Machine Learning
CS 6830

Lecture 10

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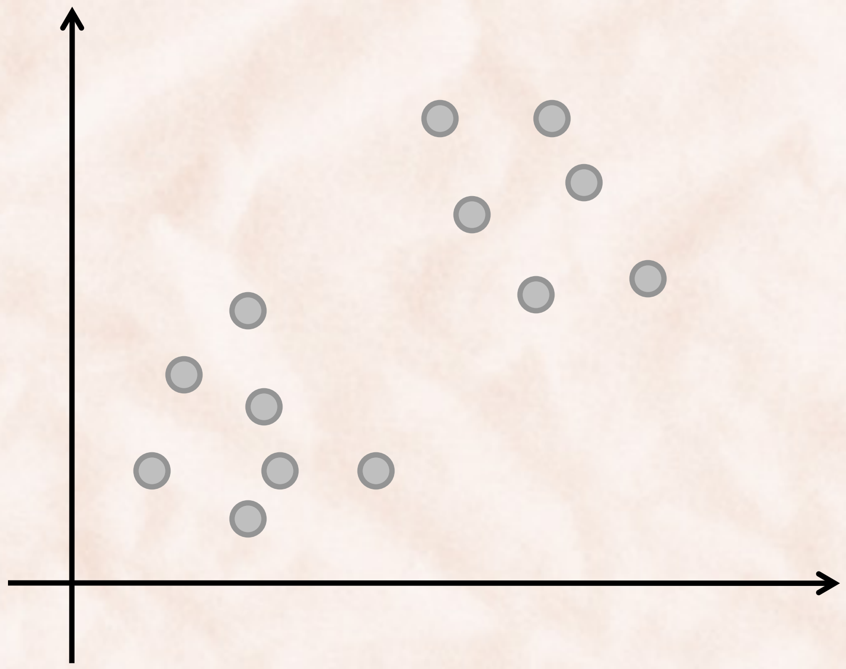
Unsupervised Learning: Clustering

- Partition unlabeled examples into disjoint clusters such that:
  - Examples in the same cluster are very similar.
  - Examples in different clusters are very different.



Unsupervised Learning: Clustering

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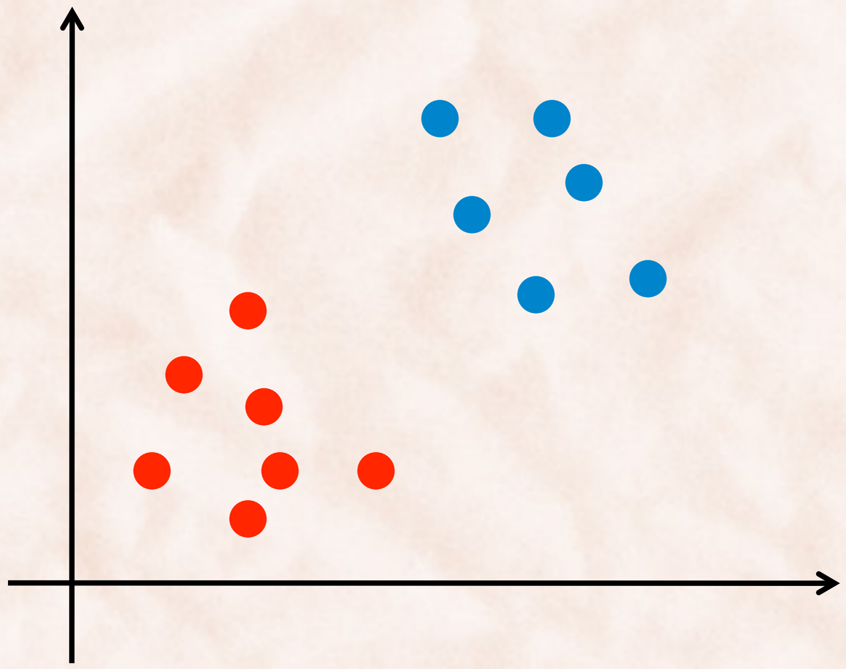


Hierarchical Agglomerative Clustering (HAC)

- Start out with *n* clusters, one example per cluster.
- At each step merge the *nearest* two clusters.
- Stop when there is only one cluster left, or:
  - there are only *k* clusters left.
  - distance is above a threshold τ.

- History of clustering decision can be represented as a binary tree.

The HAC Algorithm

```
1. let $C_i = \{\mathbf{x}_i\}$, for $i \in 1 \ldots n$
2. let $C = \{C_i\}$, for $i \in 1 \ldots n$
3. while $|C| > 1$:
4.     set $\langle C_i, C_j \rangle = \arg\min_{C_k \neq C_l} d(C_k, C_l)$
5.     replace $C_i$ , $C_j$ in $C$ with $C_i \cup C_j$
```

Q: How do we compute the distance *d* between two clusters?

Distance Measures

- Assume a distance function between any two instances:
  - Euclidean distance ||x-y||

- Single Link: $d(C_i, C_j) = \min_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} \|\mathbf{x} - \mathbf{y}\|$

- Complete Link: $d(C_i, C_j) = \max_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} \|\mathbf{x} - \mathbf{y}\|$

- Group Average: $d(C_i, C_j) = \frac{1}{|C_i| * |C_j|} \sum_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} \|\mathbf{x} - \mathbf{y}\|$

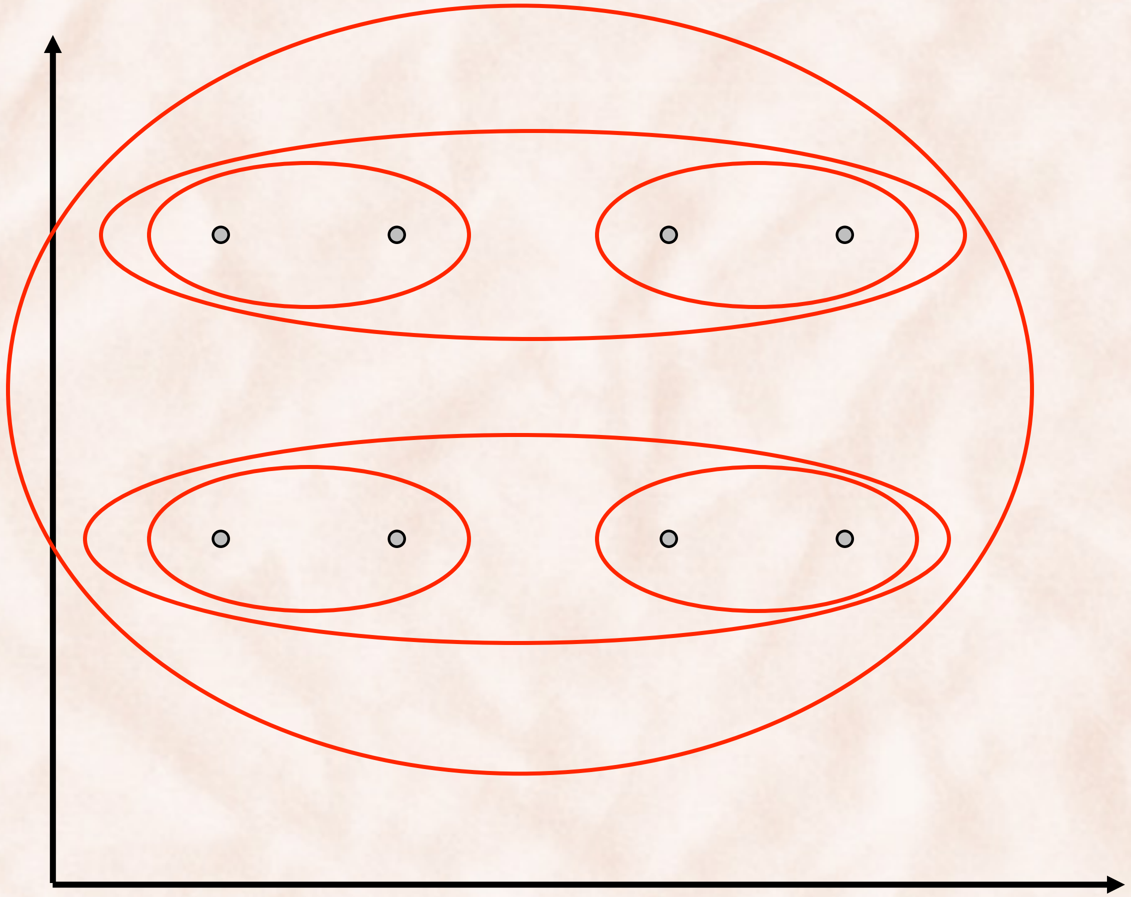
- Centroid Distance: $d(C_i, C_j) = \|\mathbf{m}_i - \mathbf{m}_j\|$

Single Link (Nearest Neighbor)

- Distance function $d(C_i, C_j) = \min_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} \|\mathbf{x} - \mathbf{y}\|$

- It favors elongated clusters.
- Equivalent with Kruskal’s MST algorithm.

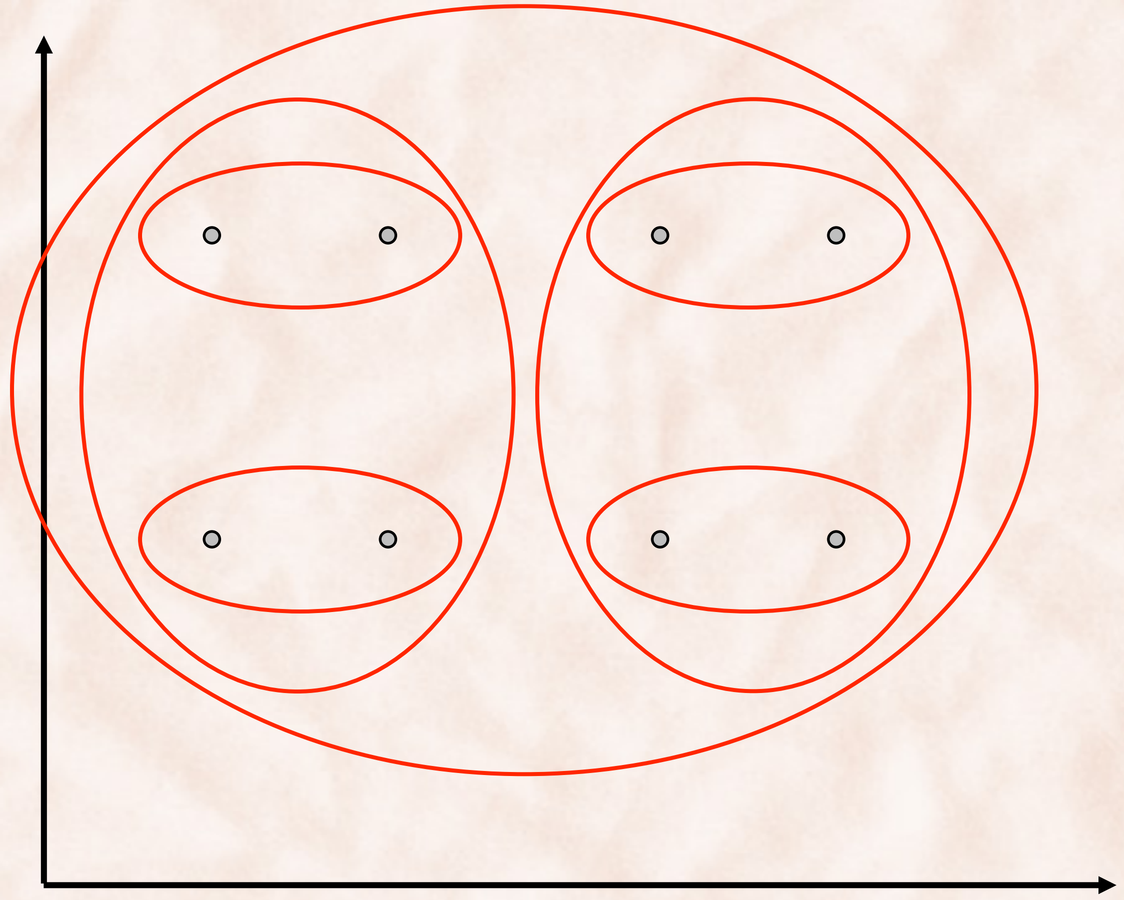
Single Link



Complete Link (Farthest Neighbor)

- Distance function $d(C_i, C_j) = \max_{\mathbf{x} \in C_i, \mathbf{y} \in C_j} \|\mathbf{x} - \mathbf{y}\|$
- It favors tight, spherical clusters.
- $d(C_i,C_j)$ is the *diameter* of the cluster $C_i \cup C_j$.

Complete Link



Divisive Clustering with *k*-Means

- The goal is to produce *k* clusters such that instances are close to the cluster centroids:
  - The cluster centroid is the mean of all instances in the cluster.

- Optimization problem:

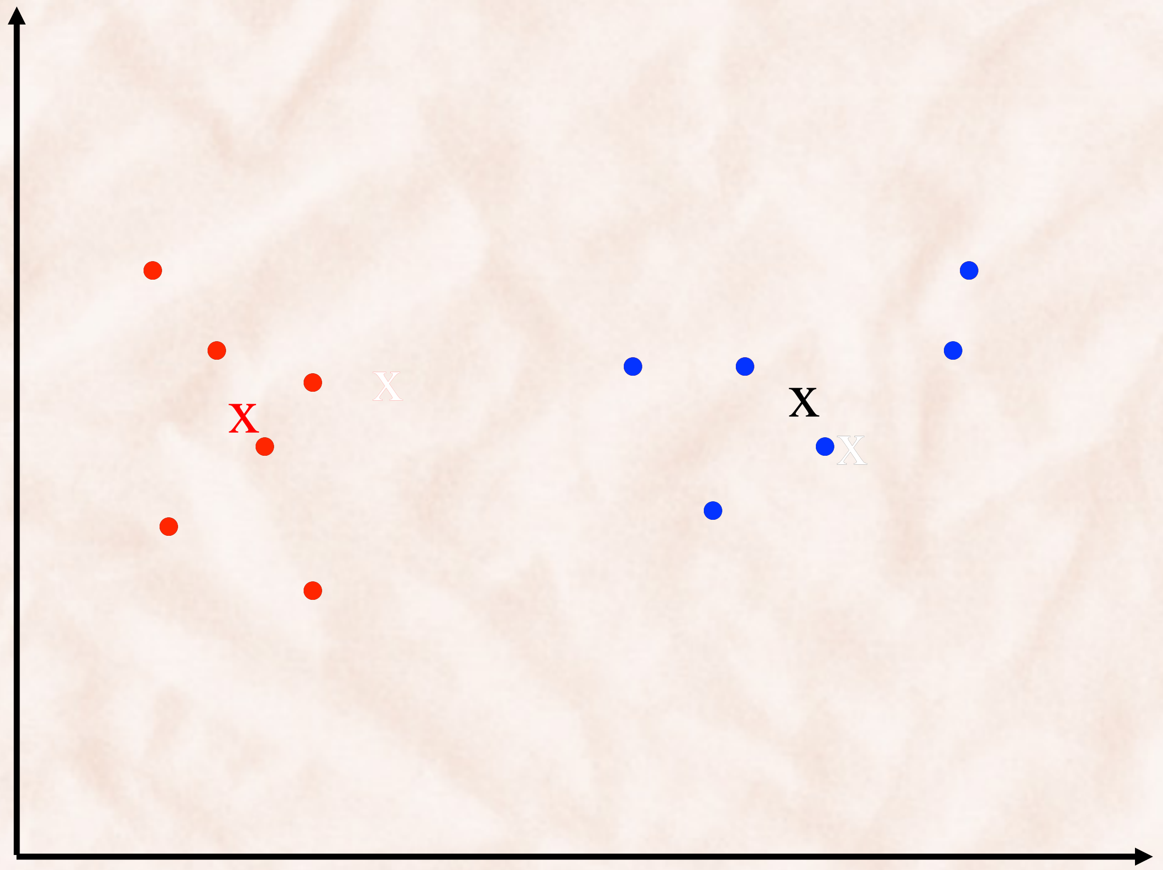
$$\hat{C} = \arg\min_{C} J(C)$$

$$J(C) = \sum_{i=1}^{k} \sum_{\mathbf{x} \in C_i} \| \mathbf{x} - \mathbf{m}_i \|^2$$

The *k*-Means Algorithm

```
1. start with some seed centroids $\mathbf{m}_1^{(0)}, \mathbf{m}_2^{(0)}, \ldots, \mathbf{m}_k^{(0)}$
2. set $t \leftarrow 0$.
3. while not converged:
4.     for each $\mathbf{x}$:
5.         set $\mathbf{m}^{(t)}(\mathbf{x}) \leftarrow \arg\min_{\mathbf{m}_i^{(t)}} \left\| \mathbf{x} - \mathbf{m}_i^{(t)} \right\|$   ← [E] step
6.     set $C_i^{(t+1)} \leftarrow \left\{ \mathbf{x} \mid \mathbf{m}^{(t)}(\mathbf{x}) = \mathbf{m}_i^{(t)} \right\}$
7.     set $\mathbf{m}_i^{(t+1)} \leftarrow \frac{1}{\left| C_i^{(t+1)} \right|} \sum_{\mathbf{x} \in C_i^{(t+1)}} \mathbf{x}$   ← [M] step
8.     set $t \leftarrow t + 1$
```

The *k*-Means Algorithm (*k* = 2)



Pick seeds

Reassign clusters

Compute centroids

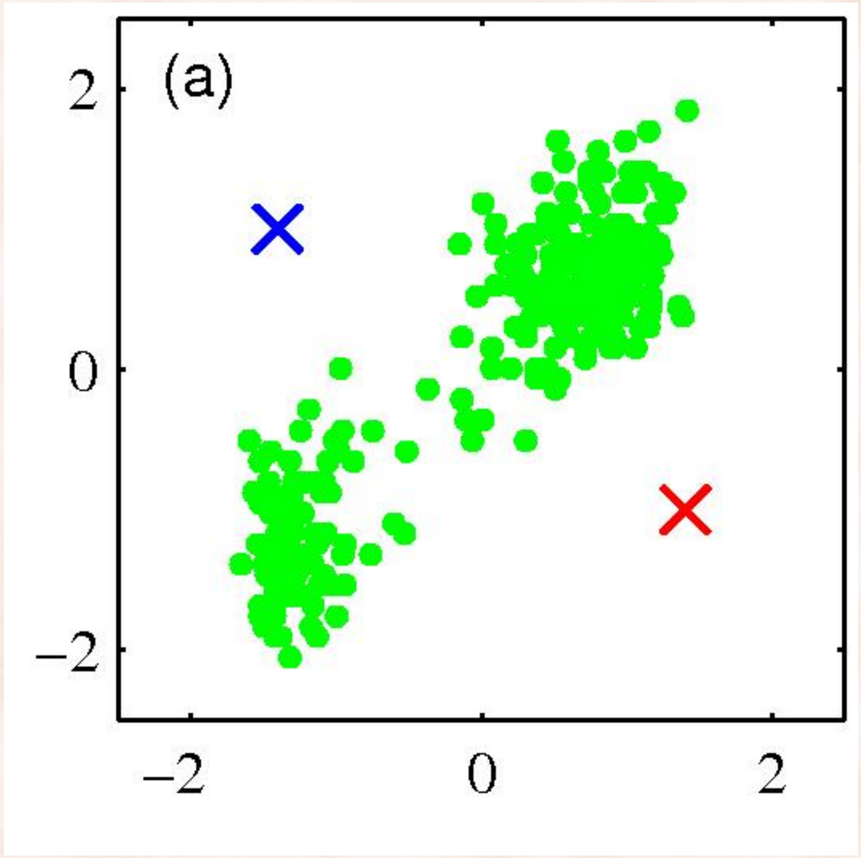
Reasssign clusters

Compute centroids

Reassign clusters

Converged!

The k-Means Algorithm ($k = 2$)



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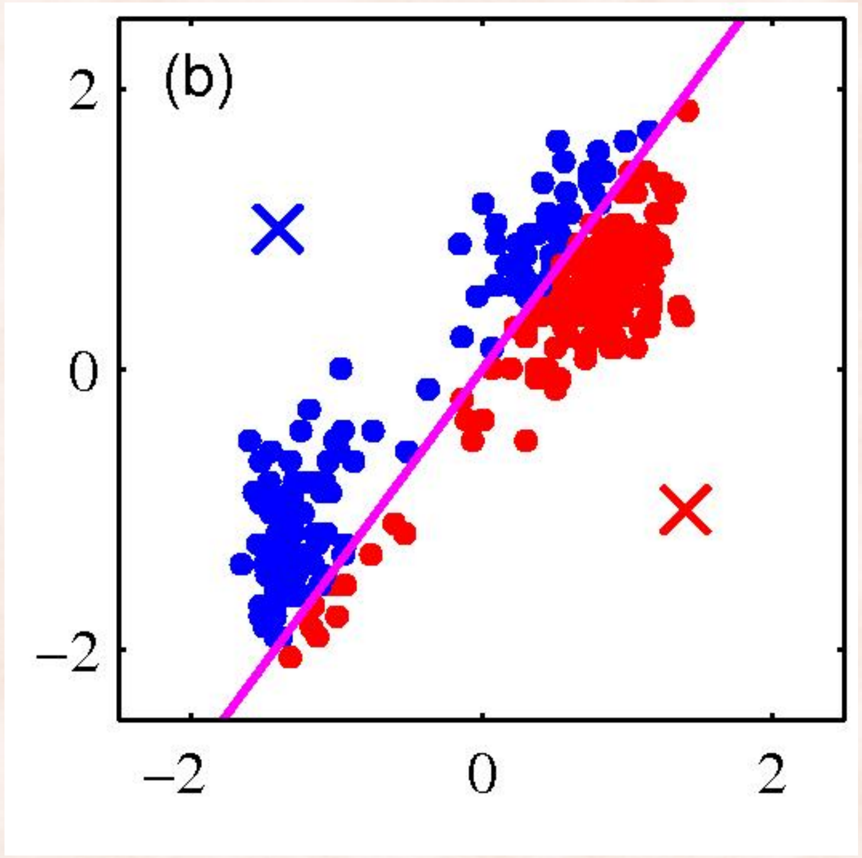

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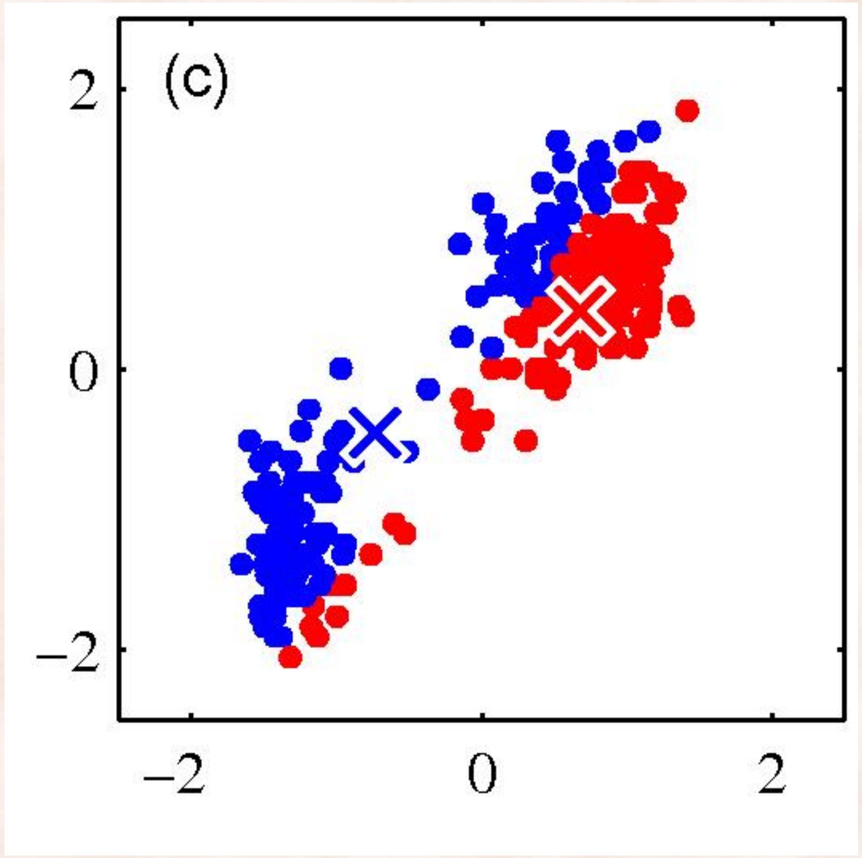

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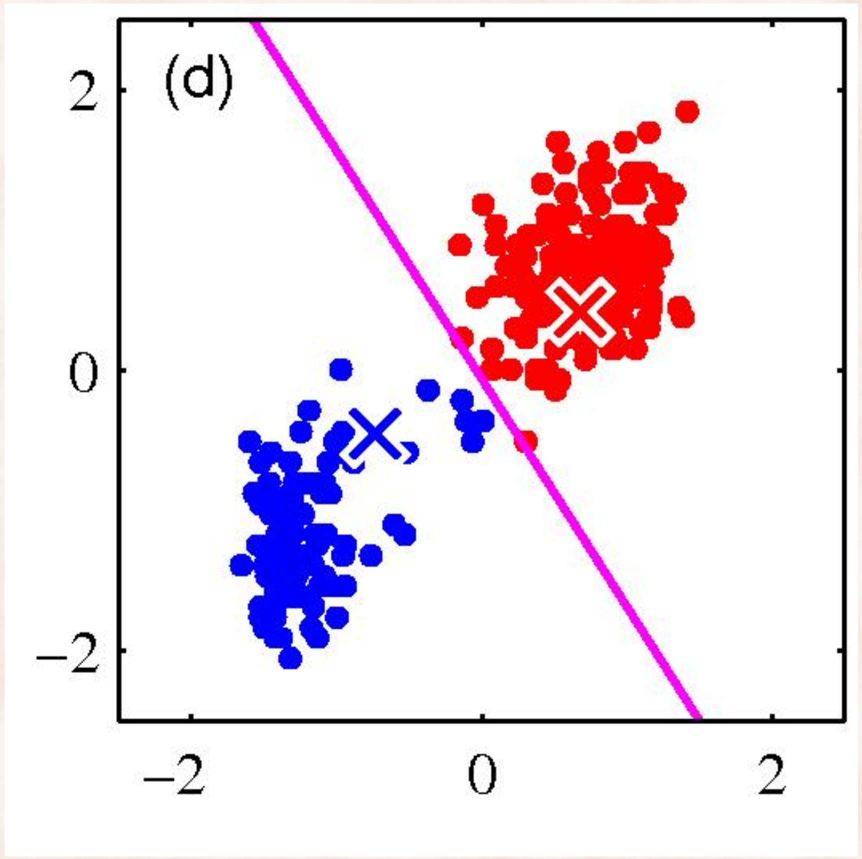

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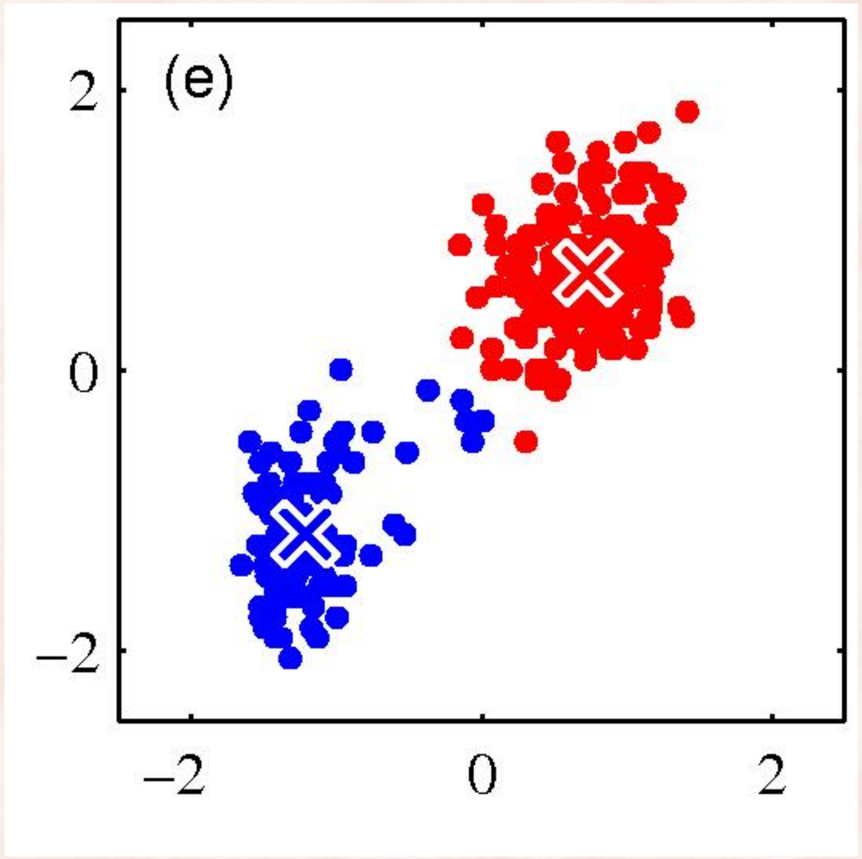

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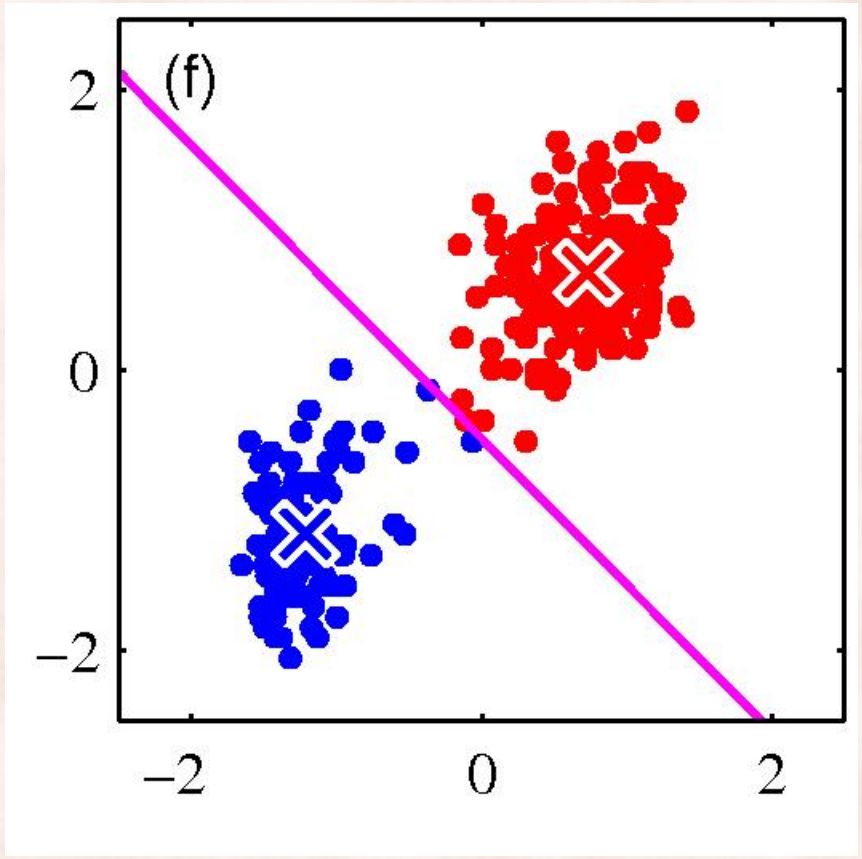

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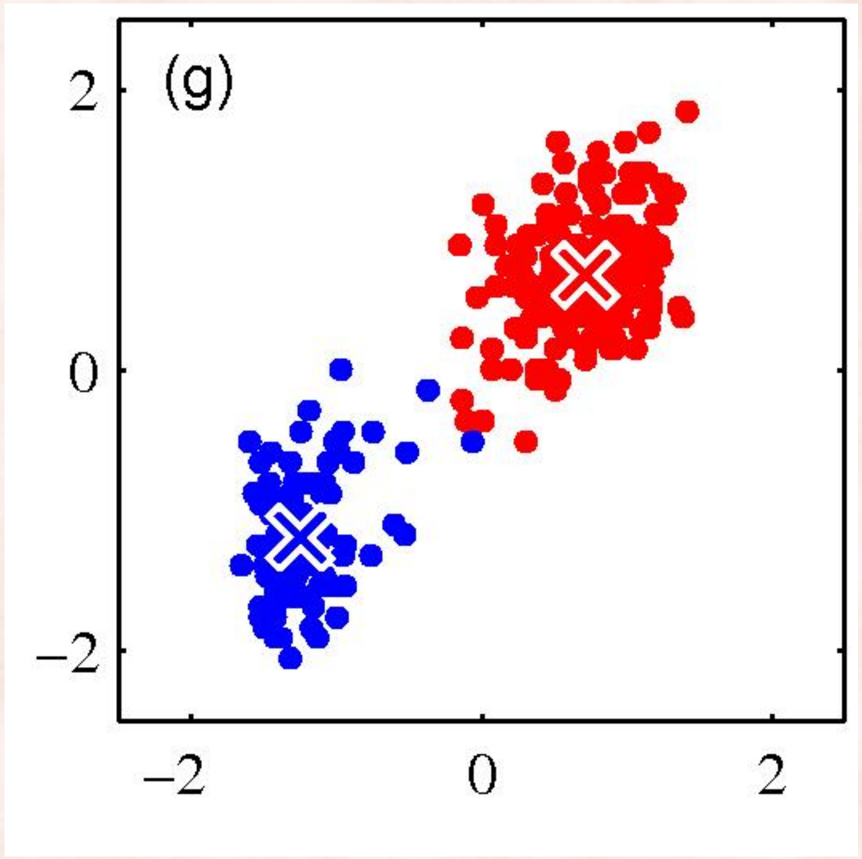

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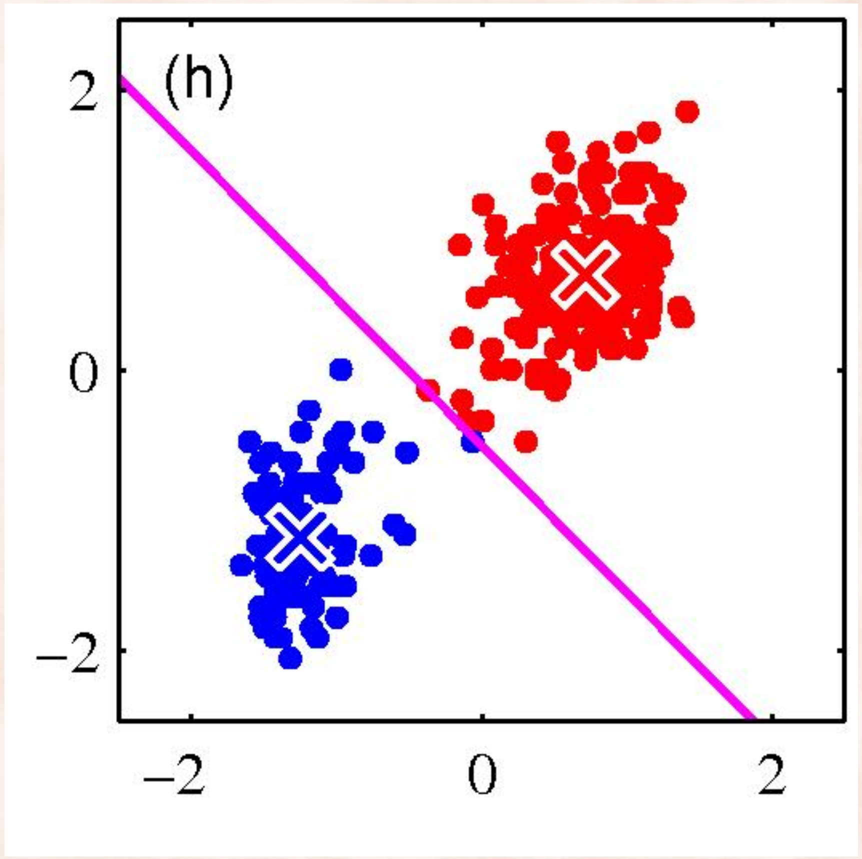

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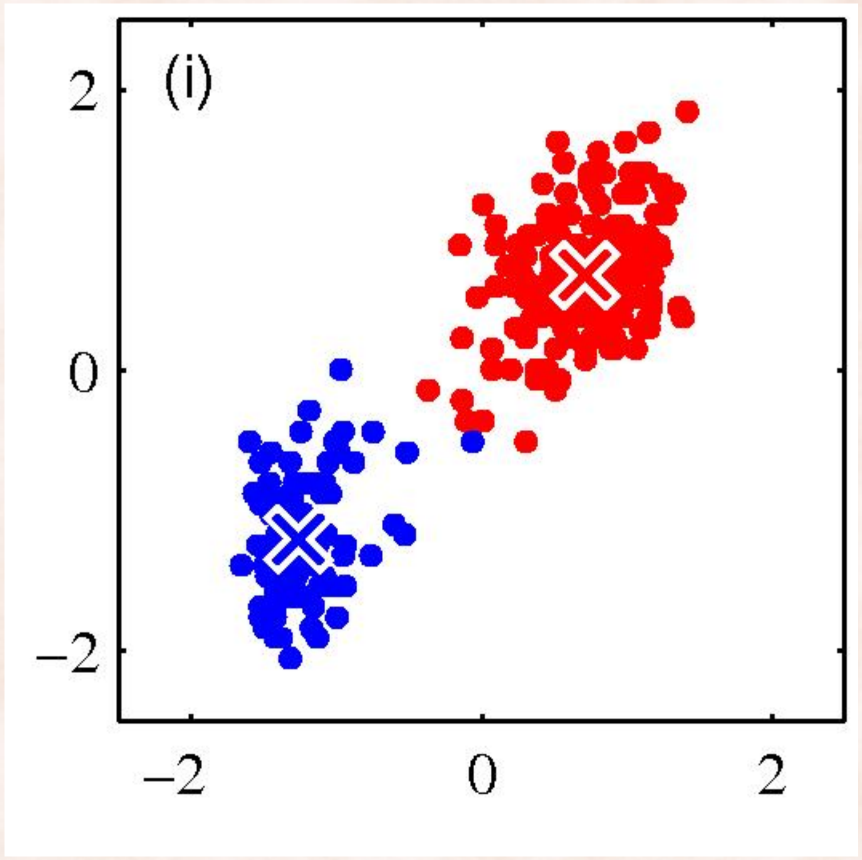


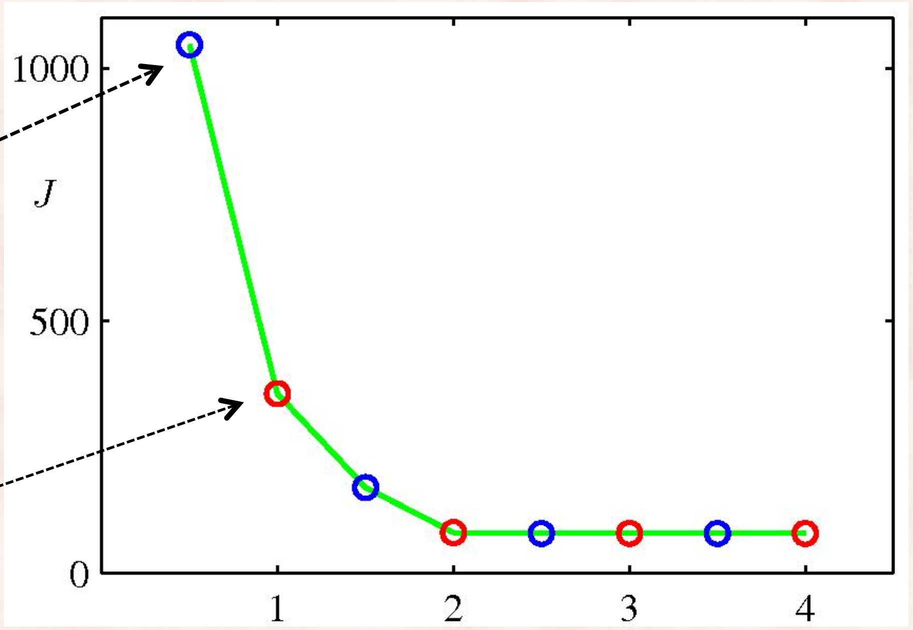
The *k*-Means Algorithm

- The objective function monotonically decreases at every iteration:

$$J^{(t)} \geq J^{(t+1)}$$

[**E**] step

[**M**] step



The *k*-Means Algorithm

- Optimization problem is NP-hard:
  - Results depend on seed selection.
  - Improve performance by providing *must-link* and/or *cannot-link* constraints $\Rightarrow$ semi-supervised clustering.

- Time complexity for each iteration is O(knm):
  - number of clusters is k.
  - feature vectors have dimensionality m.
  - total number of instances is n.

Soft Clustering

- **Clustering** typically assumes that each instance is given a "hard" assignment to exactly one cluster.
- Does not allow uncertainty in class membership or for an instance to belong to more than one cluster.

- **Soft clustering** gives probabilities that an instance belongs to each of a set of clusters.
- Each instance is assigned a probability distribution across a set of discovered categories.

Soft Clustering with EM

- Soft version of *k*-means.
- Assumes a probabilistic model of categories that allows computing $P(c_{\mathrm{i}} \mid \mathbf{x})$ for each category, c_{i}, for a given example $\mathbf{x}$.
  - For text, typically assume a naïve-Bayes category model.
    - Parameters $\theta = \{P(c_i), P(w_j \mid c_i) \mid i \in \{1, \ldots k\}, j \in \{1, \ldots, |V|\}\}$

Soft Clustering with EM

- Iterative method for learning probabilistic categorization model from unsupervised data.
- Initially assume random assignment of examples to categories.
- Learn an initial probabilistic model by estimating model parameters θ from this randomly labeled data.
- Iterate following two steps until convergence:
  - Expectation (E-step): Compute $P(c_i \mid \mathbf{x})$ for each example given the current model, and probabilistically re-label the examples based on these posterior probability estimates.
  - Maximization (M-step): Re-estimate the model parameters, θ, from the probabilistically re-labeled data.

Learning with Probabilistic Labels

- Instead of training data labeled with “hard” category labels, training data is labeled with “soft” probabilistic category labels.
- When estimating model parameters θ from training data, weight counts by the corresponding probability of the given category label.
- For example, if $P(c_1 \mid \mathbf{x}) = 0.8$ and $P(c_2 \mid \mathbf{x}) = 0.2$, each word w_j in **x** contributes only 0.8 towards the counts n_1 and n_{1j}, and 0.2 towards the counts n_2 and n_{2j}.

Naïve Bayes EM

1. Randomly assign examples probabilistic category labels.
2. Use standard naïve-Bayes training to learn a probabilistic model with parameters θ from the labeled data.
3. Until convergence or until maximum number of iterations reached:
   - E-Step: Use the naïve Bayes model θ to compute $P(c_i \mid \mathbf{x})$ for each category and example, and re-label each example using these probability values as soft category labels.
   - M-Step: Use standard naïve-Bayes training to re-estimate the parameters θ using these new probabilistic category labels.

The *k*-Means Algorithm

```
1. start with some seed centroids $\mathbf{m}_1^{(0)}, \mathbf{m}_2^{(0)}, \ldots, \mathbf{m}_k^{(0)}$
2. set $t \leftarrow 0$.
3. while not converged:
4.     for each $\mathbf{x}$:
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7.     set $\mathbf{m}_i^{(t+1)} \leftarrow \frac{1}{\left|C_i^{(t+1)}\right|} \sum_{\mathbf{x} \in C_i^{(t+1)}} \mathbf{x}$ <------ [M] step
8.     set $t \leftarrow t + 1$
```

The *k*-Medoids Algorithm

```
1.  start with some random seed centroids $\mathbf{m}_1^{(0)}, \mathbf{m}_2^{(0)}, \ldots, \mathbf{m}_k^{(0)}$
2.  set $t \leftarrow 0$.
3.  while not converged:
4.      for each x:
5.          set $\mathbf{m}^{(t)}(\mathbf{x}) \leftarrow \arg\min_{\mathbf{m}_i^{(t)}} d\left(\mathbf{x} - \mathbf{m}_i^{(t)}\right)$ ←------ [E] step
6.      set $C_i^{(t+1)} \leftarrow \left\{\mathbf{x} \mid \mathbf{m}^{(t)}(\mathbf{x}) = \mathbf{m}_i^{(t)}\right\}$
7.      set $\mathbf{m}_i^{(t+1)} \leftarrow \arg\min_{\mathbf{x} \in C_i^{(t+1)}} \sum_{\mathbf{y} \in C_i^{(t+1)}} d(\mathbf{x}, \mathbf{y})$ ←------ [M] step
8.      set $t \leftarrow t + 1$
```

Principal Component Analysis (PCA)

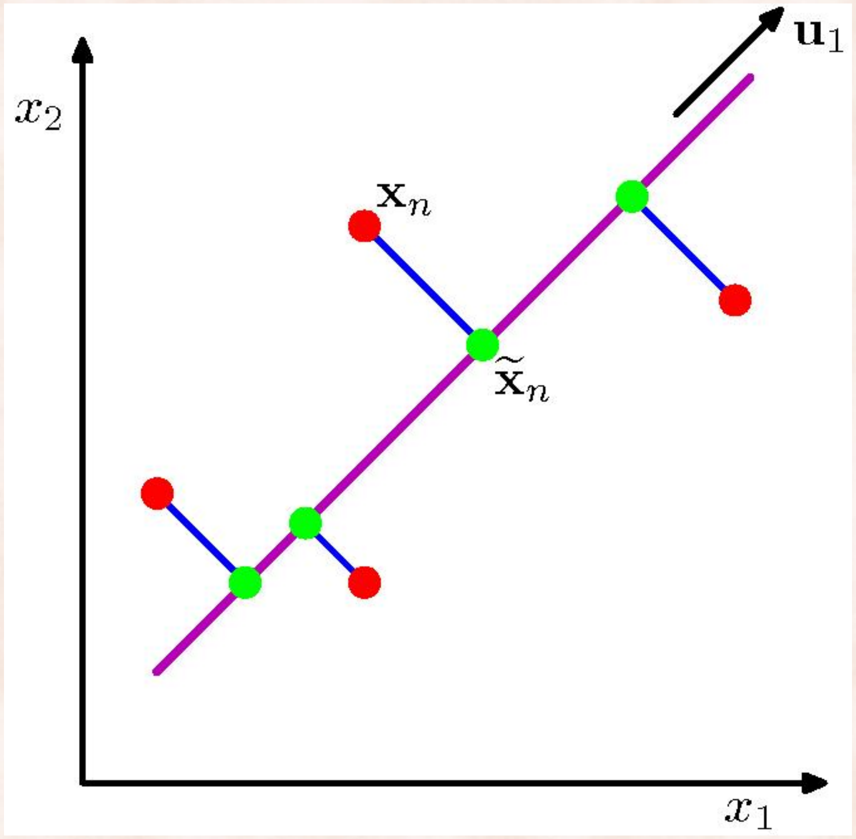
- A technique widely used for:
  - dimensionality reduction.
  - data compression.
  - feature extraction.
  - data visualization.

maximum variance

- Two equivalent definitions of PCA:
  1) Project the data onto a lower dimensional space such that the variance of the projected data is *maximized*.
  2) Project the data onto a lower dimensional space such that the mean squared distance between data points and their projections (average projection cost) is *minimized*.

minimum error

Principal Component Analysis (PCA)



PCA (Maximum Variance)

- Let $X = \{\mathbf{x}_n\}_{1 \leq n \leq N}$ be a set of observations:
  - Each $\mathbf{x}_n \in R^D$ (D is the dimensionality of $\mathbf{x}_n$).
- Project X onto an M dimensional space ($M < D$) such that the *variance* of the projected X is *maximized*.
- Work out solution for $M = 1$, then generalize to any $M < D$.

PCA (Maximum Variance, $M = 1$)

- The lower dimensional space is defined by a vector $\mathbf{u}_1 \in \mathrm{R}^D$.
  - Show that only direction is important $\Rightarrow$ choose $\|\mathbf{u}_1\| = 1$.
- Each $\mathbf{x}_n$ is projected onto a scalar $\mathbf{u}_1^T \mathbf{x}_n$
- The (sample) mean of the data is:

$$\overline{\mathbf{x}} = \frac{1}{N} \sum_{n=1}^{N} \mathbf{x}_n$$

- The (sample) mean of the projected data is $\mathbf{u}_1^T \overline{\mathbf{x}}$

PCA (Maximum Variance, $M = 1$)

- The (sample) variance of the projected data:

$$\frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{u}_1^T\mathbf{x}_n - \mathbf{u}_1^T\overline{\mathbf{x}}\right)^2 = \mathbf{u}_1^T\mathbf{S}\mathbf{u}_1$$

where **S** is the data covariance matrix:

$$\mathbf{S} = \frac{1}{N}\sum_{n=1}^{N}\left(\mathbf{x}_n - \overline{\mathbf{x}}\right)\left(\mathbf{x}_n - \overline{\mathbf{x}}\right)^T$$

- Optimization problem is:

minimize:

$$\mathbf{u}_1^T\mathbf{S}\mathbf{u}_1$$

subject to:

$$\mathbf{u}_1^T\mathbf{u}_1 = 1$$

PCA (Maximum Variance, $M = 1$)

- Lagrangian function:

$$L_P(\mathbf{u}_1, \lambda_1) = \mathbf{u}_1^T \mathbf{S} \mathbf{u}_1 + \lambda_1 (1 - \mathbf{u}_1^T \mathbf{u}_1)$$

where λ_1 is the *Lagrangian multiplier* for constraint $\mathbf{u}_1^T \mathbf{u}_1 = 1$

- Solve:

$$\frac{\partial L_P}{\partial \mathbf{u}_1} = 0 \Rightarrow \mathbf{S}\mathbf{u}_1 = \lambda_1 \mathbf{u}_1 \Rightarrow \left\{ \begin{array}{l} \mathbf{u}_1 \text{ is an eigenvector of } \mathbf{S} \\ \lambda_1 \text{ is an eigenvalue of } \mathbf{S} \end{array} \right.$$

$$\Rightarrow \mathbf{u}_1^T \mathbf{S} \mathbf{u}_1 = \lambda_1 \mathbf{u}_1^T \mathbf{u}_1 = \lambda_1$$

$\Rightarrow \lambda_1$ is the largest eigenvalue of **S**.

PCA (Maximum Variance, $M = 1$)

- λ_1 is the largest eigenvalue of $\mathbf{S}$.
- $\mathbf{u}_1$ is the eigenvector corresponding to λ_1:
  - also called the *first principal component*.

- For $M < D$ dimensions:
  - $\mathbf{u}_1\ \mathbf{u}_2 \ldots \mathbf{u}_M$ are the eigenvectors corresponding to the largest eigenvalues $\lambda_1\ \lambda_2 \ldots \lambda_M$ of $\mathbf{S}$.
  - proof by induction.

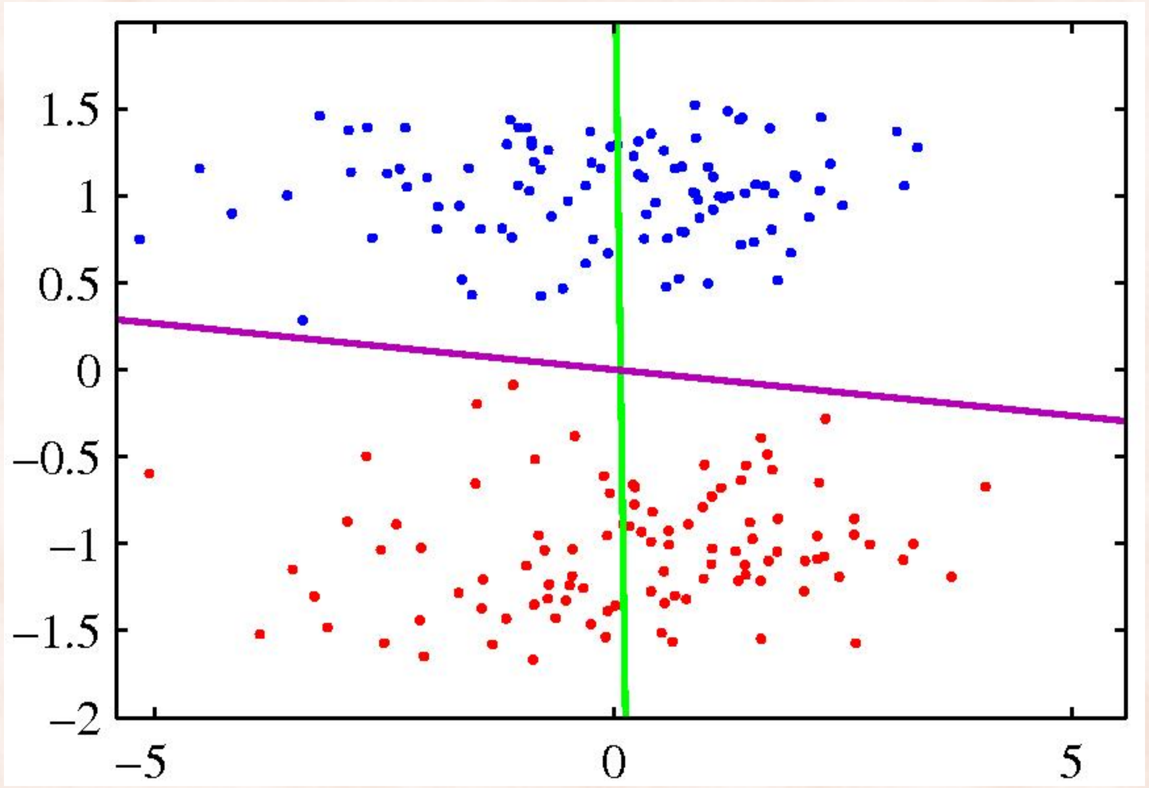
Principal Component Analysis vs. Fisher Linear Discriminant

- Both methods can be used for linear dimensionality reduction.

- PCA is unsupervised:
  - it depends only on the values $\mathbf{x}_n$.

- Fisher linear discriminant is supervised:
  - it depends on both the observations and the labels $(\mathbf{x}_n, t_n)$.

Principal Component Analysis vs. Fisher Linear Discriminant



PCA for High-Dimensional Data

- If $N < D$, it does not make sense to use PCA for $M > N$-1:
  - The set of N points define a linear subspace with dimensionality at most N-1.
  - PCA will find at least D-N+1 eigenvalues that are 0.
  - Typical algorithms for finding eigenvalues are O(D^3).

- Solution:
  - Let $\mathbf{X}$ by the N×D matrix with nth row given by $(\mathbf{x}_n - \overline{\mathbf{x}})^T$
  - Then the sample covariance matrix $\mathbf{S}$ can be written as:

$$\mathbf{S} = \frac{1}{N}\mathbf{X}^T\mathbf{X}$$

PCA for High-Dimensional Data

$$\mathbf{S}\mathbf{u}_i = \lambda_i \mathbf{u}_i \Rightarrow \frac{1}{N}\mathbf{X}^T\mathbf{X}\mathbf{u}_i = \lambda_i \mathbf{u}_i$$

$$\Rightarrow \frac{1}{N}\mathbf{X}\mathbf{X}^T\left(\mathbf{X}\mathbf{u}_i\right) = \lambda_i\left(\mathbf{X}\mathbf{u}_i\right)$$

Define $\mathbf{v}_i = \mathbf{X}\mathbf{u}_i$

$$\Rightarrow \underbrace{\left(\frac{1}{N}\mathbf{X}\mathbf{X}^T\right)}\mathbf{v}_i = \lambda_i \mathbf{v}_i$$

an N×N matrix $\Rightarrow O(N^3)$ instead of $O(D^3)$ cost.

- Same eigenvalues as original problem, but what are the original, principal eigenvectors?

PCA for High-Dimensional Data

$$\left(\frac{1}{N}\mathbf{X}\mathbf{X}^T\right)\mathbf{v}_i = \lambda_i \mathbf{v}_i \Rightarrow \left(\frac{1}{N}\mathbf{X}^T\mathbf{X}\right)\left(\mathbf{X}^T\mathbf{v}_i\right) = \lambda_i\left(\mathbf{X}^T\mathbf{v}_i\right)$$

$\Rightarrow \mathbf{X}^\mathrm{T}\mathbf{v}_i$ is an eigenvector of **S** with eigenvalue λ_i.

$$\Rightarrow \mathbf{u}_i = \frac{\mathbf{X}^T\mathbf{v}_i}{\left\|\mathbf{X}^T\mathbf{v}_i\right\|}$$

- Summary of solution:
  1. evaluate $\mathbf{X}^\mathrm{T}\mathbf{X}$.
  2. find its eigenvectors and eigenvalues.
  3. compute the eigenvectors in the original dataspace.

PCA, Fisher & Kernels

- Minimum error formulation leads to the same solution [12.1.2].
  - shows how PCA can be used for compression.

- Kernel PCA [12.3].

- Kernel Fisher linear discriminant [Mika et al., 1999]