Sapienza University of Rome

Master in Engineering in Computer Science

Machine Learning

A.Y. 2022/2023

Prof. Luca locchi

Luca locchi

7. Linear models for classification

1/61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

7. Linear models for classification

Luca locchi

Luca locchi

7. Linear models for classification

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

Luca locchi

7. Linear models for classification

3/61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Linear Models for Classification

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

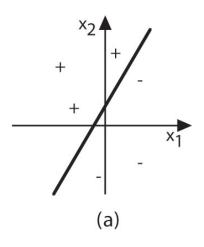
•
$$X \subset \Re^d$$

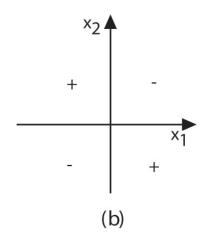
•
$$Y = \{C_1, \ldots, C_k\}$$

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





Luca locchi

7. Linear models for classification

5/61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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:

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

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

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

Luca locchi

7. Linear models for classification

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:

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

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

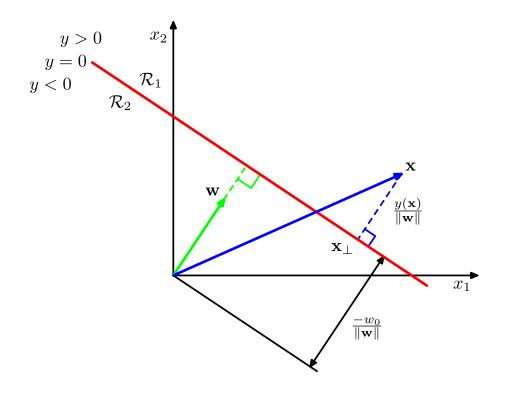
Luca locchi

7. Linear models for classification

7/61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Linear discriminant functions



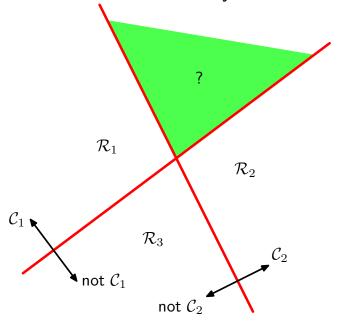
Luca locchi

7. Linear models for classification

Multiple classes

Cannot use combinations of binary linear models.

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



Luca locchi

7. Linear models for classification

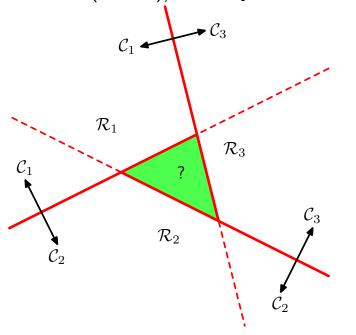
9/61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Multiple classes

Cannot use combinations of binary linear models.

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



Luca locchi

7. Linear models for classification

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}):

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

Luca locchi

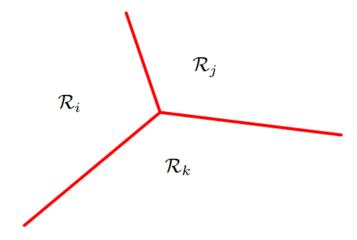
7. Linear models for classification

11/61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Multiple classes

Example of K-class discriminant



Luca locchi

7. Linear models for classification

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.

Luca locchi

7. Linear models for classification

13 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Approaches to learn linear discriminants

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

Luca locchi

7. Linear models for classification

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., $\mathbf{t}_n = (0, \dots, 1, \dots, 0)^T$

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

Luca locchi

7. Linear models for classification

15 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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:

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

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

Luca locchi

7. Linear models for classification

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:

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

Luca locchi

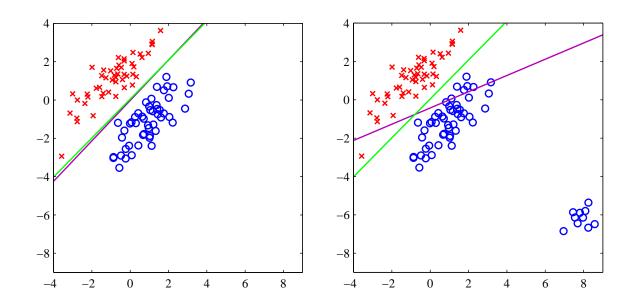
7. Linear models for classification

17 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Issues with least squares

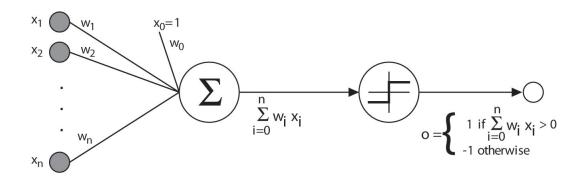
Assume Gaussian conditional distributions. Not robust to outliers!



Luca locchi

7. Linear models for classification

Perceptron



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

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

Luca locchi

Luca locchi

7. Linear models for classification

19/61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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)

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

7. Linear models for classification 20 / 61

Perceptron training rule

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

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

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

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

Luca locchi

7. Linear models for classification

21 / 61

22 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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*

Luca locchi 7. Linear models for classification

Perceptron training rule

Thresholded unit:

Update of weights w

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

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

Luca locchi

7. Linear models for classification

23 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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

Luca locchi

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.

Luca locchi

7. Linear models for classification

25 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Perceptron algorithm

Termination conditions

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

Luca locchi

7. Linear models for classification

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 $\Delta w_i=-0.16$

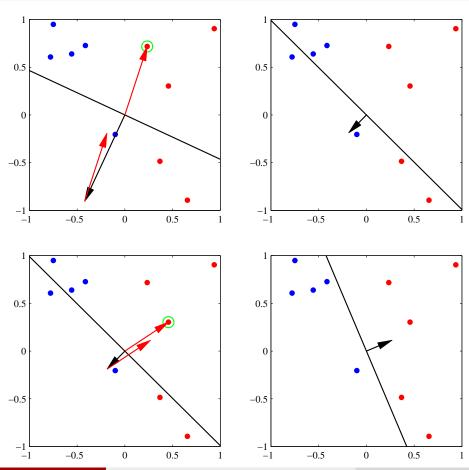
Luca locchi

7. Linear models for classification

27 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Perceptron training rule



Luca locchi

7. Linear models for classification

Perceptron training rule

Can prove it will converge:

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

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

Luca locchi

7. Linear models for classification

29 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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**

Luca locchi

7. Linear models for classification

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} .

Luca locchi

7. Linear models for classification

31 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Fisher's linear discriminant

Adjusting w to find a direction that maximizes class separation.

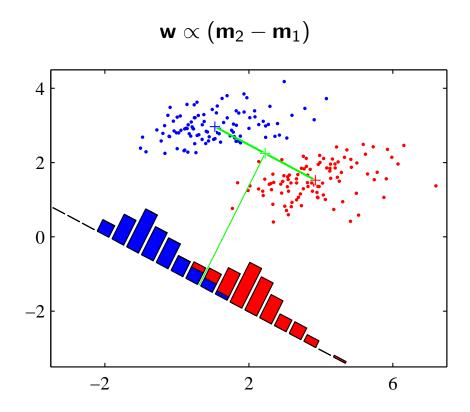
Consider a data set with N_1 points in C_1 and N_2 points in C_2

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

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

Luca locchi

7. Linear models for classification



Luca locchi

7. Linear models for classification

33 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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 $J(\mathbf{w})$.

Luca locchi

7. Linear models for classification

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 $_1$)

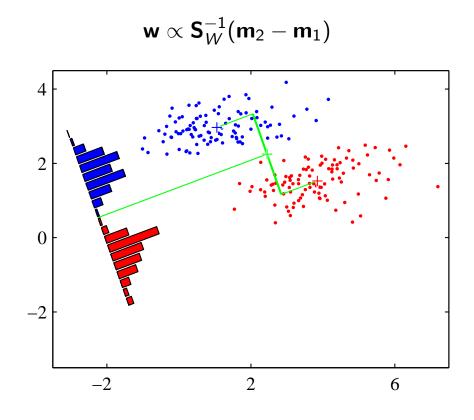
Luca locchi

7. Linear models for classification

35 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Fisher's linear discriminant



Luca locchi

7. Linear models for classification

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.

Luca locchi

7. Linear models for classification

37 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Fisher's linear discriminant

Multiple classes.

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

Maximizing

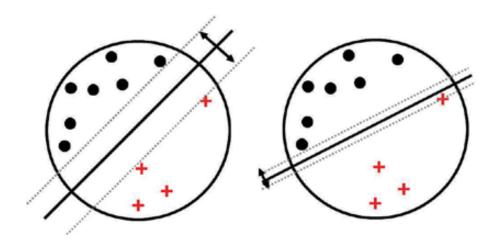
$$J(\mathbf{W}) = Tr\left\{ (\mathbf{W}\mathbf{S}_W\mathbf{W}^T)^{-1}(\mathbf{W}\mathbf{S}_B\mathbf{W}^T) \right\}$$

. . .

Luca locchi 7. Linear mod

7. Linear models for classification

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



Luca locchi

7. Linear models for classification

39 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Support Vector Machines

Let's consider binary classification $f: X \to \{+1, -1\}$ 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

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

Luca locchi

7. Linear models for classification

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

Luca locchi

7. Linear models for classification

41 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Support Vector Machines

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

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

Luca locchi

7. Linear models for classification

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:

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

Luca locchi

7. Linear models for classification

43 / 61

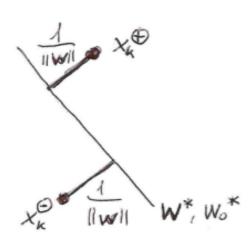
Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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.

Luca locchi

7. Linear models for classification

45 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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

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

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

Luca locchi

7. Linear models for classification

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 $a_k^* > 0$

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

Luca locchi

7. Linear models for classification

47 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Support Vector Machines

Hyperplanes expressed with support vectors

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

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

Luca locchi

7. Linear models for classification

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 $t_k^2 = 1$

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

Luca locchi

7. Linear models for classification

49 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Support Vector Machines

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

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

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

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

Luca locchi 7. Linear models for classification

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

Classification of a new instance \mathbf{x}'

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

Luca locchi

7. Linear models for classification

51 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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.

Luca locchi

7. Linear models for classification

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 $\xi_n \geq 0$ $n = 1, \dots, N$

Luca locchi

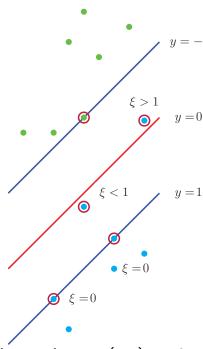
7. Linear models for classification

53 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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

Luca locchi

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)

Luca locchi

7. Linear models for classification

55 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

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.

Luca locchi

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} .

Luca locchi

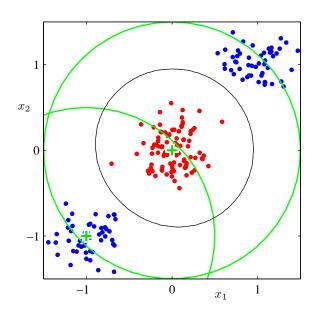
7. Linear models for classification

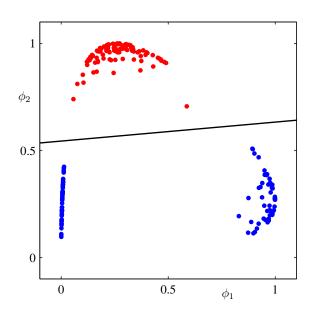
57 / 61

58 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Basis functions example





Luca locchi

7. Linear models for classification

Basis functions examples

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

Luca locchi

7. Linear models for classification

59 / 61

Sapienza University of Rome, Italy - Machine Learning (2022/2023)

Linear models for non-linear functions

Learning non-linear function

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

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)

Luca locchi

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

Luca locchi

7. Linear models for classification