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Optimization
and
Data Analytics

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Nearest Prototype Classification

Given a set of N samples, each represented by a vector $\mathbf{x}_i \in \mathbb{R}^D$, and the corresponding labels l_i, we can define the class mean vectors:

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i, l_i = k} \mathbf{x}_i, \; k = 1, \ldots, K$$

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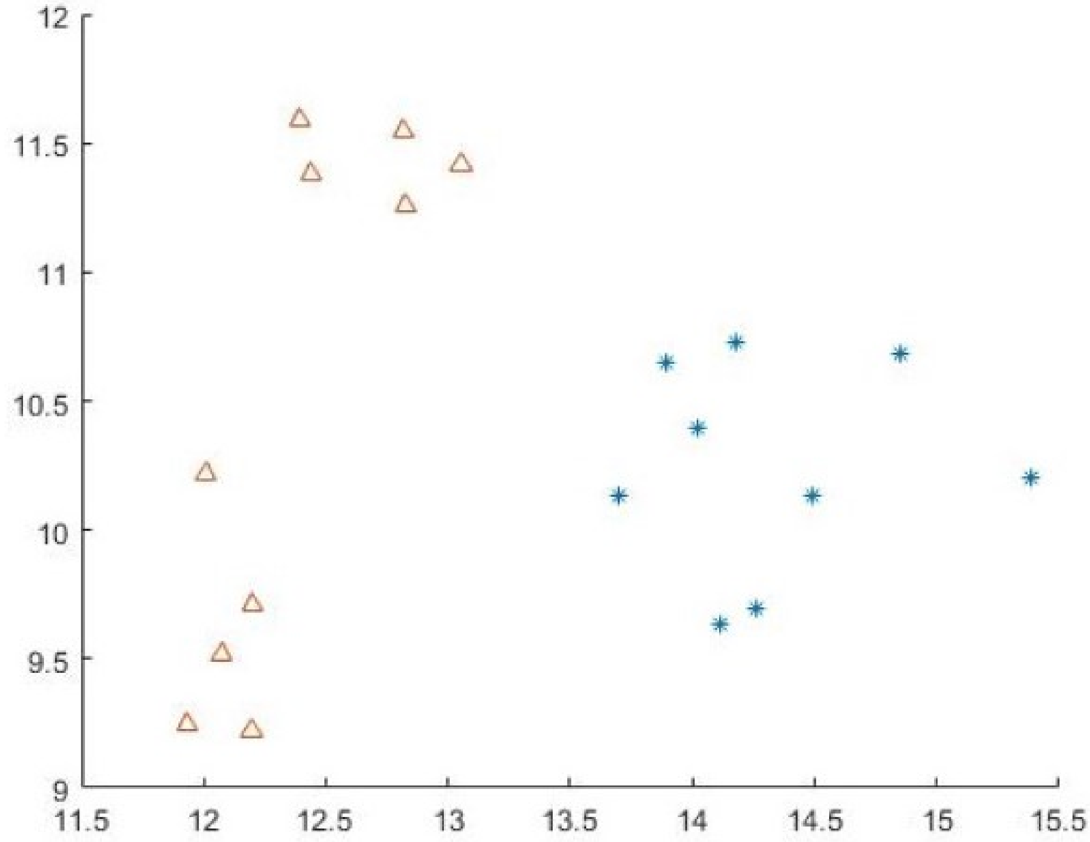
Then, a new vector $\mathbf{x}_*$ can be classified based on the minimal distance from $\boldsymbol{\mu}_k$

$$d(\mathbf{x}_*, \boldsymbol{\mu}_k) = \|\mathbf{x}_* - \boldsymbol{\mu}_k\|_2^2$$

This can be interpreted as a probalistic classifcation if we say that p(x|c_k) is defined in such a way that the Sigma is identity and all prior probabilities P(c_k) are the same. If P(c_k) is larger than any of the other classes then naturally it will have more influence which moves the decision boundary!

Nearest Prototype Classification

Example



Nearest Prototype Classification

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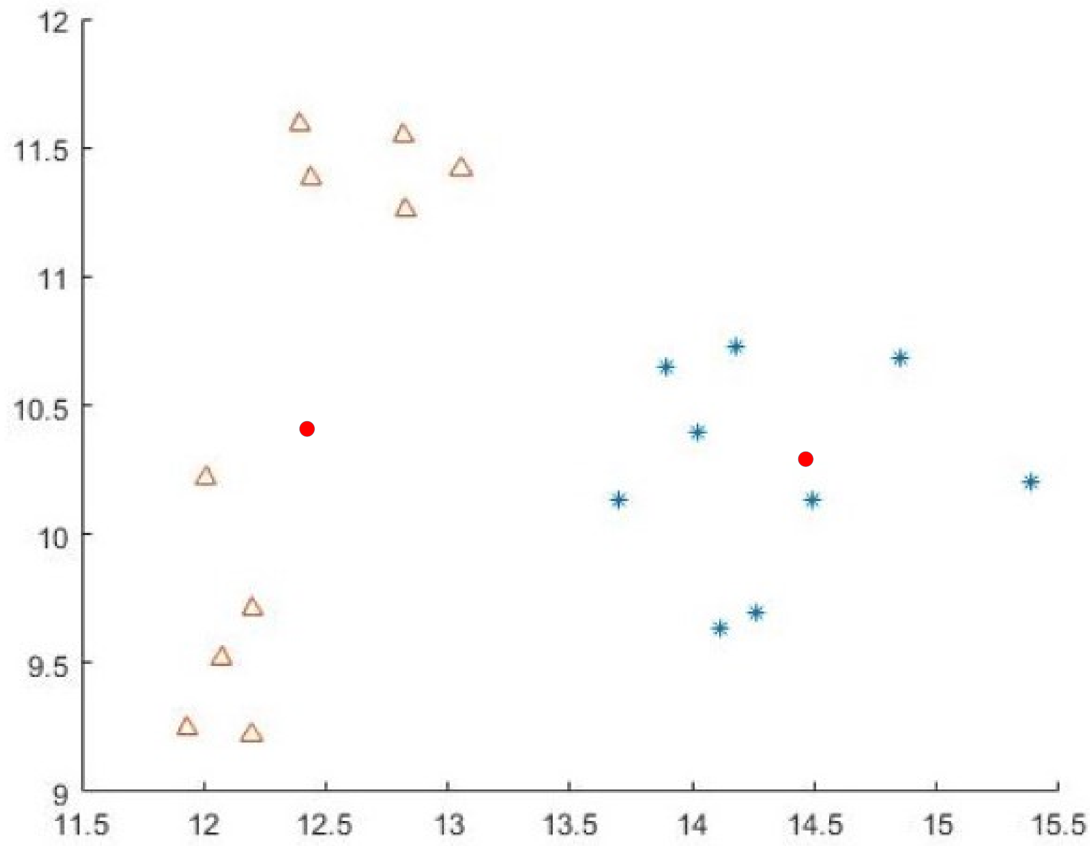

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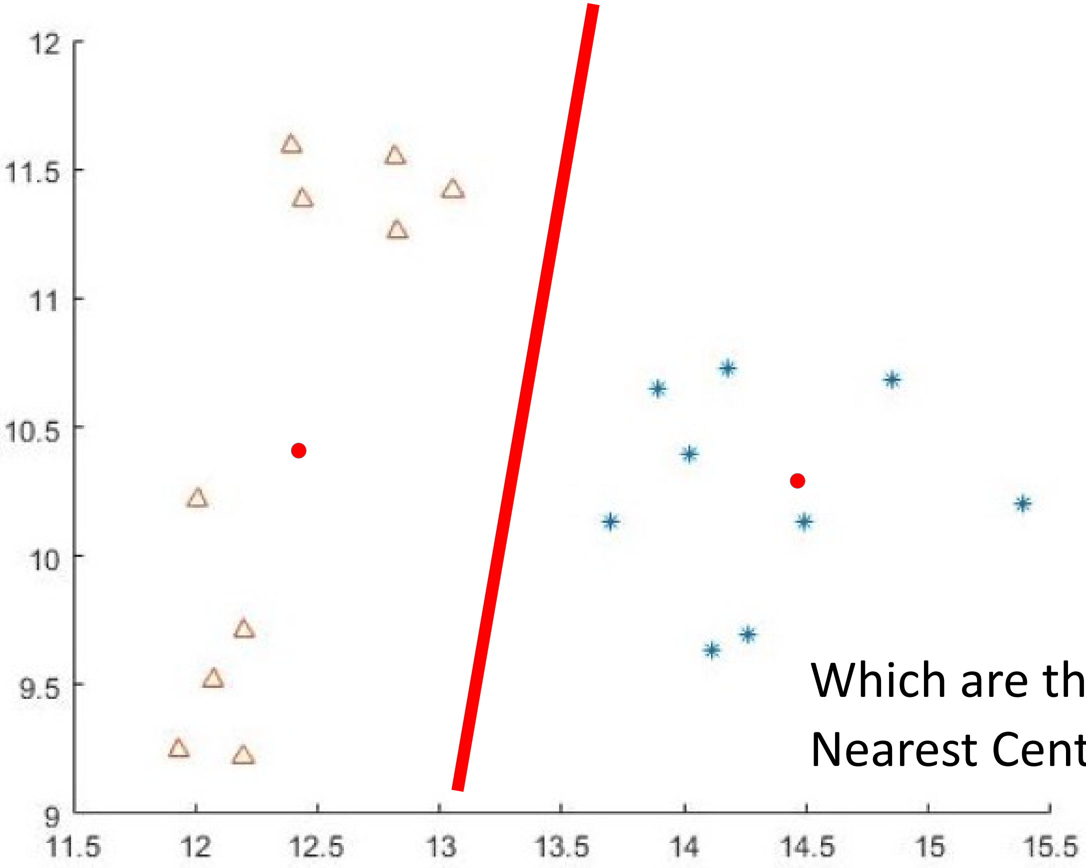

Which are the assumptions of Nearest Centroid classifier?

Nearest Prototype Classification

Given a set of N samples, each represented by a vector $\mathbf{x}_i \in \mathbb{R}^D$, and the corresponding labels l_i, we can define the class mean vectors, we can define clusters on each class.

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We obtain multiple prototypes for each class

$$\boldsymbol{\mu}_{km} = \frac{1}{N_{km}} \sum_{i, l_i = k, q_i = m} \mathbf{x}_i$$

Then, a new vector $\mathbf{x}_*$ can be classified based on the minimal distance from $\boldsymbol{\mu}_{km}$

$$d(\mathbf{x}_*, \boldsymbol{\mu}_{km}) = \|\mathbf{x}_* - \boldsymbol{\mu}_{km}\|_2^2$$

Nearest Prototype Classification

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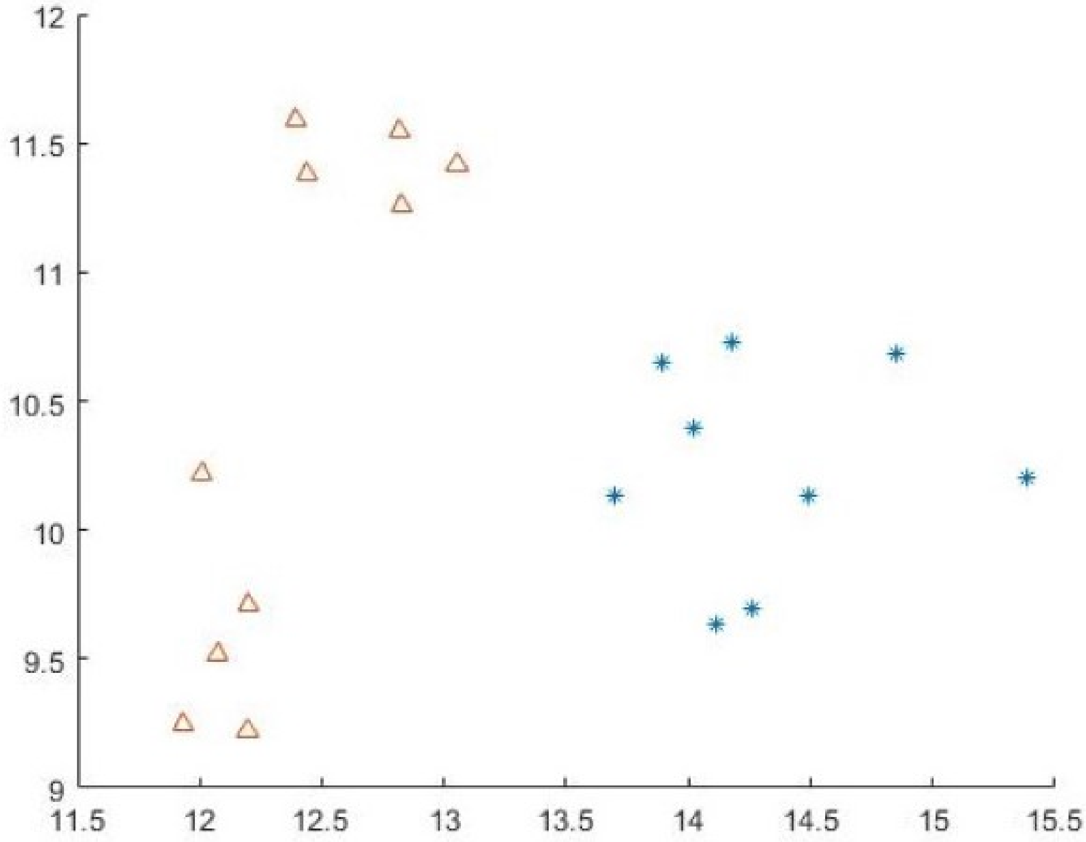
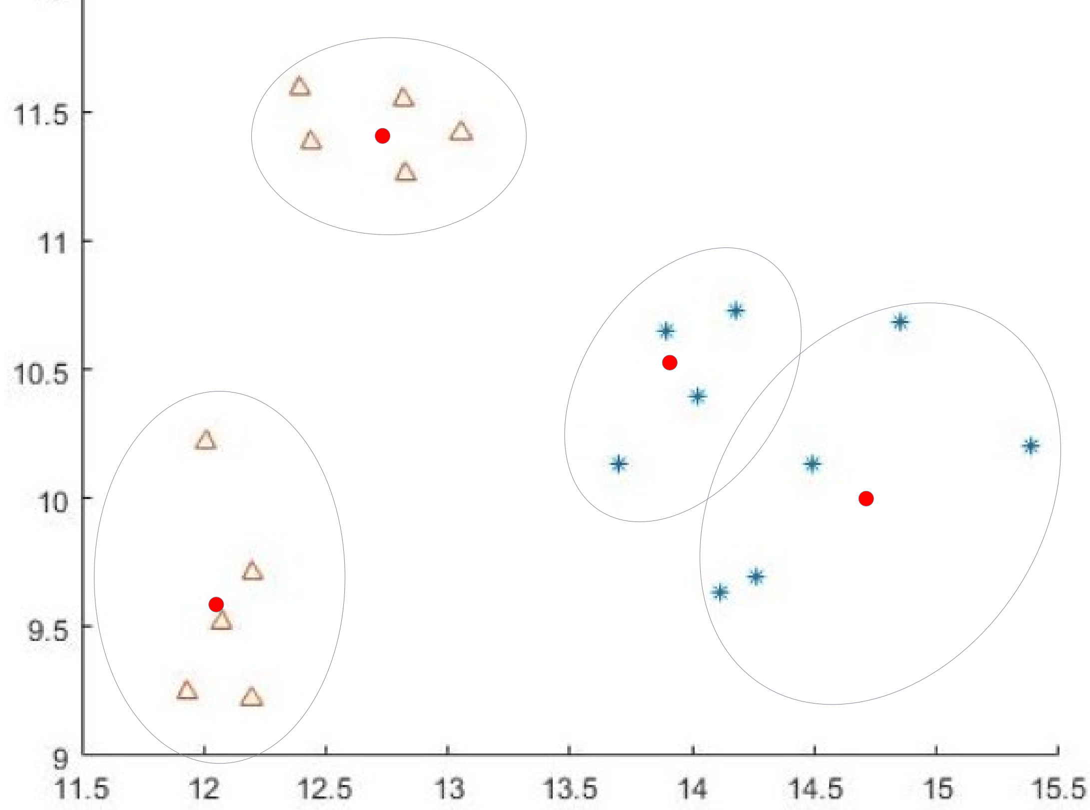


Nearest Prototype Classification

Interpreting this as probability-based classifier is complicated because we do not know the mean vectors.
The mean vectors are found by applying k-means. Applying k-means more than once, we get different resuts.
p(x|c1) = integral of N(mu,) * P(x)

Example

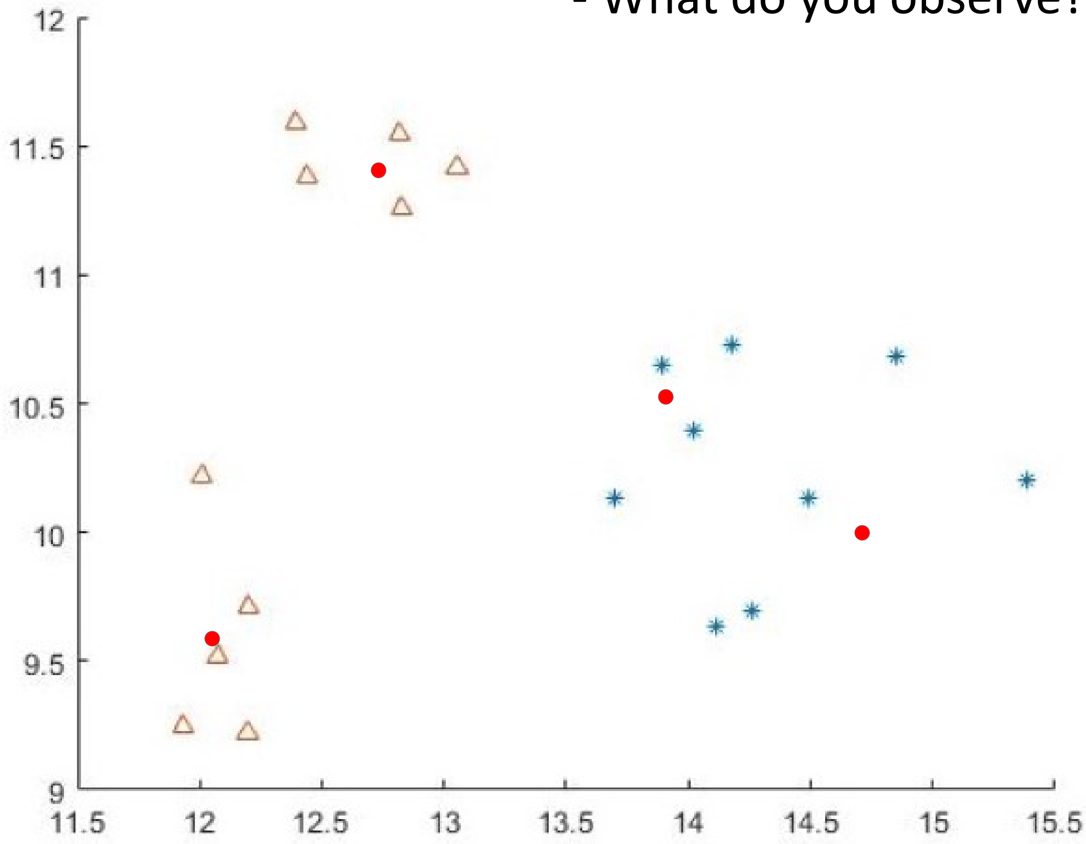
The mean vectors of each class is drawn from a probability distribution.
We need to estimate the mean vectors.



Nearest Prototype Classification

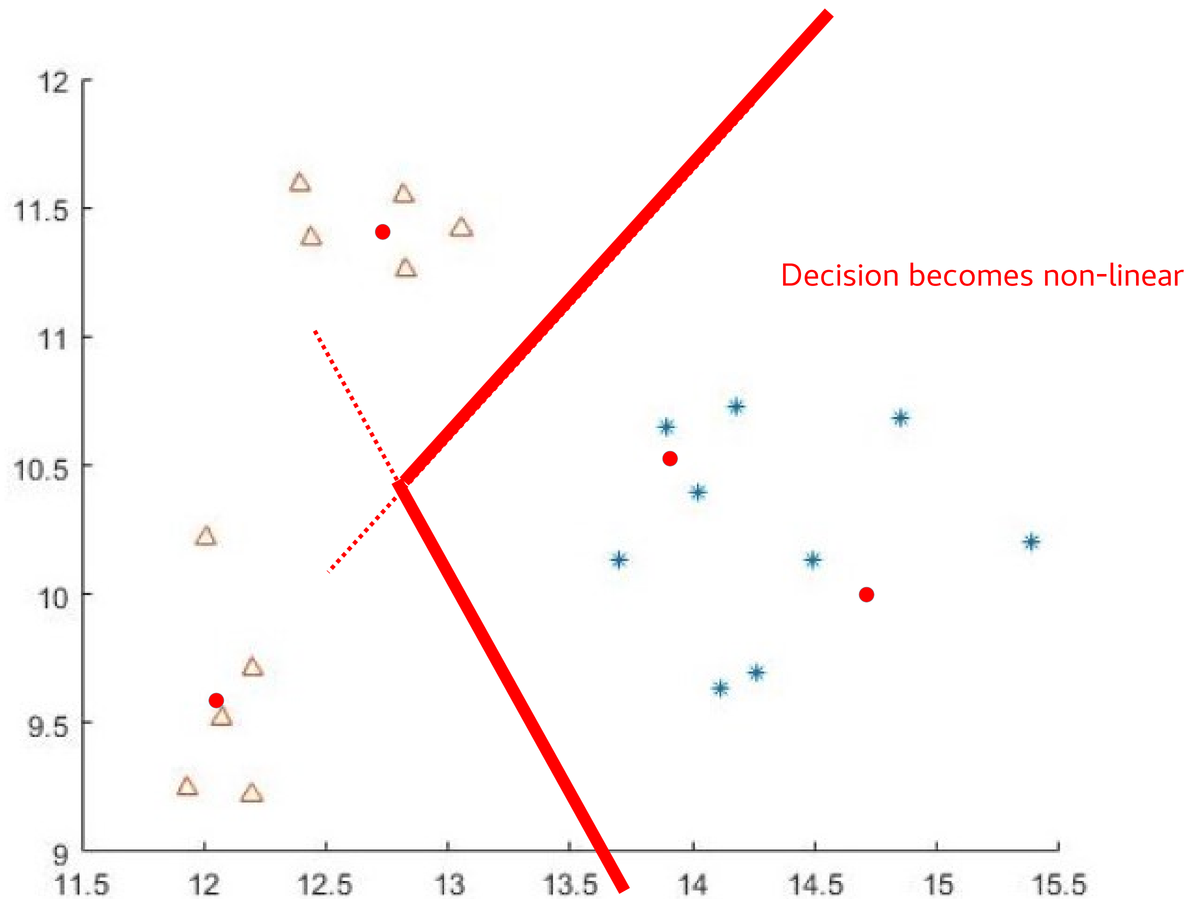
Example

- Which will be the decision hyperplane?
- What do you observe?



Nearest Prototype Classification

Example



Nearest Neighbor-based Classification

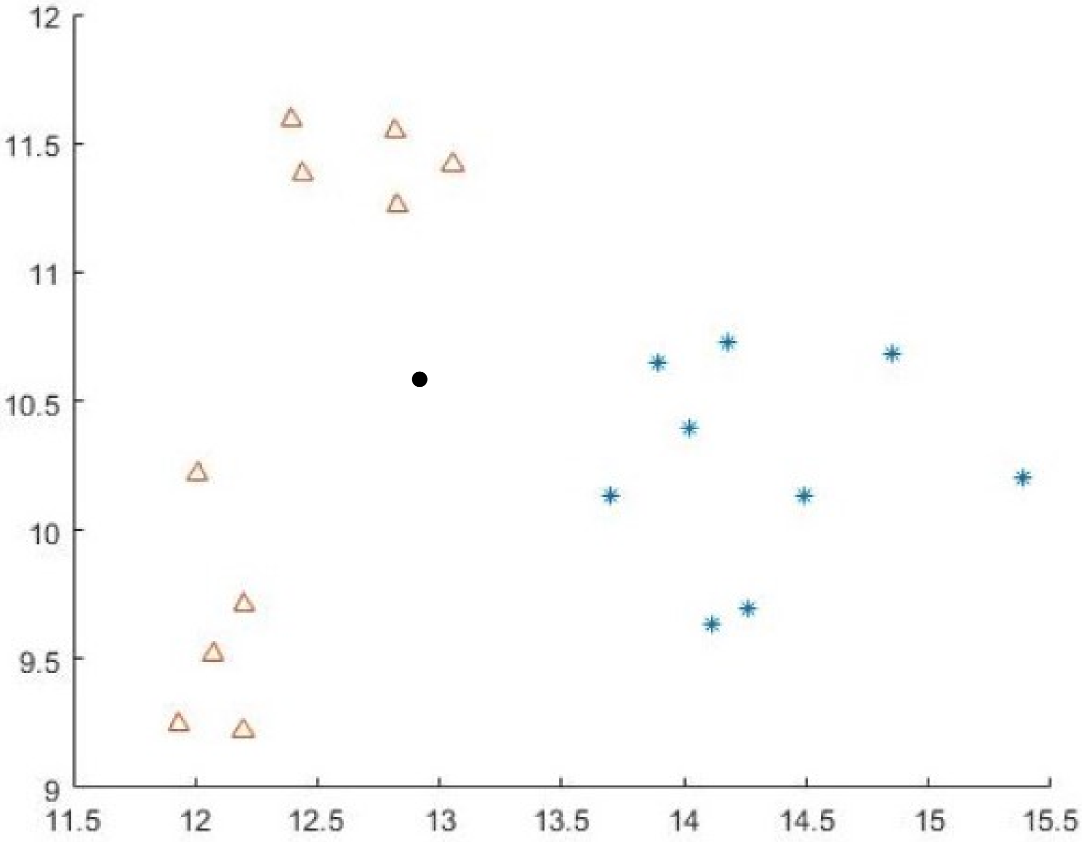
In the limit case where we assume that each training sample is a prototype, we end up calculating the distance of $\mathbf{x}_*$ with all training vectors $\mathbf{x}_i$, i=1,…,N and classify it to the class of the closest training sample.

How can we use multiple nearest neighbors for classification?

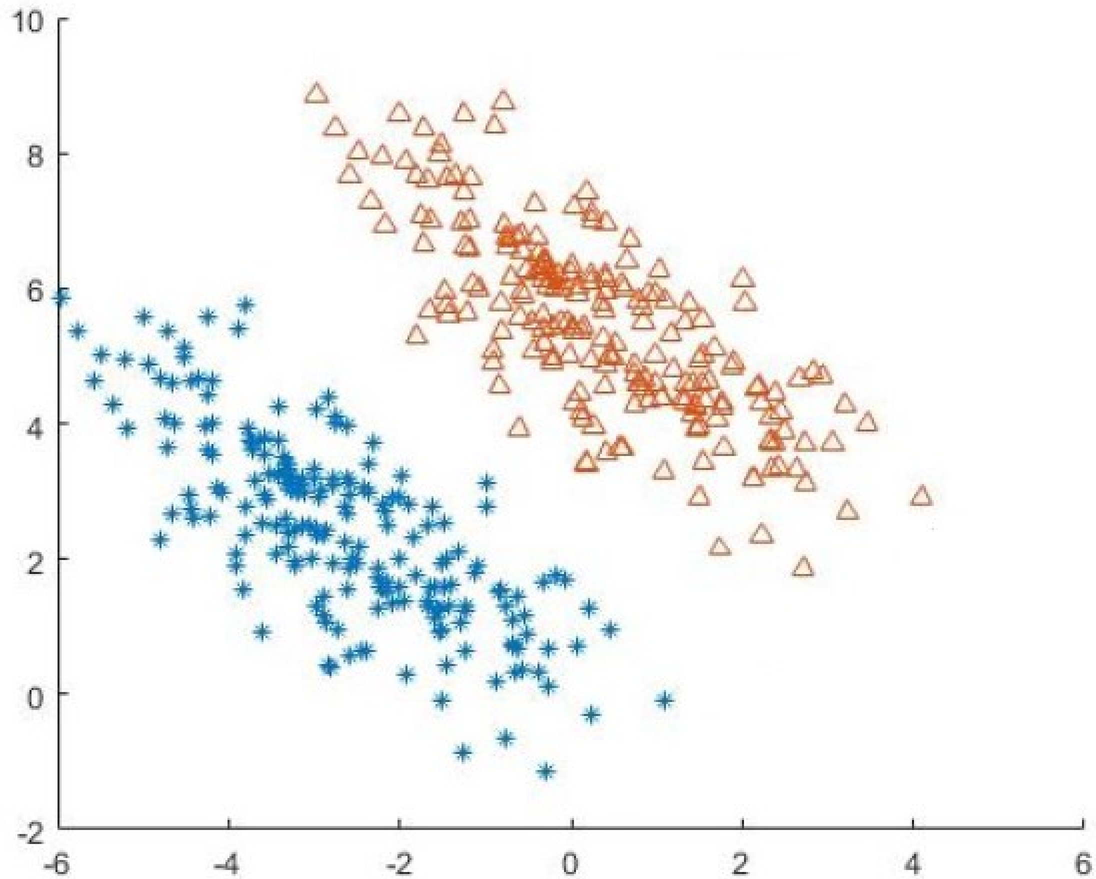
Demo: http://vision.stanford.edu/teaching/cs231n-demos/knn/

Nearest Neighbor-based Classification

Example



Fisher Discriminant Analysis



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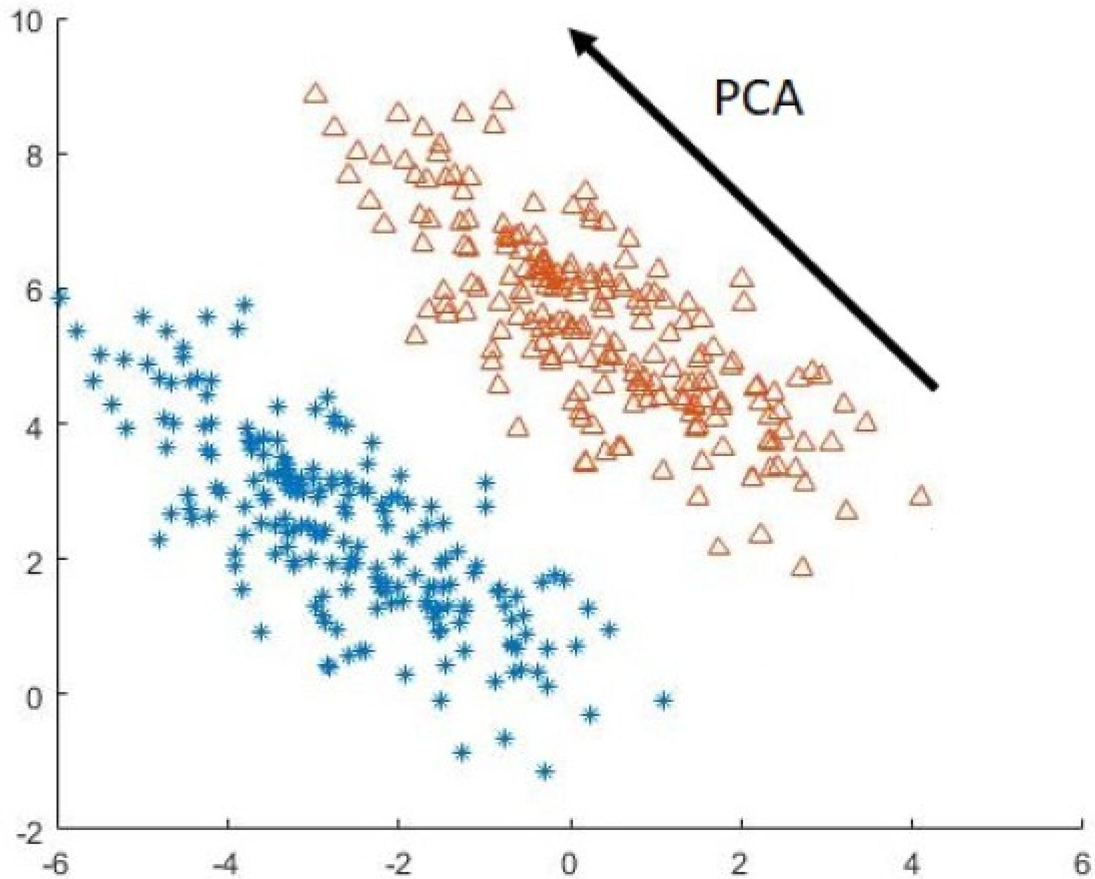

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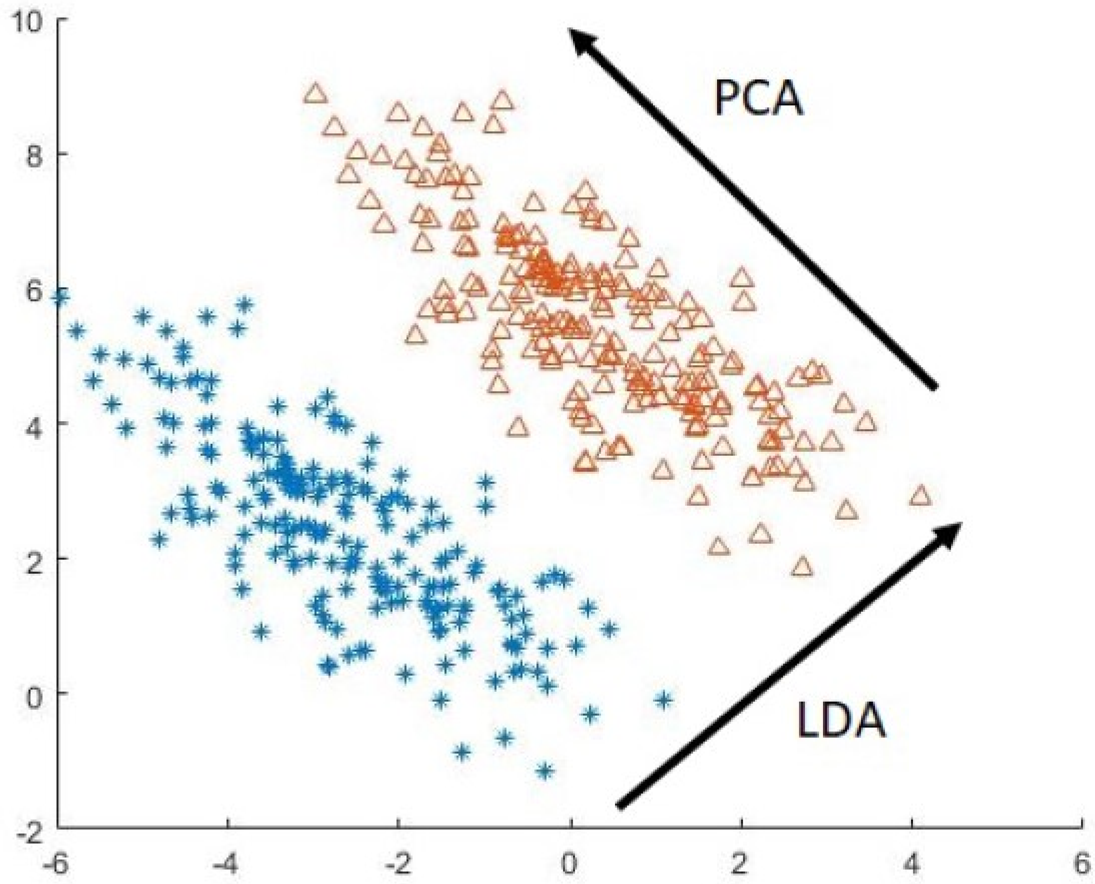

Fisher Discriminant Analysis

Given a set of N samples, each represented by a vector $\mathbf{x}_i \in \mathbb{R}^D$, and the corresponding labels $l_i = \{1,2\}$ we can define a linear projection of the form

$$y_i = \mathbf{w}^T \mathbf{x}_i$$

where $\mathbf{w} \in \mathbb{R}^D$ is a (projection) vector mapping the D-dimensional space to a line.

Demo: https://calerga.com/projects/fm20170202/lda.html

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Assuming that each class is unimodal and follows a Normal Distribution, how can we define the optimal vector **w**?

The mean vector

Fisher Discriminant Analysis

We define the class mean vectors $\boldsymbol{\mu}_k \in \mathbb{R}^D$, k=1,…,K

$$\boldsymbol{\mu}_k = \frac{1}{N_k} \sum_{i,l_i=k} \mathbf{x}_i$$

Then, the mean values of each class in the projection space (line) are

$$m_k = \frac{1}{N_k} \sum_{i,l_i=k} y_i = \frac{1}{N_k} \sum_{i,l_i=k} \mathbf{w}^T \mathbf{x}_i = \mathbf{w}^T \boldsymbol{\mu}_k$$

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The variance of each class in the line is

$$\sigma_k^2 = \frac{1}{N_k} \sum_{i, l_i = k} (y_i - m_k)^2$$

Fisher Discriminant Analysis

Since classes are unimodal and follow a Normal Distribution, they are better discriminated when:

1. The two mean values are as far as possible, i.e. their distance is as large as possible
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The distance of the centers can be expressed as a function of **w**

Similar to the expressing the objective function in PCA

$$\begin{aligned}(m_1 - m_2)^2 &= (\mathbf{w}^T \boldsymbol{\mu}_1 - \mathbf{w}^T \boldsymbol{\mu}_2)^2 \\ &= \mathbf{w}^T (\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)^T \mathbf{w} \\ &= \mathbf{w}^T \mathbf{S}_b \mathbf{w}\end{aligned}$$

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The variance can be written as

$$\begin{aligned}\sigma^2 &= \sigma_1^2 + \sigma_2^2 = \sum_{k=1}^{2} \sum_{i, l_i = k} (\mathbf{w}^T \mathbf{x}_i - \mathbf{w}^T \boldsymbol{\mu}_k)^2 \\ &= \sum_{k=1}^{2} \sum_{i, l_i = k} \mathbf{w}^T (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T \mathbf{w} = \mathbf{w}^T \mathbf{S}_w \mathbf{w}\end{aligned}$$

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After expressing the two objectives above as functions of **w**, we can formulate an optimization problem which is a function of **w**

$$\mathcal{J}(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_b \mathbf{w}}{\mathbf{w}^T \mathbf{S}_w \mathbf{w}}$$

maximise the numerator
while
minimising the denominator

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The above optimization problem is equivalent to the following problem

We can arrive at the next expressiong if we set the derivative of J(w) = 0. Once we take the derivative then the denominator cannot be zero. Look at the camera picture.

$$\mathbf{S}_b \mathbf{w} = \lambda \mathbf{S}_w \mathbf{w}$$

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$$\mathbf{S}_b \mathbf{w} = \lambda \mathbf{S}_w \mathbf{w}$$

Notice that w has not the same scale here. Therefore, w must be normalised

Assuming that $\mathbf{S}_w$ is non-singular

$$\mathbf{S}_w^{-1} \mathbf{S}_b \mathbf{w} = \lambda \mathbf{w} \Longrightarrow \mathbf{w} = \mathbf{S}_w^{-1}(\boldsymbol{\mu}_1 - \boldsymbol{\mu}_2)$$

Linear Discriminant Analysis

Linear Discriminant Analysis (LDA) is the extension of Fisher Discriminant Analysis for the case where $K > 2$.

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In LDA, $\mathbf{S}_w$ is a straightforward extension of the one used in FDA

$$\mathbf{S}_k = \sum_{i,l_i=k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$$

$$\mathbf{S}_w = \sum_{k=1}^{K} \sum_{i,l_i=k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$$

Linear Discriminant Analysis

In order to define the between-class scatter, we have

Total scatter matrix? Scatter matrix of all samples!

$$
\begin{aligned}
\mathbf{S}_T &= \sum_{k=1}^{K} \sum_{i,l_i=k} (\mathbf{x}_i - \boldsymbol{\mu})(\mathbf{x}_i - \boldsymbol{\mu})^T \\
&= \sum_{k=1}^{K} \sum_{i,l_i=k} (\mathbf{x}_i - \boldsymbol{\mu}_k + \boldsymbol{\mu}_k - \boldsymbol{\mu})(\mathbf{x}_i - \boldsymbol{\mu}_k + \boldsymbol{\mu}_k - \boldsymbol{\mu})^T \\
&= \sum_{k=1}^{K} \sum_{i,l_i=k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T + \sum_{k=1}^{K} \sum_{i,l_i=k} (\boldsymbol{\mu}_k - \boldsymbol{\mu})(\boldsymbol{\mu}_k - \boldsymbol{\mu})^T \\
&= \mathbf{S}_w + \sum_{k=1}^{K} N_k (\boldsymbol{\mu}_k - \boldsymbol{\mu})(\boldsymbol{\mu}_k - \boldsymbol{\mu})^T \\
&= \mathbf{S}_w + \mathbf{S}_b.
\end{aligned}
$$

N_k is because we have double sum here
Essentially,

Linear Discriminant Analysis

Linear Discriminant Analysis (LDA) is the extension of Fisher Discriminant Analysis for the case where K > 2.

Thus, the within-class and between-class scatter matrices are defined as

$$\mathbf{S}_k = \sum_{i, l_i = k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$$

$$\mathbf{S}_w = \sum_{k=1}^{K} \sum_{i, l_i = k} (\mathbf{x}_i - \boldsymbol{\mu}_k)(\mathbf{x}_i - \boldsymbol{\mu}_k)^T$$

$$\mathbf{S}_b = \sum_{k=1}^{K} N_k (\boldsymbol{\mu}_k - \boldsymbol{\mu})(\boldsymbol{\mu}_k - \boldsymbol{\mu})^T$$

Linear Discriminant Analysis

Linear Discriminant Analysis (LDA) is the extension of Fisher Discriminant Analysis for the case where K > 2.

The optimization problem of LDA is

$$\mathcal{J}(\mathbf{W}) = \frac{Tr(\mathbf{W}^T \mathbf{S}_b \mathbf{W})}{Tr(\mathbf{W}^T \mathbf{S}_w \mathbf{W})}$$

What are the dimensions of **W**?

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W is obtained by solving for: $\mathbf{S}_b \mathbf{w} = \lambda \mathbf{S}_w \mathbf{w}$

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Solving this eigenproblem we get K-1 eigenvectors because the rank of S_b is K-1

We usually add a constraint $\mathbf{W}^T\mathbf{W} = \mathbf{I}$, why?

Because we need the vectors in W to be orthonormal. The practical problem that we are solving is we don't want to have irrelavent information.