Introduction to machine-learning using scikit-learn

QLSC612

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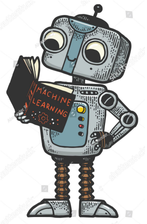
By

Mohammad Torabi & Michelle Wang

McGill UNIVERSITY

ORIGAMI Lab

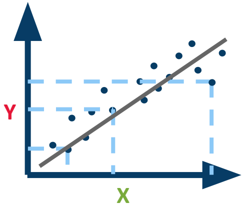
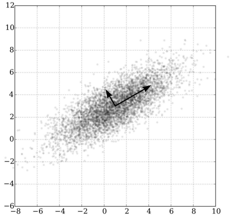
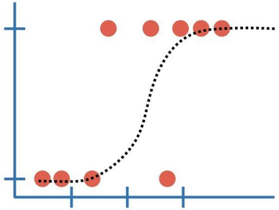
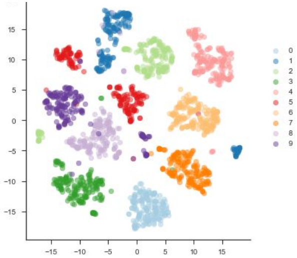
neuro Montreal Neurological Institute-Hospital



Objectives

- Part 2: Unsupervised learning
    - Dimensionality reduction
    - Clustering
    - *Coding example: PCA, k-means*
    - *Coding example: fMRI site prediction*

Types of ML Algorithms

Outcome	Supervised Learning	Unsupervised Learning
Continuous	Regression  	Principal Component 
Categorical	Classification 	Clustering 

Types of ML Algorithms

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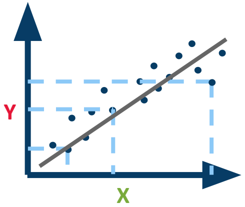
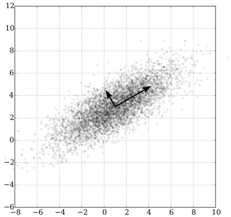
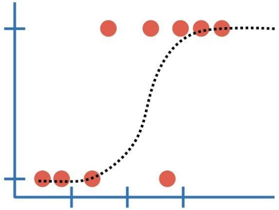
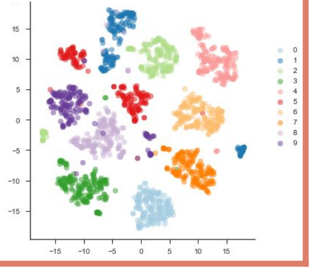
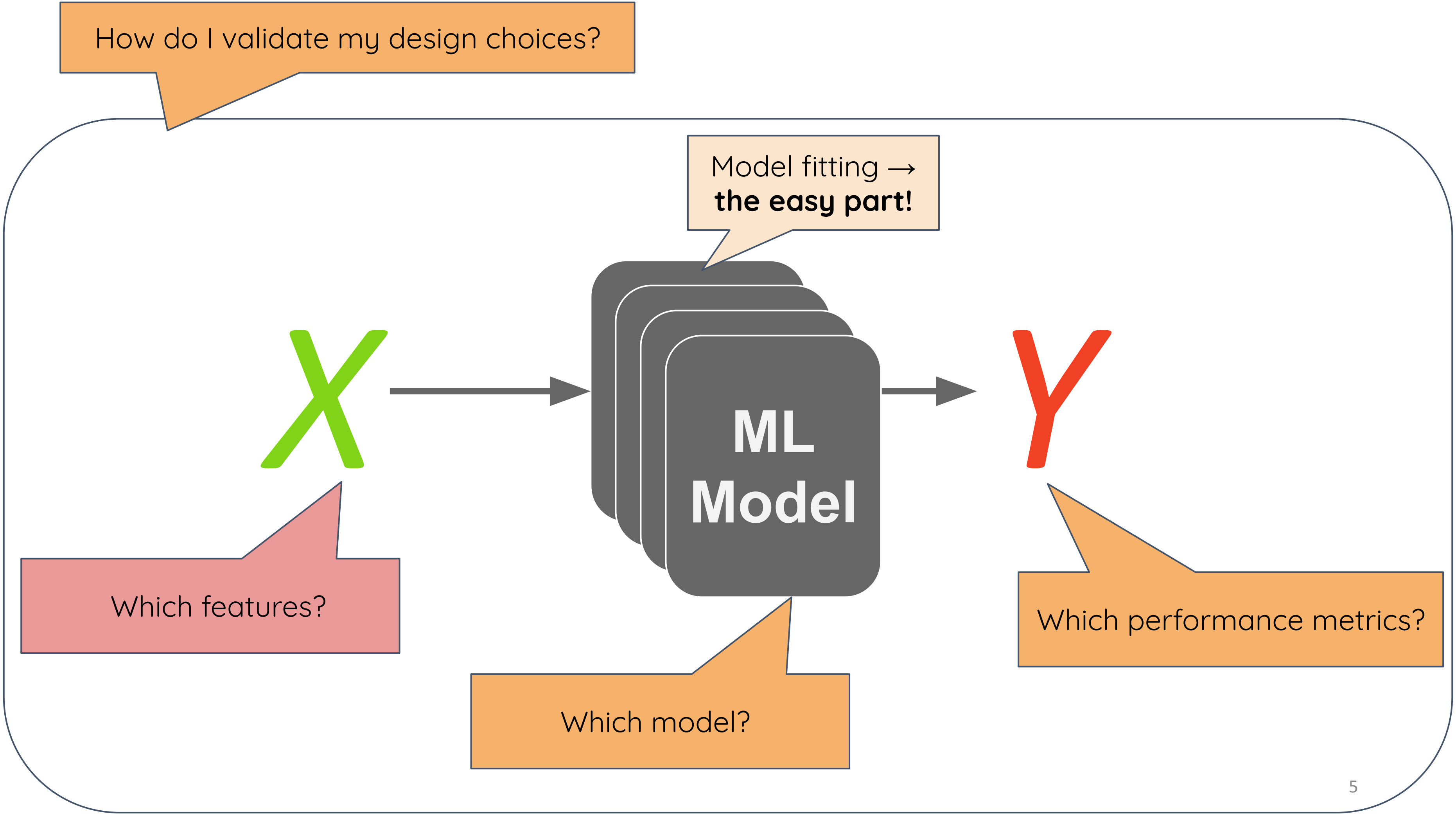
Continuous	Regression  	Principal Component 
Categorical	Classification 	Clustering 



How do I validate my design choices?

Model fitting →
the easy part!

Which features?

Which model?

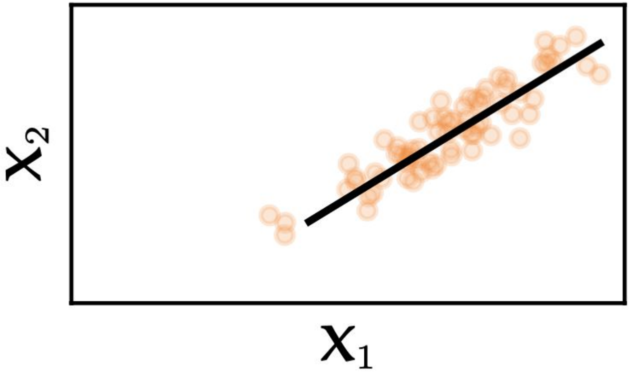
Which performance metrics?

Unsupervised learning

- Learning without knowing the true labels
- Objectives
  - Dimensionality reduction of features through **transformation** rather than **selection**
  - Grouping of samples based on **“similarity”**
- Techniques
  - Feature Transformation/Projection
  - Clustering

Dimensionality Reduction

Data is almost 1-dimensional
BUT represented as
2-dimensional

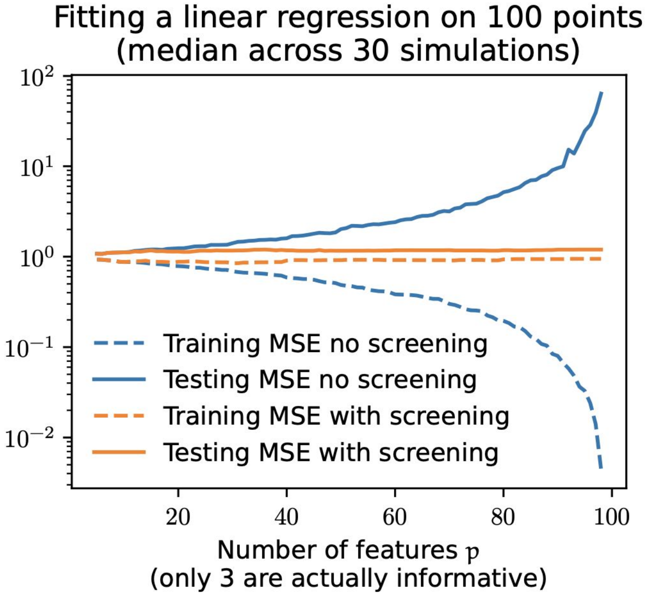


Dimensionality Reduction

- **Curse of Dimensionality:** large number of input features can dramatically impact the performance of ML algorithms
- Techniques:
  - Feature selection (usually supervised)
  - Feature transformation (usually unsupervised)
- Feature transformation is useful for
  - Information compression
  - Data artifact clean-up
  - Visualization

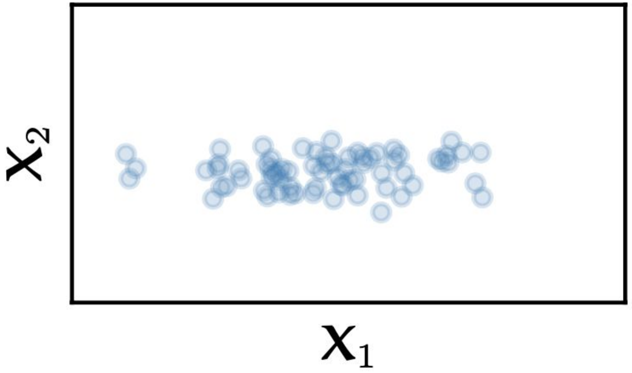
Dimensionality Reduction

- High dimensional data:
  - Model complexity increases -> unstable solution
  - Risk of overfitting: fitting exactly training data but failing on test data

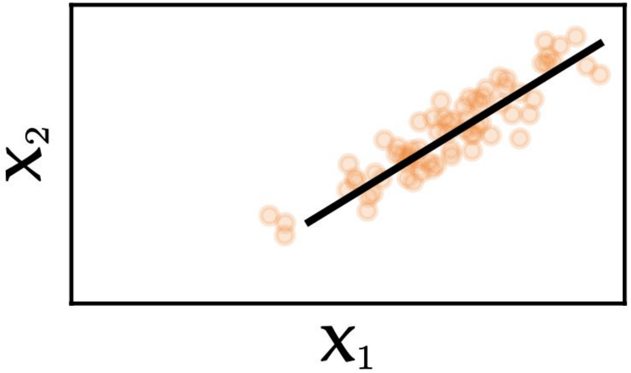


Feature Transformation vs. Feature Selection

Maybe OK to drop X2

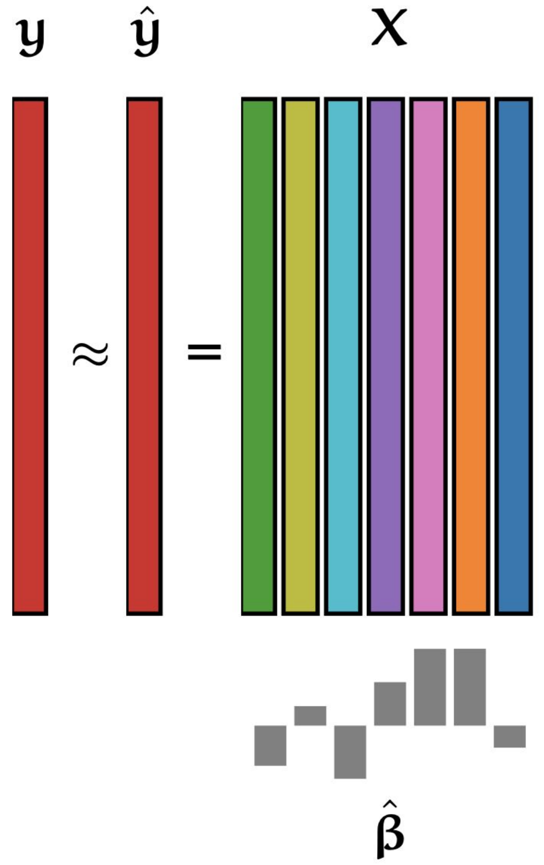


Data is low-dimensional BUT no feature can be dropped



Feature Transformation vs. Feature Selection

$$\hat{\mathbf{y}} = \mathbf{X}\,\hat{\boldsymbol{\beta}}$$



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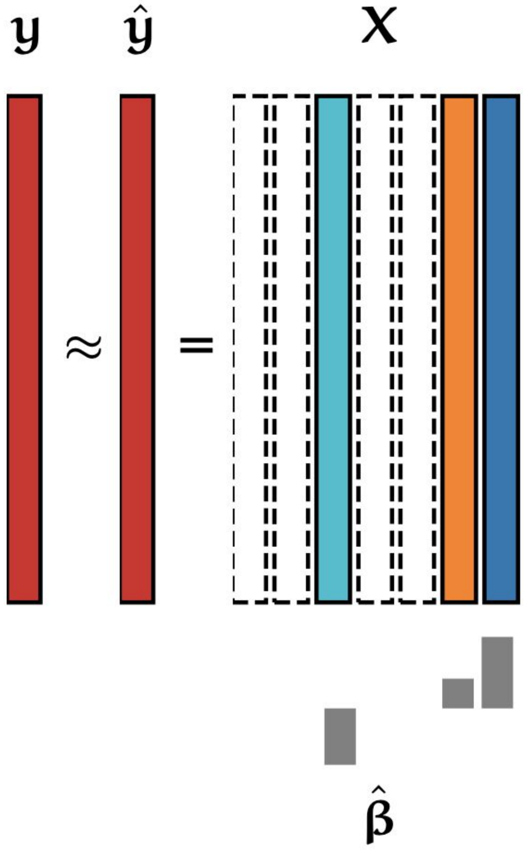
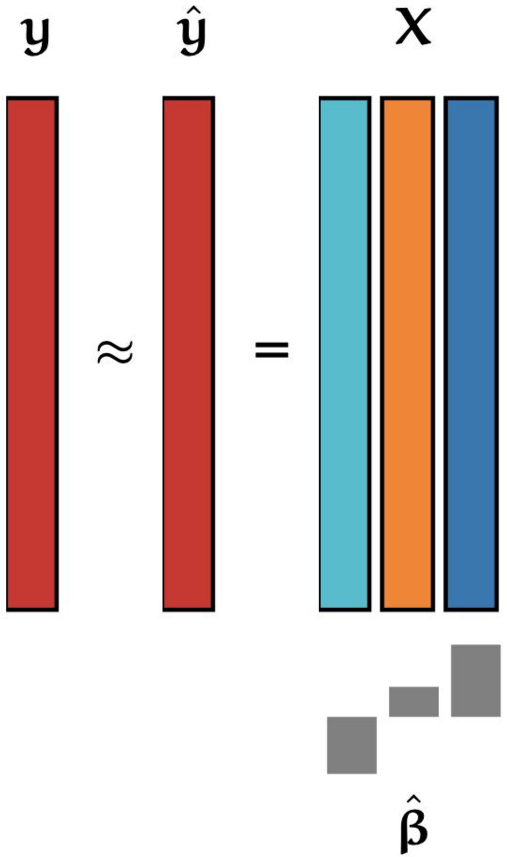


Feature Transformation vs. Feature Selection



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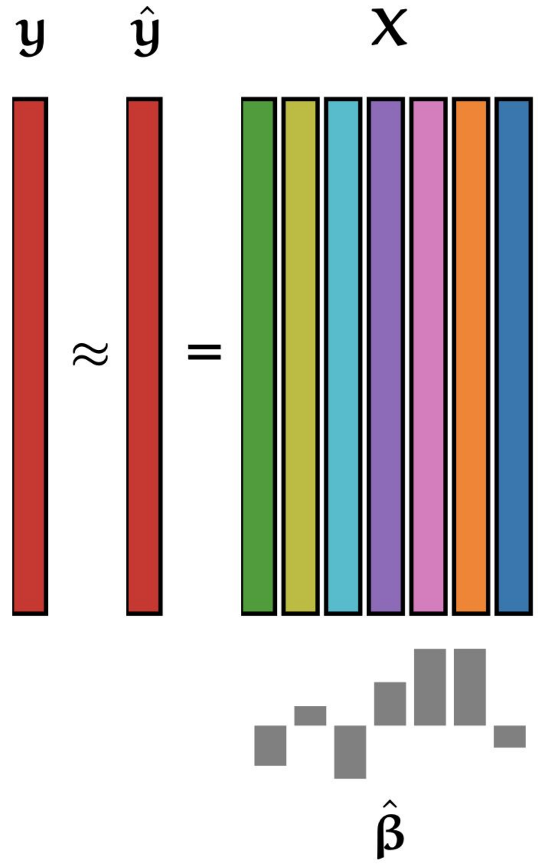
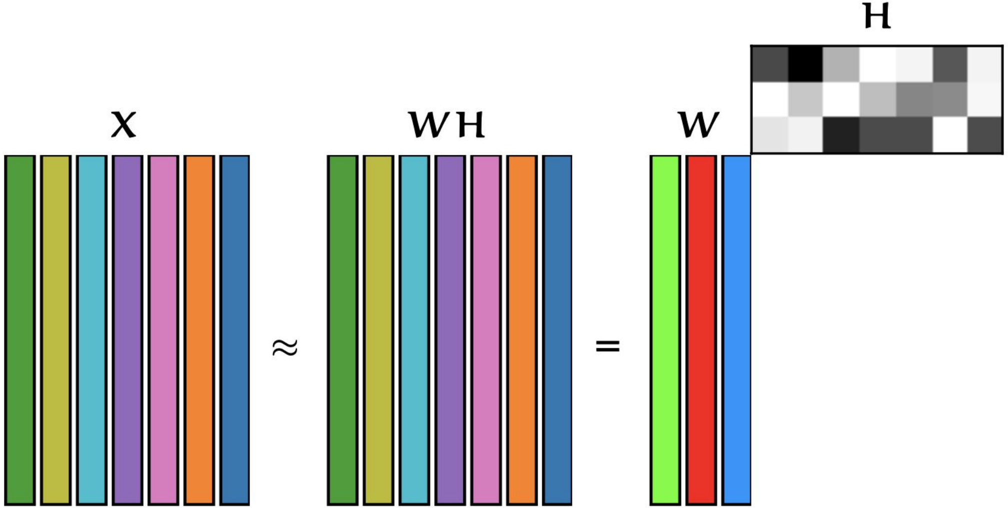


Feature Transformation vs. Feature Selection

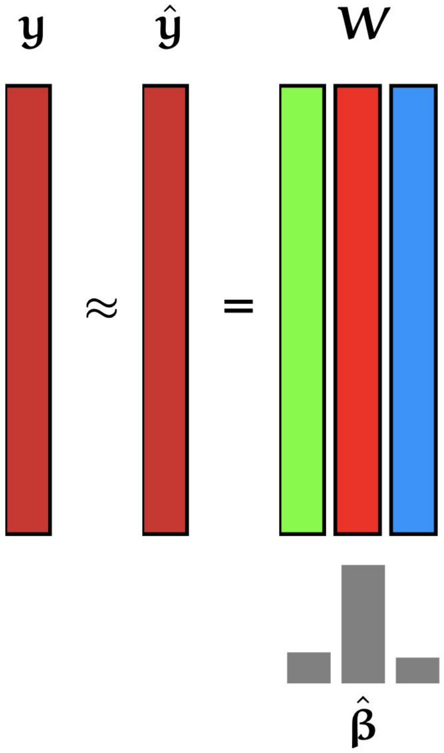
Minimize

$$\|\mathbf{X} - \mathbf{W}\mathbf{H}\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - (\mathbf{W}\mathbf{H})_{i,j})^2$$



Feature Transformation vs. Feature Selection

$$\hat{\mathbf{y}} = \boldsymbol{W}\hat{\boldsymbol{\beta}}$$

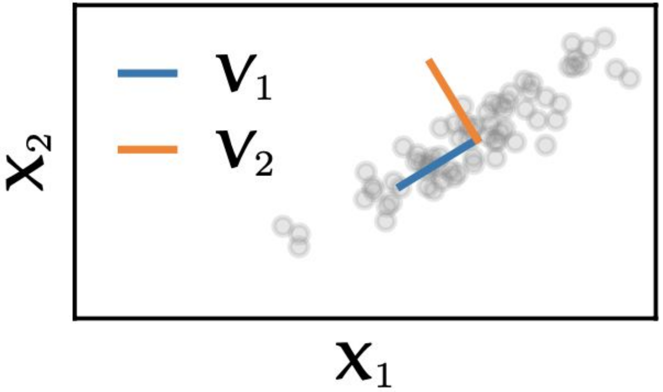


Feature Transformation

- Change of basis (i.e. “perspective”) for data representation
- Priors on data generation process
    - Singular Value Decomposition (SVD)
    - Principal Component Analysis (PCA)
    - Independent Component Analysis (ICA)
    - Non-negative Matrix Factorization (NMF)

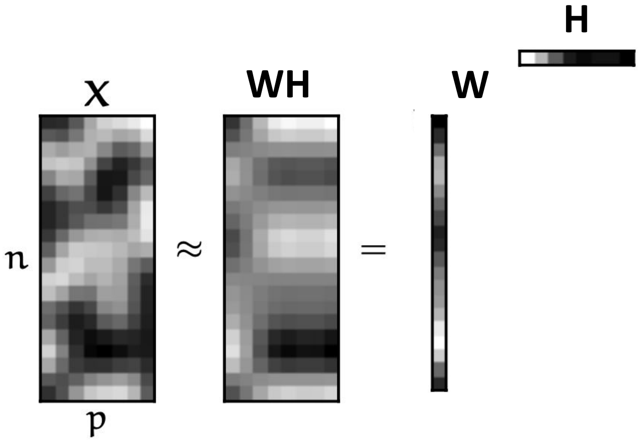
Principal Component Analysis (PCA)

- PCA finds the components (eigenvectors) that are orthogonal and capture the maximum variance in data.
- These components form the basis of the new space that the data will be transformed to
- Truncating the components to keep only the first k components gives the best rank-k approximation of X and transforms X to k-dim space



Principal Component Analysis (PCA)

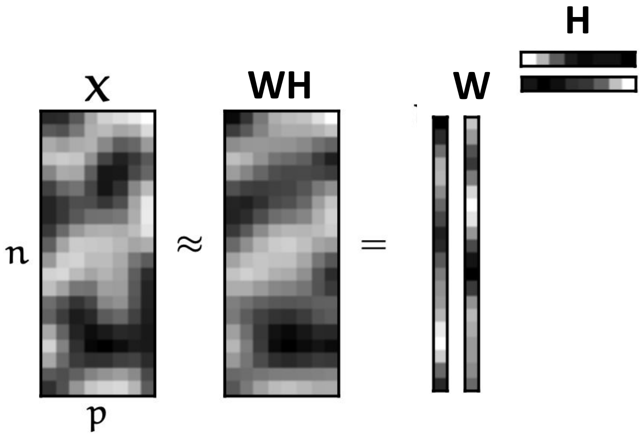
Reconstructing with 1 principal component:



Explained variance: 0.53

Principal Component Analysis (PCA)

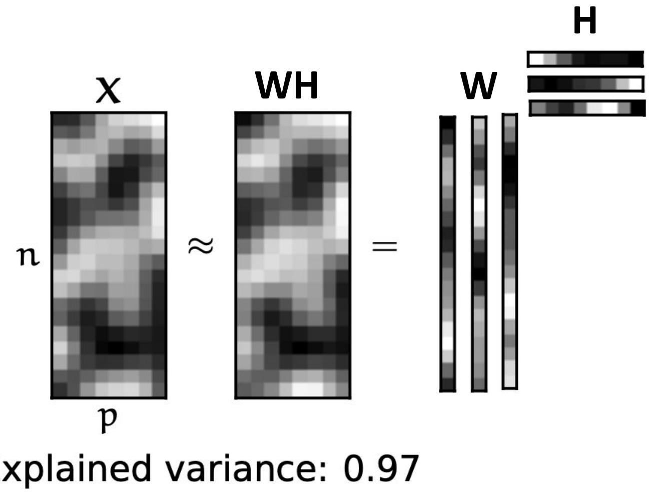
Reconstructing with 2 principal components:



Explained variance: 0.84

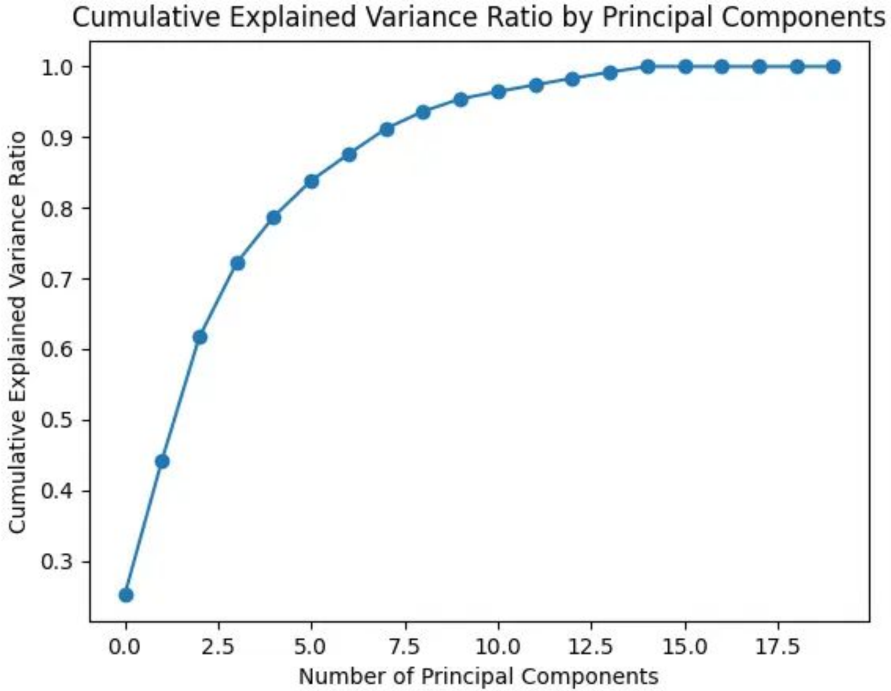
Principal Component Analysis (PCA)

Reconstructing with 3 principal components:

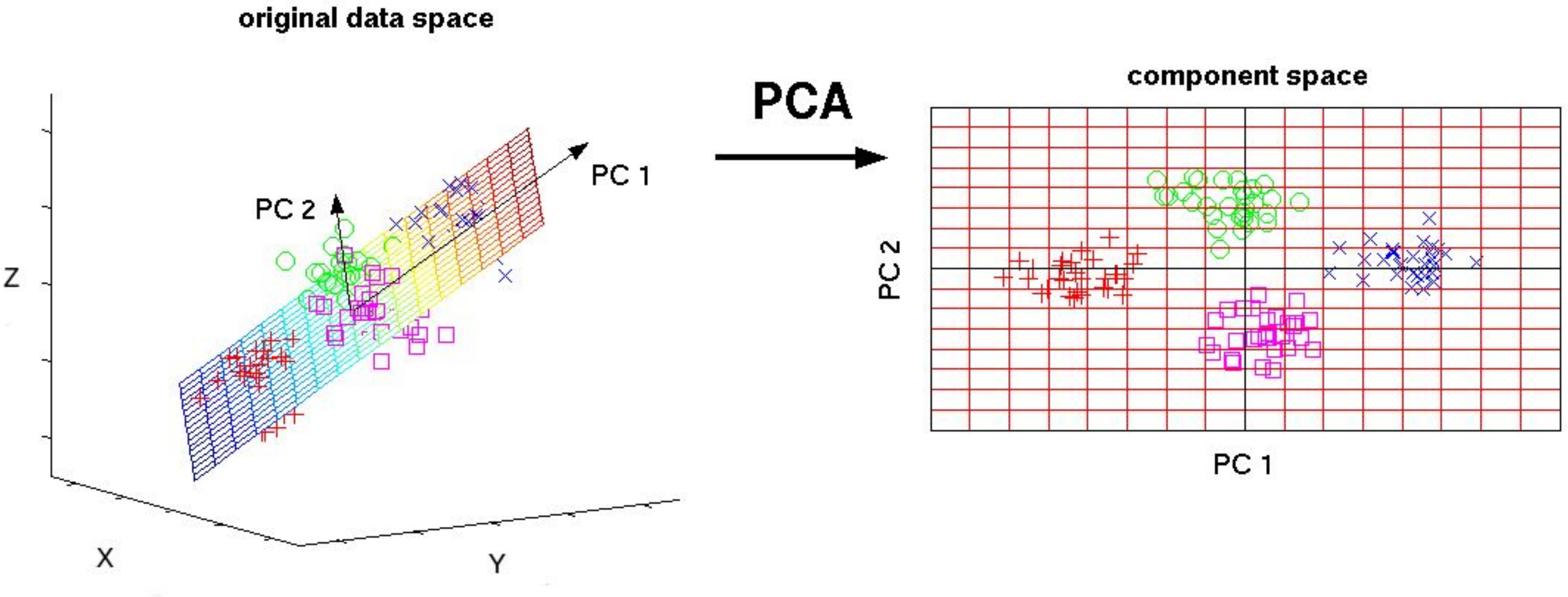


Principal Component Analysis

- Variance explained

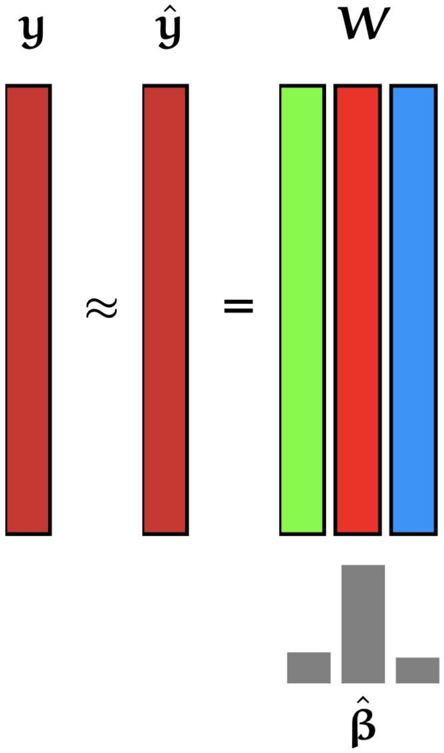


Principal Component Analysis (PCA)



Principal Component Analysis (PCA)

$$\hat{\mathbf{y}} = \boldsymbol{W}\hat{\boldsymbol{\beta}}$$



Principal Component Analysis

- sklearn

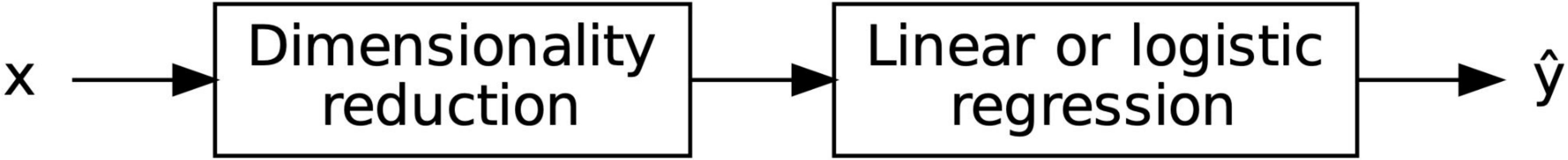
```
transformer = PCA(n_components=N)
transformer.fit(X)
transformed_X = transformer.transform(X)
print(transformed_X.shape) #(n_samples, n_components)
```

```
transformer = PCA(n_components=N)
transformed_X = transformer.fit_transform(X)
```

sklearn.decomposition.PCA

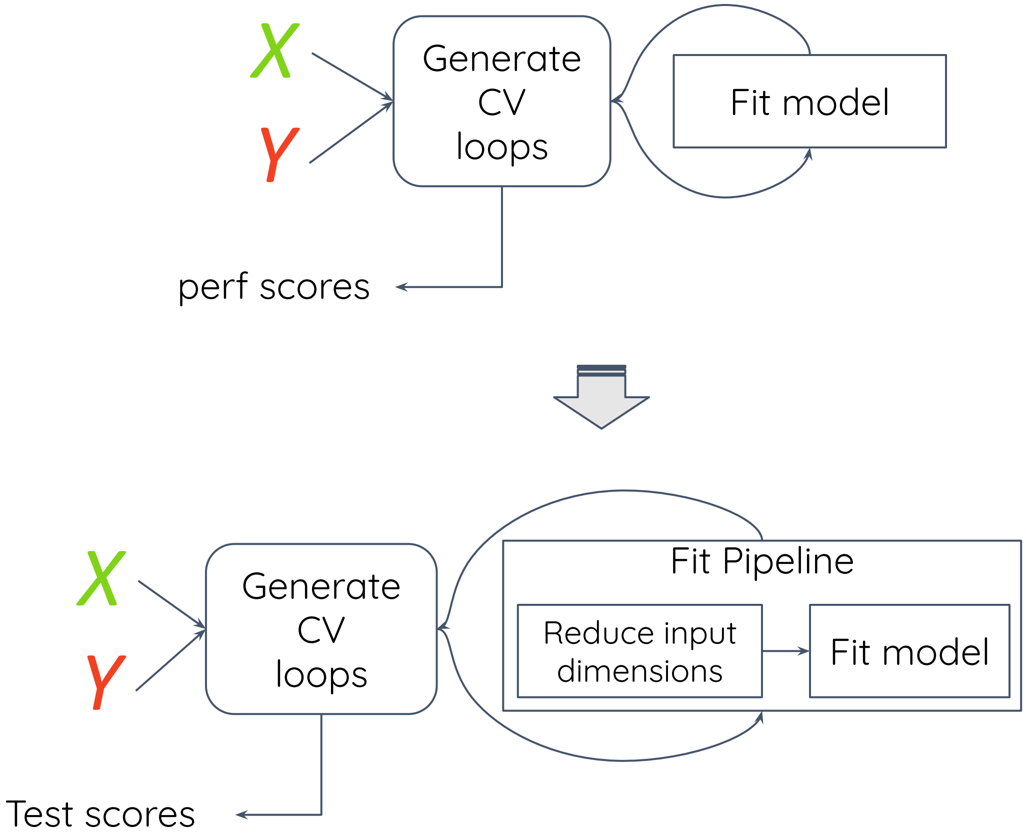
Dimensionality Reduction

- A preprocessing step



Pipelines

- Chain various “preprocessing” tasks in your analysis
    - Feature scaling
    - Dimensionality reduction
- Avoids mistakes e.g. double dipping
- Simplifies changes to your analysis



Pipelines

- Feature selection / transformation only on the training data!

```
transformer = PCA(n_components=N)
transformed_train = transformer.fit_transform(X_train)
Transformed_test = transformer.transform(X_test)
```

`sklearn.pipeline.make_pipeline`

Pipelines

```
pipeline = make_pipeline(PCA(n_components=N), LinearRegression())
pipeline.fit(X_train, y_train)
y_test_predicted = pipeline.predict(X_test)
```

sklearn.pipeline.make_pipeline

Clustering

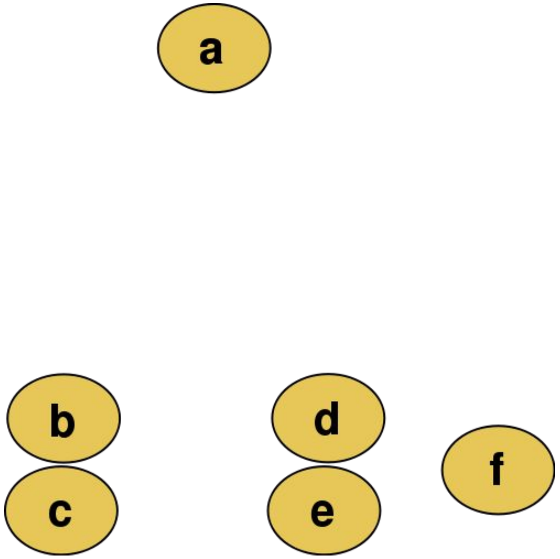
- Grouping observations together without knowing their true labels
- Use distance (i.e. similarity) between samples (often in a high-dimensional space!)
- Things to consider
  - Priors on parameters (e.g. n_clusters)
  - Scalability

Clustering

Method name	Parameters	Scalability	Usecase	Geometry (metric used)
K-Means	number of clusters	Very large `n_samples`, medium `n_clusters` with MiniBatch code	General-purpose, even cluster size, flat geometry, not too many clusters, inductive	Distances between points
Agglomerative clustering	number of clusters or distance threshold, linkage type, distance	Large `n_samples` and `n_clusters`	Many clusters, possibly connectivity constraints, non Euclidean distances, transductive	Any pairwise distance
Gaussian mixtures	many	Not scalable	Flat geometry, good for density estimation, inductive	Mahalanobis distances to centers

Clustering

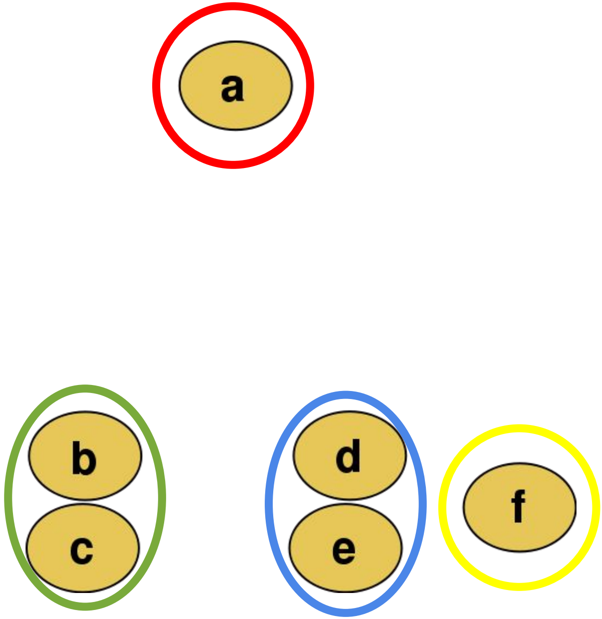
- Which samples will cluster together?



Sample space

Clustering

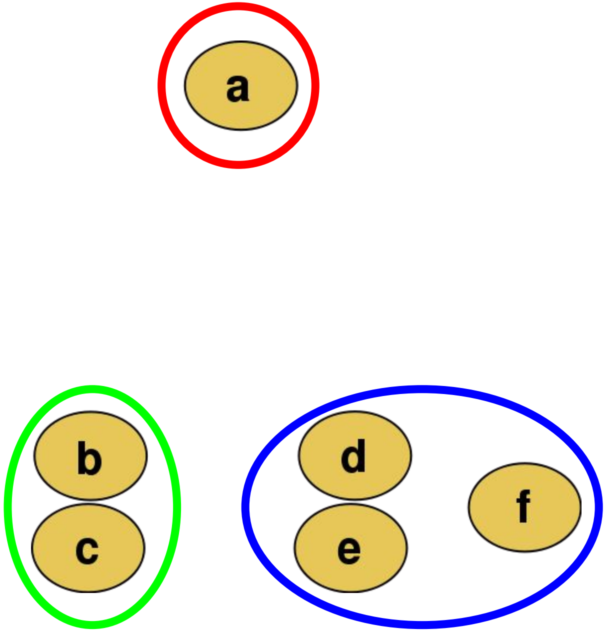
- Which samples will cluster together if n_clusters=4?



Sample space

Clustering

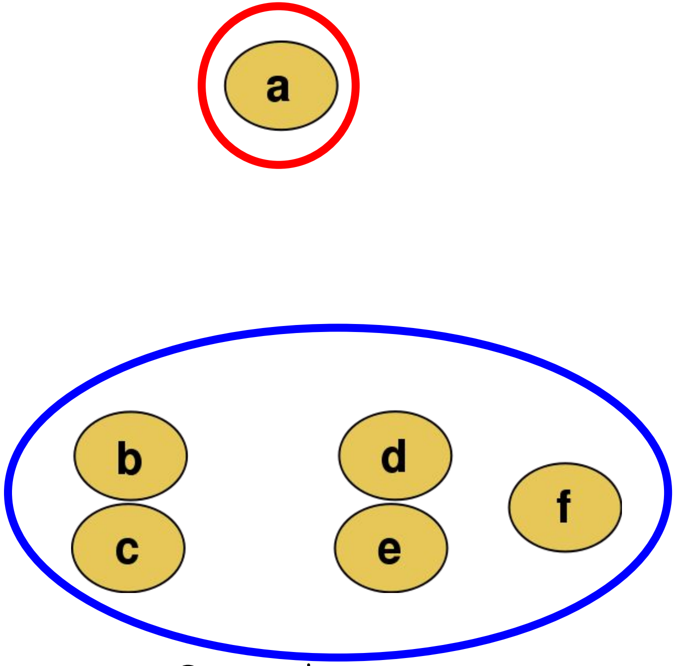
- Which samples will cluster together if n_clusters=3?



Sample space

Clustering

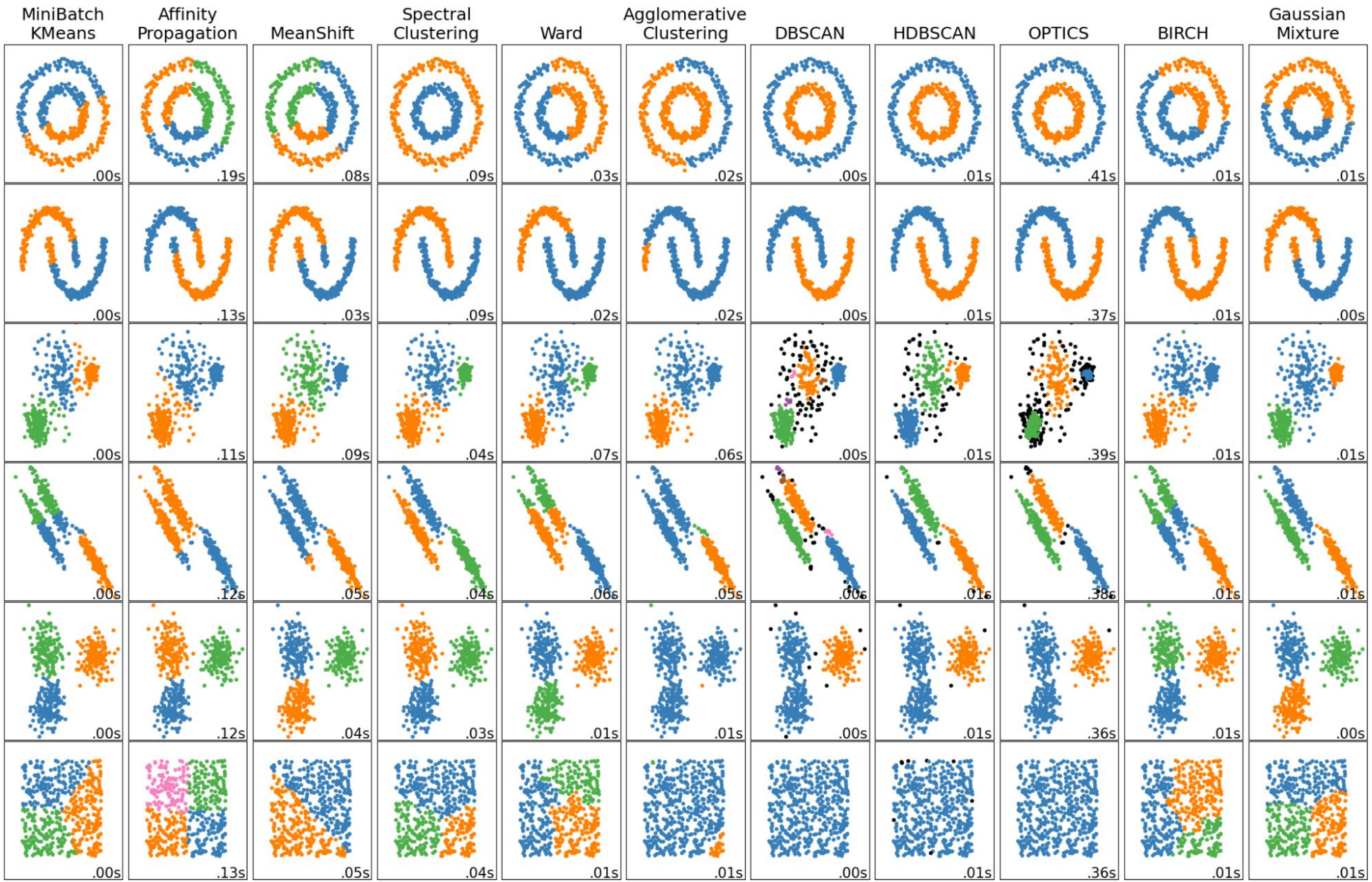
- Which samples will cluster together if n_clusters=2?



Sample space

Clustering

… is in the eyes of the beholder



K-means Clustering

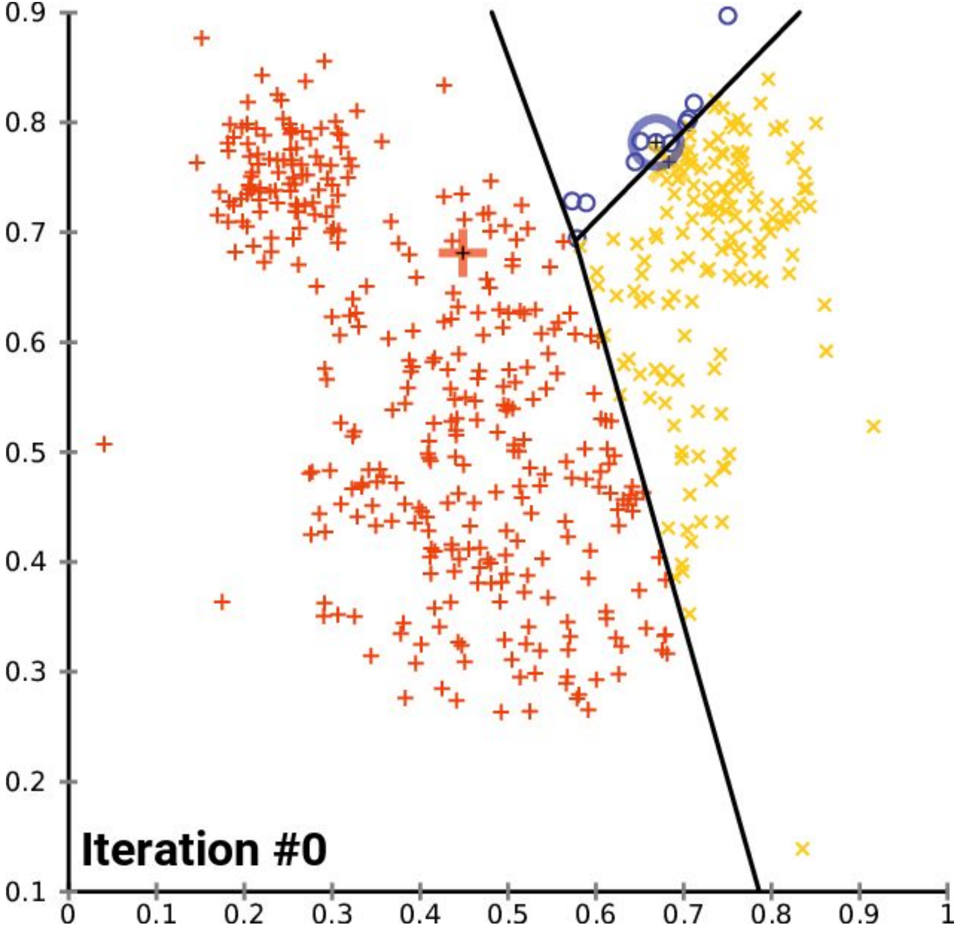
- The K-means algorithm aims to choose centroids that minimise the inertia, or within-cluster sum-of-squares criterion
- Each centroid represents a cluster
- This algorithm requires the number of clusters to be specified
- Very high-dimensional spaces result in inflated Euclidean distances (an instance of curse of dimensionality)
    - Run a dimensionality reduction algorithm (e.g. PCA) prior to k-means clustering

$$\sum_{i=0}^{n} \min_{\mu_j \in C}(||x_i - \mu_j||^2)$$

K-means Clustering

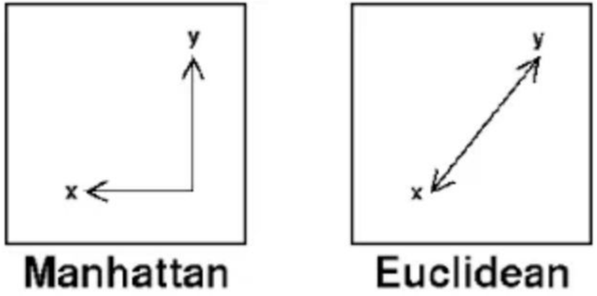
Steps:

1. **Initialization:** Choose k random centroids
2. **Assignment step:** Assign each observation to the cluster with the nearest mean.
3. **Update step:** Recalculate means (centroids) for observations assigned to each cluster.



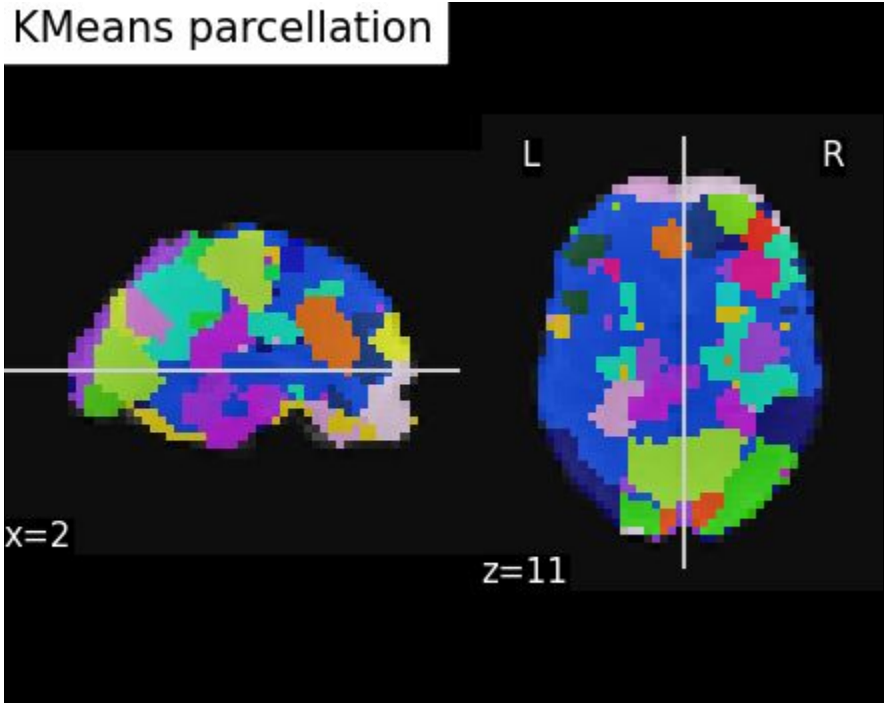
Distance Metrics

- Euclidean distance
- Manhattan distance
- Hamming distance
- Correlation (1 - corr)



Biological Example

- Parcellate brain voxels based on their fMRI signals
- How do we know if the clustering is done well?
- What metrics do we have?



Clustering methods to learn a brain parcellation from fMRI

Evaluation of clusters

- Internal validation (without true labels):
    - Silhouette Coefficient

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

- external validation
    - With true labels:
        - Rand Index (RI) and Adjusted Rand Index (ARI)
        - Mutual Information

$$\text{RI} = \frac{a + b}{C_2^{n_{samples}}}$$

$$\text{ARI} = \frac{\text{RI} - E[\text{RI}]}{\max(\text{RI}) - E[\text{RI}]}$$

Clustering Performance Evaluation

Project

- **Data:** X: connectivity features derived from fMRI data, y: fMRI site label for each participant.
- **Visualize the data:** you have to apply dimensionality reduction first
- **Classification (supervised learning):** Use different models to classify and predict the fMRI site using the connectivity features and compare their performance. We will use scikit-learn pipeline for this purpose, which chains different transformations. Then we will fit the whole pipeline on our data using cross-validation.
- **Clustering (unsupervised learning):** use K-means clustering to cluster the participants. Find the best number of clusters and evaluate the clustering performance.