

Faculty of Electrical Engineering Department of Cybernetics

# **Linear Methods for Regression and Classification**

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**Regression task** is a supervised learning task, i.e.

- a training (multi)set  $T = \{(x^{(1)}, y^{(1)}), \dots, (x^{(|T|)}, y^{(|T|)})\}$  is available, where
- the labels  $y^{(i)}$  are *quantitative*, often *continuous* (as opposed to classification tasks where  $y^{(i)}$  are nominal).
- Its purpose is to model the relationship between independent variables (inputs)  $x = (x_1, ..., x_D)$  and the dependent variable (output) *y*.

Linear regression

- Regression
- Notation remarks
- Train, apply
- 1D regression
- LSM
- Minimizing J(w, T)
- Gradient descent
- Multivariate linear regression

Linear classification

Perceptron

Logistic regression

Optimal separating hyperplane



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Linear regression is a particular regression model which assumes (and learns) linear relationship between the inputs and the output:

$$\widehat{y} = h(\mathbf{x}) = w_0 + w_1 x_1 + \ldots + w_D x_D = w_0 + \langle \mathbf{w}, \mathbf{x} \rangle = w_0 + \mathbf{x} \mathbf{w}^T,$$

where

- $\hat{y}$  is the model *prediction* (*estimate* of the true value y),
- $h(\mathbf{x})$  is the linear model (a *hypothesis*),
- $w_0, \ldots, w_D$  are the coefficients of the linear function,  $w_0$  is the *bias*, organized in a row vector w,
- $\langle w, x \rangle$  is a *dot product* of vectors w and x (scalar product),
- which can be also computed as a matrix product  $xw^T$  if w and x are row vectors.

Linear regression Regression

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#### **Notation remarks**

**Homogeneous coordinates**: If we add "1" as the first element of *x* so that  $x = (1, x_1, ..., x_D)$ , then we can write the linear model in an even simpler form (without the explicit bias term):

$$\widehat{y} = h(\mathbf{x}) = w_0 \cdot 1 + w_1 x_1 + \ldots + w_D x_D = \langle \mathbf{w}, \mathbf{x} \rangle = \mathbf{x} \mathbf{w}^T.$$

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Optimal separating hyperplane Summary Matrix notation: If we organize the data into matrix *X* and vector *y*, such that



and similarly with  $\hat{y}$ , then we can write a batch computation of predictions for all data in X as

 $\widehat{y} = Xw^T.$ 



Any ML model has 2 operation modes:

- 1. learning (training, fitting) and
- 2. application (testing, making predictions).



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- Minimizing J(w,T) The model *h* can be viewed as a function of 2 variables: h(x,w).
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- Multivariate linear
- regression
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- Summary





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The model *h* can be viewed as a function of 2 variables: h(x, w).

**Model application:** If the model is given (*w* is fixed), we can manipulate *x* to make predictions:

$$\widehat{y} = h(\mathbf{x}, \mathbf{w}) = h_{\mathbf{w}}(\mathbf{x})$$



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$$\widehat{y} = h(x, w) = h_w(x).$$

• **Model learning:** If the data is given (*T* is fixed), we can manipulate the model parameters • *w* to fit the model to the data:

 $w^* = \underset{w}{\operatorname{argmin}} J(w, T).$ 



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#### How to train the model?



### Simple (univariate) linear regression

**Simple (univariate) regression** deals with cases where  $x^{(i)} = x^{(i)}$ , i.e. the examples are described by a single feature (they are 1-dimensional).

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## Simple (univariate) linear regression

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#### Fitting a line to data:

- find parameters  $w_0$ ,  $w_1$  of a linear model  $\hat{y} = w_0 + w_1 x$
- given a training (multi)set  $T = \{(x^{(i)}, y^{(i)})\}_{i=1}^{|T|}$ .



## Simple (univariate) linear regression

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#### Linear regression

Regression

• Train, apply • 1D regression

• LSM

#### Fitting a line to data: Notation remarks

- find parameters  $w_0, w_1$  of a linear model  $\hat{y} = w_0 + w_1 x$
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How to fit a line depending on the number of training examples |T|:

- Given a single example (1 equation, 2 parameters)  $\Rightarrow$  infinitely many linear functions can be fitted.
- Given 2 examples (2 equations, 2 parameters)  $\Rightarrow$  exactly 1 linear function can be fitted.

Given 3 or more examples (> 2 equations, 2 parameters)

- $\Rightarrow$  no line can be fitted with zero error
- $\Rightarrow$  a line which minimizes the "size" of error  $y \hat{y}$  can be fitted:

$$w^* = (w_0^*, w_1^*) = \operatorname*{argmin}_{w_0, w_1} J(w_0, w_1, T).$$

#### • Gradient descent • Multivariate linear

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• Minimizing J(w, T)

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#### The least squares method

The **least squares method (LSM)** suggests to choose such parameters *w* which minimize the *mean squared error* (MSE)

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#### The least squares method

 $(x^{(1)}, \hat{y}^{(1)})$ 

 $(x^{(1)}, y^{(1)})$ 

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1

 $|y^{(1)} - \hat{y}^{(1)}|$ 

#### **Explicit solution:**

0

 $w_0$ 

x

## Universal fitting method: minimization of cost function J

The landscape of *J* in the space of parameters  $w_0$  and  $w_1$ :



Gradually better linear models found by an optimization method (BFGS):





#### Gradient descent algorithm

- Given a function  $J(w_0, w_1)$  that should be minimized,
- start with a guess of  $w_0$  and  $w_1$  and
- change it, so that  $J(w_0, w_1)$  decreases, i.e.
- update our current guess of *w*<sup>0</sup> and *w*<sup>1</sup> by taking a step in the direction opposite to the gradient:

$$w \leftarrow w - \alpha \nabla J(w_0, w_1)$$
, i.e.  
 $w_d \leftarrow w_d - \alpha \frac{\partial}{\partial w_d} J(w_0, w_1)$ ,

where all  $w_i$ s are updated simultaneously and  $\alpha$  is a **learning rate** (step size). For the cost function

$$J(w_0, w_1) = \frac{1}{|T|} \sum_{i=1}^{|T|} \left( y^{(i)} - h_w(x^{(i)}) \right)^2 = \frac{1}{|T|} \sum_{i=1}^{|T|} \left( y^{(i)} - (w_0 + w_1 x^{(i)}) \right)^2,$$

the gradient can be computed as

$$\begin{aligned} \frac{\partial}{\partial w_0} J(w_0, w_1) &= -\frac{2}{|T|} \sum_{i=1}^{|T|} \left( y^{(i)} - h_w(x^{(i)}) \right) = \frac{2}{|T|} \sum_{i=1}^{|T|} \left( h_w(x^{(i)}) - y^{(i)} \right) \\ \frac{\partial}{\partial w_1} J(w_0, w_1) &= -\frac{2}{|T|} \sum_{i=1}^{|T|} \left( y^{(i)} - h_w(x^{(i)}) \right) x^{(i)} = \frac{2}{|T|} \sum_{i=1}^{|T|} \left( h_w(x^{(i)}) - y^{(i)} \right) x^{(i)} \end{aligned}$$

Linear regression **chang** 

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#### **Multivariate linear regression**

**Multivariate linear regression** deals with cases where  $x^{(i)} = (x_1^{(i)}, \ldots, x_D^{(i)})$ , i.e. the examples are described by more than 1 feature (they are *D*-dimensional).

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#### **Model fitting:**

- find parameters  $w = (w_1, \ldots, w_D)$  of a linear model  $\hat{y} = xw^T$
- **given the training (multi)set**  $T = \{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}_{i=1}^{|T|}$ .
- The model is a *hyperplane* in the D + 1-dimensional space.

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#### Fitting methods:

- 1. Numeric optimization of J(w, T):
  - Works as for simple regression, it only searches a space with more dimensions.
  - Sometimes one needs to tune some parameters of the optimization algorithm to work properly (learning rate in gradient descent, etc.).
  - May be slow (many iterations needed), but works even for very large *D*.
  - 2. Normal equation:
    - $\boldsymbol{w}^* = (\boldsymbol{X}^T \boldsymbol{X})^{-1} \boldsymbol{X}^T \boldsymbol{y}$
    - Method to solve for the optimal  $w^*$  analytically!
    - No need to choose optimization algorithm parameters.
    - No iterations.
    - Needs to compute  $(X^T X)^{-1}$ , which is  $O(D^3)$ . Slow, or intractable, for large *D*.

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# **Linear classification**



Linear classification • Binary class.

• Naive approach

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hyperplane

Summary

## **Binary classification task (dichotomy)**

Let's have the training dataset  $T = \{(x^{(1)}, y^{(1)}), \dots, (x^{(|T|)}, y^{(|T|)})\}$ :

- each example is described by a vector of features  $x = (x_1, ..., x_D)$ ,
- each example is labeled with the correct class  $y \in \{+1, -1\}$ .

**Discrimination function:** a function allowing us to *decide* to which class an example *x* belongs.

- For 2 classes, 1 discrimination function is enough.
- Decision rule:

$$\begin{cases} f(\mathbf{x}) > 0 \iff \widehat{y} = +1 \\ f(\mathbf{x}) < 0 \iff \widehat{y} = -1 \end{cases}$$
 i.e.  $\widehat{y} = \operatorname{sign}(f(\mathbf{x}))$ 

**Decision boundary:**  $\{x : f(x) = 0\}$ 

*Learning* then amounts to finding (parameters of) function *f*.







## Naive approach

**Problem:** Learn a linear discrimination function *f* from data *T*.

Linear regression

Linear classification

• Binary class.

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Linear classification • Binary class. • Naive approach

## Naive approach

**Problem:** Learn a linear discrimination function f from data T.

Naive solution: fit linear regression model to the data!

Use cost function

$$J_{MSE}(w,T) = \frac{1}{|T|} \sum_{i=1}^{|T|} \left( y^{(i)} - f(w, x^{(i)}) \right)^2,$$

Optimal separating hyperplane

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minimize it with respect to w,

and use  $\widehat{y} = \operatorname{sign}(f(x))$ .

I Issue: Points far away from the decision boundary have *huge effect* on the model!



Linear classificationBinary class.Naive approach

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- minimize it with respect to w,
- and use  $\widehat{y} = \operatorname{sign}(f(x))$ .
- Issue: Points far away from the decision boundary have *huge effect* on the model!

**Better solution:** fit a linear discrimination function which minimizes the number of errors!

2

Cost function:

$$J_{01}(\boldsymbol{w},T) = \frac{1}{|T|} \sum_{i=1}^{|T|} \mathbb{I}(y^{(i)} \neq \hat{y}^{(i)}),$$

where  $\mathbb{I}$  is the indicator function:  $\mathbb{I}(a)$  returns 1 iff *a* is True, 0 otherwise.

■ The cost function is non-smooth, contains plateaus, not easy to optimize, but there are algorithms which attempt to solve it, e.g. perceptron, Kozinec's algorithm, etc.



# Perceptron



Linear classification

## **Perceptron algorithm**

Perceptron [Ros62]:

- a simple model of a neuron
- a linear classifier (in this case, a classifier with a linear discrimination function)

Perceptron			
<ul><li>Algorithm</li><li>Demo</li></ul>		Algorithm 1: Perceptron algorithm	
<ul><li>Features</li><li>Result</li></ul>		<b>Input:</b> Linearly separable training dataset: $\{x^{(i)}, y^{(i)}\}, x^{(i)} \in \mathbb{R}^{D+1}$ (homogeneous coordinates), $y^{(i)} \in \{+1, -1\}$	
Logistic regression		<b>Output:</b> Weight vector $w$ such that $x^{(i)}w^T > 0$ iff $y^{(i)} = +1$ and $x^{(i)}w^T < 0$ iff $y^{(i)} = -1$	
Optimal separating hyperplane	1 2	<b>begin</b>   Initialize the weight vector, e.g. $w = 0$ .	
Summary	3	Invert all examples <i>x</i> belonging to class -1: $x^{(i)} = -x^{(i)}$ for all <i>i</i> , where $y^{(i)} = -1$ .	
	4	Find an incorrectly classified training vector, i.e. find <i>j</i> such that $\mathbf{x}^{(j)}\mathbf{w}^T \leq 0$ , e.g. the worst classified vector: $\mathbf{x}^{(j)} = \operatorname{argmin}_{\mathbf{x}^{(i)}} (\mathbf{x}^{(i)}\mathbf{w}^T)$ .	
	5	if all examples classified correctly then	
	6	Return the solution <i>w</i> . Terminate.	
	7	else	
	8	Update the weight vector: $w = w + x^{(j)}$ .	
	9	Go to 4.	

Instead of using the worst classified point, the algorithm may go over the training set (several times) and use all encountered wrongly classified points to update w.

Frank Rosenblatt. Principles of Neurodynamics: Perceptron and the Theory of Brain Mechanisms. Spartan Books, Washington, D.C., 1962. [Ros62]



#### **Demo: Perceptron**



1.2



Perceptron
 Algorithm

DemoFeatures

Result

hyperplane

Summary

Logistic regression

Optimal separating

Linear classification

## Features of the perceptron algorithm

Perceptron convergence theorem [Nov62]:

- Perceptron algorithm eventually finds a hyperplane that separates 2 classes of points in a finite number of steps, if such a hyperplane exists.
  - If no separating hyperplane exists, the algorithm does not converge and will iterate forever.
- Possible solutions:
- Pocket algorithm track the error the perceptron makes in each iteration and store the best weights found so far in a separate memory (pocket).
  - Use a different learning algorithm, which finds an approximate solution, if the classes are not linearly separable.



## The hyperplane found by perceptron

#### The perceptron algorithm

finds a separating hyperplane, if it exists;

Linear regression

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Perceptron

- Algorithm
- Demo
- Features
- Result

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Optimal separating hyperplane

Summary





■ and perceptron finds *any* of them!

Which separating hyperplane is the optimal one? What does "optimal" actually mean?



# **Logistic regression**



#### Logistic regression model

have a huge impact on *f*. How to limit their influence?

**Problem:** Learn a binary classifier for the dataset  $T = \{(x^{(i)}, y^{(i)})\}$ , where  $y^{(i)} \in \{0, 1\}$ .<sup>1</sup>

To reiterate: when using linear regression, the examples far from the decision boundary

Linear regression

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Model

• Cost function

Optimal separating hyperplane



### Logistic regression model

**Problem:** Learn a binary classifier for the dataset  $T = \{(x^{(i)}, y^{(i)})\}$ , where  $y^{(i)} \in \{0, 1\}$ .<sup>1</sup>

Linear regression
Linear classification

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Logistic regression

• Model

• Cost function

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Summary

To reiterate: when using linear regression, the examples far from the decision boundary have a huge impact on f. How to limit their influence?

**Logistic regression** uses a discrimination function which is a nonlinear transformation of the values of a linear function

$$f_{\boldsymbol{w}}(\boldsymbol{x}) = g(\boldsymbol{x}\boldsymbol{w}^T) = \frac{1}{1 + e^{-\boldsymbol{x}\boldsymbol{w}^T}},$$

where  $g(z) = \frac{1}{1 + e^{-z}}$  is the **sigmoid** function (a.k.a **logistic** function).



## Logistic regression model

**Problem:** Learn a binary classifier for the dataset  $T = \{(x^{(i)}, y^{(i)})\}$ , where  $y^{(i)} \in \{0, 1\}$ .<sup>1</sup>

Linear regression

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where  $g(z) = \frac{1}{1 + e^{-z}}$  is the **sigmoid** function (a.k.a **logistic** function).

#### Interpretation of the model:

- $f_w(x)$  is interpretted as an estimate of the probability that *x* belongs to class 1.
- The decision boundary is defined using a different level-set:  $\{x : f_w(x) = 0.5\}$ .
- Logistic *regression* is a *classification model*!
- The discrimination function  $f_w(x)$  itself is not linear anymore; but the *decision boundary is still linear*!
- Thanks to the sigmoidal transformation, logistic regression is much less influenced by examples far from the decision boundary!

<sup>&</sup>lt;sup>1</sup>Previously, we have used  $y^{(i)} \in \{-1, +1\}$ , but the values can be chosen arbitrarily, and  $\{0, 1\}$  is convenient for logistic regression.



### **Cost function**

To train the logistic regression model, one can use the  $J_{MSE}$  criterion:

However, this results in a non-convex multimodal landscape which is hard to optimize.

 $J(w,T) = \frac{1}{|T|} \sum_{i=1}^{|T|} \left( y^{(i)} - f_w(x^{(i)}) \right)^2.$ 

Linear regression

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## **Cost function**

To train the logistic regression model, one can use the  $J_{MSE}$  criterion:

However, this results in a non-convex multimodal landscape which is hard to optimize.

Logistic regression uses a modified cost function (sometimes called *cross-entropy*):

$$J(w,T) = \frac{1}{|T|} \sum_{i=1}^{|T|} \left( y^{(i)} - f_w(x^{(i)}) \right)^2.$$

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$$J(\boldsymbol{w},T) = \frac{1}{|T|} \sum_{i=1}^{|T|} \operatorname{cost}(y^{(i)}, f_{\boldsymbol{w}}(\boldsymbol{x}^{(i)})), \text{ where}$$
$$\operatorname{cost}(y,\widehat{y}) = \begin{cases} -\log(\widehat{y}) & \text{if } y = 1\\ -\log(1-\widehat{y}) & \text{if } y = 0 \end{cases},$$

which can be rewritten in a single expression as

$$\operatorname{cost}(y,\widehat{y}) = -y\log(\widehat{y}) - (1-y)\log(1-\widehat{y}).$$

#### Such a cost function is simpler to optimize for numerical solvers.



# **Optimal separating hyperplane**

## **Optimal separating hyperplane (separable case)**

#### Margin (cz:odstup):

"The width of the band in which the decision boundary can move (in the direction of its normal vector) without touching any data point."

#### Maximum margin linear classifier



Plus 1 level:  $\{x : xw^T + w_0 = 1\}$ Minus 1 level:  $\{x : xw^T + w_0 = -1\}$ Decision boundary (separating hyperplane):  $\{x : xw^T + w_0 = 0\}$ 

#### Support vectors:

- Data points *x* lying at the plus 1 level or minus 1 level.
- Only these points influence the decision boundary!

Why we would like to maximize the margin?

- Intuitively, it is safe.
- If we make a small error in estimating the boundary, the classification will likely stay correct.
- The model is invariant with respect to the training set changes, except the changes of support vectors.
- There are sound theoretical results that having a maximum margin classifier is good.
- Maximal margin works well in practice.



#### Margin size

We know that:

Linear regression

Linear classification

Perceptron

Logistic regression

Optimal separating hyperplane

- Optimal SH
- Margin size
- OSH learning
- Non-separable case
- OSH learning (2)
- OSH: remarks

• Demo

Summary





$$M = \|x^{+} - x^{-}\| = \|\lambda w\| = \lambda \|w\| = \frac{2}{\|w\|^{2}} \|w\| = \frac{2}{\|w\|}$$

How to compute the margin *M* given  $w = (w_1, ..., w_D)$ ,  $w_0$  of certain sep. hyperplane?

- Let's choose two points  $x^+$  and  $x^-$ , lying in the plus 1 level and minus 1 level, respectively.
- Let's compute the margin *M* as their distance.



And we can derive:

$$(x^{+} - x^{-})w^{T} = 2$$
$$(x^{-} + \lambda w - x^{-})w^{T} = 2$$
$$\lambda ww^{T} = 2$$
$$\lambda = \frac{2}{ww^{T}} = \frac{2}{\|w\|^{2}}$$



## **Optimal separating hyperplane learning**

We want to maximize margin  $M = \frac{2}{\|w\|}$  subject to the constraints ensuring correct classification of the training set *T*. This optimization problem can be formulated as a *quadratic programming* (QP) task.

Linear regression

Linear classification

Perceptron

Logistic regression

Optimal separating hyperplane

- Optimal SH
- Margin size
- OSH learning
- Non-separable case
- OSH learning (2)
- OSH: remarks
- Demo



Linear classification

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Summary

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Primary QP task:

minimize  $ww^T$  with respect to  $w_0, \ldots, w_D$ 

subject to 
$$y^{(i)}(\mathbf{x}^{(i)}\mathbf{w}^T + w_0) \ge 1 \quad \forall i \in 1, \dots, |T|.$$



Perceptron

hyperplane • Optimal SH • Margin size

Linear classification

Logistic regression

Optimal separating

## **Optimal separating hyperplane learning**

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Summary

Dual QP task:

maximize 
$$\sum_{i=1}^{|T|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|T|} \sum_{j=1}^{|T|} \alpha_i \alpha_j y^{(i)} y^{(j)} x^{(i)} x^{(j)^T}$$
 with respect to  $\alpha_1, \ldots, \alpha_{|T|}$ 

subject to  $\alpha_i \ge 0$ 

and 
$$\sum_{i=1}^{|T|} \alpha_i y^{(i)} = 0.$$



Perceptron

hyperplane

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Summary

Dual QP task:

maximize  $\sum_{i=1}^{|I|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|I|} \sum_{i=1}^{|I|} \alpha_i \alpha_j y^{(i)} y^{(j)} x^{(i)} x^{(j)^T}$  with respect to  $\alpha_1, ..., \alpha_{|T|}$ 

subject to 
$$\alpha_i \ge 0$$
  
and  $\sum_{i=1}^{|T|} \alpha_i y^{(i)} = 0$ 

From the solution of the dual task, we can compute the solution of the primal task:

where  $(x^{(k)}, y^{(k)})$  is any *support vector*, i.e.  $\alpha_k > 0$ .



#### Non-separable case

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Summary

**Soft margin:** Allows for incorrect classification of some data points.

**Slack variables**  $\xi_i$ : The shortest distances of data points to their correct "place":

0 for correctly classified data "outside the margin",

positive for incorrectly classified data and data "inside the margin".



Primary QP task with slack variables:

minimize 
$$(ww^T + C\sum_{i=1}^{|T|} \xi_i)$$
 with respect to  $w_0, \dots, w_D, \xi_1, \dots, \xi_{|T|}$   
subject to  $y^{(i)}(x^{(i)}w^T + w_0) \ge 1 - \xi_i \quad \forall i \in 1, \dots, |T|,$   
and  $\xi_i \ge 0 \quad \forall i \in 1, \dots, |T|.$ 

Primary QP task with slack variables:

minimize 
$$(ww^T + C\sum_{i=1}^{|T|} \xi_i)$$
 with respect to  $w_0, \dots, w_D, \xi_1, \dots, \xi_{|T|}$   
subject to  $y^{(i)}(x^{(i)}w^T + w_0) \ge 1 - \xi_i \quad \forall i \in 1, \dots, |T|,$   
and  $\xi_i \ge 0 \quad \forall i \in 1, \dots, |T|.$ 

Dual QP task:

maximize 
$$\sum_{i=1}^{|T|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|T|} \sum_{j=1}^{|T|} \alpha_i \alpha_j y^{(i)} y^{(j)} x^{(i)} x^{(j)^T}$$
 with respect to  $\alpha_1, \dots, \alpha_{|T|}, \mu_1, \dots, \mu_{|T|}$ , subject to  $\alpha_i \ge 0$ ,  $\mu_i \ge 0$ ,  $\alpha_i + \mu_i = C$ ,  
and 
$$\sum_{i=1}^{|T|} \alpha_i y^{(i)} = 0.$$

Primary QP task with slack variables:

minimize 
$$(ww^T + C\sum_{i=1}^{|T|} \xi_i)$$
 with respect to  $w_0, \dots, w_D, \xi_1, \dots, \xi_{|T|}$   
subject to  $y^{(i)}(x^{(i)}w^T + w_0) \ge 1 - \xi_i \quad \forall i \in 1, \dots, |T|,$   
and  $\xi_i \ge 0 \quad \forall i \in 1, \dots, |T|.$ 

Dual QP task:

maximize 
$$\sum_{i=1}^{|T|} \alpha_i - \frac{1}{2} \sum_{i=1}^{|T|} \sum_{j=1}^{|T|} \alpha_i \alpha_j y^{(i)} x^{(i)} x^{(j)^T}$$
 with respect to  $\alpha_1, \dots, \alpha_{|T|}, \mu_1, \dots, \mu_{|T|},$   
subject to  $\alpha_i \ge 0$ ,  $\mu_i \ge 0$ ,  $\alpha_i + \mu_i = C$ ,  
and 
$$\sum_{i=1}^{|T|} \alpha_i y^{(i)} = 0.$$

Variables  $\alpha_i$  are more constrained than in the separable case, but the solution is the same:

$$\boldsymbol{w} = \sum_{i=1}^{|T|} \alpha_i y^{(i)} \boldsymbol{x}^{(i)}, \qquad \qquad \boldsymbol{w}_0 = y^{(k)} - \boldsymbol{x}^{(k)} \boldsymbol{w}^T,$$

where  $(\mathbf{x}^{(k)}, \mathbf{y}^{(k)})$  is any *support vector*, i.e.  $\alpha_k > 0$ .



Perceptron

hyperplaneOptimal SH

• Demo

Summarv

Margin sizeOSH learning

• Non-separable case

OSH learning (2)OSH: remarks

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Optimal separating

#### The importance of dual formulation:

- The QP task in dual formulation is easier to solve for QP solvers than the primal formulation.
  - New, unseen examples can be classified using function

$$f(\boldsymbol{x}, \boldsymbol{w}, w_0) = \operatorname{sign}(\boldsymbol{x}\boldsymbol{w}^T + w_0) = \operatorname{sign}\left(\sum_{i=1}^{|T|} \alpha_i \boldsymbol{y}^{(i)} \boldsymbol{x}^{(i)} \boldsymbol{x}^T + w_0\right),$$

i.e. the discrimination function contains the examples *x* only in the form of dot products (which will be useful later).

- The examples with  $\alpha_i > 0$  are *support vectors*, thus the sums may be carried out only over the support vectors.
- The dual formulation contains the data only in the form of dot products which allows for other tricks you will learn later.
- The primal task with soft margin has double the number of constraints, the task is more complex, but
- the results for the QP task with soft margin are of the same type as in the separable case.



#### **Optimal separating hyperplane: demo**







#### Competencies

After this lecture, a student shall be able to ...

- define and recognize linear regression model (with scalar parameters, in scalar product form, in matrix form, non-homogenous and homogenous coordinates);
- define the loss function suitable for fitting a regression model;
- explain the least squares metod, draw an illustration;
- compute coefficients of simple (1D) linear regression by hand, write a computer program computing coefficients for multiple regression;
- explain the concept of discrimination function for binary and multinomial classification;
- define a loss function suitable for fitting a classification model;
- describe a perceptron algorithm, perform a few iterations by hand;
- explain the characteristics of perceptron algorithm;
- describe logistic regression, the interpretation of its outputs, and why we classify it as a linear model;
- define loss functions suitable for fitting logistic regression;
- define optimal separating hyperplane, explain in what sense it is optimal;
- define what a margin is, what support vectors are, and explain their relation;
- compute the margin given the parameters of separating hyperplane for which  $\min_{i:y^{(i)}=+1}(x^{(i)}w^T + w_0) = 1$  and  $\max_{i:y^{(i)}=-1}(x^{(i)}w^T + w_0) = -1$ ;
- formulate the primary quadratic programming task which results in the optimal separating hyperplane (including the soft-margin version);
- compute the parameters of optimal hyperplane given the set of support vectors and their weights.