

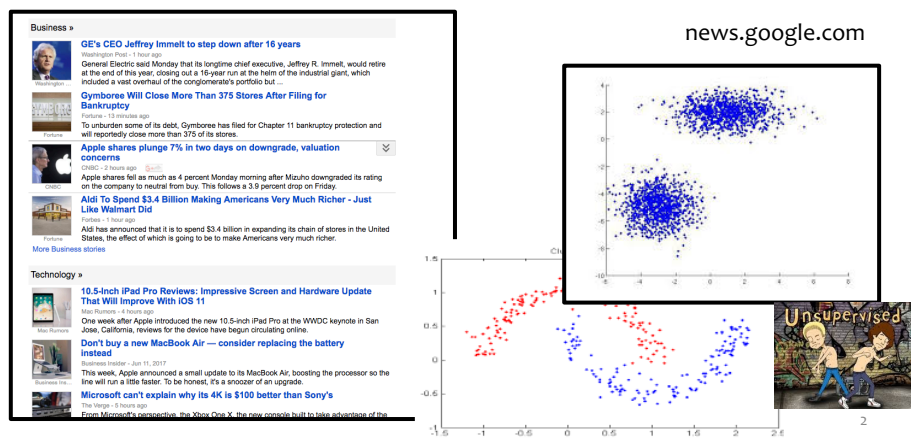
Unsupervised Learning

Stephan Robert

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Unsupervised Learning

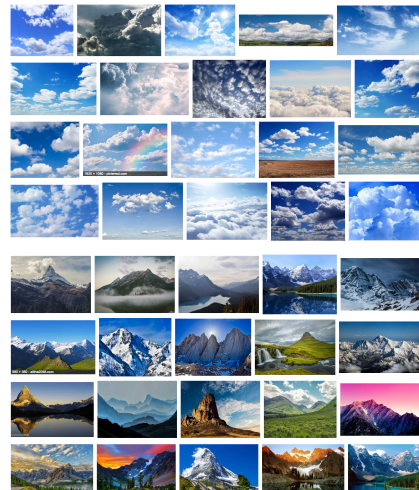
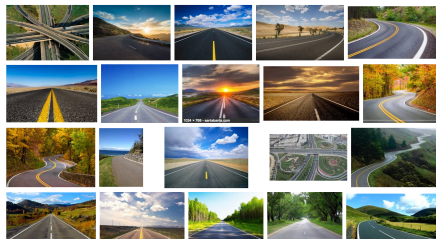
- Learning without the presence of an expert (e.g k-means, clustering approaches ,...)



Unsupervised Learning

- **Clustering** images,
group as:

- ✦ Clouds
- ✦ Mountains
- ✦ Roads



- Users on Web sites (groups, activities)
- Words (First names, last names, location words, ...)

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Unsupervised Learning

- Supervised Learning. Training set:

$$\{((x)_1, (y)_1), ((x)_2, (y)_2), ((x)_3, (y)_3), \dots, ((x)_m, (y)_m)\}$$

- Unsupervised Learning. Training set:

$$\{(x)_1, (x)_2, (x)_3, \dots, (x)_m\}$$

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Algorithms

- K-Means
- Principal Component Analysis (PCA)

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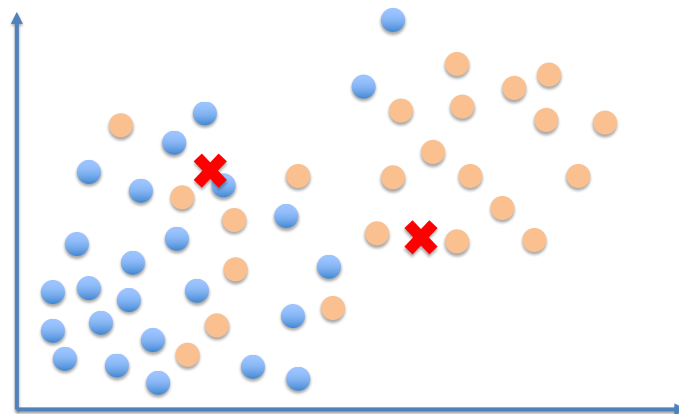
K-Means Algorithm

- Randomly chose K examples as initial centroids
- While true:
 - create k clusters by assigning each example to closest centroid
 - compute k new centroids by averaging examples in each cluster
 - if centroids don't change:
- Break

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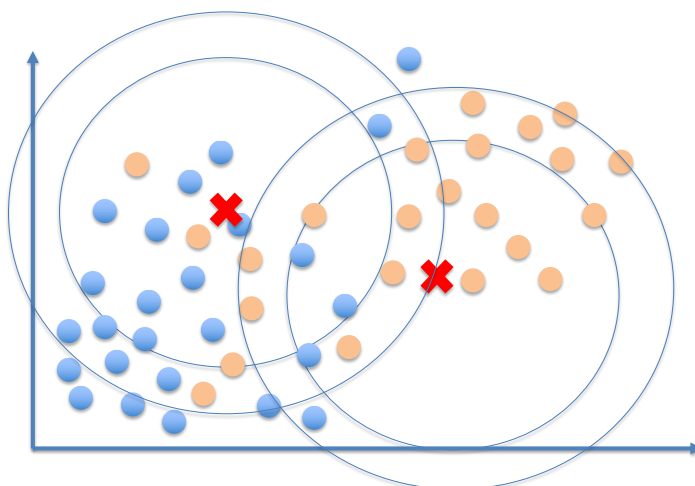
K-Means Algorithm

Random placement of the centroids



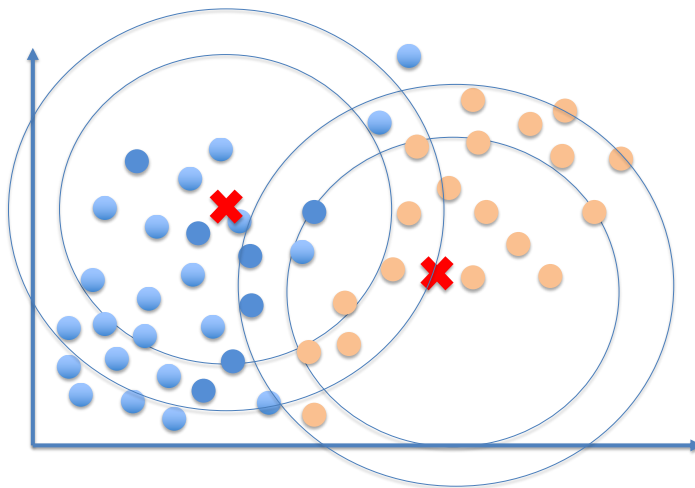
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K-Means Algorithm: iteration 1



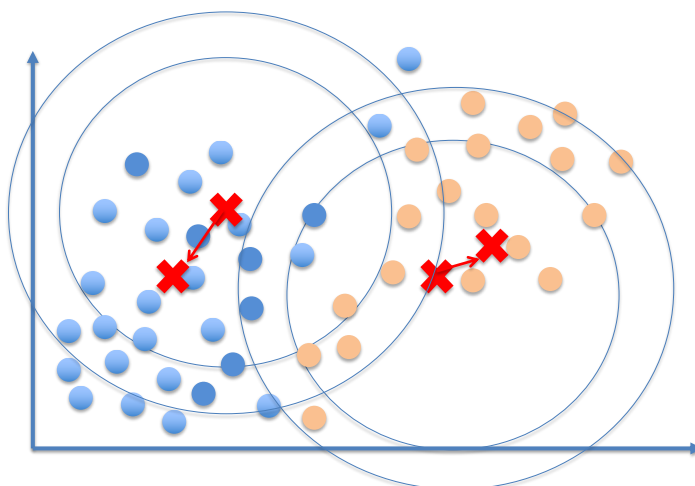
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K-Means Algorithm: iteration 1



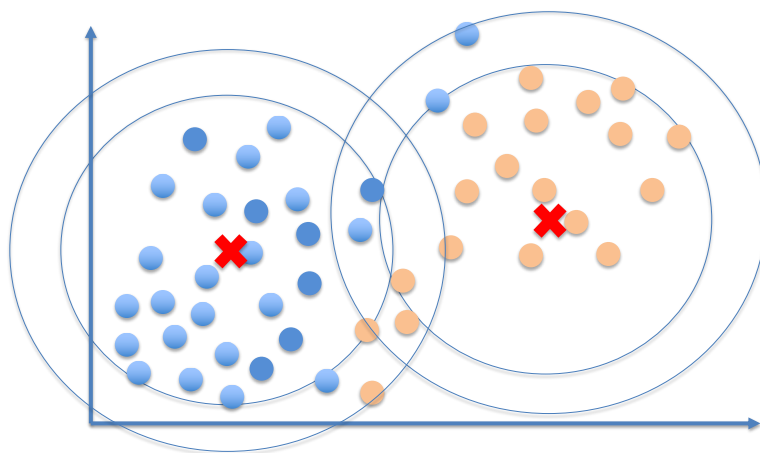
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K-Means Algorithm: iteration 2



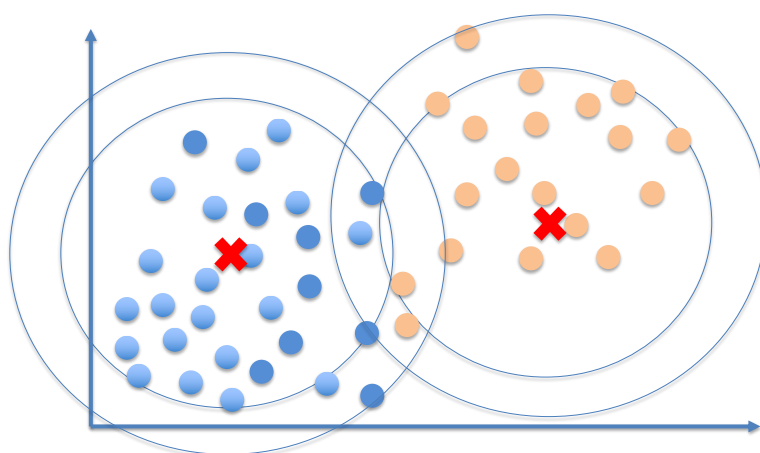
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K-Means Algorithm: iteration 3



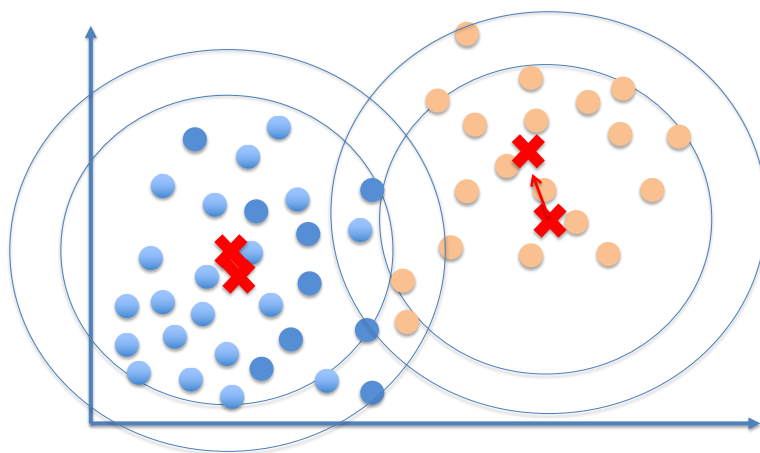
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K-Means Algorithm: iteration 3



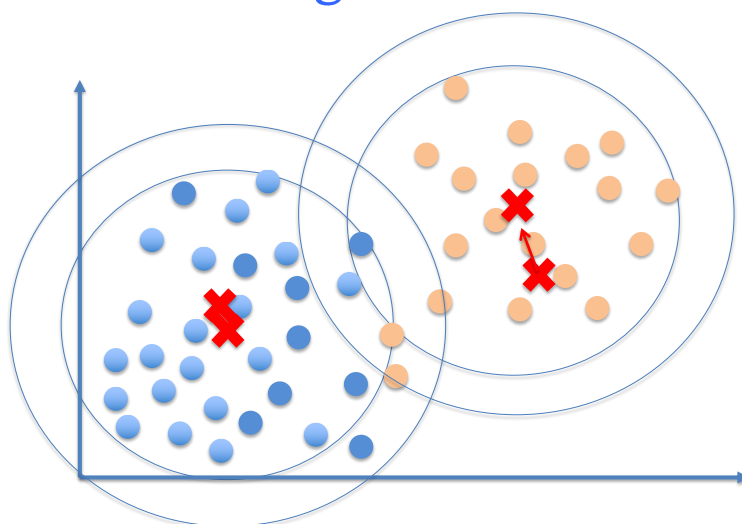
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K-Means Algorithm: iteration 4



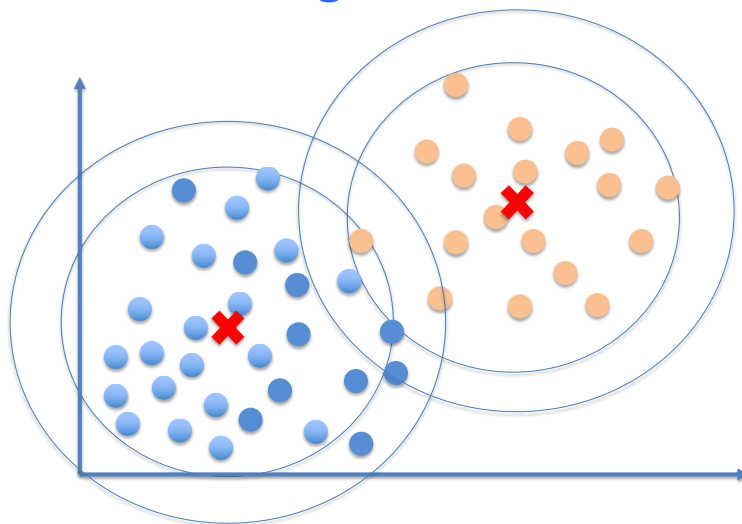
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K-Means Algorithm: iteration 4



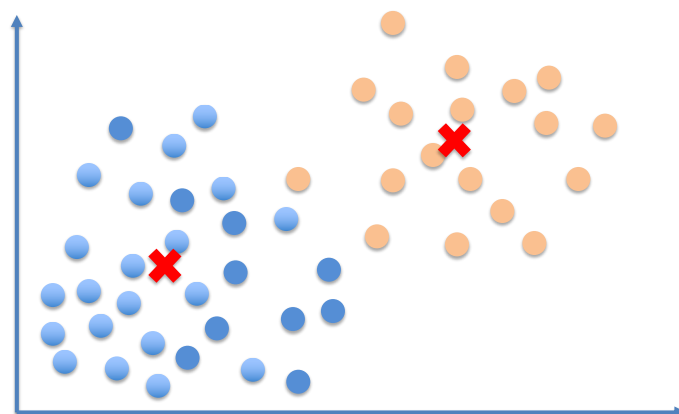
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K-Means Algorithm: iteration 5



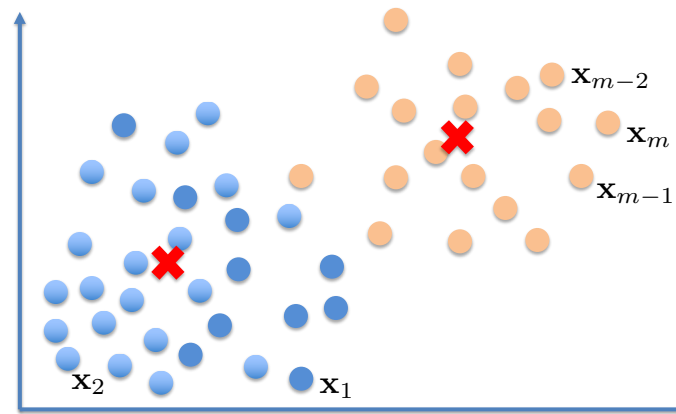
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K-Means Algorithm: iteration 5



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K-Means Algorithm: stop



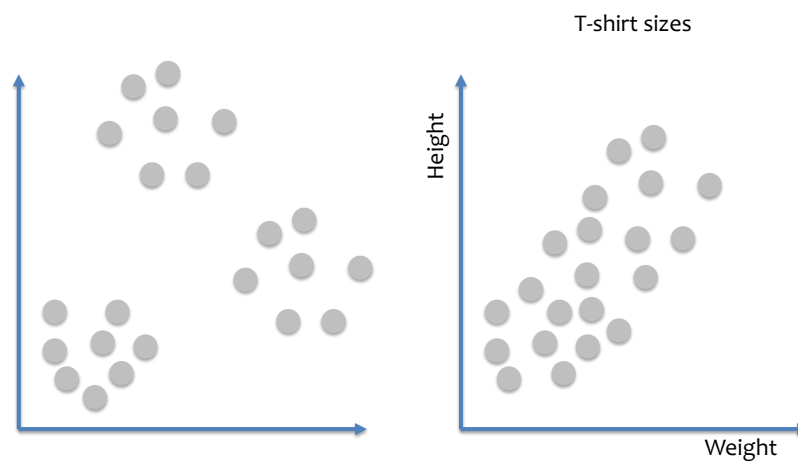
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K-Means Algorithm

- randomly chose K examples as initial centroids
- for $i=1$ to m (number of vectors \mathbf{x}):
 - Create K clusters by assigning each example to closest centroid. Label each \mathbf{x} with $(c)_i \in \mathbb{N}^K$
- For $k=1$ to K
 - compute k new centroids by averaging examples in each cluster (l is the number of \mathbf{x} associated to the centroid)
$$\mu_k = \frac{1}{l} \sum_{i=1}^l \mathbf{x}_i \in \mathbb{R}^n$$
- Repeat if centroids do change, else finished

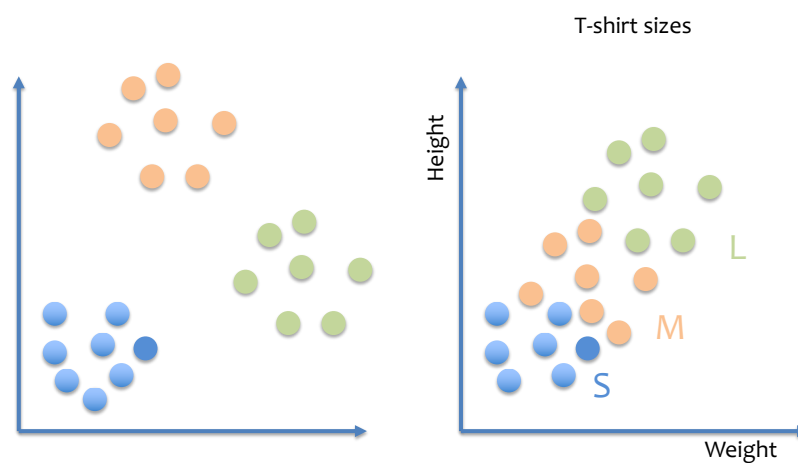
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Clusters for non-separated clusters



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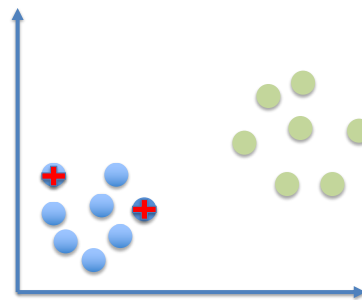
Clusters for non-separated clusters



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Random initialisation

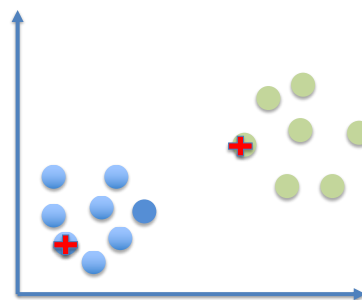
- Should have $K < m$!
- Randomly pick K training examples
- Set $\mu_1, \mu_2, \dots, \mu_k$ equal to these K examples



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Random initialisation

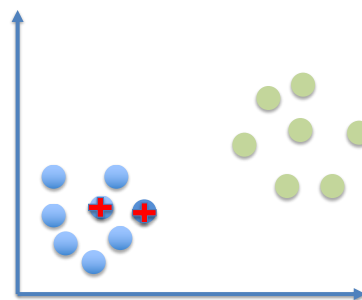
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Random initialisation

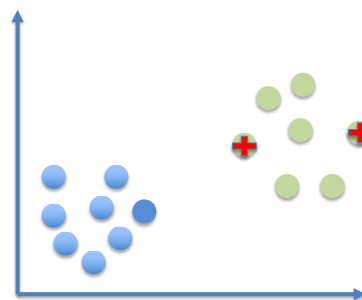
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Random initialisation

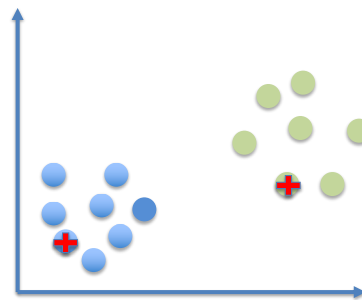
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Random initialisation

- Should have $K < m$!
- Randomly pick K training examples
- Set $\mu_1, \mu_2, \dots, \mu_k$ equal to these K examples



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Choosing the number of clusters

- Cost function:

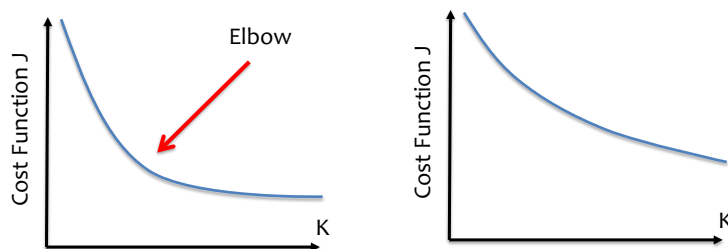
$$J = \frac{1}{m} \sum_{i=1}^m \|\mathbf{x}_i - \mu_{(c)_i}\|$$

$(c)_i$ is the index of the cluster to which \mathbf{x}_i is assigned, $= 1, 2, \dots, K$

$$\min_{\substack{(c)_1, (c)_2, \dots, (c)_m \\ \mu_1, \mu_2, \dots, \mu_K}} J$$

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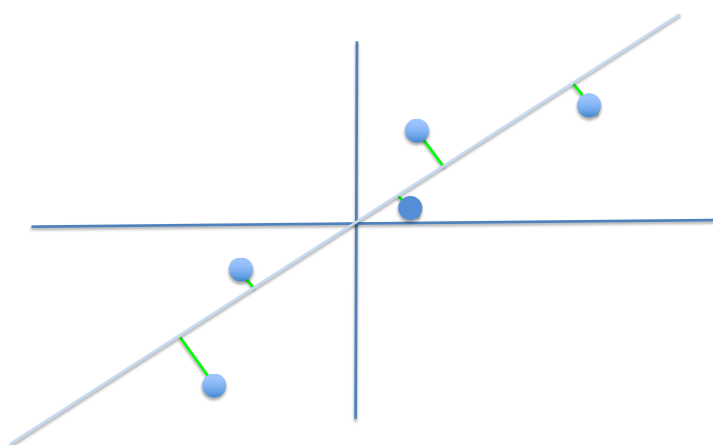
Choosing the number of clusters



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Principal Component Analysis (PCA)

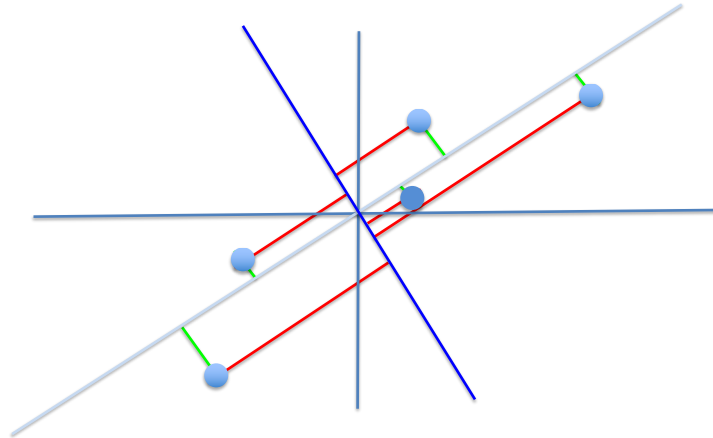
Problem Formulation



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Principal Component Analysis (PCA)

Problem Formulation

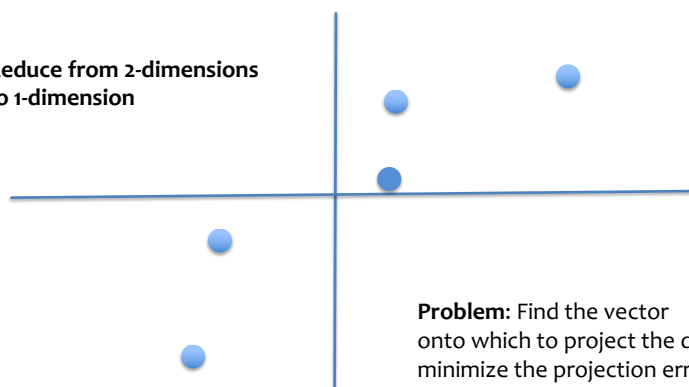


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Principal Component Analysis (PCA)

Problem Formulation

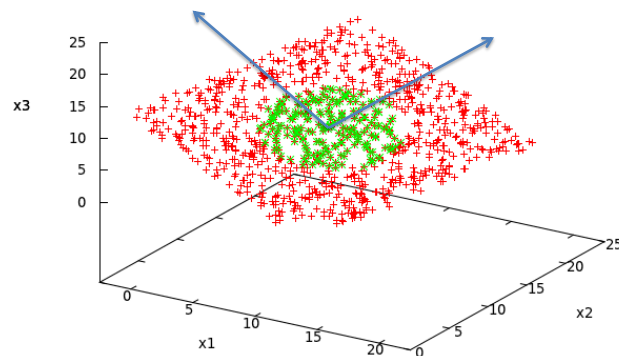
Reduce from 2-dimensions
to 1-dimension



Problem: Find the vector
onto which to project the data to
minimize the projection error

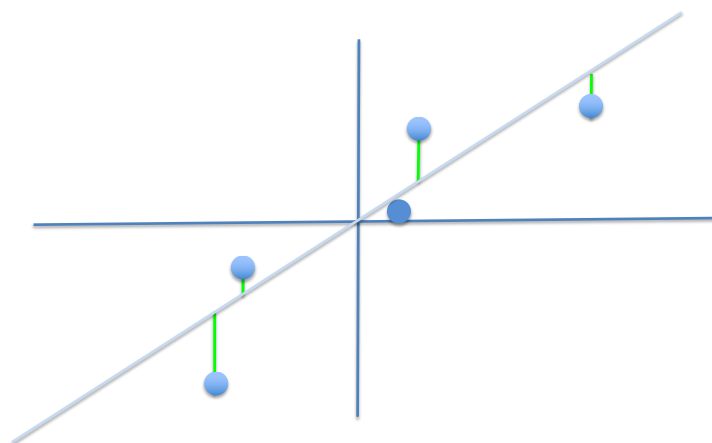
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PCA: 3D \rightarrow 2D



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PCA: **Not** a linear regression



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PCA: data preprocessing

- Training set: $(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_m)$

- Preprocessing:
$$\mu_0 = \frac{1}{m} \sum_{i=1}^m (x_0)_i$$

$$\mu_1 = \frac{1}{m} \sum_{i=1}^m (x_1)_i$$

$$\vdots$$

- Replace each $(x_j)_i$ with $(x_j)_i - \mu_j$
- Eventually scaling: replace each $(x_j)_i$ with

$$\frac{(x_j)_i - \mu_j}{\sigma_j}$$

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PCA Algorithm

- Reduce data from n -dimension to k -dimension

- Covariance matrix:

$$(\mathbf{x})_i = \mathbf{x}_i = \begin{pmatrix} (x_0)_i \\ (x_1)_i \\ \vdots \\ (x_n)_i \end{pmatrix}$$

$$\Sigma = \frac{1}{m} \sum_{i=1}^m (\mathbf{x}_i \mathbf{x}_i^t) =$$

$$\begin{pmatrix} \frac{1}{m} \sum_{i=1}^m (x_0)_i (x_0)_i & \frac{1}{m} \sum_{i=1}^m (x_0)_i (x_1)_i & \dots & \frac{1}{m} \sum_{i=1}^m (x_0)_i (x_n)_i \\ \frac{1}{m} \sum_{i=1}^m (x_1)_i (x_0)_i & \frac{1}{m} \sum_{i=1}^m (x_1)_i (x_1)_i & \dots & \frac{1}{m} \sum_{i=1}^m (x_1)_i (x_n)_i \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{m} \sum_{i=1}^m (x_n)_i (x_0)_i & \frac{1}{m} \sum_{i=1}^m (x_n)_i (x_1)_i & \dots & \frac{1}{m} \sum_{i=1}^m (x_n)_i (x_n)_i \end{pmatrix}$$

- Compute the eigenvectors of Σ $\Sigma \in \mathbb{R}^{n \times n}$

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PCA Algorithm

- Eigenvectors: $\mathbf{u}_i, i = 1, \dots, n$

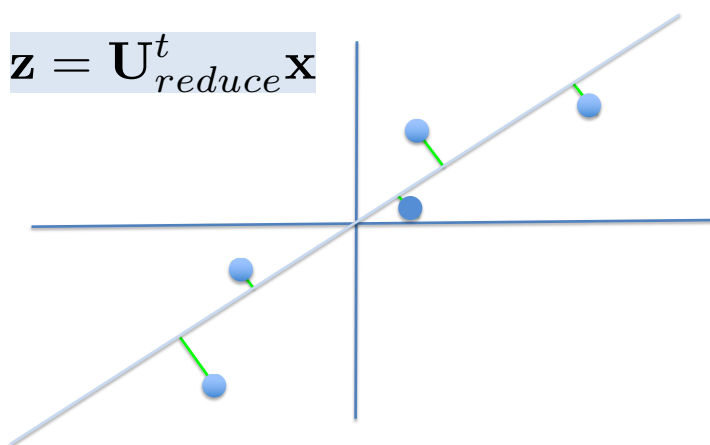
$$\mathbf{U} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \dots \ \mathbf{u}_n]$$
- We construct a matrix $\mathbf{U} \in \mathbb{R}^{n \times n}$ with the eigenvectors and another one with the k first eigenvectors: $\mathbf{U}_{reduce} \in \mathbb{R}^{n \times k}$

$$\mathbf{U}_{reduce} = [\mathbf{u}_1 \ \mathbf{u}_2 \ \dots \ \mathbf{u}_k]$$
- Notice: Normalize and scale eventually!
 Every feature should be 0-mean.

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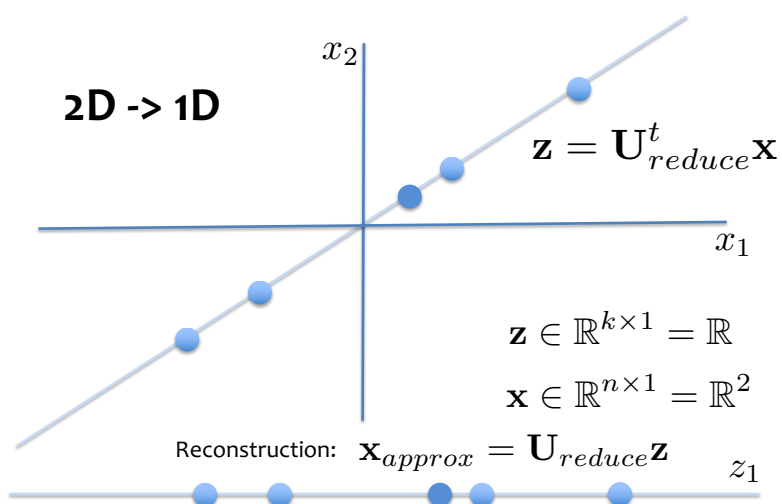
Principal Component Analysis (PCA)

$$\mathbf{z} = \mathbf{U}_{reduce}^t \mathbf{x}$$



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Principal Component Analysis (PCA)



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How many principal components?

- Average squared projection error:

$$\frac{1}{m} \sum_{i=1}^m \|(\mathbf{x})_i - (\mathbf{x}_{approx})_i\|^2$$

- Total variation in the data:

$$\frac{1}{m} \sum_{i=1}^m \|(\mathbf{x})_i\|^2$$

- Choose k to be the smallest value so that

$$\frac{\frac{1}{m} \sum_{i=1}^m \|(\mathbf{x})_i - (\mathbf{x}_{approx})_i\|^2}{\frac{1}{m} \sum_{i=1}^m \|(\mathbf{x})_i\|^2} \leq 0.01$$

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Number of principal components

- Algorithm

- Try PCA for $k = 1, 2, 3, 4, \dots$

- Compute

$$\mathbf{U}_{reduce}, (\mathbf{z})_1, (\mathbf{z})_2, \dots, (\mathbf{z})_m,$$

$$(\mathbf{x}_{approx})_1, (\mathbf{x}_{approx})_2, \dots, (\mathbf{x}_{approx})_m$$

- Check if

$$\frac{\frac{1}{m} \sum_{i=1}^m \|(\mathbf{x})_i - (\mathbf{x}_{approx})_i\|^2}{\frac{1}{m} \sum_{i=1}^m \|(\mathbf{x})_i\|^2} \leq 0.01$$

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