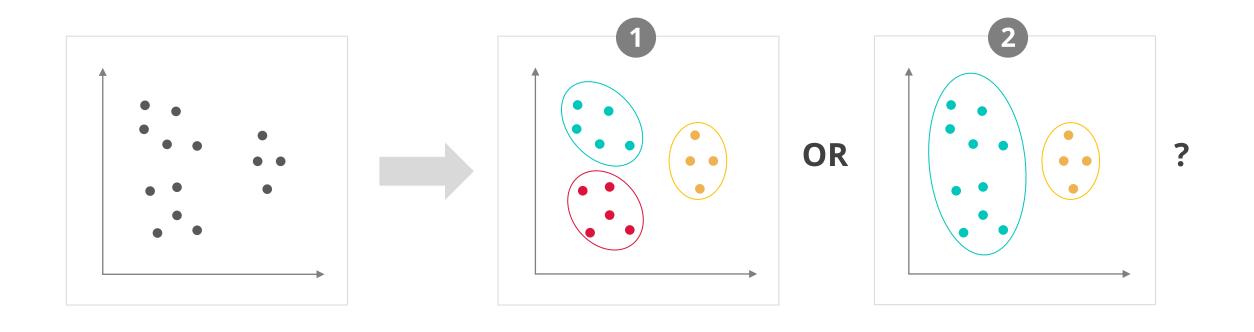
Hierarchical (Agglomerative) Clustering



Distance-Based Clustering

How to define **similarity**

between data points (and clusters)?



Similarity Measures

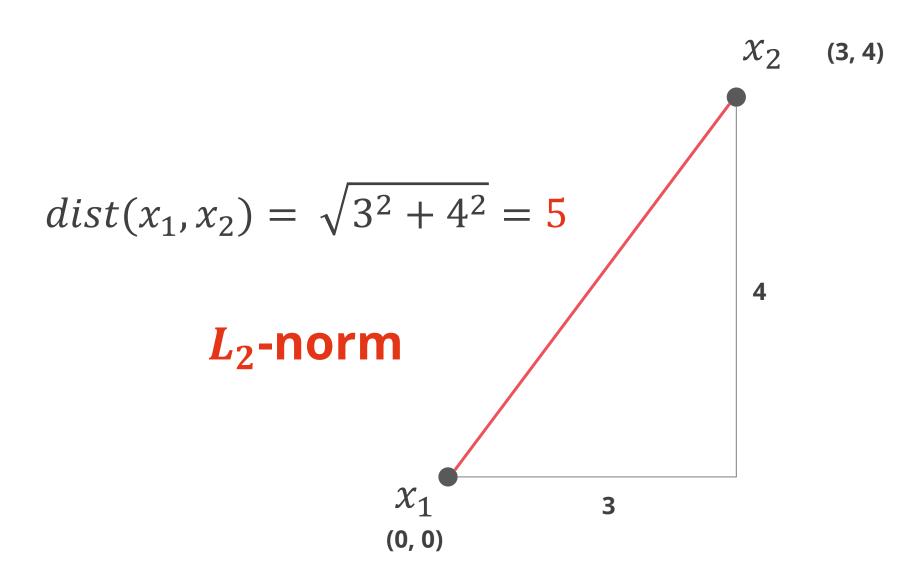
1 Similarity between data points.

2 Similarity between **clusters**.

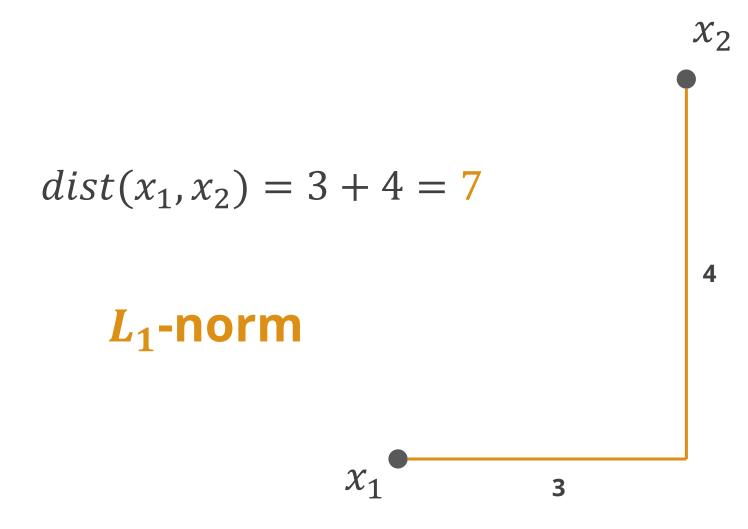
Similarity Measures

1 Similarity between data points.

2 Similarity between clusters.



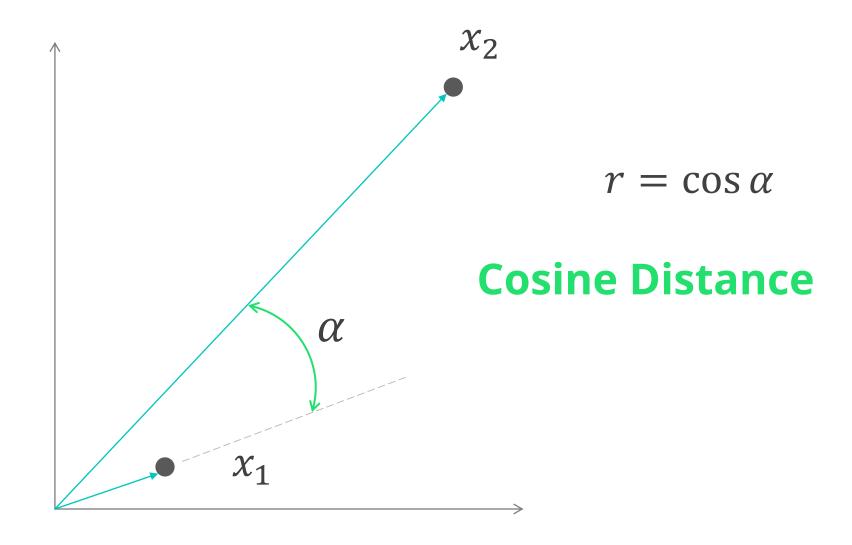
This is the most common notion of "distance".



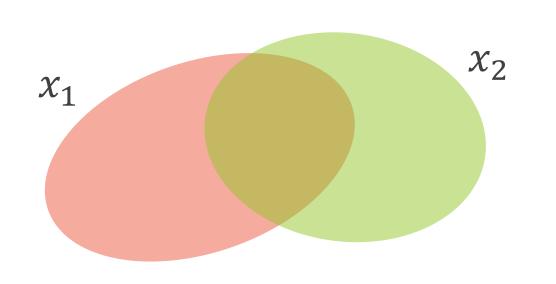


 L_1 -norm

*L*₁-norm is also known as the Manhattan distance – the distance if you had to travel along the coordinates only.



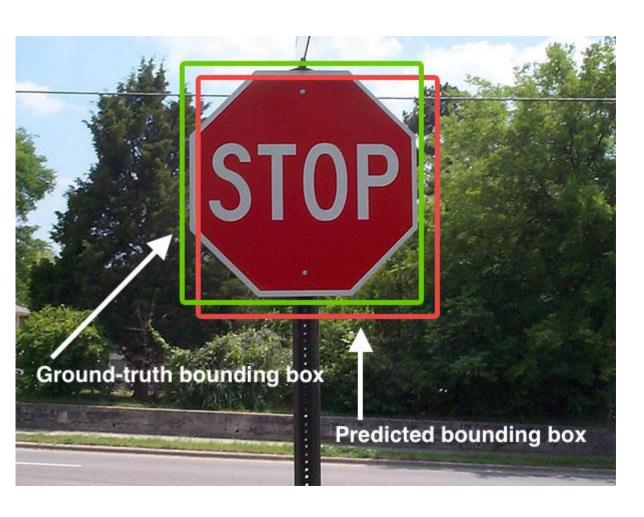
The correlation coefficient can be rescaled to distance measure of range 0 – 1 by $r_{distance} = (1-r)/2$



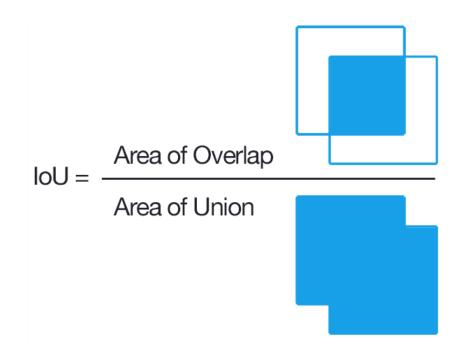
Jaccard Similarity =
$$\frac{|x_1 \cap x_2|}{|x_1 \cup x_2|}$$

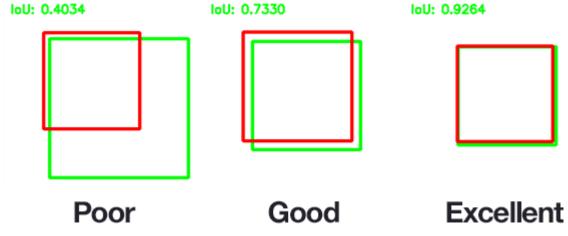
Jaccard Distance =
$$1 - \frac{|x_1 \cap x_2|}{|x_1 \cup x_2|}$$

Jaccard distance (dissimilarity) is the proportion of the combined abundance that is not shared.[†]



https://en.wikipedia.org/wiki/Jaccard index

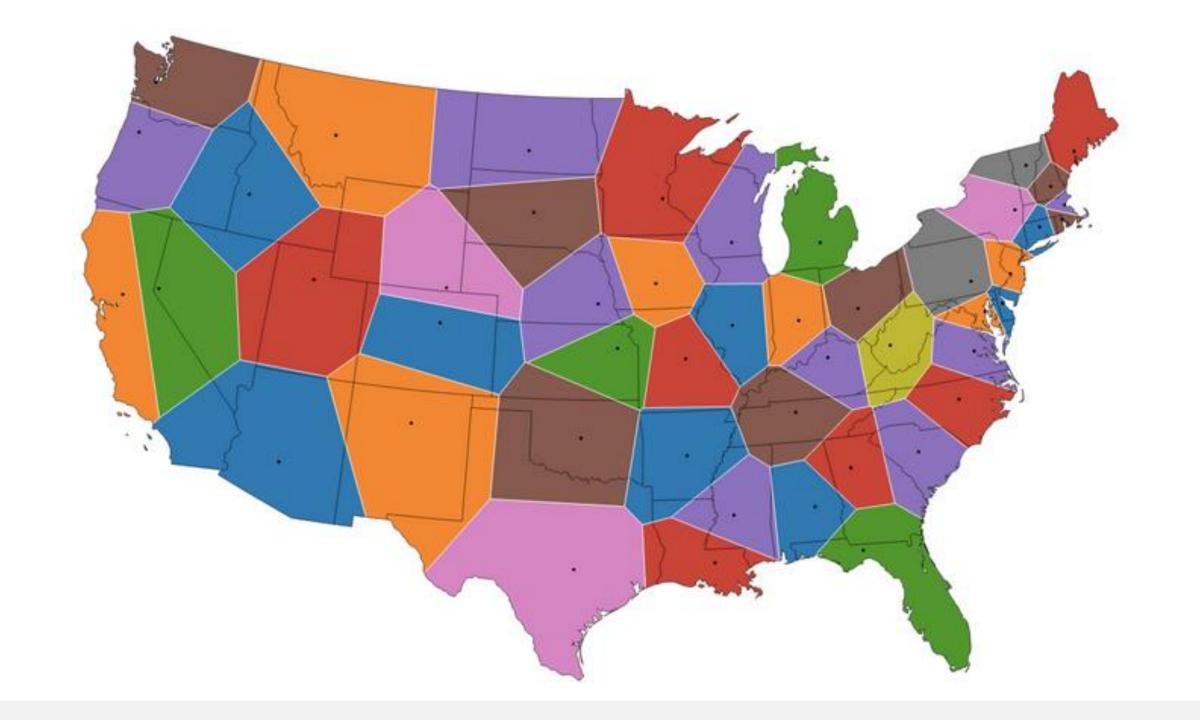






A **Voronoi diagram** of people enjoying the sun in Bryant Park.

(by @RodBogart)



Similarity Measures

1 Similarity between data points.

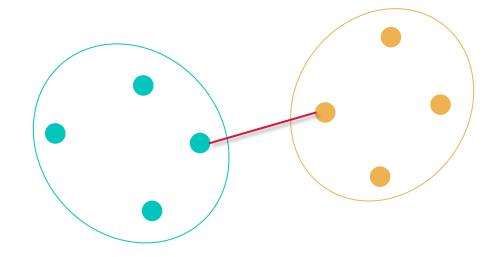
2 Similarity between **clusters**.

Hierarchical Clustering

Distance Between Clusters:

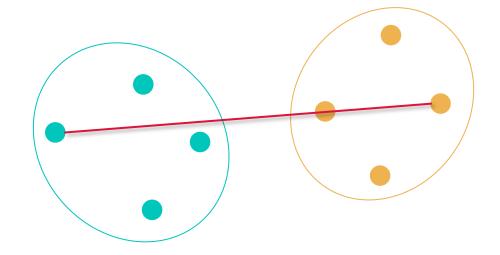
- 1. Single link = Smallest dissimilarity
- 2. Complete link = Largest dissimilarity
- **3. Average link** = Average dissimilarity
- **4. Centroid method** = Distance between centroids
- 5. Ward's method = Sum of squared distances of points in clusters

- 1. Single link
- 2. Complete link
- 3. Average link
- 4. Centroid method
- 5. Ward's method



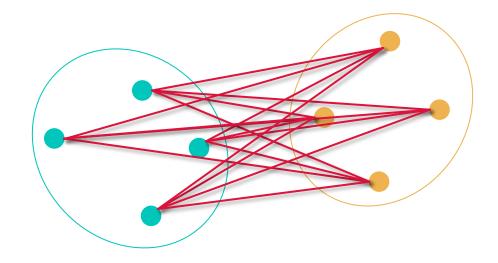
<u>Minimal</u> intercluster dissimilarity: Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B and record the smallest of these dissimilarities.[†]

- 1. Single link
- 2. Complete link
- 3. Average link
- 4. Centroid method
- 5. Ward's method



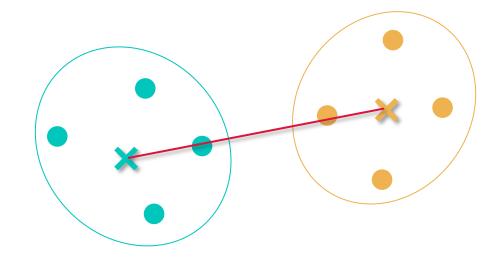
<u>Maximal</u> intercluster dissimilarity: Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B and record the largest of these dissimilarities.[†]

- 1. Single link
- 2. Complete link
- 3. Average link
- 4. Centroid method
- 5. Ward's method



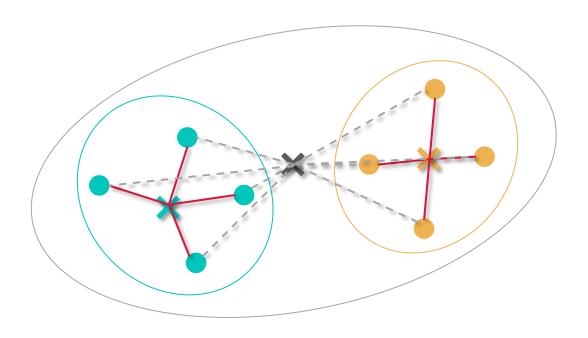
Mean intercluster dissimilarity: Compute all pairwise dissimilarities between the observations in cluster A and the observations in cluster B and record the average of these dissimilarities.[†]

- 1. Single link
- 2. Complete link
- 3. Average link
- 4. Centroid method
- 5. Ward's method



Dissimilarity between the centroid for cluster A and the centroid for cluster B.[†]

- 1. Single link
- 2. Complete link
- 3. Average link
- 4. Centroid method
- 5. Ward's method



Minimum variance: The dissimilarity between two clusters, **A** and **B**, is how much **the sum of squares** will increase when we merge them.

$$\Delta(A,B) = \sum_{i \in A \cup B} \|x_i - \mu_{A \cup B}\|^2 - \sum_{i \in A} \|x_i - \mu_A\|^2 - \sum_{i \in B} \|x_i - \mu_B\|^2$$

	BOS	NY	CHI	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
NY		0	802	1,771	2,934	2,815
CHI			0	966	1,242	2,103
DEN				0	1,235	1,307
SF					0	808
SEA						0



(DOC)	(NIV)	(CLII)	(הבעו)	(CE)	(CEA)
{BO2}	{INY}	{CHI}	{DEN}	{SF}	{SEA}

	BOS	NY	CHI	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
NY		0	802	1,771	2,934	2,815
CHI			0	966	1,242	2,103
DEN				0	1,235	1,307
SF					0	808
SEA						0

?

{BOS	5, NY}	{CHI}	{DEN}	{SF}	{SEA}
{BOS}	{NY}	{CHI}	{DEN}	{SF}	{SEA}

	BOS	NY	СНІ	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
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CHI			0	966	1,242	2,103
DEN				0	1,235	1,307
SF					0	808
SEA						0

?

{BOS, NY, CHI}			{DEN}	{SF}	{SEA}
{BOS	5, NY}	{CHI}	{DEN}	{SF}	{SEA}
{BOS}	{NY}	{CHI}	{DEN}	{SF}	{SEA}

	BOS	NY	CHI	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
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CHI			0	966	1,242	2,103
DEN				0	1,235	1,307
SF					0	808
SEA						0

{BOS, NY, CHI}			{DEN}	{SF,	SEA}
{BOS, NY, CHI}			{DEN}	{SF}	{SEA}
{BOS	5, NY}	{CHI}	{DEN}	{SF}	{SEA}
{BOS}	{NY}	{CHI}	{DEN}	{SF}	{SEA}

	BOS	NY	CHI	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
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DEN				0	1,235	1,307
SF					0	808
SEA						0

?

{BOS, NY, CHI}			{DEN}	{SF,	SEA}
{BOS, NY, CHI}			{DEN}	{SF}	{SEA}
{BOS	{BOS, NY} {CHI}		{DEN}	{SF}	{SEA}
{BOS}	{NY}	{CHI}	{DEN}	{SF}	{SEA}

	BOS	NY	CHI	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
NY		0	802	1,771	2,934	2,815
CHI			0	966	1,242	2,103
DEN				0	1,235	1,307
SF					0	808
SEA						0

Single Linkage



{BOS, NY, CHI}			{DEN}	{SF,	SEA}
{BOS, NY, CHI}			{DEN}	{SF}	{SEA}
{BOS	{BOS, NY} {({DEN}	{SF}	{SEA}
{BOS}	{NY}	{CHI}	{DEN}	{SF}	{SEA}

	BOS	NY	CHI	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
NY		0	802	1,771	2,934	2,815
СНІ			0	966	1,242	2,103
DEN				0	1,235	1,307
SF					0	808
SEA						0

Single Linkage

{	BOS, NY,	{SF, SEA}			
{B	OS, NY, CI	HI}	{DEN}	{SF, SEA}	
{BOS, NY, CHI}			{DEN}	{SF}	{SEA}
{BOS, NY} {CHI}		{DEN}	{SF}	{SEA}	
{BOS}	{NY}	{CHI}	{DEN}	{SF}	{SEA}

	BOS	NY	CHI	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
NY		0	802	1,771	2,934	2,815
CHI			0	966	1,242	2,103
DEN				0	1,235	1,307
SF					0	808
SEA						0

Complete Linkage



{BOS, NY, CHI}			{DEN}	{SF, SEA}	
{BOS, NY, CHI}			{DEN}	{SF}	{SEA}
{BOS, NY}		{CHI}	{DEN}	{SF}	{SEA}
{BOS}	{NY}	{CHI}	{DEN}	{SF}	{SEA}

	BOS	NY	CHI	DEN	SF	SEA
BOS	0	206	963	1,949	3,095	2,979
NY		0	802	1,771	2,934	2,815
CHI			0	966	1,242	2,103
DEN				0	1,235	1,307
SF					0	808
SEA						0

Complete Linkage

{BOS, NY, CHI}			{DEN, SF, SEA}			
{BOS, NY, CHI}			{DEN}	{SF, SEA}		
{BOS, NY, CHI}			{DEN}	{SF}	{SEA}	
{BOS, NY} {CHI}			{DEN}	{SF}	{SEA}	
{BOS}	{NY}	{CHI}	{DEN}	{SF}	{SEA}	

Hierarchical Clustering

Pros

- 1. Intuitive
- 2. More informative than "flat clustering"
- 3. Deterministic
- **4.** Does not require *k* to be pre-specified

Cons

1. Computationally expensive

```
class sklearn.cluster.AgglomerativeClustering (
    n_clusters=2,
    affinity='euclidean',
    memory=None,
    connectivity=None,
    compute_full_tree='auto',
    linkage='ward')
```

Agglomerative Clustering

Recursively merges the pair of clusters that minimally increases a given linkage distance.

class sklearn.cluster.AgglomerativeClustering (

```
n_clusters=2,
affinity='euclidean',
memory=None,
connectivity=None,
compute_full_tree='auto',
linkage='ward')
```

The number of clusters to find.

Similarity Measures

1 Similarity between data points.

AFFINITY

2 Similarity between **clusters**.

LINKAGE

```
class sklearn.cluster.AgglomerativeClustering (
    n_clusters=2,
    affinity='euclidean',
    memory=None,
    connectivity=None,
    compute_full_tree='auto',
```

linkage='ward')

Metric used to compute the linkage.

Can be "euclidean", "l1", "l2", "manhattan", "cosine", or "precomputed".

```
class sklearn.cluster.AgglomerativeClustering (
    n_clusters=2,
    affinity='euclidean',
    memory=None,
    connectivity=None,
    compute_full_tree='auto',
    linkage='ward')
```

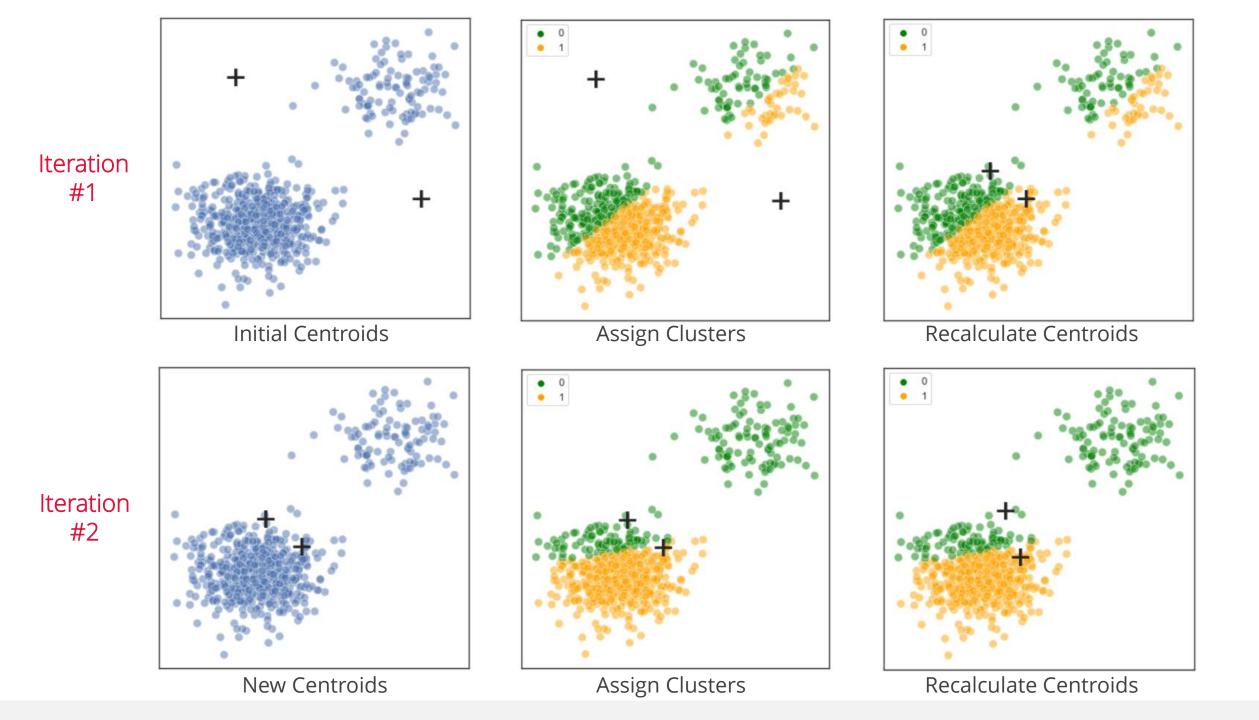
The linkage criterion determines which distance to use between sets of observation.

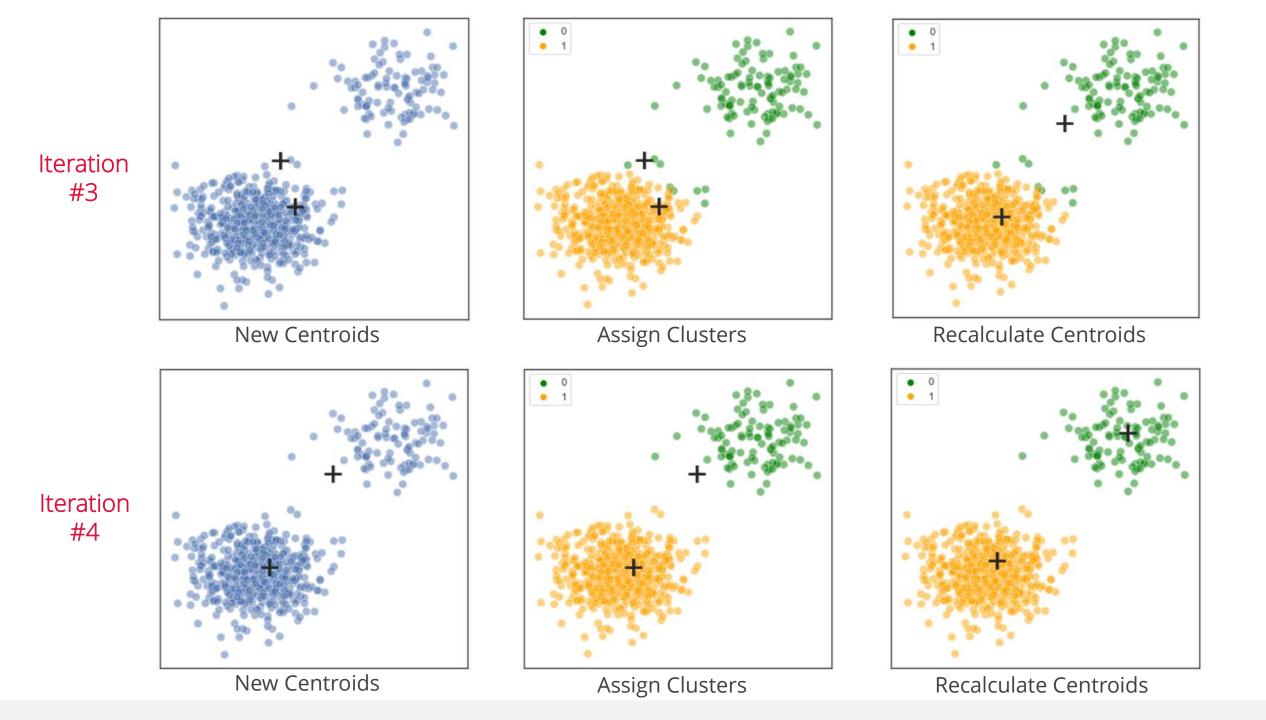
Supported criteria are "ward", "complete", "average", and "single".

→ → Agglomerative Clustering Tutorial

13_clustering_intro.ipynb

k-means Clustering





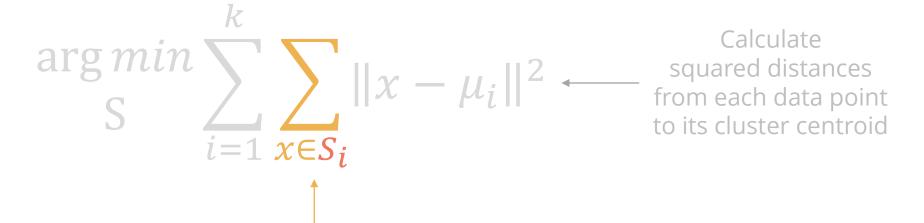
k-means Clustering: Steps

- 1. Provide the number of clusters (k).
- 2. Randomly initialize k centroids.
- 3. Assign data points to the nearest centroid.
- 4. Update the centroids.
- 5. Repeat steps 3 and 4.

$$\arg\min_{S} \sum_{i=1}^{\kappa} \sum_{x \in S_i} ||x - \mu_i||^2$$

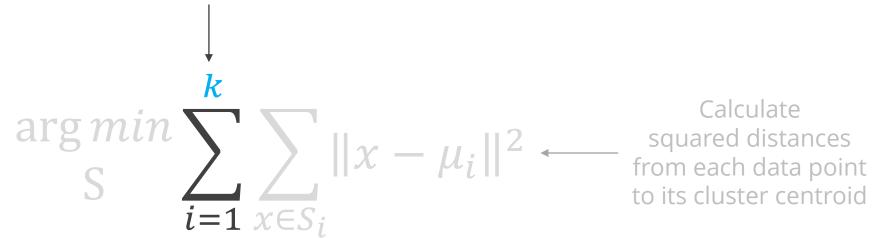
Given a set of observations $(x_1, x_2, ..., x_n)$, where each observation is a d-dimensional real vector, k-means clustering aims to partition the n observations into $k (\leq n)$ sets $S = \{S1, S2, ..., Sk\}$ so as to minimize the within-cluster sum of squares (WCSS). [Wikipedia]

arg
$$\min_{S} \sum_{i=1}^{K} \|x - \mu_i\|^2 \leftarrow \text{Calculate squared distances from each data point to its cluster centroid}$$



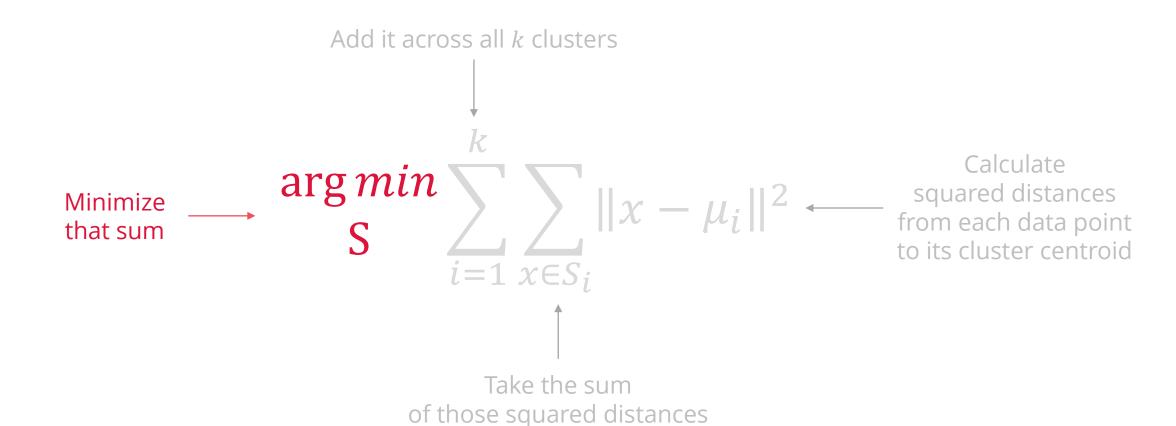
Take the sum of those squared distances within each cluster

Add it across all clusters



Calculate

Take the sum of those squared distances within each cluster



within each cluster

$$\underset{S}{\operatorname{arg}\,min} \sum_{i=1}^{R} \sum_{x \in S_i} ||x - \mu_i||^2$$

Given a set of observations $(x_1, x_2, ..., x_n)$, where each observation is a d-dimensional real vector, k-means clustering aims to partition the n observations into $k (\leq n)$ sets $S = \{S1, S2, ..., Sk\}$ so as to minimize the within-cluster sum of squares (WCSS).

k-means Clustering

Pros

- 1. Intuitive
- 2. Widely used and understood
- 3. Quick to execute

Cons

- 1. Assumes spherical clusters
- 2. Challenging to determine *k*
- 3. Initialization is important

```
class sklearn.cluster.KMeans (
    n_clusters=8,
   init='k-means++',
    n_init=10,
    max_iter=300,
    tol=0.0001,
    precompute_distances='auto',
    verbose=0,
    random_state=None,
    copy_x=True,
    algorithm='lloyd')
```

k-means Clustering

class sklearn.cluster.KMeans (n_clusters=8, init='k-means++', n_init=10, max_iter=300, tol=0.0001, precompute_distances='auto', verbose=0, random_state=None, copy_x=True, algorithm='lloyd')

The number of clusters to form as well as the number of centroids to generate.

```
class sklearn.cluster.KMeans (
    n_clusters=8,
   init='k-means++',
   n_init=10,
    max_iter=300,
    tol=0.0001,
    precompute_distances='auto',
    verbose=0,
    random_state=None,
    copy_x=True,
    algorithm='lloyd')
```

Number of time the *k*-means algorithm will be run with different centroid seeds.

The final results will be the best output of n_init consecutive runs in terms of inertia (i.e., how much distance did the clusters move).

```
class sklearn.cluster.KMeans (
    n_clusters=8,
   init='k-means++',
    n_init=10,
   max_iter=300,
    tol=0.0001,
    precompute_distances='auto',
    verbose=0,
    random_state=None,
    copy_x=True,
    algorithm='lloyd')
```

Maximum number of iterations of the k-means algorithm for a single run.

```
class sklearn.cluster.KMeans (
   n_clusters=8,
   init='k-means++',
   n_init=10,
    max_iter=300,
   tol=0.0001,
    precompute_distances='auto',
   verbose=0,
   random_state=None,
    copy_x=True,
    algorithm='lloyd')
```

Set a user-defined seed for reproducible results.

If int, random_state is the seed used by the random number generator.

Recommendation: Always set a seed (e.g., 314) to ensure reproducible results.

\rightarrow \rightarrow \rightarrow k-means Clustering Tutorial

13_clustering_intro.ipynb

DBSCAN

Density-Based Clustering: DBSCAN

Density-Based Spatial Clustering of Applications with Noise

E (eps)

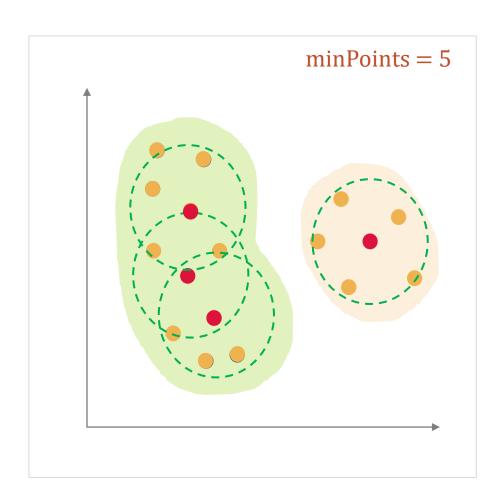
The minimum distance between two points for them to be considered **neighbors**.

minPoints

The minimum number of points to form a dense **region**.

- 1. Find **core points**: points with at least minPoints points in their neighborhood (as defined by ε).
- 2. Find **boundary points**: points in the neighborhood of core points.
- 3. If two core points are near each other, assign them and all of their boundary points to the same cluster.

DBSCAN



- 1. Find **core points**: points with at least five points in their neighborhood (as defined by ε).
- 2. Find **boundary points**: points in the neighborhood of core points.
- 3. If two or more **core** points are near each other, assign them and all of their boundary points to the same cluster.



DBSCAN

Pros

- 1. Deterministic
- 2. Robust to noise
- 3. Can handle clusters of arbitrary shapes

Cons

- 1. Driven by density; requires connected regions to be of sufficiently high density
- 2. Difficulty in dealing with datasets with varying density

class sklearn.cluster.DBSCAN (eps=0.5, min_samples=5, metric='euclidean', metric_params=None, algorithm='auto', leaf_size=30, p=None, n_jobs=None)

Perform DBSCAN clustering from vector array or distance matrix.

class sklearn.cluster.DBSCAN (eps=0.5, min_samples=5, metric='euclidean', metric_params=None, algorithm='auto', leaf_size=30, p=None, n_jobs=None)

The maximum distance (ε)
between two samples
for them to be considered
as in the same neighborhood.

```
class sklearn.cluster.DBSCAN (
   eps=0.5,
   min_samples=5,
   metric='euclidean',
   metric_params=None,
   algorithm='auto',
   leaf_size=30,
   p=None,
   n_jobs=None)
```

The number of samples
in a neighborhood
for a point to be considered
as a core point.

→ → → DBSCAN Clustering Tutorial

13_clustering_intro.ipynb

Clustering Methods: Summary

1

Distance-Based

Bad for:

- Non-globular clusters
- Clusters with different numbers of points

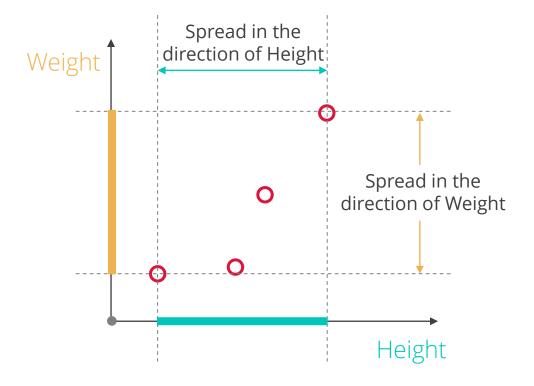
2

Density-Based

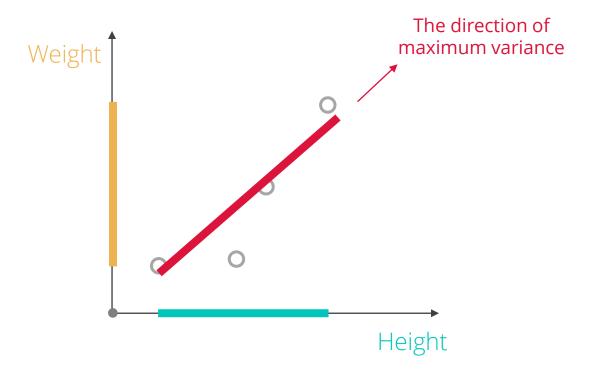
Bad for:

- Overlapping distributions
- Clusters with different densities

Principal Component Analysis

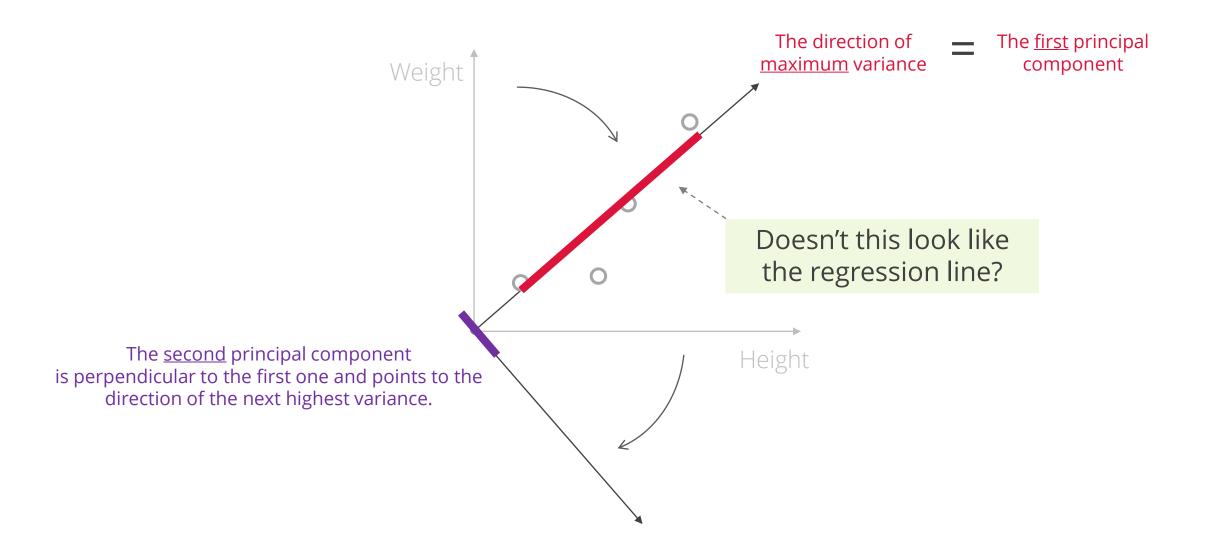


What is the direction of maximum spread?

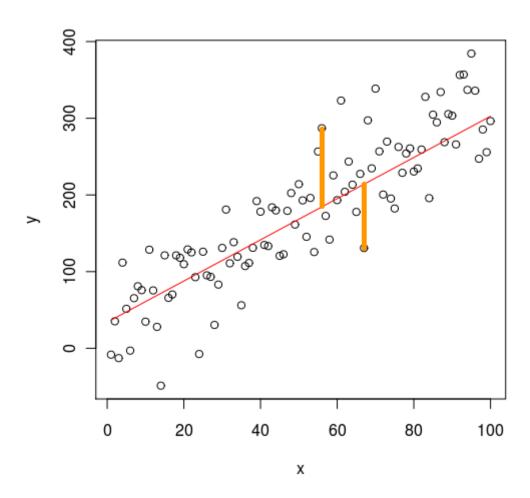


What is the direction of maximum spread?

A Change in Perspective

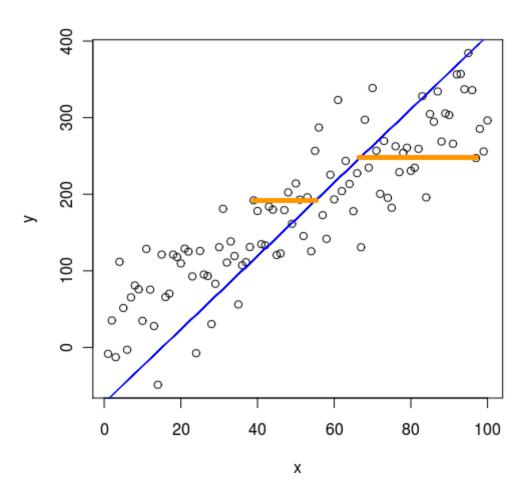


Regression Model: y ~ x



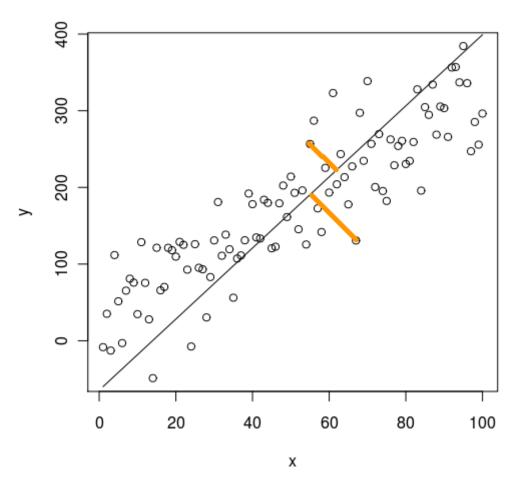
The $y \sim x$ regression model minimizes the error in the vertical (y) direction.

Regression Model: x ~ y



The $x \sim y$ regression model minimizes the error in the horizontal (x) direction.

PCA



PCA minimizes the error orthogonal (perpendicular) to the model line!

Rotation of the Axes [ILLUSTRATIVE]

Height	Weight
1.74	59
1.69	75
1.75	55
1.50	51

In the original data set, each row is expressed in terms of the following two dimensions (axes):

Height and Weight.

PC1	PC2
0.14	0.91
-0.78	0.08
0.65	0.18
0.13	-0.76

After the PCA is performed, the data set is expressed in terms of the two new dimensions (axes):

Principal Component #1 and #2.

You can now choose to drop the second Principal Component if it doesn't help explain much variance.

Feature Reduction

Chaining PCA with a Model



Classifier, Clustering, etc.

```
class sklearn.decomposition.PCA (
   n_components=None,
   copy=True,
   whiten=False,
   svd_solver='auto',
   tol=0.0,
   iterated_power='auto',
   random_state=None)
```

Linear dimensionality reduction using Singular Value Decomposition of the data to project it to a lower dimensional space.

class sklearn.decomposition.PCA (

n_components=None,

```
copy=True,
whiten=False,
svd_solver='auto',
tol=0.0,
iterated_power='auto',
random_state=None)
```

Number of components to keep.

If n_components is not set then all components are kept

class sklearn.decomposition.PCA (n_components=None, copy=True, whiten=False, svd_solver='auto', tol=0.0, iterated_power='auto', random_state=None)

Set a user-defined seed for reproducible results.

If int, random_state is the seed used by the random number generator.

Recommendation: Always set a seed (e.g., 314) to ensure reproducible results.

\rightarrow \rightarrow PCA Tutorial

14_pca.ipynb

Evaluating Clusters



1 The observer's vantage point



1 The observer's vantage point

The projection space (number of dimensions)

Bellatrix 245 light years

Betelgeuse 624 light years

Alnilam 1,342 light years

> **Rigel** 772 light years

Reification

Pure Fiction

Objective Truth

Convenient ways of summarizing data, with no other meaning

Reflections of the real divisions of the world into distinct types

- 1 Clusters should generalize well.
- 2 Clusters should generalize to new features.
- Clusters should fit into a theory or narrative.

Evaluating Clusters

- 1. Silhouette scores
- 2. Segment (Cluster) profile
- 3. ANOVA and MANOVA
- 4. Cubic Clustering Criterion (CCC)
- 5. Predict cluster membership using classification

Silhouette Score



 α = Average distance to all data points within its own cluster

This is a measure of how well a point is assigned to its cluster. The smaller the value, the better the assignment.

b = Average distance to all data points within the closest cluster

Silhouette Score

$$s = \frac{b - a}{\max(a, b)}$$

 α = Average distance to all data points within its own cluster

b = Average distance to all data points within the closest cluster

Silhouette Score

$$s = \frac{b - a}{\max(a, b)}$$

a = Average distanceto all data pointswithin its own cluster

b = Average distance
 to all data points within
 the closest cluster

$$s = \begin{cases} 1 - \frac{a}{b}, & \text{if } a < b \\ 0, & \text{if } a = b \\ \frac{b}{a} - 1, & \text{if } a > b \end{cases}$$

Therefore:
$$-1 < s < 1$$

For *S* to be close to 1 we require $a \ll b$.

→ → → PCA + Clustering Tutorial

15_clustering.ipynb

\rightarrow \rightarrow Homework

DAPT-631 Homework Assignment #4

Due date: 12-MAY-2024