Linear models

Alessio Micheli

micheli@di.unipi.it

Dipartimento di Informatica
Università di Pisa - Italy

Computational Intelligence &
Machine Learning Group

Sept, 2025

ML Course structure
Where we go

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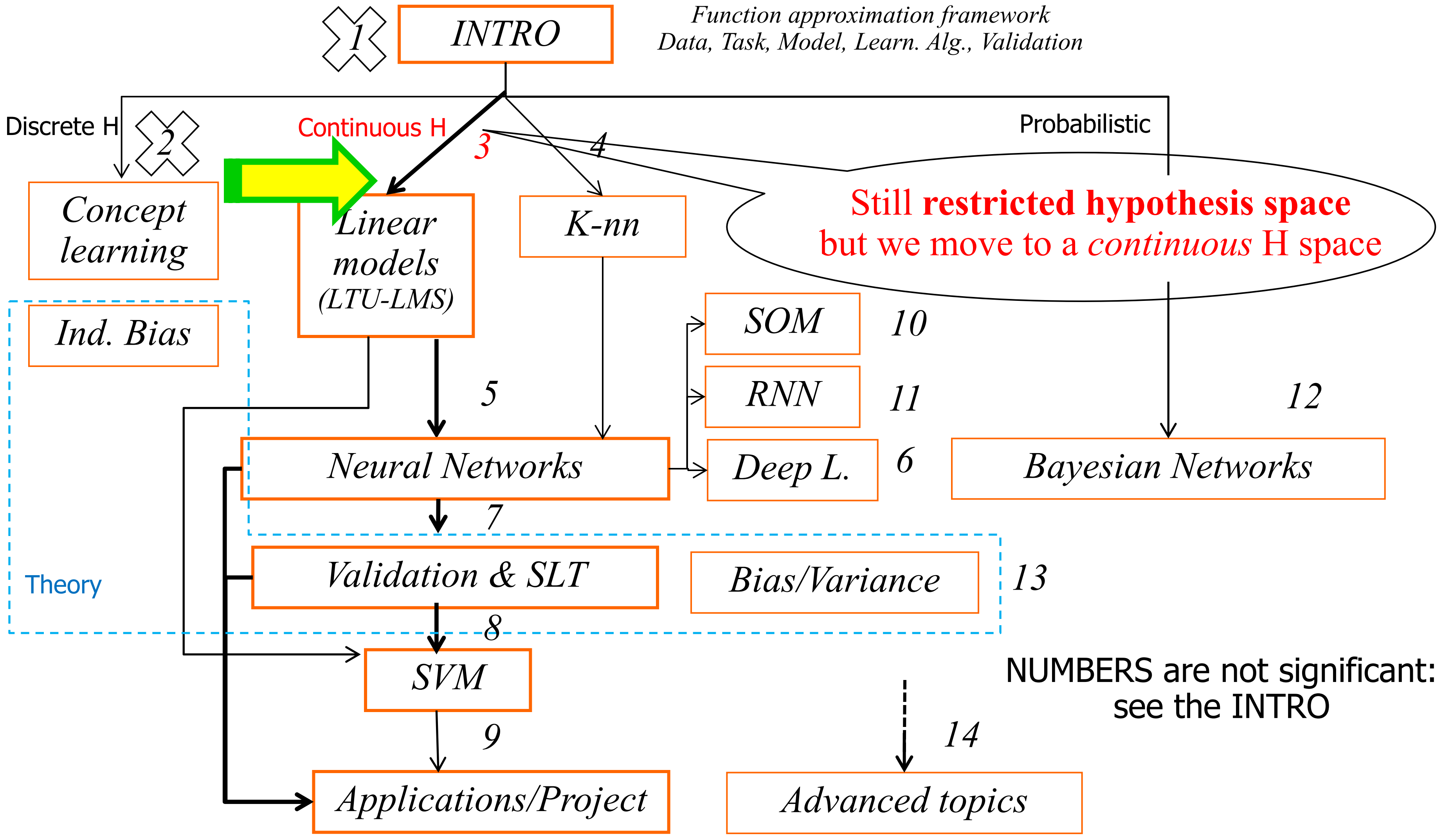
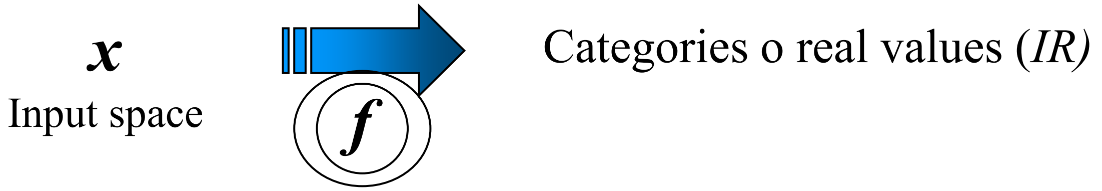


NUMBERS are not significant:
see the INTRO

Tasks: Supervised Learning

- Given: Training examples as <*input,output*>=($\mathbf{x}$,*d*) (***labeled* examples**) for an unknown function *f* (known only at the given points of example)
  - Target value: desiderate value *d* or *t* or *y* … is given by the teacher according to *f*($\mathbf{x}$).
- Find: A *good* approximation to *f* (a hypothesis *h* that can used for prediction on unseen data *x'*, i.e. that is able to generalize)



- Target *d* (or *t or y*): a categorical or numerical *label*
  - ***Classification:*** discrete value outputs:
    $f(\mathbf{x}) \in \{1,2,\dots,K\}$ *classes (discrete-valued function*)
  - ***Regression:*** real continuous output values (approximate a real-valued target function)

Both as a *task of function approximation*

A premise on DATA notation

Pattern	x_1	x_2	x_i	x_n
Pat 1	$x_{1,1}$	$x_{1,2}$		$x_{1,n}$
…				
Pat *p*	$x_{p,1}$	$x_{p,2}$	$\boxed{x_{p,i}}$	$x_{p,n}$
…				

$\boldsymbol{X}$ is a matrix $\boldsymbol{l} \times \boldsymbol{n}$

$\boldsymbol{l}$ rows, $\boldsymbol{n}$ columns

$p=1..l, \quad i=1..n$

We often need to omit some indices when the context is clear, e.g.:

- Each row, generic $\boldsymbol{x}$ (vector - bold), a raw in the table: (input) example, pattern, instance, sample ,…, input vector, …
- x_i or x_j (scalar): component *i* or *j* (given a pattern $\boldsymbol{x}$, i.e. omitting p)
- $\boldsymbol{x}_p$ or $\boldsymbol{x}_i$ (vector – bold) *p-th* or *i-th* raw in the table = pattern p or *i*
- $\boxed{x_{p,i}}$ (scalar) also as $(\boldsymbol{x}_p)_i$: component *i* of the pattern p
  or also, often, $\boldsymbol{x}_{p,j}$ for the component j, etc.
- For the target y we will typically use just y_p with $p=1..l$ (the same for *d* or *t*)

Linear models

- Regression
- Classification

Linear models

The linear model has been the mainstay of statistics

- "*Despite the great inroads made by modern nonparametric regression techniques, linear models remain important, and so we need to understand them well*". (Hastie)

Plenty of studies and in many books (mathematics, statistics, numerical analysis, applicative fields, ML, …)

- We start with the simplest form, linear in the input variables
- A baseline for learning (first: is it a linear problem?)

Regression

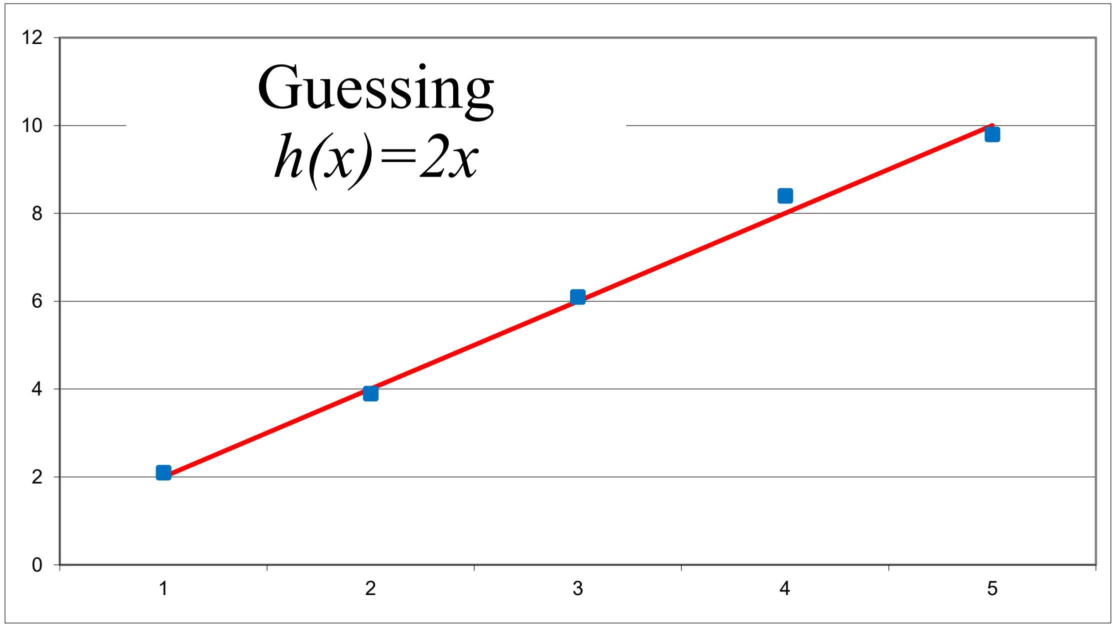
- **Just to see how formulate the *learning problem* as a LMS on the R_{emp}**
  - Then (next lecture) we will consider also the control of complexity
- **We formulate a first derivation in a simplified setting (univariate case)**

Repetita: regression: example

- Process of estimating of a real-value function on the basis of a finite set of noisy samples
  - known pairs$(x\ ,\ f(x){+}random\ noise)$

Task (exercise): find f for the data in the following table:

x	$target$
1	2.1
2	3.9
3	6.1
4	8.4
5	9.8
…	…



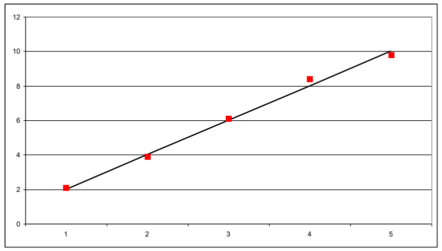
Now, we want to solve it (how to find $\boldsymbol{w}$) in a «systematic» way

Univariate Linear Regression

- Univariate case, simple linear regression :
- We start with 1 input variable x, 1 output variable y
- We assume a model $h_{\mathbf{w}}(x)$ expressed as $\boxed{out=w_1 x+w_0}$

$$\begin{tikzcd} {} \arrow[r, "x"] & \boxed{h} \arrow[r] & {} \end{tikzcd}$$

- *where* $\mathbf{w}$ *are real-valued coefficients/free parameters (weights)*
- ***Fitting*** the data by a "straight line"



- Infinite hp space (continuous w values) but we have nice solution from classical math (going back to Gauss/Legendre ~1795!)
  - Surprisingly we can "learn" by this basic tool
  - Although simple it includes many relevant concept of modern ML and it is a basis of evolved methods in the field

Build it: Learning via LMS (I)

- Training → find $\boldsymbol{w}$ such that minimize **error**/empirical **loss** (best data fitting – on the training set with l examples): i.e. we are now focusing on the R_{emp}
- **Given** a set of l training examples $(\boldsymbol{x}_p, y_p)$ $p=1..l$
- **Find**: $h_w(x)$ in the form w_1x+w_0 (hence the values of $\boldsymbol{w}$) that minimizes the expected loss on the training data.

- For the loss we use the square of errors:
- Least (Mean) Square: Find $\boldsymbol{w}$ to *minimize* the residual sum of squares $[argmin_{\mathbf{w}}\ Error(\mathbf{w})\ in\ L_2]$:

p runs over patterns/examples

$$Loss(h_{\mathbf{w}}) = E(\boldsymbol{w}) = \sum_{p=1}^{l} (y_p - h_{\mathbf{w}}(x_p))^2 = \sum_{p=1}^{l} (y_p - (w_1 x_p + w_0))^2$$

where x_p is p-th input/pattern/example, y_p the output for p, w free par., l num. of examples

Note: to have the mean divide by l

On the notation: Indeed for the univariate case, with 1 variable: $x_p = x_{p,1} = (\boldsymbol{x}_p)_1$

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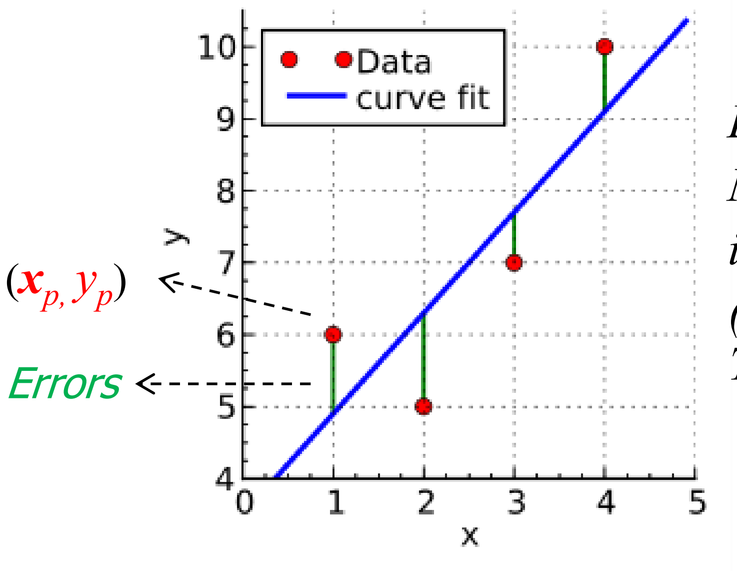
Build it: Learning via LMS (II)

Why LMS to fit the data with *h* ?

- Least (Mean) Square: Find $\boldsymbol{w}$ to *minimize* the residual sum of squares $\left[argmin_{\mathbf{w}}\ Error(\mathbf{w})\ in\ L_2 \right]$:

$$\boxed{h_{\mathbf{w}}(x)}$$

$$y = w_1 x + w_0 + noise$$



Different blue lines will have different green bars.
Minimizing the green bars (residuals /errors)
is a way to find the best approximation/fitting of the data
(i.e. our $h_{\mathbf{w}}(x)$ or blue line).
*The squares of errors E(**w**) quantify such green bars:*

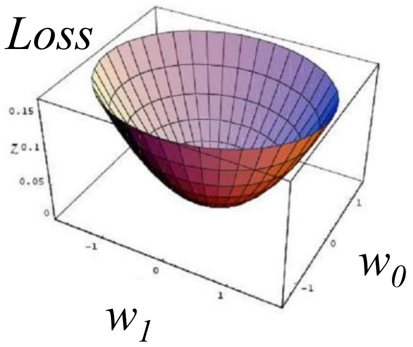
$$E(\mathbf{w}) = \sum_{p=1}^{l} \left(y_p - h_{\mathbf{w}}(x_p) \right)^2$$

- The method of **least squares** is a standard approach to the approximate solution of over-determined systems, i.e., sets of equations in which there are more equations than unknowns.

How to solve?

- Remember: local minimum as stationary point: the gradient is zero

$$\frac{\partial E(\mathbf{w})}{\partial w_i} = 0, \qquad i = 1,\dots,\mathrm{dim\_}input + 1 = 1,\dots,n+1$$



- For the simple Lin. Regr. (2 free parameters)

Search the w such that $\dfrac{\partial E(\mathbf{w})}{\partial w_0} = 0 \quad \dfrac{\partial E(\mathbf{w})}{\partial w_1} = 0$

Convex loss function → *we have the following solution (no local minima)*

(just to know that it exists!)

$$\boxed{w_1 = \frac{\sum x_p y_p - \frac{1}{l}\sum x_p \sum y_p}{\sum\limits_{p:1\to l} x_p^2 - \frac{1}{l}(\sum x_p)^2}} = \frac{\mathrm{Cov}[x,y]}{\mathrm{Var}[x]}, \quad \boxed{w_0 = \bar{y} - w_1 \bar{x}}$$

$$\bar{y} = \frac{1}{l}\sum_{p\to l} y_p \qquad \bar{x} = \frac{1}{l}\sum_{p\to l} x_p$$

Exercise: *compute w_0 and w_1 according to the next slide results for the gradient (extended to l patterns)*

Compute the gradient for 1 (each) pattern *p*

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Redo this by yourself as an *Exercise*

Basic rules:

$$\frac{\partial}{\partial w} k = 0, \frac{\partial}{\partial w} w = 1, \frac{\partial}{\partial w} w^2 = 2w$$

$$\frac{\partial (f(w))^2}{\partial w} = 2 f(w) \frac{\partial (f(w))}{\partial w}$$

Der. sum = sum of der.

We will call (y-$h(x)$) "delta"

$$\frac{\partial E(\mathbf{w})}{\partial w_i} = \frac{\partial (y - h_{\mathbf{w}}(x))^2}{\partial w_i} =$$

$$= 2(y - h_{\mathbf{w}}(x)) \frac{\partial (y - h_{\mathbf{w}}(x))}{\partial w_i} = 2(y - h_{\mathbf{w}}(x)) \frac{\partial (y - (w_1 x + w_0))}{\partial w_i}$$

$$\boxed{\frac{\partial E(\mathbf{w})}{\partial w_0} = -2(y - h_{\mathbf{w}}(x))} \qquad \boxed{\frac{\partial E(\mathbf{w})}{\partial w_1} = -2(y - h_{\mathbf{w}}(x)) \cdot x}$$

Then we will sum up for l patterns (x_p, y_p) …

And we will extend to multidimensional $\boldsymbol{x}$ and $\boldsymbol{w}$ *(n=1 here)* …

Linear model: notation for multidimensional inputs

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- Assuming column vector for $\boldsymbol{x}$ and $\boldsymbol{w}$ *(in bold)*
- Number of data l, dimension of input vector n, y_p *(targets)* $p=1..l$

d_p or t_p

$$\boldsymbol{w}^T\boldsymbol{x} + w_0 = w_0 + w_1x_1 + w_2x_2 + \cdots + w_nx_n = w_0 + \sum_{i=1}^{n} w_ix_i \qquad \text{(eq. 1)}$$

- Note that sometimes (in NN) the transpose notation T in $\boldsymbol{w}^T$ is omitted

- w_0 is the *intercept, threshold, bias, offset.....*

Often it is convenient to include the constant $x_0 = 1$ so that we can write eq.1 as :

$$\boldsymbol{w}^T\boldsymbol{x} = \boxed{\boldsymbol{x}^T\boldsymbol{w}}$$

Inner product

$$\boldsymbol{x}^T = [1, x_1, x_2, \ldots, x_n]$$

$$\boldsymbol{w}^T = [w_0, w_1, w_2, \ldots, w_n]$$

So, the "linear "model can be written as a function that for each $\boldsymbol{x}_p$ compute:

$$h(\boldsymbol{x}_p) = \boldsymbol{x}_p{}^T\boldsymbol{w} = \sum_{i=0}^{n} x_{p,i}\, w_i$$

***w*: continuous (free) parameters: "weights"**

Learning algorithm: just wait!

- For the learning algorithm in the multidimensional case for linear regression: please wait.
- We will provide it along with the learning algorithm of the linear classifier in the next few slides.

Summing up:

- Given the data set and the linear model, we can state the learning problem as LMS problem
- Once we find the best $\boldsymbol{w}$ parameters values, we have our $h_{\boldsymbol{w}}(x)$ for regression purposes

- For students that need a soft intro to just LMS Regression:
  - https://svivek.com/teaching/machine-learning/lectures/slides/linear-models/lms-regression.pdf

Classification

What we are looking at

1. The classification by hyperplanes

2. See how the model works after training ("use it" slides)

3. How to state/formulate a (regression)/classification learning problem for a linear model by LMS

4. How to derive the learning algorithm

5. Proposing two learning algorithms to build a linear classifier

Problem: example

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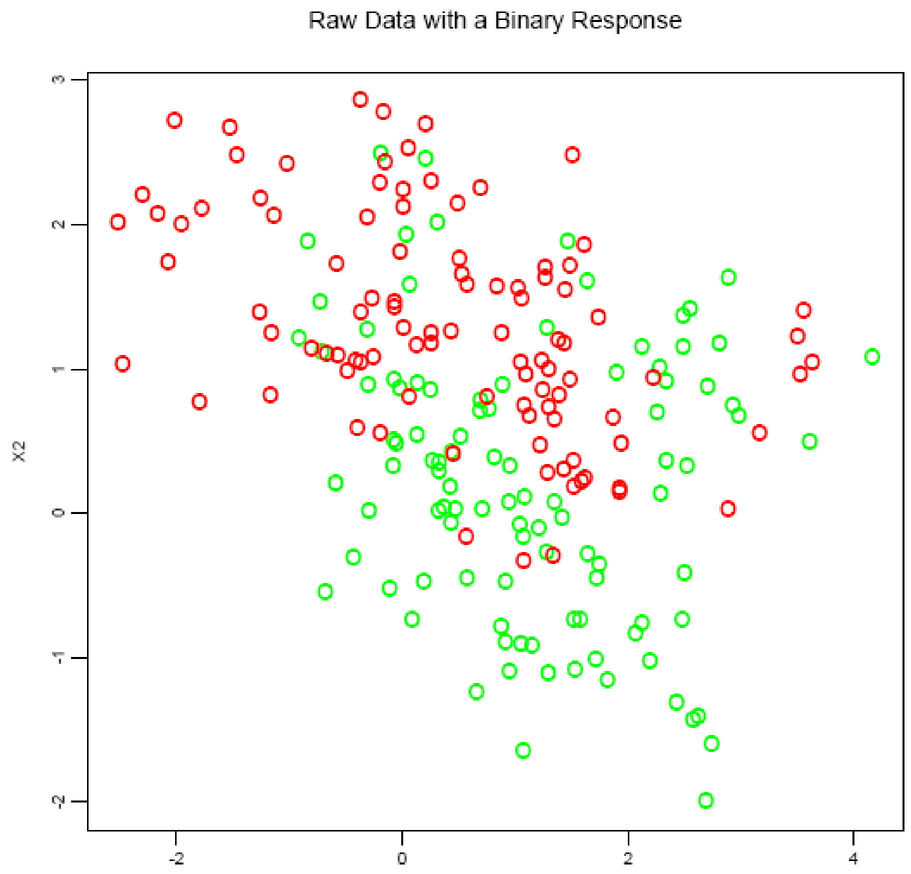

200 points generated in IR^2 from an unknown distribution; 100 in each of two classes.

Can we build a rule to predict the color of future points?

Data may be generated by gaussian distribution (for each class) with different means

or by a mixture of different low variance gaussian distributions.

We reuse the linear model

- The same models (used for regression) can be used for **classification**: categorical targets (*y* or *d*), **e.g. 0/1 or -1/+1.**

  - In this case we use a hyperplane ($\boldsymbol{w}^T\boldsymbol{x}$) assuming negative or positive values
  - We exploit such models to decide if a point $\boldsymbol{x}$ belong to positive or negative zone of the hyperplane (to classify it)
  - So we want to set $\boldsymbol{w}$ (by learning) s.t. we get good classification accuracy

Geometrical view: hyperplane

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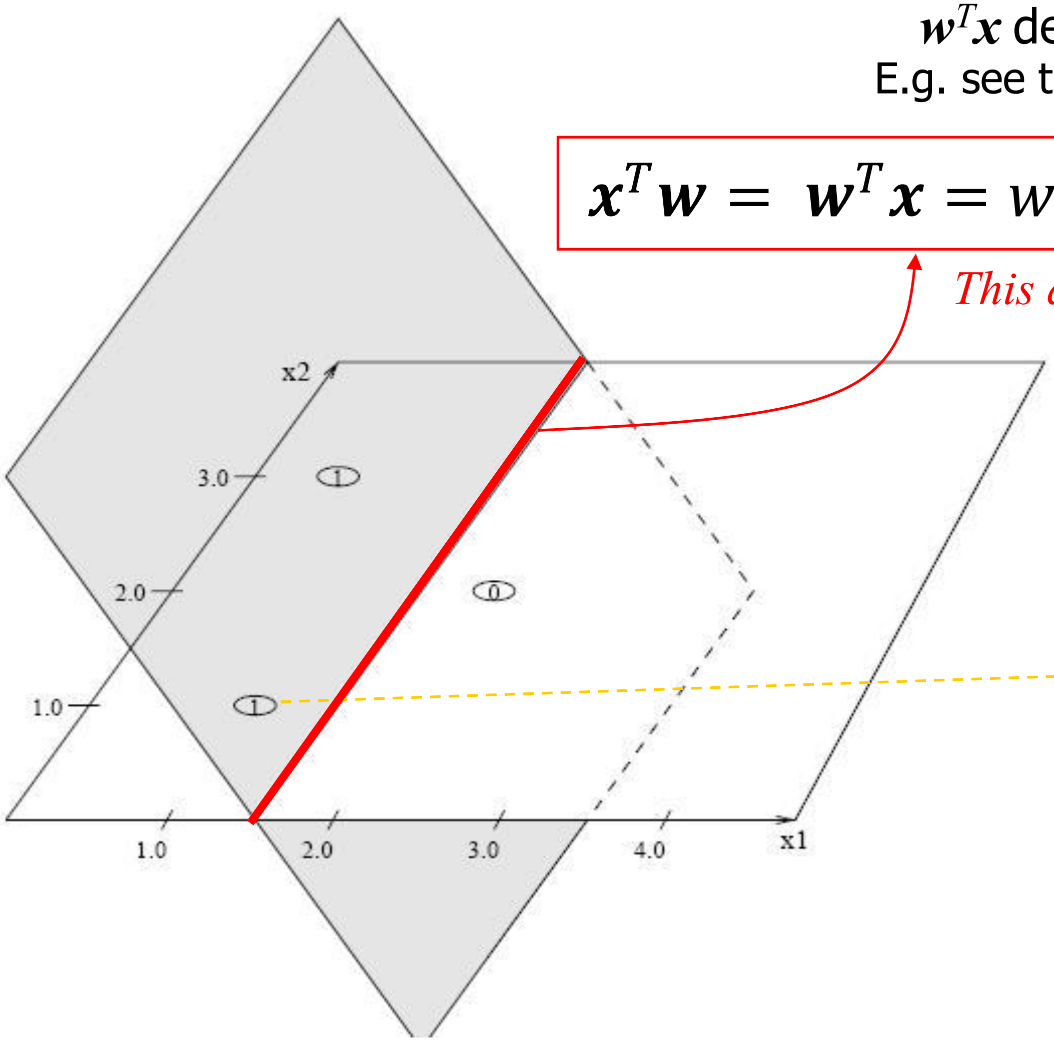
$\boldsymbol{w}^T\boldsymbol{x}$ define an hyperplane.
E.g. see the picture for 2 variables

$$\boxed{\boldsymbol{x}^T\boldsymbol{w} = \boldsymbol{w}^T\boldsymbol{x} = w_0 + w_1x_1 + w_2x_2 = 0}$$

This defines the decision boundary



Can be used to classify:

Examples <*(x*$_1$,*x*$_2$*), y*>:

<(1.0, 1.0), 1>

<(0.5, 3.0), 1>

<(2.0, 2.0), 0>

Geometrical view: classifier

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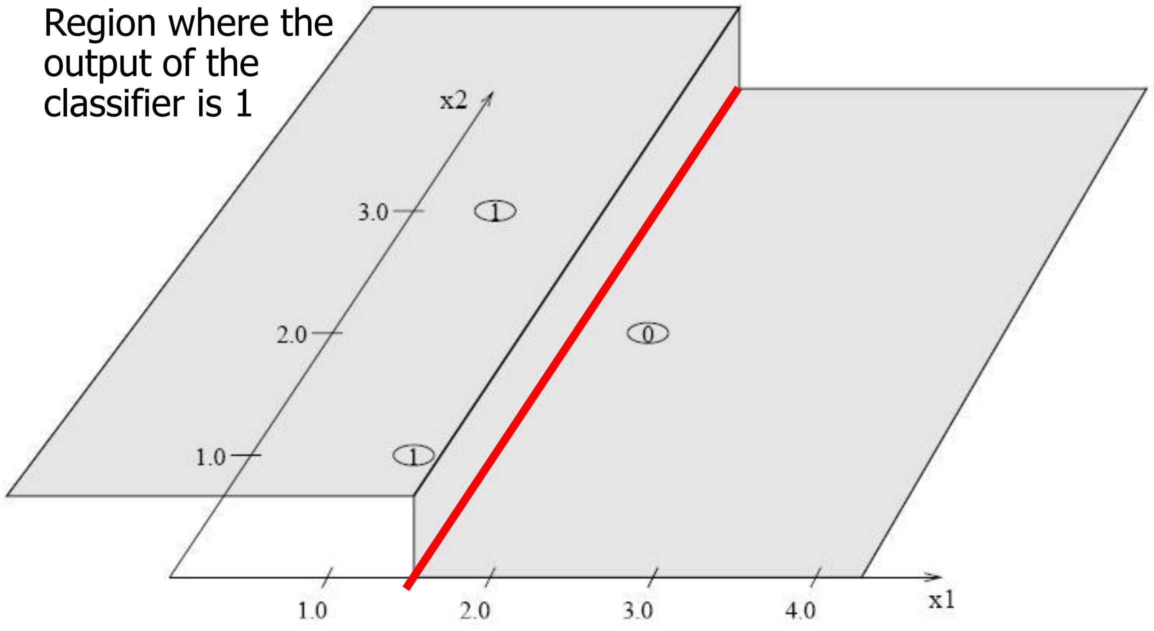
Introducing a threshold function

Region where the output of the classifier is 1



Examples:

<(1.0, 1.0), 1>

<(0.5, 3.0), 1>

<(2.0, 2.0), 0>

[0,1] output range

$$h(\boldsymbol{x}) = \begin{cases} 1 & \_if \quad \boldsymbol{w}^T\boldsymbol{x} + w_0 \geq 0 \\ 0 & \_\_\_\_\_\_otherwise \end{cases}$$

or

[-1,+1] output range

$$h(\boldsymbol{x}) = sign(\boldsymbol{w}^T\boldsymbol{x} + w_0)$$

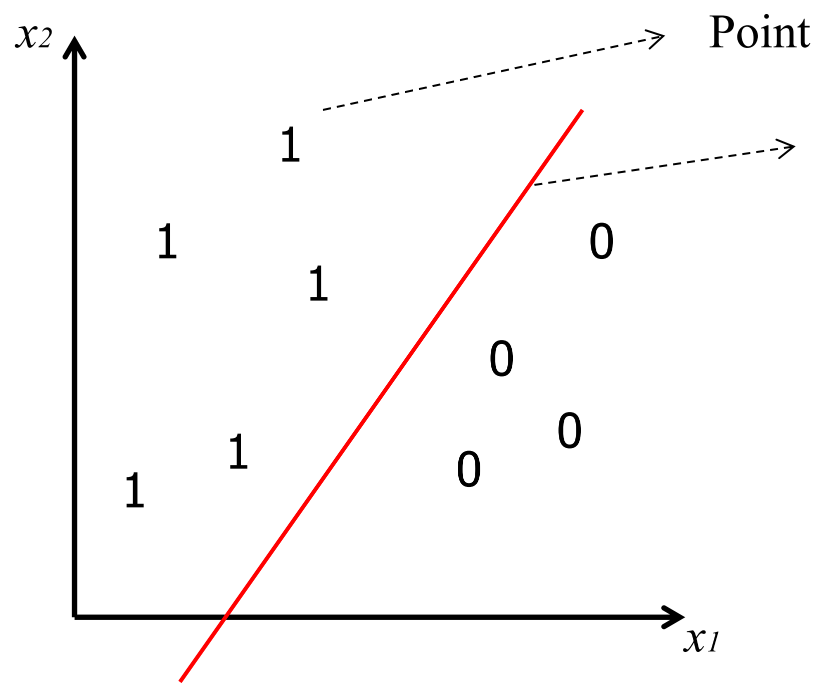
Using $\boldsymbol{x}_p$ *and including* w_0 *in* $\boldsymbol{w}$

$$h(\mathbf{x}_p) = sign(\mathbf{x}_p^T\mathbf{w}) = sign\left(\sum_{i=0}^{n} x_{p,i} w_i\right)$$

In this slide $\boldsymbol{w}$ *is omitted from* $h_{\boldsymbol{w}}$ *(we use just h)*

Classification by linear decision boundary [repetita]

The classification may be viewed as the allocation of the input space in decision regions (e.g. **0/1**)
Example: linear separator on
2-dim instance space $\boldsymbol{x}=(x_1,x_2)$ *in* IR^2, $f(\boldsymbol{x})=0/1$ (or $-1/+1$)



Point belonging to class 1

Separating (hyper)plane : $\boldsymbol{x}$ s.t.

$$\boldsymbol{w}^T\boldsymbol{x} + w_0 = w_1x_1 + w_2x_2 + w_0 = 0$$

$$\boxed{h(\boldsymbol{x}) = \begin{cases} 1 & if \quad \boldsymbol{w}^T\boldsymbol{x} + w_0 \geq 0 \\ 0 & otherwise \end{cases}}$$

[0,1]
output range

or

$$\boxed{h(\boldsymbol{x}) = sign(\boldsymbol{w}^T\boldsymbol{x} + w_0)}$$

[-1,+1]
output range

Linear threshold unit (LTU)

Indicator functions

How many? (H): set of dichotomies induced by hyperplanes

Threshold (bias w_0)

Note that, given the bias w_0, in the LTU

saying $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x} + w_0 \geq 0$

is equivalent to say $h(\mathbf{x}) = \mathbf{w}^T\mathbf{x} \geq -w_0$

with $-w_0$ as the «threshold» value

- The two forms identify the same positive zone of the classifier
- The second one emphasizes the role of the bias as a threshold value to "activate" the +1 output of the classifier.

Use it: Example (AIMA)
Classify a new data (x_1,x_2)

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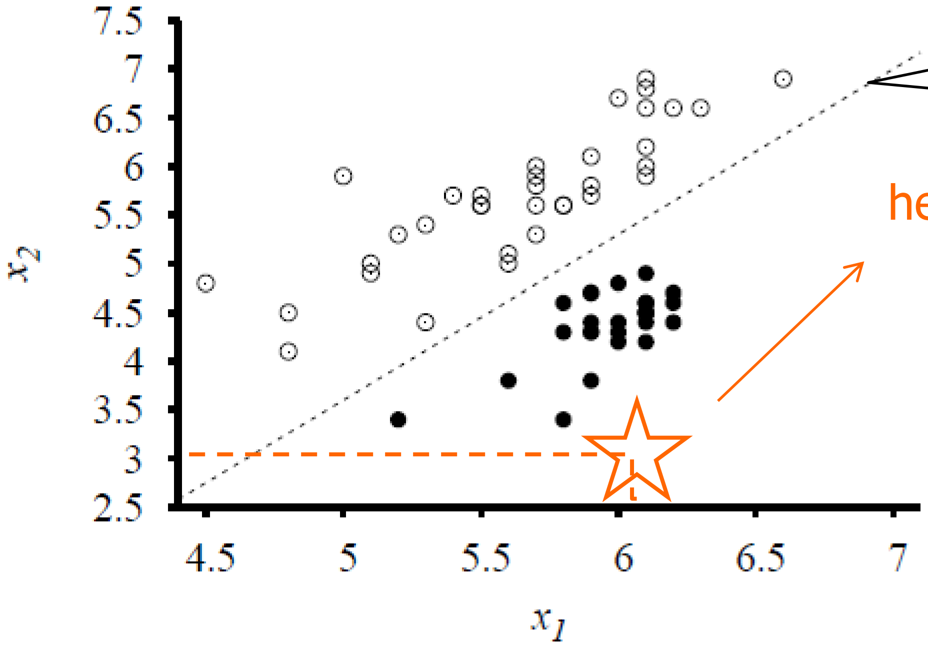
Find h s.t. given (x_1,x_2) return 0/-1 for *Earthquakes* and 1 for *Nuclear Explosion*

Some alg. finds this decision boundary:



Seismic data.

x_1 body wave magnitude, x_2 surface wave magnitude

Earthquakes (white) Nuclear Explosion (black) 1982-1990 Asia

$$w_0 + w_1 x_1 + w_2 x_2 = 0$$

$$\Updownarrow \quad \Updownarrow \quad \Updownarrow$$

$$-4.9 + 1.7 x_1 - 1 x_2 = 0$$

hence $h(6,3) = sign(w_0 + w_1 * 6 + w_2 * 3) =$

$= sign(-4.9 + 1.7 * 6 - 1 * 3)$

$= sign(2.3) = +1 \rightarrow$ *nuclear expl.*

Getting new examples is expensive;-)

Use it: Example (Spam)

- Find $h(mail)$ +1 for *spam*, -1 *not-spam*
  - Features Phi(*mail*) = words [0/1] or phrases ("free money") [0/1] or length [integer]
  - e.g $\phi_k(\mathbf{x}) = contain(word_k)$ [*bag of words* representation]
- $w \rightarrow$ weight contribution of the input features to prediction
  - e.g. positive weight for "free money", negative for ".edu" or "unipi"
- $\boldsymbol{x}^T\boldsymbol{w}$ is the weight combination
- $h_{\mathbf{w}}(x)$ provides the threshold to decide spam/not spam

$$h_{\mathbf{w}}(\mathbf{x}) = sign\left(\sum_k w_k \phi_k(\mathbf{x})\right)$$ $>0 \rightarrow +1 = Spam\ !$

Some useful properties
(we will use them in future lectures)

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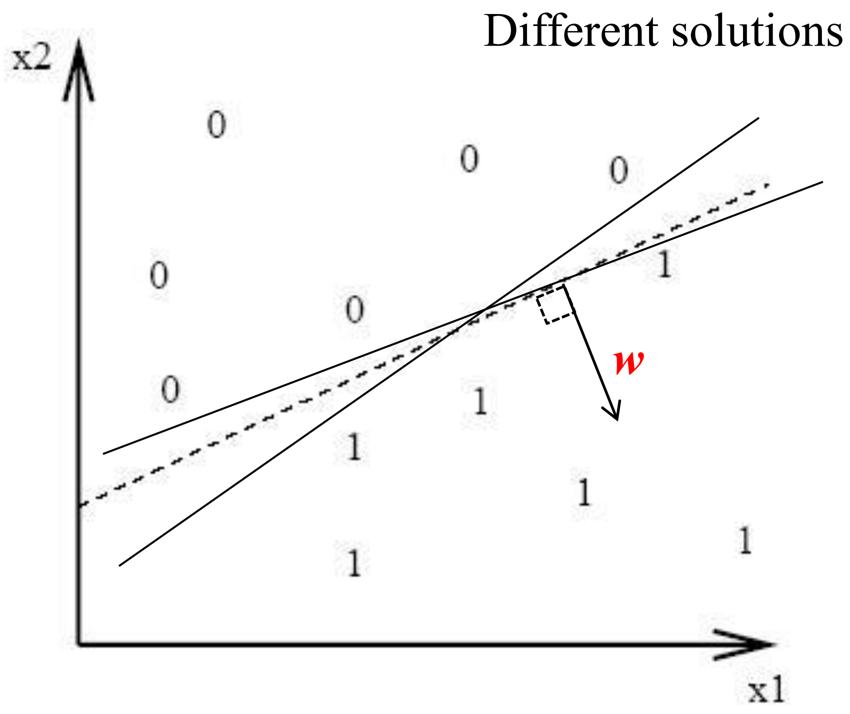
$$\boldsymbol{w}^T\boldsymbol{x} = w_1x_1 + w_2x_2 + w_0 = 0$$

Exercise: Draw $x_2 = -\, x_1\, w_1/w_2 - w_0/w_2$ with different $\boldsymbol{w}$ values



A linearly separable problem

- If w_0=0 the line goes through the *origin* of the coordinate system.
- If $n > 2$ → *hyperplane (decision boundary)*
- *Scaling freedom*: the same decision boundary multiplying $\boldsymbol{w}$ by K
- $\boldsymbol{w}$ is a vector *orthogonal* to the hyperplane:

Given $\boldsymbol{x}_a, \boldsymbol{x}_b$ ***(belonging to the sep. hyperplane):***
$\boldsymbol{w}^T\boldsymbol{x}_a + w_0 = 0$; $\boldsymbol{w}^T\boldsymbol{x}_b + w_0 = 0$ *(take the diff.)* →
$\boldsymbol{w}^T(\boldsymbol{x}_a - \boldsymbol{x}_b) = 0$ → ***orthogonal vectors*** *(dot prod. 0)*

- If it exist, there are many possible hyperplanes separating these points: also many ML alg.!!!

Learning Algorithms

- We are going to introduce 2 learning algorithms
for the regression and for the classification task using a linear model, both based on LMS:

  1. A direct approach based on **normal equation** solution
  2. An iterative approach based on **gradient descent**

- We start redefining the learning problem and the loss for them (for l data and multidimensional inputs)

The learning problem (classification tasks)

- **Given** a set of l training examples $(\boldsymbol{x}_p, y_p)$ and a loss function (measure) *L*

  $y_p = \{0,1\}$ or $y_p = \{-1,+1\}$

- **Find**: The weight vector $\boldsymbol{w}$ that minimizes the expected loss on the training data

$$R_{emp} = \frac{1}{l}\sum_{p=1}^{l} L(h(\boldsymbol{x}_p), y_p)$$

- For classification: Using a piecewise constant (over $sign(\boldsymbol{w}^T\boldsymbol{x})$) for the loss can make this a difficult problem.

- Assume we still use the *least squares (as for the regression case)*

$$E(\boldsymbol{w}) \propto \sum_{p=1}^{l}(y_p - \boldsymbol{x}_p{}^T\boldsymbol{w})^2 = \sum_{p=1}^{l}(y_p - \boldsymbol{w}^T\boldsymbol{x}_p)^2$$

Approximating expected loss by a smooth function (#)

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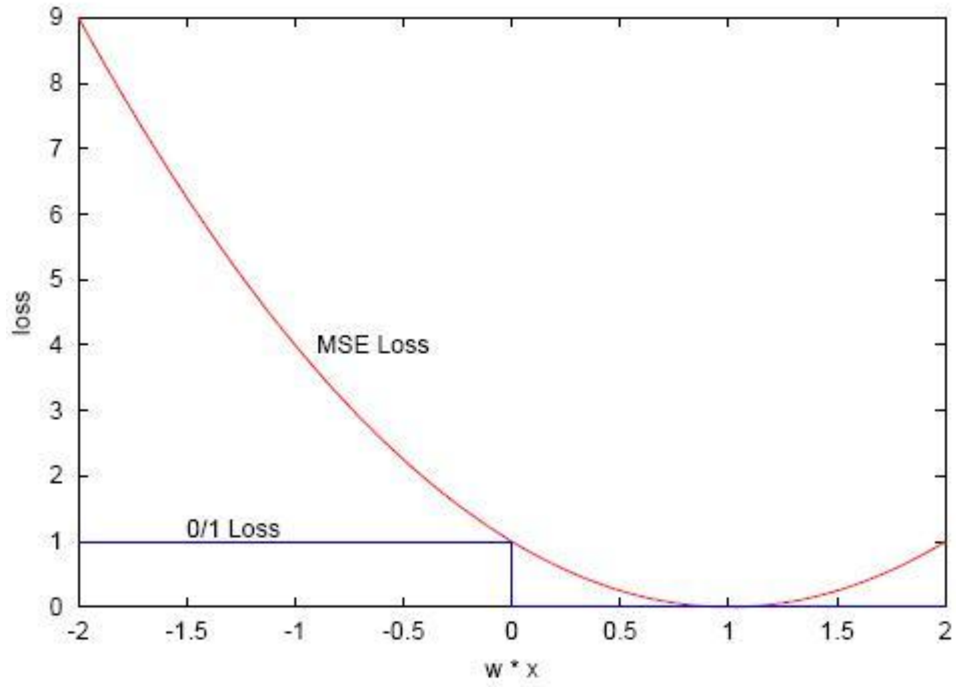
- Initially, we can make the optimization problem easier by replacing the original objective function *L (0/1 loss)* by **a smooth, *differentiable function***. For example, consider the popular *mean squared error (MSE loss)*:

Both losses satisfy the minimization of error *(*)*,
Let us start with LMS avoiding to introduce combinatorial problems



(*) Example: y (target)=1,
*h(**x**)=1 if $\mathbf{w}^T\mathbf{x}>0$,*
→ No err. when $\mathbf{w}^T\mathbf{x}>0$ for the classifier

Hence no classif. error minimizing either
- *0/1 loss*
- *or MSE loss*

(solution is for both on the right part in the plot)

Learning (a classifier) by Least Squares

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- Find optimal values for $\boldsymbol{w}$ (for fitting of training (TR) data) by *least squares*:
- **Given** a set of l training examples $(\boldsymbol{x}_p, y_p)$, **find** $\boldsymbol{w}$ to *minimize* the residual sum of squares:

$$E(\boldsymbol{w}) = \sum_{p=1}^{l} (y_p - \underline{\boldsymbol{x}_p{}^T \boldsymbol{w}})^2 = \quad ||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{w}||^2$$

Where $\boldsymbol{x}_p$ is p-th input vector, y_p the output for p, $\boldsymbol{w}$ free par., l num. of examples, n input dim.

Min error: if $y_p = 1$ then $\boldsymbol{x}_i^T\boldsymbol{w}$ go toward 1 → *no class. error* ;
if $y_p = -1$ then $\boldsymbol{x}_p^T\boldsymbol{w}$ go toward -1 → *no class. Error*

Note: *in E(**w**) we do **not** use h(**x**), as for regression, to hold a continuous **differentiable** loss (because h(**x**)=sign(**w**^{T}**x**) for classification) !!!*

- This is a quadratic function → minimum always exists (but may be not unique) [see course of CM or O4DS (@DSBI)]
- $\boldsymbol{X}$ is a matrix $\boldsymbol{l} \times \boldsymbol{n}$ with a row for each input vector $\boldsymbol{x}_p$
- Note: The same approach is used for a *regression problem*

Learning Algorithms

- We will introduce 2 learning algorithms
for the regression and for the classification tasks using a linear model, both based on LMS

1. A direct approach based on **normal equation** solution

2. An iterative approach based on **gradient descent**

Normal equation & direct approach solution

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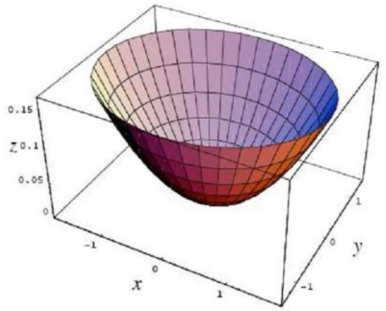
- Differentiate *E(w)* with respect to ***w***: Blackboard or Exercise (a next slide).

Result synthesis:

- In the derivation we find that
$$\frac{\partial E(\boldsymbol{w})}{\partial w_j} = -2\sum_{p=1}^{l} \left(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w}\right) x_{p,j}$$

- We can get the **normal equation** (point with gradient of E w.r.t $\boldsymbol{w}$ =0):
$$(\boldsymbol{X}^T\boldsymbol{X})\boldsymbol{w} = \boldsymbol{X}^T\boldsymbol{y}$$



See also CM course

- If X^TX is not singular the unique solution is given by
$$\boldsymbol{w} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y} \quad = \boldsymbol{X}^+\boldsymbol{y}$$
`+` Moore-Penrose *pseudoinverse* (also if X is not invertible)

- Else the solution are infinite (satisfying the normal equation): we can choose the *min norm* ($\boldsymbol{w}$) solution

Direct approach by SVD

- The *Singular Value Decomposition (SVD)* can be used for computing the pseudoinverse of a matrix ($\boldsymbol{X}^+$)

$$\boldsymbol{X} = \boldsymbol{U}\underset{\text{diagonal}}{\underset{\downarrow}{\boldsymbol{\Sigma}}}\boldsymbol{V}^T \Rightarrow \boldsymbol{X}^+ = \boldsymbol{V}\boldsymbol{\Sigma}^+\boldsymbol{U}^T$$

by replacing every nonzero entry by its reciprocal

- Moreover we can apply directly SVD to compute $\boldsymbol{w} = \boldsymbol{X}^+\boldsymbol{y}$

obtaining the minimal norm (on $\boldsymbol{w}$) solution of least squares problem.

- Note: THIS IS the learning alg. for the ***direct*** approach solution on $\boldsymbol{w}$ (or say in *closed form*)

- A practical tool. E.g. see "numerical recipes" in C and many numerical/statistical tools and scientific library (also in R, Octave, Matlab,…)
  - e.g. ARMADILLO: since 2011/12 C++ linear algebra library, NumPy etc.
- Many algorithms addressing the problems of efficiency and stability
- See also CM course (may be later) or O4DS (@DSBI)

Solution (to find the normal eq.) Make as an <u>Exercise</u> !!!(#)

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$$\frac{\partial E(\boldsymbol{w})}{\partial w_j} = \frac{\partial \sum_{p=1}^{l}(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w})^2}{\partial w_j} = \sum_{p=1}^{l} 2(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w}) \frac{\partial(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w})}{\partial w_j} =$$

$$= \sum_{p=1}^{l} 2(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w}) \left(0 - \cancel{\frac{\partial(\boldsymbol{x}_p)_1 w_1}{\partial w_j}} - \cancel{\frac{\partial(\boldsymbol{x}_p)_2 w_2}{\partial w_j}} - \ldots \frac{\partial(\boldsymbol{x}_p)_j w_j}{\partial w_j} - \cancel{\ldots}\right) =$$

Only the component j is not 0

$$= \sum_{p=1}^{l} 2(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w}) \left(-\frac{\partial(\boldsymbol{x}_p)_j w_j}{\partial w_j}\right) = -2\sum_{p=1}^{l}(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w})(\boldsymbol{x}_p)_j$$

Imposing this =0, we can easily obtain the *normal equation* (first by “sums”, then in matrix notations)

And we also obtained the gradient of *E* rewritten as:

$$\frac{\partial E(\boldsymbol{w})}{\partial w_j} = -2\sum_{p=1}^{l} \overset{\delta_p}{\boxed{(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w})}}\, x_{p,j} = -2\sum_{p=1}^{l} \delta_p\, x_{p,j}$$

(we will use this form in the future, with Neural Networks)

Other approaches to LS

Many, for instances by an **iterative/gradient descent technique** we can search for:

- More efficient solutions (previous is cubic with dim of matrix X)
- Regularization (to reduce complexity of the model)
- Better approximation with noisy data by stopping searching before the minimum

- Other approaches that can be applied also to
  NON-LINEAR models !!!

Hence, we are going to present the second (more important) learning algorithm

Learning Algorithms

- We will introduce 2 learning algorithms
for the regression and for the classification tasks using a linear model, both based on LMS

1. A direct approach based on **normal equation** solution
2. An iterative approach based on **gradient descent**

This approach will be the basis for fundamental approaches we will see later

REPETITA
Gradient on a surface

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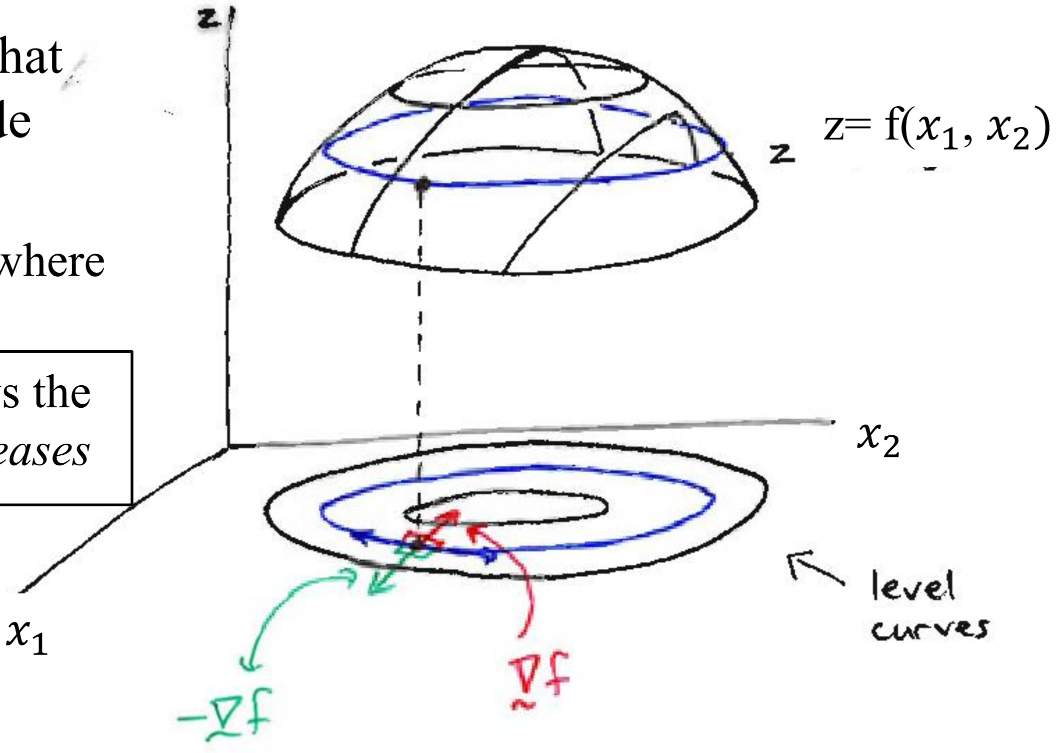
- **The gradient at a point** is a **vector** pointing in the **direction of the steepest slope** at that point.
- The steepness of the slope at that point is given by the magnitude of the gradient vector
  - The gradient shows the direction where the function grows
  - The negative of the gradient shows the direction where the function *decreases*



Gradient descent

- Previous derivation suggest the line to construct an iterative algorithm based on:

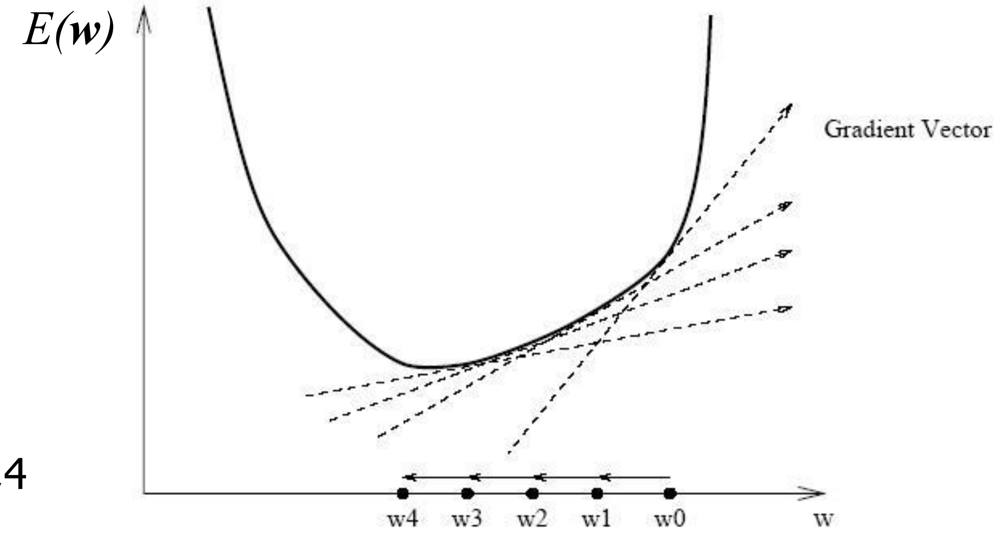
$$\frac{\partial E(\mathbf{w})}{\partial w_j} = -2\sum_{p=1}^{l}(y_p - \boldsymbol{x}_p{}^T\mathbf{w})(\boldsymbol{x}_p)_j \longrightarrow$$

*Where $\mathbf{x}_p$ is p-th input pattern, y_p the output for p, **w** free par., l num. of examples*

Component j of pattern p, also $x_{p,j}$

- **Gradient** = **ascent direction**: we can move toward the minimum with a gradient **descent** (changing w with $\Delta w = -$ gradient of $E(w)$)

  - *Local search*: it begins with an initial weight vector. We modify it iteratively to decrease up to minimize the error function (steepest descent).



A single w at step 0,1,2,3,4

Error surface for linear model with 2 weights (*w*)

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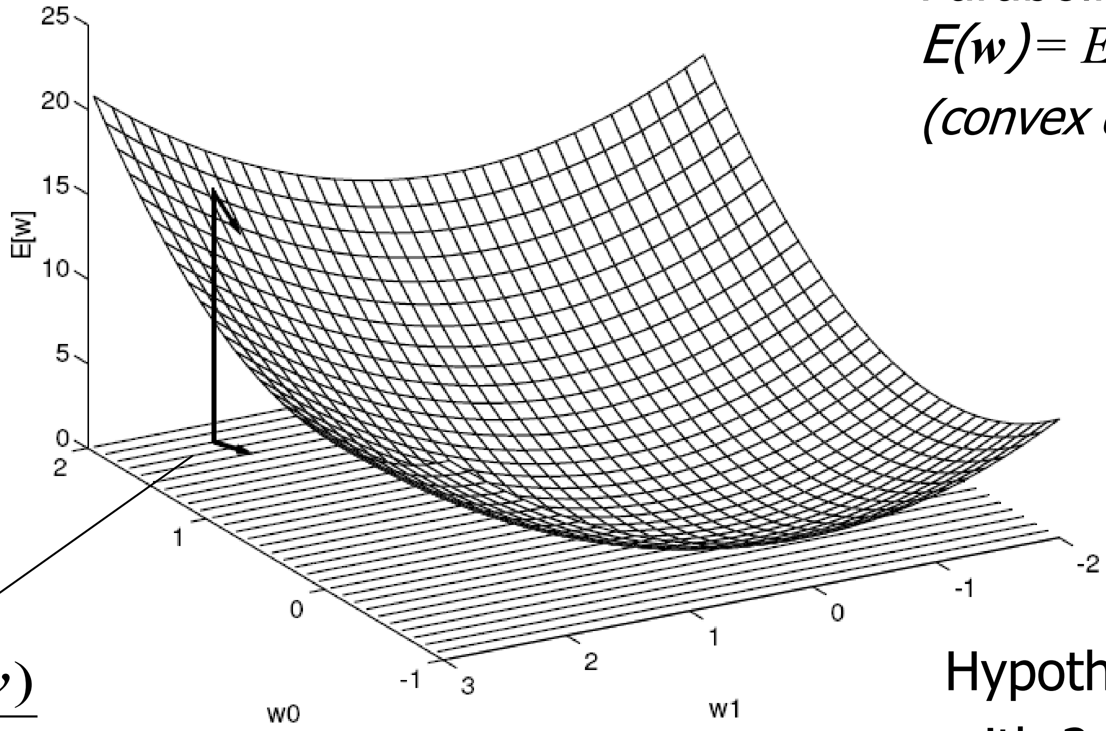

$$-\frac{\partial E(\mathbf{w})}{\partial \mathbf{w}}$$

Our "compass" to find the minimum

Parabolic for the
$E(\mathbf{w}) = E([w_0, w_1]^T)$
(convex quadratic function)

Hypothesis space with 2 parameters
w_0, w_1

The gradient vector

$$\Delta \boldsymbol{w} = -\frac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}} = \begin{bmatrix} -\frac{\partial E(\boldsymbol{w})}{\partial w_0} \\ -\frac{\partial E(\boldsymbol{w})}{\partial w_1} \\ -\frac{\partial E(\boldsymbol{w})}{\partial w_2} \\ -\frac{\partial E(\boldsymbol{w})}{\partial w_j} \\ \dots \\ -\frac{\partial E(\boldsymbol{w})}{\partial w_n} \end{bmatrix} = \begin{bmatrix} \Delta w_0 \\ \Delta w_1 \\ \Delta w_2 \\ \Delta w_j \\ \dots \\ \Delta w_n \end{bmatrix}$$

We can work in a multi-dim space without the need to visualize it

Using the Delta Rule

- Hence, as iterative approach we will move using a learning rule based on a «delta» (changing) of $\boldsymbol{w}$ proportional to the (opposite) of the local gradient
- The «movements» will be made iteratively according to

$$\boxed{\boldsymbol{w}_{\text{new}} = \boldsymbol{w} + eta * \Delta \boldsymbol{w}}$$

(or component-wise, i.e. for each w_j)

- that is the "***learning rule***"
- and *eta* (η) is the "step size" (learning rate) parameter (ruling the speed of our gradient descending)

Gradient descent algorithm

A simple algorithm:

1) Start with weight vector $\boldsymbol{w}_{\text{initial}}$ (small), fix *eta (0<eta<1)*.

2) Compute $\Delta \boldsymbol{w} = -$"gradient of $E(\boldsymbol{w})$" $= -\dfrac{\partial E(\boldsymbol{w})}{\partial \boldsymbol{w}}$ (or for each w_j)

3) Compute $\boxed{\boldsymbol{w}_{\text{new}} = \boldsymbol{w} + \eta * \Delta \boldsymbol{w}}$ (or for each w_j)

Repeat (2) until convergence or $E(\boldsymbol{w})$ is "sufficiently small"

- $\Delta \boldsymbol{w}/l$: *least mean squares* (dividing by l, that will be the standard case)
- Batch versions ($\Delta \boldsymbol{w}$ after each "epoch" of l training patterns)
- *eta* (η): step size = *learning rate*: speed/stability trade-off: can be (gradually) decreased to zero (guarantee convergence, avoiding oscillation around the min.): many variants will be introduced later

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Batch/On-line

- For **batch version** the gradient is the sum over all the *l* patterns:

$$\frac{\partial E(\boldsymbol{w})}{\partial w_j} = -2 \sum_{p=1}^{l} (y_p - \boldsymbol{x}_p{}^T \boldsymbol{w})\, x_{p,j}$$

  - provide a more "precise" evaluation of the gradient over a set of *l* data

  And we upgrade the weights after this sum

- For the **on-line/stochastic version** we upgrade the weights with the error that is computed for each pattern
  - hence, the 2nd pattern output is based on weights already updated from the 1st, and so ahead
  - It makes progress with each examples it looks at: it can be the faster, but need smaller *eta:*

$$\frac{\partial E_{p}(\boldsymbol{w})}{\partial w_j} = -2(y_p - \boldsymbol{x}_p{}^T \boldsymbol{w})x_{p,j} = -\Delta_p w_j$$

- We will see intermediate cases later (as **mini-batch**)

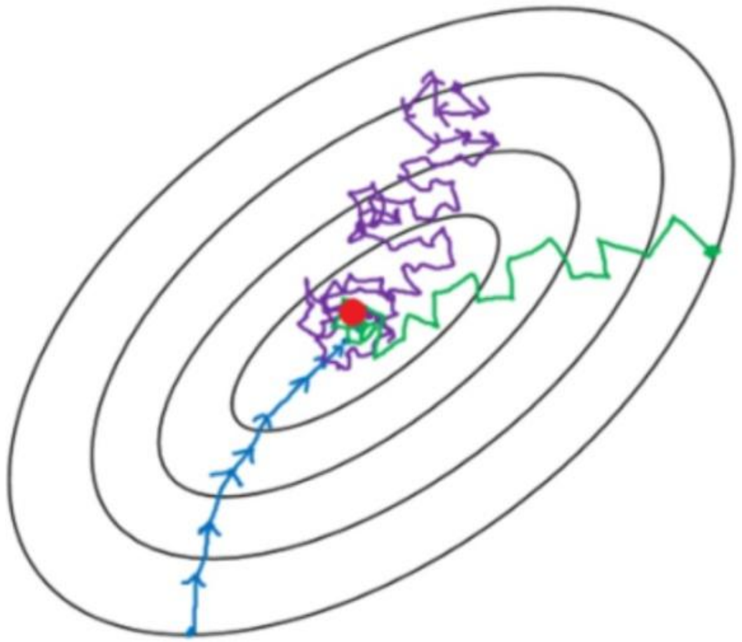
Examples

Batch algorithm

We update ***w*** after (repeating) an "epoch" of l training data → *(blu)*

On-line algorithm (stochastic gradient descent - *SGD*)

We update ***w*** after each pattern *p* ($\Delta_p \mathbf{w}$ *for each pattern*→ (purple and green)

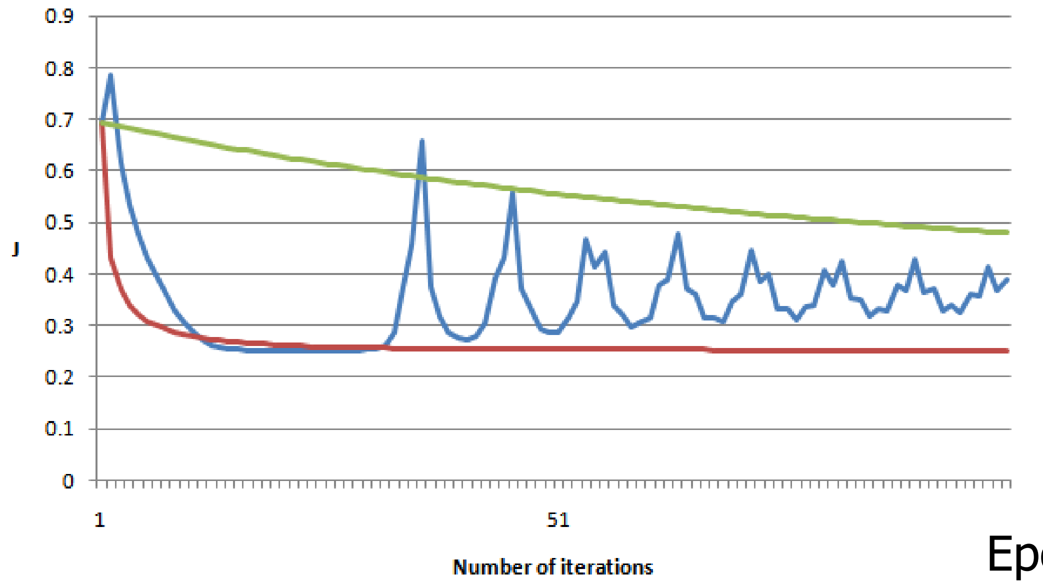


Paths over the error surface by Batch or On-line version

Learning curve examples

Error

Error vs number of iterations



Epochs

These are **learning curves**:
They show how the error decreases through gradient descent iterations

P.S. No relation with color in the previous slide!

Exercise: *1 is slow, 1 is unstable, 1 is good: which one?*
Which with high or low eta value?

Gradient descent as Error correction delta rule

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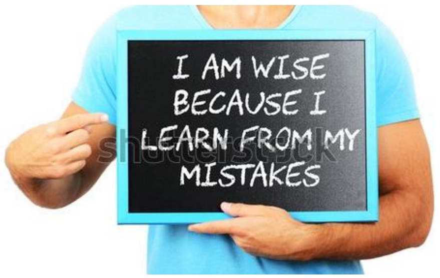
$$\Delta w_j = 2 \sum_{p=1}^{l} \overbrace{(y_p - \boldsymbol{x}_p^T \boldsymbol{w})}^{\delta_p} x_{p,j}$$

$$\boldsymbol{w}_{\text{new}} = \boldsymbol{w} + eta^* \Delta \boldsymbol{w}$$

*Where $x_{p,j}$ is the component j of the input pattern p, y_p the output for p, **w** free par., l num. of examples.*
The constant 2 can be omitted

- This is an *"error correction" rule* (Widrow-Hoff or **delta rule**) that change each w_j proportionally to the error (target y - output):
  - E.g. (target y – output) = err=0 → no correction
  - (input$_j$>0) if err + (output is too low), positive delta → increase w_j → increment the output → less err
  - (input$_j$>0) if err - (output is too high), negative delta → decrease w_j → reduce output → less err
  - ... [*exercise*: all the cases]
- We improve by learning from previous errors
  "seeking and blundering we learn (Goethe)"



Delta-W as Error Correction Learning rule (II)

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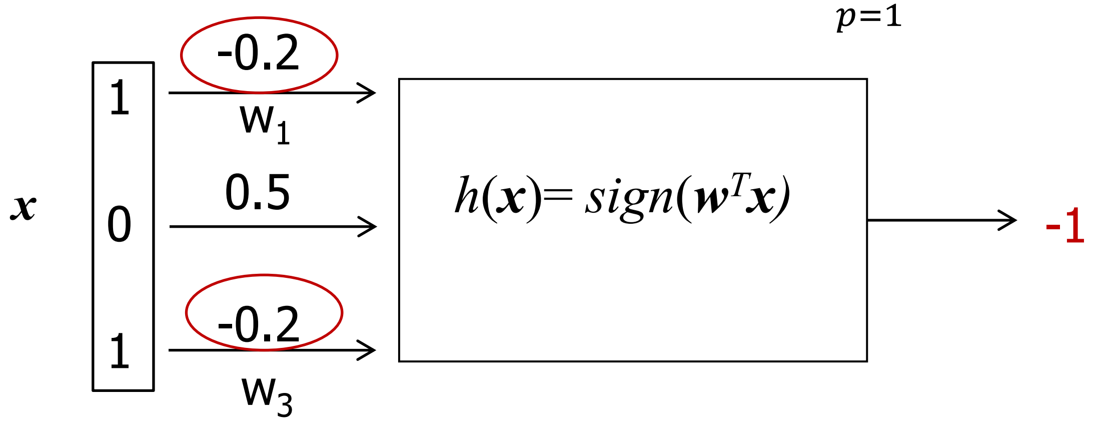
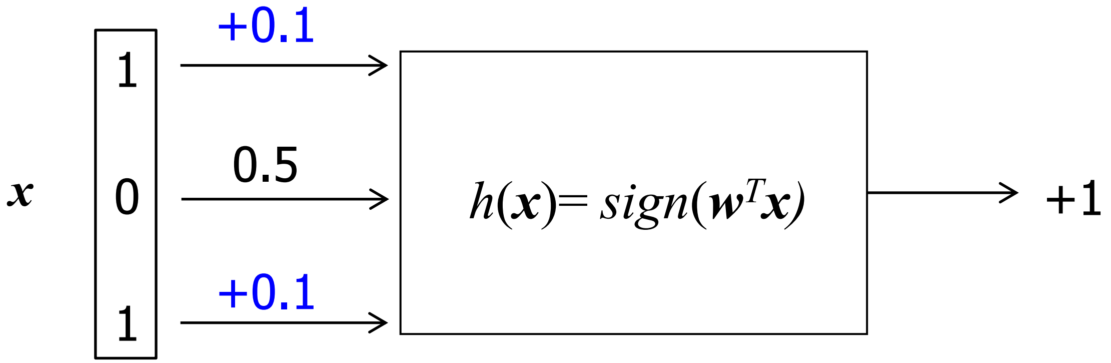
Inputs Weights $(w_0=0)$ $\Delta w_j = 2 \sum_{p=1}^{l} (y_p - \boldsymbol{x}_p{}^T \boldsymbol{w})\, x_{p,j}$



If misclassified (because target is +1) → (1-(???)) → High positive delta for w_1 and w_3 → increase them proportionally (with eta) to the *delta*, hence a positive value in this case [*error correction rule*] *!!!*



e.g. (see figure):

Now is correct !!!

Exercise: compute the values for delta (hint: see eq. above) and for also eta

Gradient descent: final discussion

Gradient descent approach it is simple and effective *local search* approach to LMS solution and

- It allows us to search through an *infinite (continuous) hypothesis* space!
- It can be easily always applied for *continues* H and *differentiable loss*
- NOT ONLY to linear models !!!! (we will see for Neural Networks and deep learning models)

- *Efficient?* Many improvements are possible, e.g. Newton & quasi-newton methods; Conjugate Gradient, …! → CM course*
(we will mention examples later, discussing Neural Networks)

Summarizing (Classification)

- Model trained (on TR set) with LS (LMS) on $\boldsymbol{w}^T\boldsymbol{x}$
  - by the simple gradient descent algorithm used for linear regression
- Model used for classification applying a threshold function, obtaining $h(\boldsymbol{x}) = sign(\boldsymbol{w}^T\boldsymbol{x})$
- The error can be computed as *classification error* or number of misclassified patterns (not only by the Mean Square Error)

0/1 Loss

$$\boxed{L(h(\mathbf{x}_p), d_p) = \begin{cases} 0 & \_if \quad h(\mathbf{x}_p) = d_p \\ 1 & \_\_\_\_\_\_\_otherwise \end{cases}}$$

$$mean\_err = \frac{1}{l} \boxed{\underbrace{\sum_{p=1}^{l} L(h(\boldsymbol{x}_p), d_p)}_{num\_err}}$$

- **ACCURACY** = mean of correctly classified = $(l\text{-}num\_err)/l$

Coming back to the problem: Linear model solution

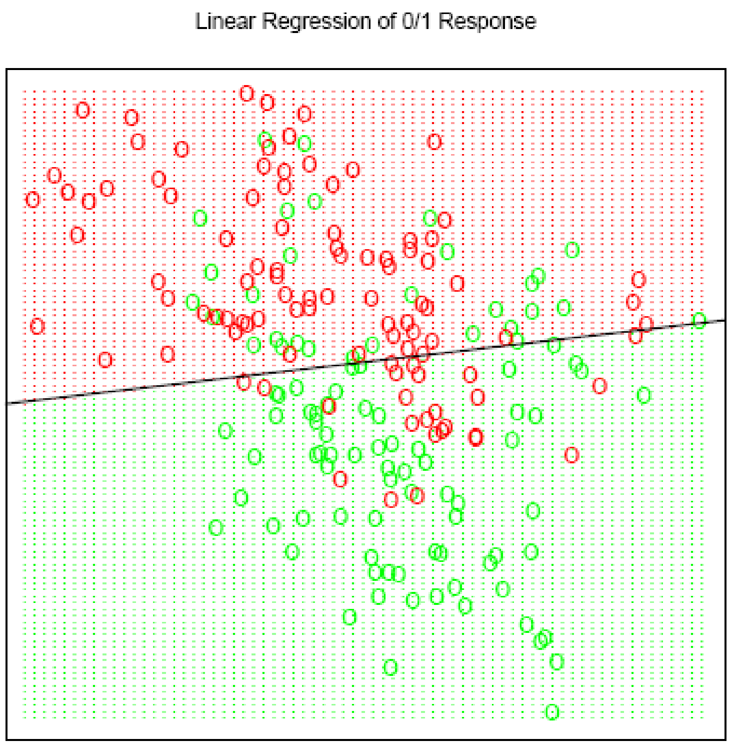


Figure 2.1 (© HTF 2001):

A classification example in two dimensions. The classes are coded as a binary variable GREEN = 0, RED = 1 *and then fit by linear regression. The line is the decision boundary defined by* $\boldsymbol{x}^T\boldsymbol{w} = 0.5$. *The red shaded region denotes that part of input space classified as* RED, *while the green region is classified as* GREEN.

$$h(\boldsymbol{x}) = \begin{cases} 1 & \_if \quad \boldsymbol{x}^T\boldsymbol{w} > 0.5 \\ 0 & \_\_\_\_\_\_ otherwise \end{cases}$$

Linear threshold unit

The *decision boundary* is $\{\boldsymbol{x} \mid \boldsymbol{x}^T\boldsymbol{w} = 0.5\}$ is linear (and seems to make many errors on the training data). Is it true?

Good or bad approximation? (#)

- Possible scenarios (we know the true target function!)
  - Scenario 1: The data in each class are generated from a Gaussian distribution with uncorrelated components, same variances, and different means.
  - Scenario 2: The data in each class are generated from a mixture of 10 gaussians in each class.

- For Scenario 1, the linear regression rule (by LS) is almost **optimal** (is the best one can do). The region of overlap is inevitable (due to errors in the input data).
- For Scenario 2, it is far too rigid: next models for it!

* Least squares corresponds to the maximum likelihood criterion if the experimental errors have a normal distribution

Linear model (in ML): Inductive Bias (alla Mitchell)

- Language bias: the H is a set of linear functions (may be very restrictive and rigid)

- Search bias: ordered search guided by the Least Squares minimization goal
  - For instance, we could prefer a different method to obtain a restriction on the values of parameters, achieving a different solutions with other properties (in particular to consider the generalization issue), …

It shows that even for a "simple" model there are many possibilities. We need a principled approach! (see theory of ML)…

Limitations: regression tasks for non linear problems

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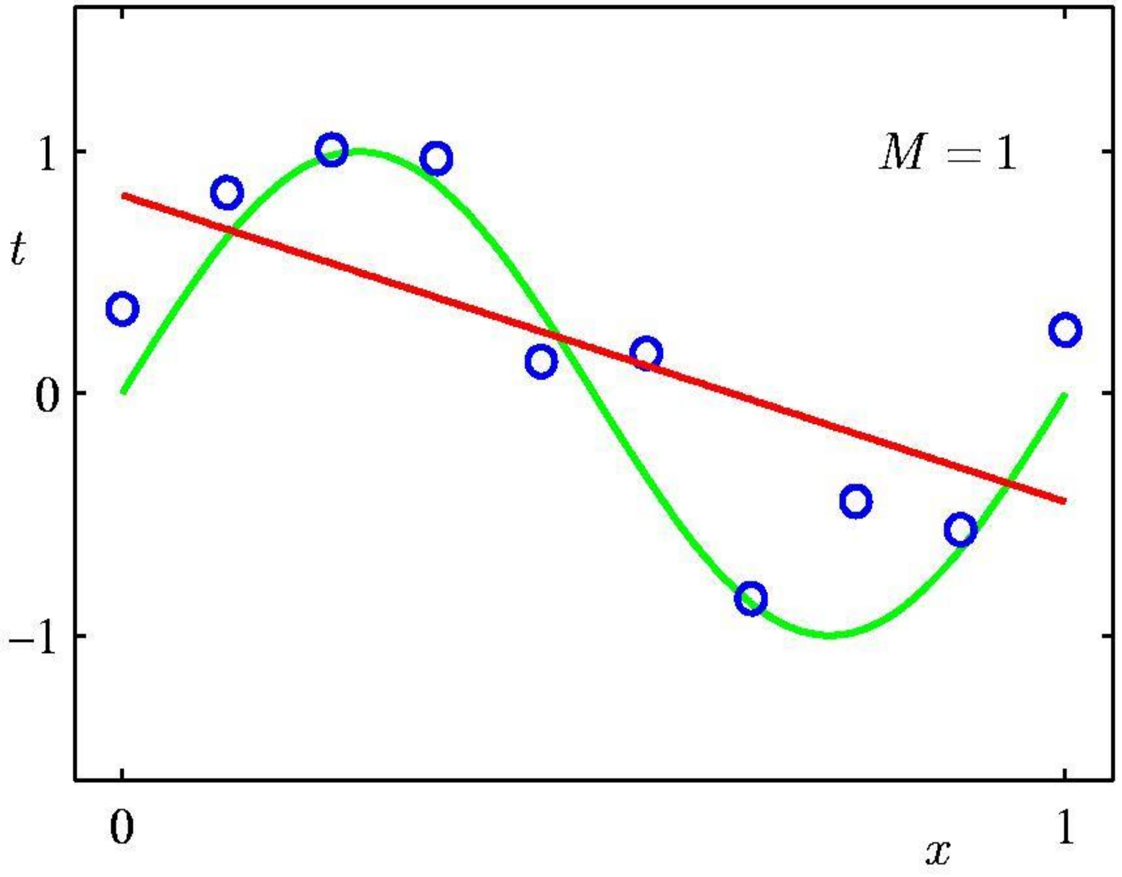

Too poor solution

Limitations (classification) (language bias)

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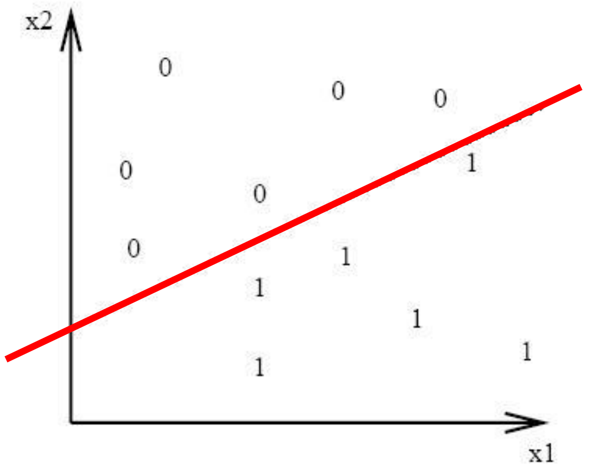
- In geometry, two set of points in a two-dimensional plot are ***linearly separable*** when the two sets of points can be completely separated by a single line
- In general, two groups are *linearly separable* in *n*-dimensional space if they can be separated by an (*n* – 1)-dimensional hyperplane.



- The linear decision boundary can provide exact solutions only for linearly separable sets of points

Example: Conjunctions

- We can represent conjunctions by the linear models, e.g.:
- **Conjunctions (**see the example in the introduction lectures**):**

4 var.: $x_1 \wedge x_2 \wedge x_4 \leftrightarrow y$

- $1\ x_1 + 1\ x_2 + 0\ x_3 + 1\ x_4 \geq 2.5$

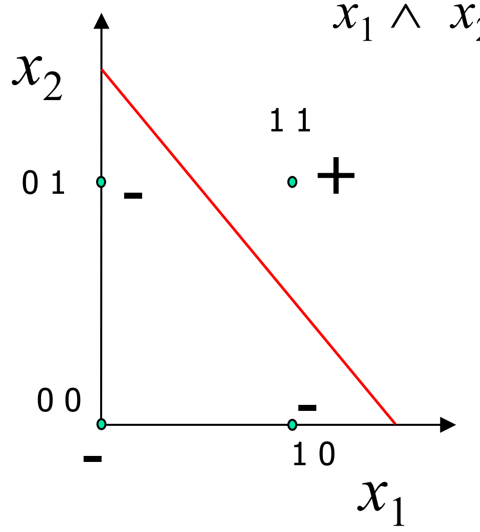
$$h(\boldsymbol{x}) = \begin{cases} 1 & \_if \quad \boldsymbol{w}^T\boldsymbol{x} + w_0 \geq 0 \\ 0 & \_\_\_\_\_\_otherwise \end{cases}$$

In the plot:

2 var.: $x_1 \wedge x_2 \leftrightarrow y$

- $1\ x_1 + 1\ x_2 \geq 1.5$

$\Rightarrow$



$x_1 \wedge x_2$	AND
00	0
01	0
10	0
11	1

w can be learned to find this solution

Limitations: classification tasks

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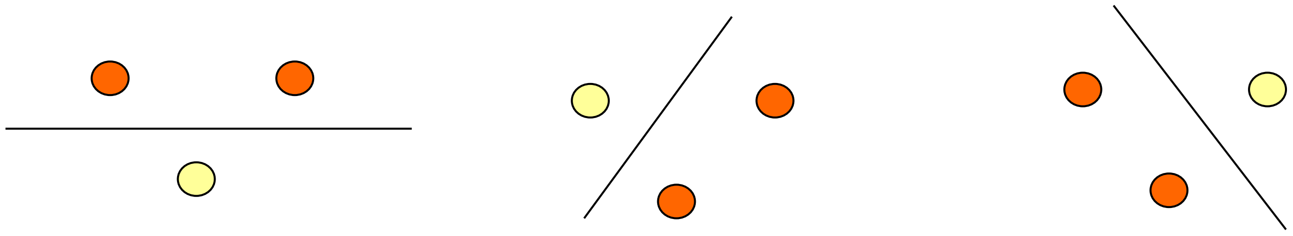
- Given **3 points**, can we always find a separation plane for every assignment of *f(**x**)*?

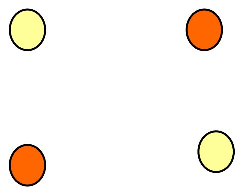
  No, 3 aligned points with 0 in the middle and others 1; yes if they are not aligned (existence!).

Here NOT complete:
There are 2^3 cases



- Given **4 points**, can we always find a separation plane for every assignment of *f(**x**)* ?
  No (XOR)

  we can find a labeling such that the linear classifier fails to be perfect



XOR	
00	0
01	1
10	1
11	0

***Exercise**: try to redo it by yourself!*

How to extend the linear model

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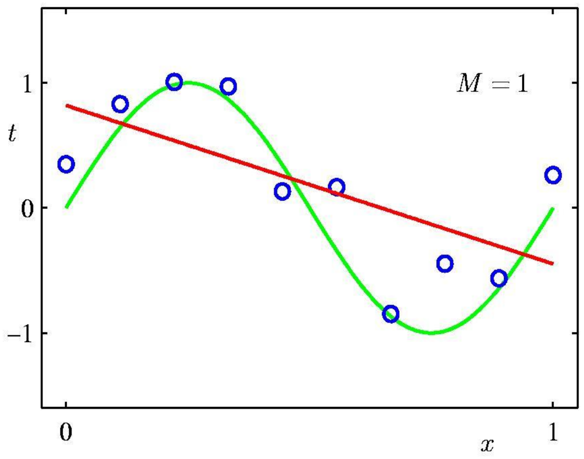
- Note that in $h_{\mathbf{w}}(x)=w_1x+w_0$ or $h_{\boldsymbol{W}}(\boldsymbol{x}) = \boldsymbol{w}^{\mathrm{T}} \cdot \boldsymbol{x}$
- As Statistical Parametric models:

  "linear" does not refer to this (red) straight line, but rather to the way in which the regression coefficients $\boldsymbol{w}$ occur in the regression equation



- Hence, we can use also transformed inputs, such are x, x^2, x^3, x^4, …. with *non-linear* relationship inputs and output, holding the learning machinery (Least Square solution) developed so far…

$$h_{\mathbf{w}}(x) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

polynomial regression

A generalization (LBE)

(shown for regression*)

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- Basis transformation: **linear *basis expansion* (LBE):**

$$h_{\boldsymbol{w}}(\boldsymbol{x}) = \sum_{k=0}^{K} w_k \phi_k(\boldsymbol{x})$$

- Augment the input vector with additional variables which are transformations of $\boldsymbol{x}$ according to a function phi (ϕ_k: $R^n \rightarrow R$)
- E.g
  - Polynomial representation of $\boldsymbol{x}$: $\phi(\boldsymbol{x}) = x_j^2$ *or* $\phi(\boldsymbol{x}) = x_j x_i$, *or* ....
  - Non-linear transformation of single inputs: $\phi(\boldsymbol{x}) = \log(x_j)$, $\phi(\boldsymbol{x}) = \mathrm{root}(x_j)$, ...
  - Non-linear transformation of multiple input: $\phi(\boldsymbol{x}) = ||\boldsymbol{x}||$
  - ***Splines, …, ….***
- Typically: Number parameters $K > n$ (before it was n)
- The model is *linear in the parameters (also in phi, not in* $\boldsymbol{x}$*): we can use the* ***same learning alg.*** *as before!*
- *Note: it can be applied for regression (here) or classification (Exercise: HOW?)*

Basis Expansion: examples

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- Basis transformation: **linear *basis expansion* :**

$$h_{\mathbf{w}}(\mathbf{x}) = \sum_{k=0}^{K} w_k \phi_k(\mathbf{x})$$

EXAMPLES:

- *[1-dim **x**]* $\phi_j(x) = x^j.$

$$h(\mathbf{x}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

1-dim polynomial regression (K=M)

Already seen in the introduction

- Or *"any other"*, *e.g.* $\phi(\mathbf{x})=\phi([x_1,x_2,x_3])$

$$h(\mathbf{x}) = w_1x_1 + w_2x_2 + w_3\log(x_2) + w_4\log(x_3) + w_5(x_2x_3) + w_0$$

Basis Expansion criticism

- Which phi (ϕ) ? Toward the so called "**dictionary**" approaches

- PROS: Can model more complicated relationships (than linear) w.r.t. the inputs: it is more expressive.
- CONS: With *large* basis of functions, we easily risk *overfitting*, hence we require methods for *controlling the complexity* (*) of the model
  - *Curse of dimensionality* (the volume of the problem space increases so fast that the available data become sparse, the data became no more sufficient to support the model complexity) → we will see later
  - Phi are *fixed before* observing training data
    - versus adaptive /non-linear in parameters e.g. NN!

- *We will see the alternative NN and SVM solutions!*

(*) Whereas **complexity** is **not** for the computational cost but a measure of the flexibility of the model to fit the data (see the VC-dim)

Improvements: How to control model complexity? Important !

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- Many approaches… e.g. coefficient shrinkage:
- **Ridge regression**: (**Tikhonov regularization**): smoothed model → possible to add constraints to the sum of value of $|w_j|$ penalizing models with high values of $|w|$, i.e. favoring "sparse" models using less terms due to weights $w_j = 0$ (or close to 0) (it means a less complex model)

"Error" data term [(M)SE] (R_{emp} in the SLT) Regularization/penalty term

$$Loss(\mathbf{w}) = \sum_{p=1}^{l} (y_p - \mathbf{x}_p{}^T \mathbf{w})^2 + \boxed{\lambda ||\mathbf{w}||^2} \longrightarrow \sum w_j{}^2$$

The sum is over the number of w

Lambda (λ): regularization (hyper)parameter
(a small positive value chosen by the "model selection" phase)

- Note that for the ***objective function*** we use here the name *Loss* (used for the model training cost function) to distinguish from the *Error E* (useful to evaluate the model error and used for the *data term* inside this Loss).
Hence, differently from previous assumptions the two terms are not more equivalent in our use (in the course).

Tikhonov Regularization: Solving it

$$Loss(\boldsymbol{w}) = \sum_{p=1}^{l} (y_p - \boldsymbol{x}_p{}^T \boldsymbol{w})^2 + \lambda ||\boldsymbol{w}||^2$$

- For the <u>direct approach</u>:

$$\mathbf{w} = \boxed{(\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}}\mathbf{X}^T\mathbf{y} \dashrightarrow$$ this matrix is always invertible

- For the <u>gradient approach</u>: we still apply **–**gradient of the Loss:
- As an **Exercise** compute the gradient of the two terms (error and penalty terms) of the *Loss*($\mathbf{w}$) w.r.t. weights w_i <u>separately</u>, using *eta* only for term *E*
- Formulate the new update rule :
- You will obtain: $\boldsymbol{w}_{\text{new}} = \boldsymbol{w} + eta * \Delta \boldsymbol{w} - 2\lambda \boldsymbol{w}$

- That is a **weight decay** technique (basically add $2\lambda w$ to the gradient)
  - E.g. with 0 gradient, it decreases the value of each w with a fraction of the old w

Andrej Nikolaevič Tikhonov

Russian mathematician
1906 –1993

Tikhonov regularization: trade-off

$$Loss(\boldsymbol{w}) = \sum_{p=1}^{l}(y_p - \boldsymbol{x}_p{}^T\boldsymbol{w})^2 + \lambda||\boldsymbol{w}||^2$$

- Note the balancing (trade-off) between the two terms:
  - Small ***lambda*** (λ) value → minimizing the loss the focus is on obtaining a small error data term (first term, minimize just the training error) with a too complex model (high norm of the weights), the risk is of ***overfitting***,
  - High ***lambda*** (λ) → minimizing the loss the focus is on the second term, hence the data error (first term) could grow too much, i.e. moving to ***underfitting***
  - The trade-off is ruled by the value of ***lambda*** (λ)
  - We will see soon some examples

- The main advantage is that we have a concrete realization of the control of model complexity, easy to be implemented and of general applicability.

Tikhonov and SLT

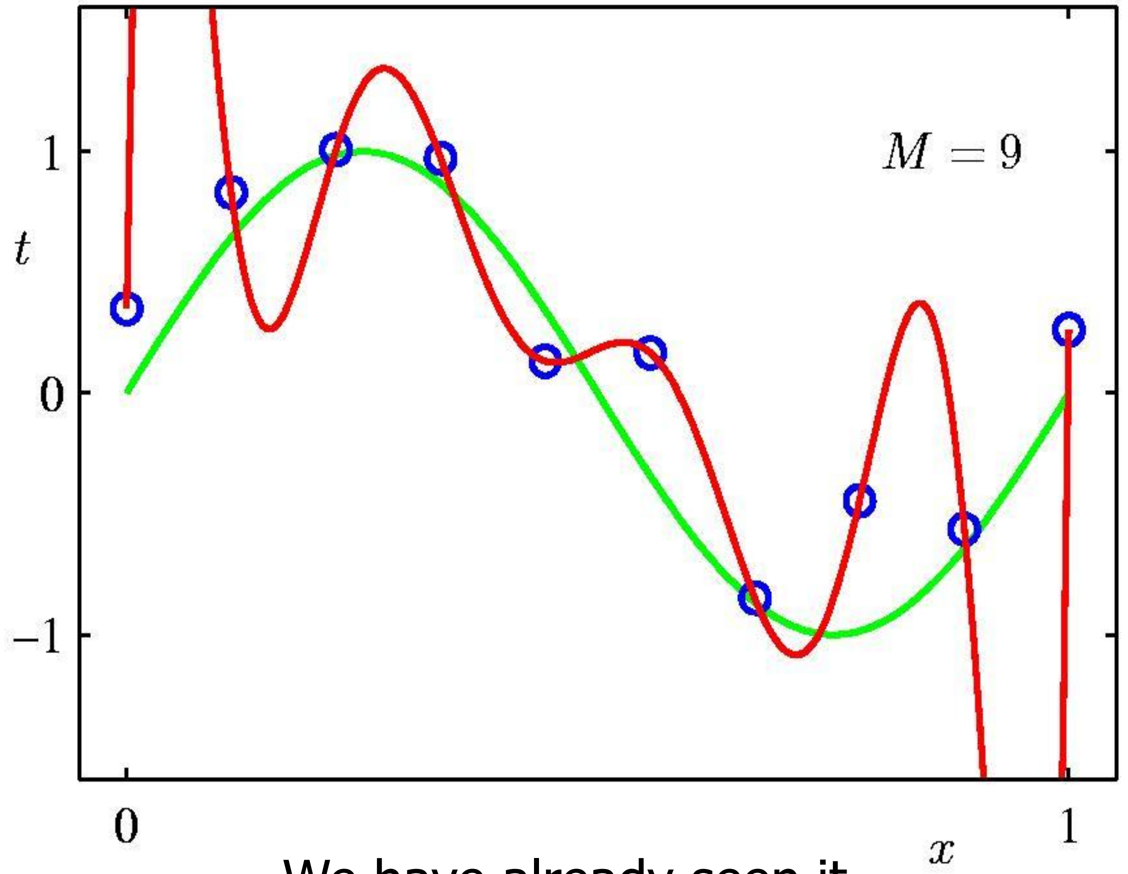
- The penalty term penalizes high value of the weights and tends to drive all the weights to smaller values
  - E.g. Some weights values can go even to zero
- It implements a control of the model complexity
- This leads to a model with less (or proper) *VC-Dim,* with a trade-off obtained through **just a (1) parameter** that you can control: the λ

- **Exercise**: connect Tikhonov regularization with the slide on SLT (see the introduction) to see
  - why this can help to have a better bound on *R*, and
  - how lambda values can rule the underfitting/overfitting cases

- **Exercise:** derive the new learning rule with weight decay using the Tikhonov loss: computing again the partial derivatives of *Loss* with respect to w, separating data term (• eta) and penalty term (• λ)

Slide from Intro slides:
9th Order Polynomial

As to have Lambda 0



We have already seen it

E(***w***)= 0 on training data and **overfitting**

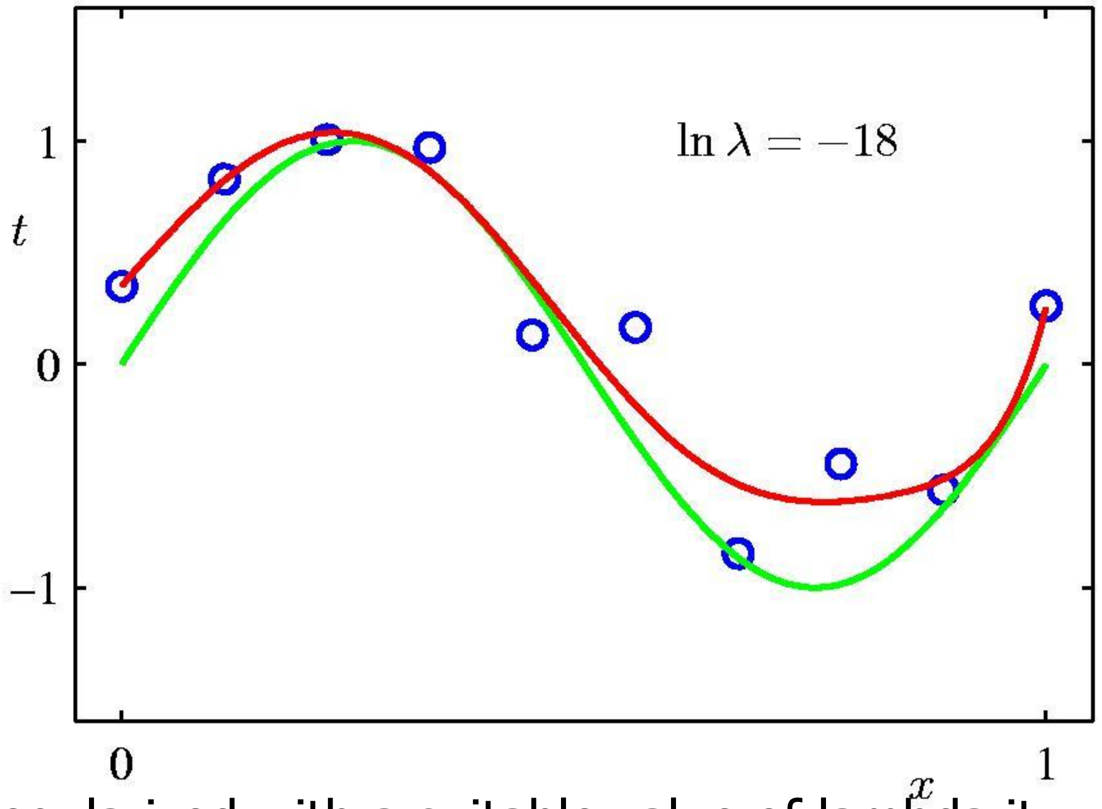
Regularization effect

$$\ln \lambda = -18$$

- 9th Order Polynomial

Lambda small positive

$\lambda = 0.0000000152$

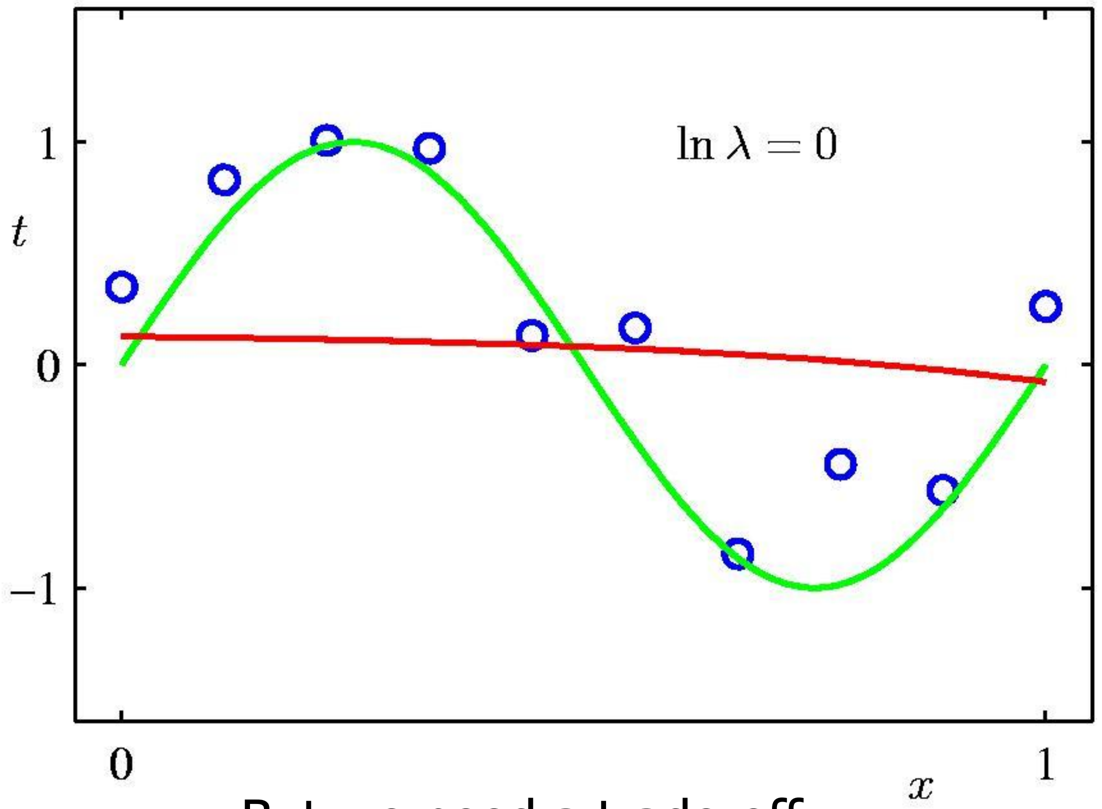


Smoothness

Once regularized with a suitable value of lambda it works well!
It is worse on training data but we reduce the **overfitting**

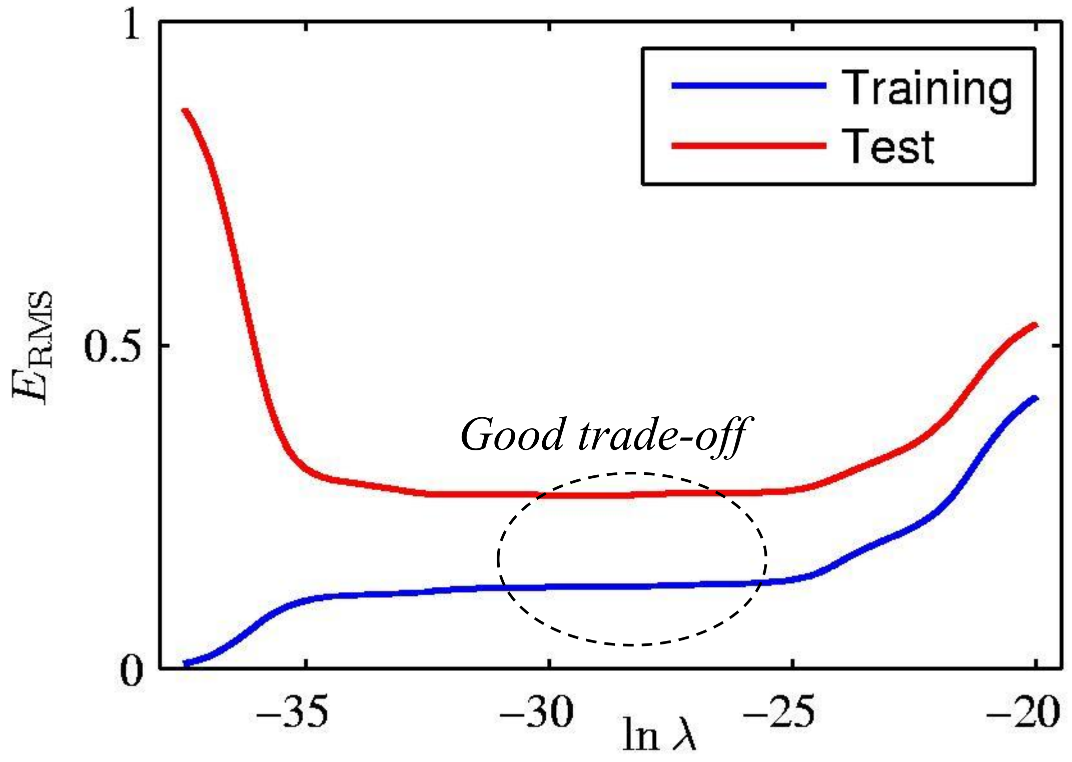
Too High lambda ($\ln \lambda = 0$)

Very high lambda, close to 1



But we need a trade-off …
(because a too high lambda leads as to **underfitting**)

Regularization: E_{RMS} vs $\ln \lambda$



Low lambda → *overfitting*

High lambda → *underfitting*

Polynomial Coefficients

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0 lambda

Very high lambda

	$\ln \lambda = -\infty$	$\ln \lambda = -18$	$\ln \lambda = 0$
$w_0^\star$	0.35	0.35	0.13
$w_1^\star$	232.37	4.74	-0.05
$w_2^\star$	-5321.83	-0.77	-0.06
$w_3^\star$	48568.31	-31.97	-0.05
$w_4^\star$	-231639.30	-3.89	-0.03
$w_5^\star$	640042.26	55.28	-0.02
$w_6^\star$	-1061800.52	41.32	-0.01
$w_7^\star$	1042400.18	-45.95	-0.00
$w_8^\star$	-557682.99	-91.53	0.00
$w_9^\star$	125201.43	72.68	0.01

Other Regularization Tech. for Linear Models

- Ridge regression ($\| \|_2$)
- Lasso ($\| \|_1$)
- Elastic nets (use both $\| \|_1$ and $\| \|_2$)

- We will introduce them later in the course (or in CM course), anyway:
- The *L2 norm* penalizes the square value of the weight and tends to drive all the weights to smaller values.
- On the other hand, the *L1 norm* penalizes the absolute value of the weights and tends to drive some weights to exactly zero (while allowing some weights to be large) → toward feature selection!
  - Unfortunately $\| \|_1$ (absolute value) introduce a non differentiable loss → needs other approaches

Other Improvements (optional)

- Data augmentation:
  - → *Inputs with added noise*: teaching models to ignore irrelevant variations, it contributes to robustness and *regularization*
  - Oversampling to address imbalanced datasets
  - …

- Derived inputs

  a small number of new variables is used in place of the ***x*** inputs, which are a linear combination of ***x***.
  - Principal Component Regression
  - Partial Least Squares

Multi-class task (#) (optional)

Two very simple approaches for multi-class:

- Class 1-of-K rep: {red, green, blue} → (0,0,1), (0,1,0), (1,0,0). → solve 3 linear models
- **OVA:** "one-vs-all": a discriminant function for each class

built on top of real-valued binary classifiers

- train K different binary classifiers, each one trained to distinguish the examples in a single class from the examples in all remaining classes.
- to classify a new example, the K classifiers are run, and the classifier which outputs the largest (most positive) value is chosen.

- AVA: "all-vs-all" = "one-versus-one":
  - each classifier separates a pair of classes. Apply it to all the pairs: K(K-1)
    [How many training?*]
  - to classify a new example, all the classifiers are run, and the winner is the one with the max sum of outputs versus all the other classes **OR** the class with most votes
  - training data set for each classifier is much smaller

Criticism (##) (optional)

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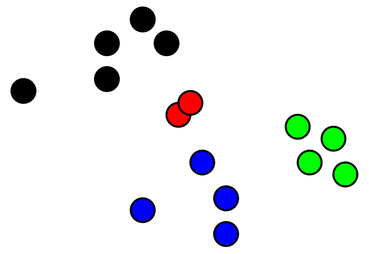
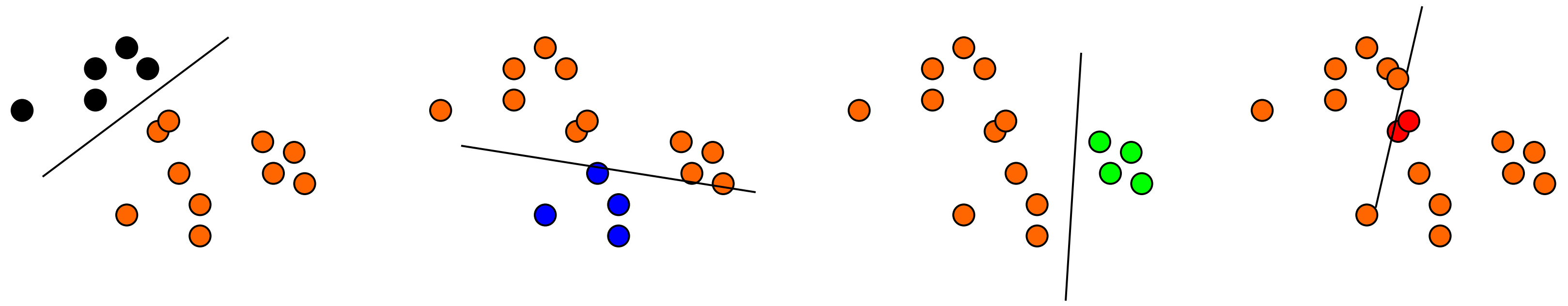
The problem can become not easy





- Masking: classes can be masked by others (for high K)
- A wide array of more sophisticated approaches for multiclass classification exists …
- Some models can deal directly with multi-output

Other learner models for classification (#) (optional)

- Linear Discriminant Analysis (also multi-class)

- Logistic regression
  - $P(y|\mathbf{x})$ starting from modeling the class density as a know density

Extensions: ML Models (pro future) (#)

In ML course (read it later!):

- Perceptron (Rosenblatt 1958, biological inspiration):
  - "minimize (only) misclassifications" algorithm
  - basis for Neural Networks (set of units with layers)
  - Adaptive *basis expansions (phi learned by training)*
    - Feature representation learning in each layer (deep learning concept)
  - Gradient descent approach for learning
- SVM (Vapnik 1996):
  - *regularization* via the concept of maximum margin: Maximize the gap (margin) between the two classes on the training data.
  - enlarge the feature space via *basis expansions* (e.g. polynomials).
- NN and SVM models realize (also) a flexible ***non-linear*** approximation for classification and regression problems

Lessons Learned

- We concretely showed that is possible to *learn* by tuning free parameters ***w***, searching over a continuous space guided by a loss f.
  - How to state/formulate a regression/classification learning problem for a linear model by LMS
  - How to derive the learning algorithm (basic univariate, direct and **gradient** based forms)
  - Two learning algorithms
  - How the model works after training
  - Linear models have limitations (strong language bias)
- How to extend to non-linear modeling (by **LBE**)
- How to implement a **regularization approach** changing the loss f.
- The role of regularization for the **control of the model complexity**

Also useful for your <u>self assessment</u> (try to check if you can answer)

ML Course structure Discussion on Linear Model

In the *file rouge* of ML, 2 main concepts up to now:

- Basis expansion → (implement) more <u>flexibility</u>
- Regularization → (implement) <u>control of complexity</u>

- The cases of the *linear models* provided an *instance* routed in the classical mathematical approaches but the we will find again <u>these concepts</u>, by different models and implemented in different/similar forms, in the modern ML (e.g. for NN & SVM in our course)!

- Now we move on the other extreme, toward a very flexible approach (K-nn)

Bibliography: Linear and K-nn (I)

- Hastie, Tibshirani, Friedman, The Elements of Statistical Learning, Springer Verlag, 2001-2017 (*check the new Ed.s*): **chap 2**

  (note: it exists an on-line pdf version)

- Mitchell:
  - Linear model and LMS alg.: chap 4.4
  - K-nn: **chap 8**

- Haykin (2nd edition):
  - Linear model and LMS alg.: chap 3 up to 3.7

    [details on Newton and Gauss-Newton methods are not strictly needed]

- Haykin (3rd edition):
  - Linear model and LMS alg.: chap 3

    [details on Newton and Gauss-Newton and other advanced approaches are not strictly needed]

Bibliography: Linear and K-nn (II)

- Moroever…
- Further readings (not mandatory!):

  – Gently introduction to linear models:

    AIMA (Russel, Norvig, Artificial Intelligence: A Modern Approach), ed .3: **chap 18.6** (18.6.1,18.6.2,18.6.3)

  – To go in deep for **Linear least squares**

  You can start from www resource as (With nice examples):

  https://en.wikipedia.org/wiki/Linear_least_squares_%28mathematics%29

  – **LS in general**

  http://en.wikipedia.org/wiki/Least_squares

For information

Alessio Micheli

micheli@di.unipi.it

www.di.unipi.it/groups/ciml

Dipartimento di Informatica
Università di Pisa - Italy

**Computational Intelligence &
Machine Learning Group**