Sapienza University of Rome

Master in Artificial Intelligence and Robotics Master in Engineering in Computer Science

Machine Learning

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Prof. Luca locchi

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7. Linear models for classification

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Overview

- Linearly separable data
- Linear models
- Least squares
- Perceptron
- Fisher's linear discriminant
- Support Vector Machines

References

- C. Bishop. Pattern Recognition and Machine Learning. Sect. 4.1, 7.1
- T. Mitchell. Machine Learning. Section 4.4

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Linear Models for Classification

Learning a function $f: X \to Y$, with ...

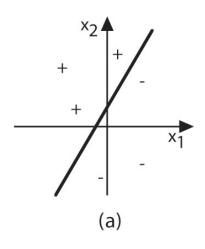
$$X \subset \mathbb{R}^d$$

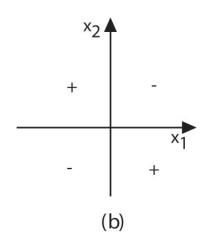
•
$$Y = \{C_1, \ldots, C_k\}$$

assuming linearly separable data.

Linearly separable data

Instances in a data set are linearly separable iff there exists a hyperplane that separates the instance space into two regions, such that differently classified instances are separated





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Linear discriminant functions

Linear discriminant function

$$y:X\to\{C_1,\ldots,C_K\}$$

Two classes:

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

K-class:

$$y_1(\mathbf{x}) = \mathbf{w}_1^T \mathbf{x} + w_{10}$$

...
 $y_K(\mathbf{x}) = \mathbf{w}_K^T \mathbf{x} + w_{K0}$

$$y_K(\mathbf{x}) = \mathbf{w}_K^T \mathbf{x} + w_{K0}$$

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Compact notation

Two classes:

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0 = \tilde{\mathbf{w}}^T \tilde{\mathbf{x}}$$
, with:

$$ilde{\mathbf{w}} = \left(egin{array}{c} w_0 \ \mathbf{w} \end{array}
ight), ilde{\mathbf{x}} = \left(egin{array}{c} 1 \ \mathbf{x} \end{array}
ight)$$

K classes:

$$\mathbf{y}(\mathbf{x}) = \begin{pmatrix} y_1(\mathbf{x}) \\ \cdots \\ y_K(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \mathbf{w}_1^T \mathbf{x} + w_{10} \\ \cdots \\ \mathbf{w}_K^T \mathbf{x} + w_{K0} \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{w}}_1^T \\ \cdots \\ \tilde{\mathbf{w}}_K^T \end{pmatrix} \tilde{\mathbf{x}} = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}, \text{ with:}$$

$$ilde{\mathbf{W}}^T = \left(egin{array}{c} ilde{\mathbf{w}}_1^T \ \cdots \ ilde{\mathbf{w}}_K^T \end{array}
ight)$$
 , i.e.: $ilde{\mathbf{W}} = (ilde{\mathbf{w}}_1, \cdots, ilde{\mathbf{w}}_K)$

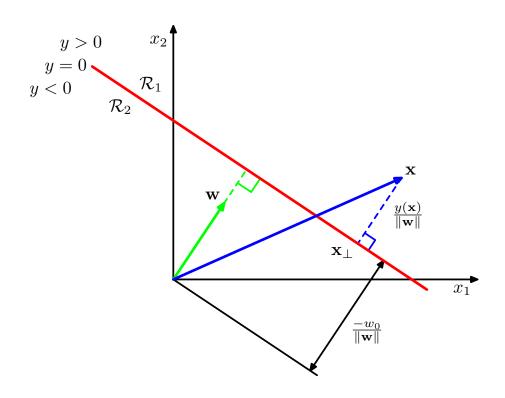
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Linear discriminant functions



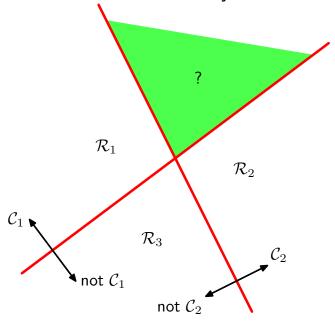
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Multiple classes

Cannot use combinations of binary linear models.

One-versus-the-rest classifiers: K-1 binary classifiers: C_k vs. not- C_k



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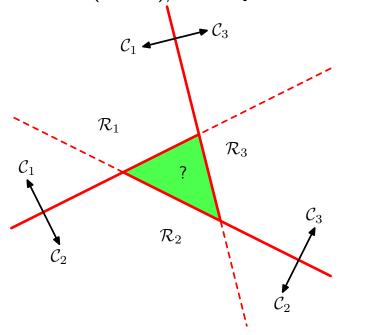
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Multiple classes

Cannot use combinations of binary linear models.

One-versus-one classifiers: K(K-1)/2 binary classifiers: C_k vs. C_j



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Multiple classes

K-class discriminant comprising K linear functions (\mathbf{x} not in dataset)

$$\mathbf{y}(\mathbf{x}) = \begin{pmatrix} y_1(\mathbf{x}) \\ \cdots \\ y_K(\mathbf{x}) \end{pmatrix} = \begin{pmatrix} \tilde{\mathbf{w}}_1^T \tilde{\mathbf{x}} \\ \cdots \\ \tilde{\mathbf{w}}_K^T \tilde{\mathbf{x}} \end{pmatrix} = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}$$

Classify **x** as C_k if $y_k(\mathbf{x}) > y_j(\mathbf{x})$ for all $j \neq k$ (j, k = 1, ..., K)

Decision boundary between C_k and C_j (hyperplane in \Re^{D-1}):

$$(\tilde{\mathbf{w}}_k - \tilde{\mathbf{w}}_j)^T \tilde{\mathbf{x}} = 0$$

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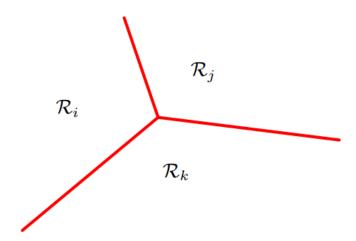
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Multiple classes

Example of K-class discriminant



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Learning linear discriminants

Given a multi-class classification problem and data set D with linearly separable data,

determine $\tilde{\mathbf{W}}$ such that $\mathbf{y}(\mathbf{x}) = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}$ is the K-class discriminant.

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Approaches to learn linear discriminants

- Least squares
- Perceptron
- Fisher's linear discriminant
- Support Vector Machines

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Least squares

Given $D = \{(\mathbf{x}_n, \mathbf{t}_n)_{n=1}^N\}$, find the linear discriminant

$$\mathbf{y}(\mathbf{x}) = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}$$

1-of-K coding scheme for \mathbf{t} : $\mathbf{x} \in C_k \to t_k = 1, t_j = 0$ for all $j \neq k$. E.g., $\mathbf{t}_n = (0, \dots, 1, \dots, 0)^T$

$$ilde{\mathbf{X}} = \left(egin{array}{c} ilde{\mathbf{x}}_1^T \ \cdots \ ilde{\mathbf{x}}_N^T \end{array}
ight) \qquad \mathbf{T} = \left(egin{array}{c} \mathbf{t}_1^T \ \cdots \ ilde{\mathbf{t}}_N^T \end{array}
ight)$$

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Least squares

Minimize sum-of-squares error function

$$E(\tilde{\mathbf{W}}) = \frac{1}{2} \operatorname{Tr} \left\{ (\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T})^T (\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T}) \right\}$$

Closed-form solution:

$$\tilde{\mathbf{W}} = \underbrace{(\tilde{\mathbf{X}}^T \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T}_{\tilde{\mathbf{X}}^\dagger} \mathbf{T}$$

$$\mathbf{y}(\mathbf{X}) = \tilde{\mathbf{W}}^T \, \tilde{\mathbf{X}} = \mathbf{T}^T (\tilde{\mathbf{X}}^\dagger)^T \tilde{\mathbf{X}}$$

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Least squares

Classification of new instance x not in dataset:

Use learnt $\tilde{\mathbf{W}}$ to compute:

$$\mathbf{y}(\mathbf{x}) = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}} = \begin{pmatrix} y_1(\mathbf{x}) \\ \cdots \\ y_K(\mathbf{x}) \end{pmatrix}$$

Assign class C_k to \mathbf{x} , where:

$$k = \underset{i \in \{1, \dots, k\}}{\operatorname{argmax}} \{ y_i(\mathbf{x}) \}$$

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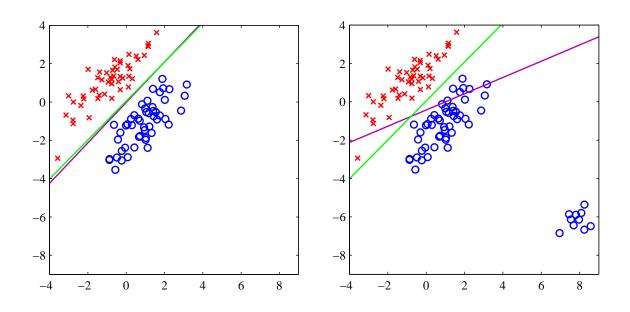
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Issues with least squares

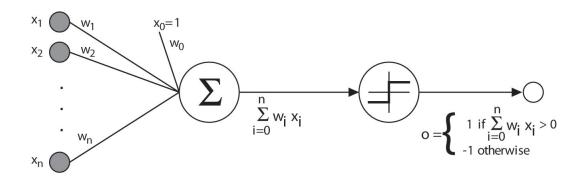
Assume Gaussian conditional distributions. Not robust to outliers!



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Perceptron



$$o(x_1,\ldots,x_d)=\left\{ egin{array}{ll} 1 & ext{if } w_0+w_1x_1+\cdots+w_dx_d>0 \ -1 & ext{otherwise}. \end{array}
ight.$$

$$o(\mathbf{x}) = \begin{cases} 1 & \text{if } \mathbf{w}^T \mathbf{x} > 0 \\ -1 & \text{otherwise.} \end{cases} = sign(\mathbf{w}^T \mathbf{x})$$

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Perceptron training rule

Consider the unthresholded linear unit, where

$$o = w_0 + w_1 x_1 + \cdots + w_d x_d = \mathbf{w}^T \mathbf{x}$$

Let's learn w_i from training examples $D = \{(\mathbf{x}_n, t_n)_{n=1}^N\}$ that minimize the squared error (loss function)

$$E(\mathbf{w}) \equiv \frac{1}{2} \sum_{n=1}^{N} (t_n - o_n)^2 = \frac{1}{2} \sum_{n=1}^{N} (t_n - \mathbf{w}^T \mathbf{x}_n)^2$$

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Perceptron training rule

$$\frac{\partial E}{\partial w_i} = \frac{\partial}{\partial w_i} \frac{1}{2} \sum_{n=1}^{N} (t_n - \mathbf{w}_n^T \mathbf{x}_n)^2 = \frac{1}{2} \sum_{n=1}^{N} \frac{\partial}{\partial w_i} (t_n - \mathbf{w}^T \mathbf{x}_n)^2$$

$$= \frac{1}{2} \sum_{n=1}^{N} 2(t_n - \mathbf{w}^T \mathbf{x}_n) \frac{\partial}{\partial w_i} (t_n - \mathbf{w}^T \mathbf{x}_n)$$

$$= \sum_{n=1}^{N} (t_n - \mathbf{w}^T \mathbf{x}_n) \frac{\partial}{\partial w_i} (t_n - \mathbf{w}^T \mathbf{x}_n)$$

$$= \sum_{n=1}^{N} (t_n - \mathbf{w}^T \mathbf{x}_n) (-x_{i,n})$$

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Perceptron training rule

Unthresholded unit:

Update of weights w

$$w_i \leftarrow w_i + \Delta w_i$$

$$\Delta w_i = -\eta \frac{\partial E}{\partial w_i} = \eta \sum_{n=1}^{N} (t_n - \mathbf{w}^T \mathbf{x}_n) x_{i,n}$$

 η is a small constant (e.g., 0.05) called *learning rate*

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Perceptron training rule

Thresholded unit:

Update of weights w

$$w_{i} \leftarrow w_{i} + \Delta w_{i}$$

$$\Delta w_{i} = -\eta \frac{\partial E}{\partial w_{i}} = \eta \sum_{n=1}^{N} (t_{n} - sign(\mathbf{w}^{T} \mathbf{x}_{n})) x_{i,n}$$

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Perceptron algorithm

Given perceptron model $o(\mathbf{x}) = sign(\mathbf{w}^T \mathbf{x})$ and data set D, determine weights \mathbf{w} .

- 1 Initialize $\hat{\mathbf{w}}$ (e.g. small random values)
- Repeat until termination condition

•
$$\hat{w}_i \leftarrow \hat{w}_i + \Delta w_i$$

Output ŵ

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Perceptron algorithm

Batch mode: Consider all dataset *D*

$$\Delta w_i = \eta \sum_{(\mathbf{x},t)\in D} (t-o(\mathbf{x})) x_i$$

Mini-Batch mode: Choose a small subset $S \subset D$

$$\Delta w_i = \eta \sum_{(\mathbf{x},t)\in S} (t-o(\mathbf{x})) x_i$$

Incremental mode: Choose one sample $(\mathbf{x}, t) \in D$

$$\Delta w_i = \eta (t - o(\mathbf{x})) x_i$$

 $o(\mathbf{x}) = \mathbf{w}^T \mathbf{x}$ for unthresholded, $o(\mathbf{x}) = sign(\mathbf{w}^T \mathbf{x})$ for thresholded Incremental and mini-batch modes speed up convergence and are less sensitive to local minima.

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Perceptron algorithm

Termination conditions

- Predefined number of iterations
- Threshold on changes in the loss function $E(\mathbf{w})$

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Perceptron training rule

Example:

$$\eta = 0.1$$
, $x_i = 0.8$

- if t=1 and o=-1 then $\Delta w_i=0.16$
- ullet if t=-1 and o=1 then $\Delta w_i=-0.16$

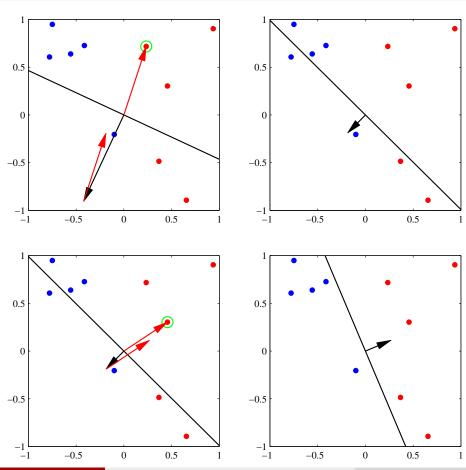
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Perceptron training rule



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Perceptron training rule

Can prove it will converge:

- if training data is linearly separable
- ullet and η sufficiently small

Small $\eta \to \text{slow convergence}$.

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Perceptron: Prediction

Classification of new instance x not in dataset:

Classify **x** as C_k , for $k = sign(\mathbf{w}^T \mathbf{x})$, using learnt **w**

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Consider two classes case.

Determine $y = \mathbf{w}^T \mathbf{x}$ and classify $\mathbf{x} \in C_1$ if $y \ge -w_0$, $\mathbf{x} \in C_2$ otherwise.

Corresponding to the projection on a line determined by \mathbf{w} .

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Fisher's linear discriminant

Adjusting w to find a direction that maximizes class separation.

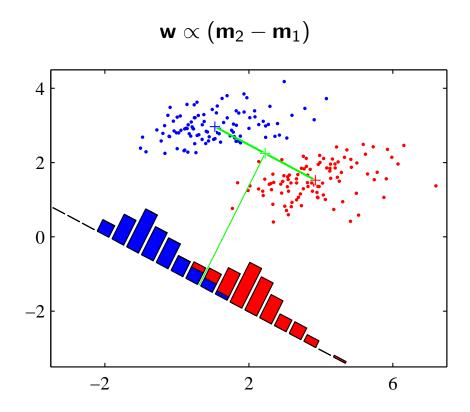
Consider a data set with N_1 points in C_1 and N_2 points in C_2

$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{n \in C_1} \mathbf{x}_n \qquad \mathbf{m}_2 = \frac{1}{N_2} \sum_{n \in C_2} \mathbf{x}_n$$

Choose **w** that maximizes $J(\mathbf{w}) = \mathbf{w}^T(\mathbf{m}_2 - \mathbf{m}_1)$, subject to $||\mathbf{w}|| = 1$.

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Fisher's linear discriminant

Fisher criterion

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

with

$$\mathbf{S}_B = (\mathbf{m}_2 - \mathbf{m}_1)(\mathbf{m}_2 - \mathbf{m}_1)^T$$

Between class scatter

$$\mathbf{S}_W = \sum_{n \in C_1} (\mathbf{x}_n - \mathbf{m}_1) (\mathbf{x}_n - \mathbf{m}_1)^T + \sum_{n \in C_2} (\mathbf{x}_n - \mathbf{m}_2) (\mathbf{x}_n - \mathbf{m}_2)^T$$

Within class scatter

Choose **w** that maximizes $J(\mathbf{w})$.

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Find w that maximizes

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

by solving

$$\frac{d}{d\mathbf{w}}J(\mathbf{w})=0$$

$$\Rightarrow$$
 w* \propto S $_W^{-1}$ (m $_2$ - m $_1$)

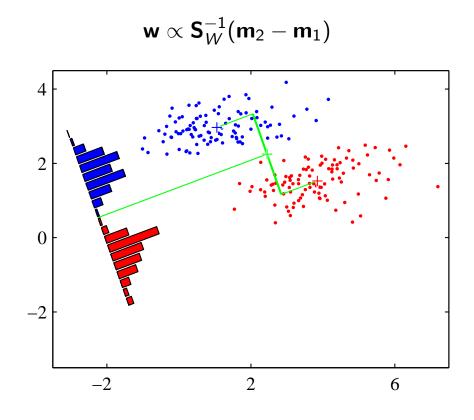
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Fisher's linear discriminant



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Summarizing, given a two classes classification problem, Fisher's linear discriminant is given by the function $y = \mathbf{w}^T \mathbf{x}$ and the classification of new instances is given by $y \ge -w_0$ where

$$\mathbf{w} = \mathbf{S}_{W}^{-1}(\mathbf{m}_2 - \mathbf{m}_1)$$

$$w_0 = \mathbf{w}^T \mathbf{m}$$

m is the global mean of all the data set.

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Fisher's linear discriminant

Multiple classes.

$$\mathbf{y} = \mathbf{W}^T \mathbf{x}$$

Maximizing

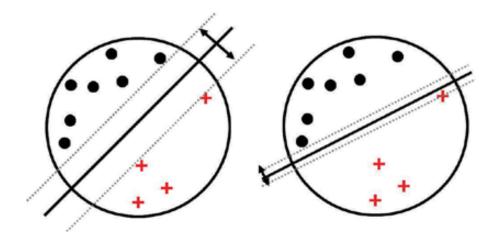
$$J(\mathbf{W}) = Tr\left\{ (\mathbf{W}\mathbf{S}_W\mathbf{W}^T)^{-1}(\mathbf{W}\mathbf{S}_B\mathbf{W}^T) \right\}$$

. . .

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Support Vector Machines (SVM) for Classification aims at maximum margin providing for better accuracy.



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Support Vector Machines

Let's consider binary classification $y: X \to \{+1, -1\}$ with data set $D = \{(\mathbf{x}_n, t_n)_{n=1}^N\}$, $t_n \in \{+1, -1\}$ and a linear model

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

Assume D is linearly separable

$$t_n y(\mathbf{x}_n) > 0 \ \forall n = 1, \dots N$$

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Let \mathbf{x}_k be the closest point of the data set D to the hyperplane $\bar{h}: \bar{\mathbf{w}}^T\mathbf{x} + \bar{w_0} = 0$

the margin (smallest distance between \mathbf{x}_k and \bar{h}) is $\frac{|y(\mathbf{x}_k)|}{||\mathbf{w}||}$

Given data set D and hyperplane \bar{h} , the margin is computed as

$$\min_{n=1,\ldots,N} \frac{|y(\mathbf{x}_n)|}{||\mathbf{w}||} = \cdots = \frac{1}{||\mathbf{w}||} \min_{n=1,\ldots,N} [t_n(\bar{\mathbf{w}}^T \mathbf{x}_n + \bar{w}_0)]$$

using the property $|y(\mathbf{x}_n)| = t_n y(\mathbf{x}_n)$

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Support Vector Machines

Given data set D, the hyperplane $h^*: \mathbf{w^*}^T \mathbf{x} + w_0^* = 0$ with maximum margin is computed as

$$\mathbf{w}^*, w_0^* = \operatorname*{argmax}_{\mathbf{w}, w_0} \frac{1}{||\mathbf{w}||} \min_{n=1,\dots,N} [t_n(\mathbf{w}^T \mathbf{x}_n + w_0)]$$

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Rescaling all the points does not affect the solution.

Rescale in such a way that for the closet point \mathbf{x}_k we have

$$t_k(\mathbf{w}^T\mathbf{x}_k+w_0)=1$$

Canonical representation:

$$t_n(\mathbf{w}^T\mathbf{x}_n + w_0) \ge 1 \ \forall n = 1, \dots, N$$

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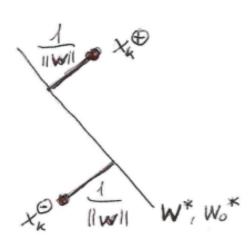
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Support Vector Machines

When the maximum margin hyperplane \mathbf{w}^* , w_0^* is found, there will be at least 2 closest points \mathbf{x}_k^{\oplus} and \mathbf{x}_k^{\ominus} (one for each class).

$$\mathbf{w}^{*T}\mathbf{x}_{k}^{\oplus}+w_{0}^{*}=+1$$

$$\mathbf{w}^{*T}\mathbf{x}_{k}^{\ominus}+w_{0}^{*}=-1$$



In the canonical representation of the problem the maximum margin hyperplane can be found by solving the optimization problem

$$\mathbf{w}^*, w_0^* = \operatorname{argmax} \frac{1}{||\mathbf{w}||} = \operatorname{argmin} \frac{1}{2} ||\mathbf{w}||^2$$

subject to

$$t_n(\mathbf{w}^T\mathbf{x}_n + w_0) \geq 1 \ \forall n = 1, \dots, N$$

Quadratic programming problem solved with Lagrangian method.

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Support Vector Machines

Solution

$$\mathbf{w}^* = \sum_{n=1}^N a_n^* t_n \mathbf{x}_n$$

 a_i^* (Lagrange multipliers): results of the Lagrangian optimization problem

$$\tilde{L}(\mathbf{a}) = \sum_{n=1}^{N} a_n - \frac{1}{2} \sum_{n=1}^{N} \sum_{m=1}^{N} a_n a_m t_n t_m \mathbf{x}_n^T \mathbf{x}_m$$

subject to

$$a_n \geq 0 \ \forall n = 1, \dots, N$$

$$\sum_{n=1}^{N} a_n t_n = 0$$

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Note:

samples \mathbf{x}_n for which $a_n^* = 0$ do not contribute to the solution

Karush-Kuhn-Tucker (KKT) condition:

for each $\mathbf{x}_n \in D$, either $a_n^* = 0$ or $t_n y(\mathbf{x}_n) = 1$

thus $t_n y(\mathbf{x}_n) > 1$ implies $a_n^* = 0$

Support vectors: x_k such that $t_k y(\mathbf{x}_k) = 1$ and $a_k^* > 0$

$$SV \equiv \{\mathbf{x}_k \in D \mid t_k y(\mathbf{x}_k) = 1\}$$

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Support Vector Machines

Hyperplanes expressed with support vectors

$$y(\mathbf{x}) = \sum_{\mathbf{x}_j \in SV} a_j^* t_j \mathbf{x}^T \mathbf{x}_j + w_0^* = 0$$

Note: other vectors $\mathbf{x}_n \not\in SV$ do not contribute $(a_n^* = 0)$

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To compute w_0^* :

Support vector $\mathbf{x}_k \in SV$ satisfies $t_k y(\mathbf{x}_k) = 1$

$$t_k \left(\sum_{\mathbf{x}_j \in SV} a_j^* t_j \mathbf{x}_k^T \mathbf{x}_j + w_0^*
ight) = 1$$

Multiplying by t_k and using $t_k^2 = 1$

$$w_0^* = t_k - \sum_{\mathbf{x}_i \in SV} a_j^* t_j \mathbf{x}_k^T \mathbf{x}_j$$

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Support Vector Machines

Instead of using one particular support vector \mathbf{x}_k to determine w_0

$$w_0^* = t_k - \sum_{\mathbf{x}_i \in SV} a_j^* t_j \mathbf{x}_k^T \mathbf{x}_j$$

a more stable solution is obtained by averaging over all the support vectors

$$w_0^* = \frac{1}{|SV|} \sum_{\mathbf{x}_k \in SV} \left(t_k - \sum_{\mathbf{x}_j \in S} a_j^* t_j \mathbf{x}_k^T \mathbf{x}_j \right)$$

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Given the maximum margin hyperplane determined by a_k^* , w_0^*

Classification of a new instance \mathbf{x}'

$$y(\mathbf{x}') = sign\left(\sum_{\mathbf{x}_k \in SV} a_k^* t_k \mathbf{x}'^T \mathbf{x}_k + w_0^*\right)$$

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Support Vector Machines

Optimization problem for determining \mathbf{w} , w_0 (dimension d+1, with $X=\Re^d$) transformed in an optimization problem for determining \mathbf{a} (dimension |D|)

Efficient when $d \ll |D|$ (most of a_i will be zero). Very useful when d is large or infinite.

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Support Vector Machines with soft margin constraints

What if data are "almost" linearly separable (e.g., a few points are on the "wrong side")

Let us introduce slack variables $\xi_n \geq 0$ $n = 1, \dots, N$

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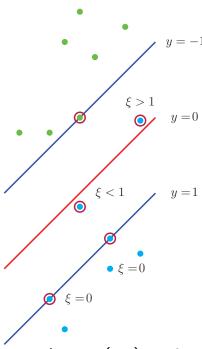
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Support Vector Machines with soft margin constraints

- $\xi_n = 0$ if point on or inside the correct margin boundary
- $0 < \xi_n \le 1$ if point inside the margin but correct side
- $\xi_n > 1$ if point on wrong side of boundary



when $\xi_n = 1$, the sample lies on the decision boundary $y(\mathbf{x}_n) = 0$ when $\xi_n > 1$, the sample will be mis-classified

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7. Linear models for classification

Support Vector Machines with soft margin constraints

Soft margin constraint

$$t_n y(\mathbf{x}_n) \geq 1 - \xi_n, \quad n = 1, \dots, N$$

Optimization problem with soft margin constraints

$$\mathbf{w}^*, w_0^* = \operatorname{argmin} \frac{1}{2} ||\mathbf{w}||^2 + C \sum_{n=1}^{N} \xi_n$$

subject to

$$t_n y(\mathbf{x}_n) \ge 1 - \xi_n, \quad n = 1, \dots, N$$

 $\xi_n \ge 0, \quad n = 1, \dots, N$

C is a constant (inverse of a regularization coefficient)

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Support Vector Machines with soft margin constraints

Solution similar to the case of linearly separable data.

$$\mathbf{w}^* = \sum_{n=1}^N a_n^* t_n \mathbf{x}_n$$

$$w_0^* =$$

with a_n^* computed as solution of a Lagrangian optimization problem.

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7. Linear models for classification

Basis functions

So far we considered models working directly on \mathbf{x} .

All the results hold if we consider a non-linear transformation of the inputs $\phi(\mathbf{x})$ (basis functions).

Decision boundaries will be linear in the feature space ϕ and non-linear in the original space ${\bf x}$

Classes that are linearly separable in the feature space ϕ may not be separable in the input space \mathbf{x} .

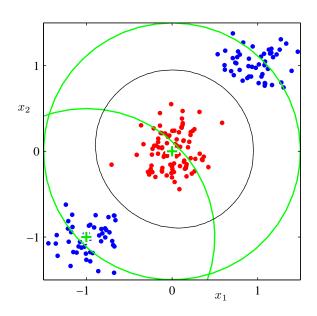
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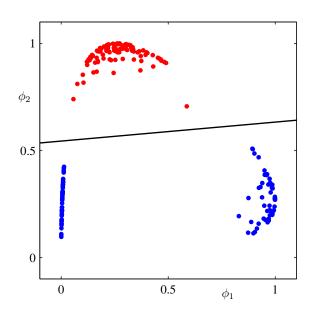
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Basis functions example





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Basis functions examples

- Linear
- Polynomial
- Radial Basis Function (RBF)
- Sigmoid
- ...

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Linear models for non-linear functions

Learning non-linear function

$$y: X \to \{C_1, \ldots, C_K\}$$

from data set D non-linearly separable.

Find a non-linear transformation ϕ and learn a linear model

$$y(\mathbf{x}) = \mathbf{w}^T \phi(\mathbf{x}) + w_0$$
 (two classes)

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \phi(\mathbf{x}) + w_{k0}$$
 (multiple classes)

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7. Linear models for classification

Summary

- Basic methods for learning linear classification functions
- Based on solution of an optimization problem
- Closed form vs. iterative solutions
- Sensitivity to outliers
- Learning non-linear functions with linear models using basis functions
- Further developed as kernel methods

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7. Linear models for classification