DM573 INTRODUCTION TO COMPUTER SCIENCE

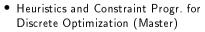
#### Classical Machine Learning: Linear Regression and Neural Networks

Marco Chiarandini

Department of Mathematics & Computer Science University of Southern Denmark

### About Me (https://imada.sdu.dk/~marco)

- Marco Chiarandini, Asc. Prof. in CS at IMADA
  - Master in Electronic Engineering, University of Udine, Italy.
  - Ph.D. in Computer Science at the Darmstadt University of Technology, Germany.
  - Post-Doc researcher at IMADA
  - Visiting Researcher, Institute of Interdisciplinary Research and Development in Artificial Intelligence, Université Libre de Bruxelles.
- Research Interests
  - Optimization (Operations Research) | Scheduling, Timetabling, Routing
  - Artificial Intelligence | Heuristics, Metaheuristics, Machine Learning
- Current Teaching in CS
  - Linear Algebra and Applications (Bachelor)
  - Linear and Integer Programming (Master)
  - Mathematical Optimization at Work (Master)



• Artificial Intelligence (Master)



Machine Learning

Group photo Cale No right): Handley, Marco Chiarandro, Anhar Zimdi, Pelan Schneider Hamp, Neri Goegabeur, Hans Christian Pelensen, Janua Hendeled Saji, Bohard Höttger, squarting The Zhang, Pernando Caleborn, Jing Qin, Agoyan Khardi La No. Outline

Machine Learning Linear Regression Artificial Neural Networks

1. Machine Learning

- 2. Linear Regression Basics Extensions
- 3. Artificial Neural Networks Single-layer Networks Multi-layer Networks

Outline

Machine Learning Linear Regression Artificial Neural Networks

#### 1. Machine Learning

#### 2. Linear Regression Basics Extensions

3. Artificial Neural Networks Single-layer Networks Multi-layer Networks

### Machine Learning

An agent is learning if it improves its performance on future tasks after making observations about the world.

Why learning instead of directly programming?

Three main situations:

- the designer cannot anticipate all possible conditions (eg, navigate in a maze)
- the designer cannot anticipate all changes over time (eg, stock price prediction)
- the designer has no idea how to program a solution (eg, face recognition)

### Forms of Machine Learning

#### • Supervised learning (this week)

the agent is provided with a series of examples with correct responses and then it generalizes from those examples to develop an algorithm that applies to new cases.

Eg: learning to recognize a person's handwriting or voice, to distinguish between junk and welcome email, or to identify a disease from a set of symptoms.

#### • Unsupervised learning (with Melih Kandemir)

Correct responses are not provided, but instead the agent tries to identify similarities between the inputs so that inputs that have something in common are categorised together.

Eg. Clustering

#### • Reinforcement learning:

the agent is given a general rule to judge for itself when it has succeeded or failed at a task during trial and error.

Sequence of decisions and assessment only at the end. The agent acts autonomously and it learns to improve its behavior over time.

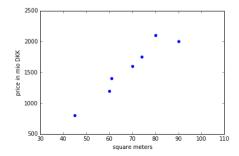
Eg: learning how to play a game like backgammon (success or failure is easy to define)

### Supervised Learning

- inputs that influence outputs inputs ≡ independent <u>variables</u>, known, predictors, features outputs ≡ dependent <u>variables</u>, unknown, responses
- goal: predict value of outputs
- supervised: we provide data set with exact answers

#### **Example:** House price prediction:

Size in m <sup>2</sup>	Price in K DKK
45	800
60	1200
61	1400
70	1600
74	1750
80	2100
90	2000

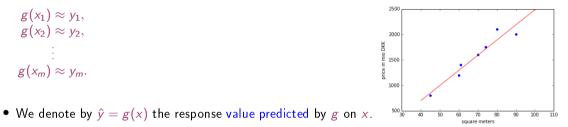


### Supervised Learning Problem

#### Machine Learning Linear Regression Artificial Neural Networks

**Given:** *m* points (pairs of numbers)  $\{(x_1, y_1), (x_2, y_2), ..., (x_m, y_m)\}$ 

**Task:** determine a model, aka a function g(x) of a simple form, such that



• The type of function (linear, polynomial, exponential, logistic, blackbox) may be suggested by the nature of the problem (the underlying physical law, the type of response). It is a form of prior knowledge.

In other words, we are fitting a function to the data

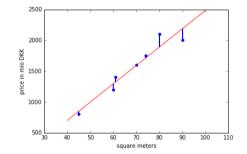
Machine Learning Linear Regression Artificial Neural Networks

### House Price Example

Size in m <sup>2</sup>	Price in M DKK
45	800
60	1200
61	1400
70	1600
74	1750
80	2100
90	2000

Training data set

$\begin{bmatrix} (x_1, y_1) \\ (x_2, y_2) \end{bmatrix}$	$\rightsquigarrow$	(45,800) (60,1200) (61,1400) (70,1600) (74,1750) (80,2100)
$\left\lfloor (x_m, y_m) \right\rfloor$		(80, 2100) (90, 2000)



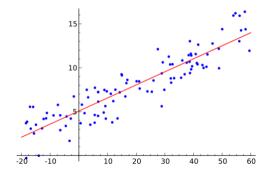
g(x) = -489.76 + 29.75x				
X	ŷ	У		
45	848.83	800		
60	1295.03	1200		
61	1324.78	1400		
70	1592.5	1600		
74	1711.48	1750		
80	1889.96	2100		
90	2187.43	2000		

### Types of Supervised Learning

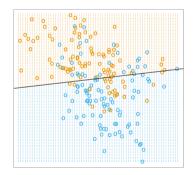
#### Machine Learning Linear Regression Artificial Neural Networks

#### Regression problem:

variable to predict is continuous/quantitative



#### Classification problem: variable to predict is discrete/qualitative



### Example: k-Nearest Neighbors

#### **Regression task**

Given:  $(x_1, y_1), \ldots, (x_m, y_m)$ Task: predict the response value  $\hat{y}$  for a new input x

Idea: Let  $\hat{y}(x)$  be the average of the k closest points:

- 1. Sort the data points  $(x_1, y_1), \ldots, (x_m, y_m)$  in increasing order of distance from x in the input space, ie,  $d(x_i, x) = |x_i x|$ .
- 2. Set the k closest points in  $N_k(x)$ .
- 3. Return the average of the y values of the k data points in  $N_k(x)$ .

In mathematical notation:

$$\hat{y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i = g(x)$$

It requires the definition of a distance metric, eg, Euclidean distance

### Example: k-Nearest Neighbors

#### **Classification task**

Given:  $(x_1, y_1), \ldots, (x_m, y_m)$ Task: predict the class  $\hat{y}$  for a new input x.

ldea: let the k closest points vote and the most popular class decide

- 1. Sort the data points  $(x_1, y_1), \ldots, (x_m, y_m)$  in increasing order of distance from  $\vec{x}$  in the input space, ie,  $d(\vec{x}_i, \vec{x}) = |x_i x|$ .
- 2. Set the k closest points in  $N_k(x)$ .
- 3. Return the class that is most represented in the k data points of  $N_k(x)$ .

In mathematical notation:

$$\hat{y}(x) = \hat{G}(x) = \operatorname{argmax}_{G \in \mathcal{G}} \sum_{x_i \in N_k(x) | y_i = G} \frac{1}{k}$$



Outline

Machine Learning Linear Regression Artificial Neural Networks

#### 1. Machine Learning

#### 2. Linear Regression

Basics Extensions

#### Artificial Neural Networks Single-layer Networks Multi-layer Networks

Outline

Machine Learning Linear Regression Artificial Neural Networks

1. Machine Learning

### 2. Linear Regression Basics

3. Artificial Neural Networks Single-layer Networks Multi-layer Networks

## Simple Linear Regression

Linear Regression with One Variable

- Let the set of models we can use (hypothesis set)  $\mathcal{H}$  be made by linear functions y = ax + b. We search in  $\mathcal{H}$  the line that fits best the data:
  - We evaluate each line by the distance of the points (x<sub>1</sub>, y<sub>1</sub>),..., (x<sub>m</sub>, y<sub>m</sub>) from the line in the vertical direction (the y-direction): Each point (x<sub>i</sub>, y<sub>i</sub>), i = 1..m would have predicted y<sub>i</sub>-value ŷ = ax<sub>i</sub> + b in the fitted line. Hence, the distance for (x<sub>i</sub>, y<sub>i</sub>) is |y<sub>i</sub> - ax<sub>i</sub> - b|.
  - 2. We define as loss (or error, or cost) function the sum of the squares of the distances from the given points  $(x_1, y_1), \ldots, (x_m, y_m)$ :

 $\hat{L}(a,b) = \sum_{i=1}^{m} (y_i - ax_i - b)^2$  sum of squared errors

 $\hat{L}$  depends on a and b, while the values  $x_i$  and  $y_i$  are given by the data available.

3. We look for the coefficients *a* and *b* that give the line of minimal loss (here, sum of squared errors, hence also known as method of least squares).

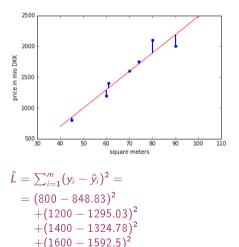
Machine Learning **Linear Regression** Artificial Neural Networks

### House Price Example

Training data set

$$\begin{bmatrix} (x_1, y_1) \\ (x_2, y_2) \\ \vdots \\ \vdots \\ (x_m, y_m) \end{bmatrix} \Longrightarrow \begin{bmatrix} (45, 800) \\ (60, 1200) \\ (61, 1400) \\ (70, 1600) \\ (74, 1750) \\ (80, 2100) \\ (90, 2000) \end{bmatrix}$$

g(x) = 29.75x - 489.76



$$(1750 - 1711.48)^2$$
  
 $(2100 - 1889.96)^2$   
 $(2000 - 2187.43)^2 = 97858.86$ 

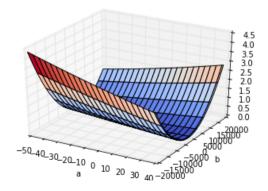
++++++

### House Price Example

For

f(x) = b + ax $\hat{L}(a, b) = \sum_{i=1}^{m} (y_i - \hat{y}_i)^2$  $= (800 - b - 45 \cdot a)^2$  $+(1200 - b - 60 \cdot a)^2$  $+(1400 - b - 61 \cdot a)^2$  $+(1600 - b - 70 \cdot a)^2$  $+(1750 - b - 74 \cdot a)^2$  $+(2100 - b - 80 \cdot a)^{2}$  $+(2000 - b - 90 \cdot a)^{2}$  Machine Learning Linear Regression Artificial Neural Networks

Plot of  $\hat{L}(a, b)$  as a function of a and b:



### **Analytical Solution**

#### Theorem (Closed form solution)

The value of the coefficients of the line that minimizes the sum of squared errors for the given points can be expressed in closed form as a function of the input data:

$$a=rac{\sum_{i=1}^m (x_i-ar{x})(y_i-ar{y})}{\sum_{i=1}^m (x_i-ar{x})^2} \qquad \qquad b=ar{y}-aar{x}$$

where:

$$\bar{x} = \frac{1}{m} \sum_{i=1}^{m} x_i \qquad \qquad \bar{y} = \frac{1}{m} \sum_{i=1}^{m} y_i$$

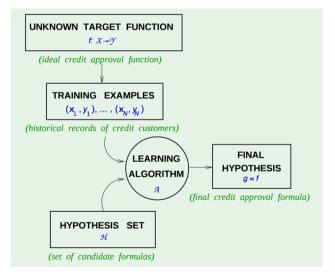
Proof not in the curriculum of DM573:

[Idea: use partial derivaties to obtain a linear system of equations that can be solved analytically]

Learning = Representation + Evaluation + Optimization

- Representation: formal language that the computer can handle. Corresponds to choosing the set of functions that can be learned, ie. the hypothesis set of the learner. How to represent the input, that is, which input variables to use.
- Evaluation: definition of a loss function
- Optimization: a method to search among the learners in the language for the one minimizing the loss.

### Learning model



Outline

Machine Learning Linear Regression Artificial Neural Networks

1. Machine Learning

#### 2. Linear Regression Basics Extensions

 Artificial Neural Networks Single-layer Networks Multi-layer Networks

#### Multiple Linear Regression Linear Regression with Multiple Variables

There can be several input variables (aka features). In practice, they improve prediction.

Size in m <sup>2</sup>	# of rooms		Price in M DKK
45	2	• • •	800
60	3		1200
61	2		1400
70	3		1600
74	3		1750
80	3		2100
90	4		2000
:	:		

In vector notation:

$$\begin{bmatrix} (\vec{x}_1, y_1) \\ (\vec{x}_2, y_2) \\ \vdots \\ (\vec{x}_m, y_m) \end{bmatrix}$$

$$\vec{x}_i = \begin{bmatrix} x_{i1} & x_{i2} & \dots & x_{ip} \end{bmatrix}$$
$$i = 1, 2, \dots, m$$

## k-Nearest Neighbors Revisited

Machine Learning **Linear Regression** Artificial Neural Networks

Case with multiple input variables

#### **Regression task**

Given:  $(\vec{x_1}, y_1), \dots, (\vec{x_m}, y_m)$ Task: predict the response value  $\hat{y}$  for a new input  $\vec{x}$ 

Idea: Let  $\hat{y}(\vec{x})$  be the average of the k closest points:

- 1. Sort the data points  $(\vec{x_1}, y_1), \dots, (\vec{x_m}, y_m)$  in increasing order of distance from x in the input space, ie,  $d(\vec{x_i}, \vec{x}) = \sqrt{\sum_j (x_{ij} x_j)^2}$ .
- 2. Set the k closest points in  $N_k(\vec{x})$ .
- 3. Return the average of the y values of the k data points in  $N_k(\vec{x})$ .

In mathematical notation:

$$\hat{y}(ec{x}) = rac{1}{k} \sum_{ec{x}_i \in N_k(ec{x})} y_i = g(ec{x})$$

It requires the redefinition of the distance metric, eg, Euclidean distance

## k-Nearest Neighbors Revisited

Case with multiple input variables

#### **Classification task**

Given:  $(\vec{x_1}, y_1), \dots, (\vec{x_m}, y_m)$ Task: predict the class  $\hat{y}$  for a new input  $\vec{x}$ .

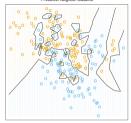
ldea: let the k closest points vote and the most popular class decide

- 1. Sort the data points  $(\vec{x}_1, y_1), \dots, (\vec{x}_m, y_m)$  in increasing order of distance from  $\vec{x}$  in the input space, ie,  $d(\vec{x}_i, \vec{x}) = \sqrt{\sum_j (x_{ij} x_j)^2}$ .
- 2. Set the k closest points in  $N_k(\vec{x})$ .
- 3. Return the class that is most represented in the k data points of  $N_k(\vec{x})$ .

Mathematical notation omitted.

Machine Learning

Linear Regression



### Linear Regression Revisited

Representation of hypothesis space if only one variable (feature):

 $h(x) = \theta_0 + \theta_1 x$  linear function

if there is another input variable (feature):

 $h(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 = h(\vec{\theta}, \vec{x})$ 

for conciseness, defining  $x_0 = 1$ .

$$h(\vec{\theta}, \vec{x}) = \vec{\theta} \cdot \vec{x} = \sum_{j=0}^{2} \theta_j x_j \qquad \qquad h(\vec{\theta}, \vec{x}_i) = \vec{\theta} \cdot \vec{x}_i = \sum_{j=0}^{p} \theta_j x_{ij}$$

Notation:

- p num. of features,  $\vec{ heta}$  vector of p+1 coefficients,  $heta_0$  is the bias
- $x_{ij}$  is the value of feature j in sample i, for i = 1..m, j = 0..p
- y<sub>i</sub> is the value of the response in sample i

#### Machine Learning Linear Regression Artificial Neural Networks

### Linear Regression Revisited

#### Evaluation

loss function for penalizing errors in prediction. Most common is squared error loss:

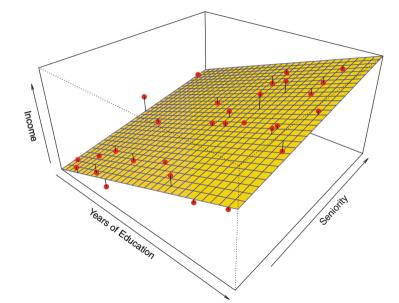
$$\hat{L}(\vec{\theta}) = \sum_{i=1}^{m} \left( y_i - h(\vec{\theta}, \vec{x}_i) \right)^2 = \sum_{i=1}^{m} \left( y_i - \sum_{j=0}^{p} \theta_j x_{ij} \right)^2 \qquad \text{loss function}$$

#### Optimization

# $\min_{\vec{\theta}} \hat{L}(\vec{\theta})$

Although not shown here, the optimization problem can be solved analytically and the solution can be expressed in closed form.

### Multiple Variables: Example



### **Polynomial Regression**

It generalizes the linear function h(x) = ax + b to a polynomial of degree k

#### Representation

 $h(x) = poly(\vec{\theta}, x) = \theta_0 + \theta_1 x + \dots + \theta_k x^k$ 

where  $k \leq m-1$  (*m* number of training samples). Each term acts like a different variable in the previous case.

 $\vec{x} = \begin{bmatrix} 1 \ x \ x^2 \ \dots \ x^k \end{bmatrix}$ 

Evaluation Again, we use the loss function defined as the sum of squared errors:

$$\hat{L}(\vec{\theta}) = \sum_{i=1}^{m} \left( y_i - \operatorname{poly}(\vec{\theta}, \vec{x}_i) \right)^2 = \sum_{i=1}^{m} \left( y_i - \theta_0 - \theta_1 x_i - \dots - \theta_k x_i^k \right)^2$$

### **Polynomial Regression**

Machine Learning Linear Regression Artificial Neural Networks

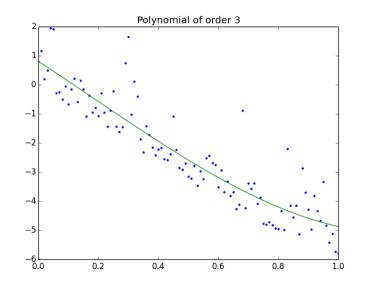
#### **Optimization**:

$$\min_{\vec{\theta}} L(\vec{\theta}) = \min \sum_{i=1}^{m} \left( y_i - \text{poly}(\vec{\theta}, \vec{x}_i) \right)^2$$
$$= \min \sum_{i=1}^{m} \left( y_i - \theta_0 - \theta_1 x_i - \dots - \theta_k x_i^k \right)^2$$

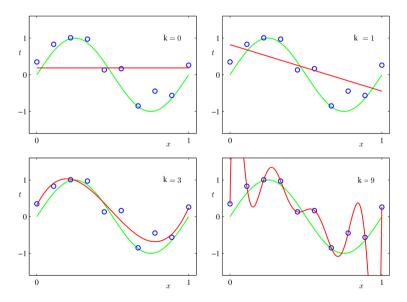
this is a function of k + 1 coefficients  $\theta_0, \dots, \theta_k$ .

Although not shown here, also this optimization problem can be solved analytically and the solution can be expressed in closed form.

### Polynomial Regression: Example



### Overfitting



### **Training and Assessment**

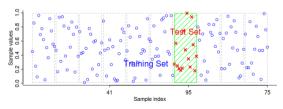
Avoid peeking: use different data for different tasks:

Training + Validation + Test data

- Coefficients learned on Training data
- Coefficients and Models compared on Validation data
- Final assessment on Test data

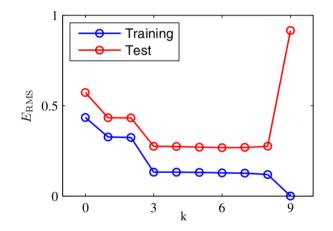
Techniques:

- Holdout method
- If small data:
  k-fold cross validation



### **Model Comparison**

k number of coefficients, eg, in polynomial regression the order of the polynomial  $E_{RMS}$  root mean squares of errors



Outline

Machine Learning Linear Regression Artificial Neural Networks

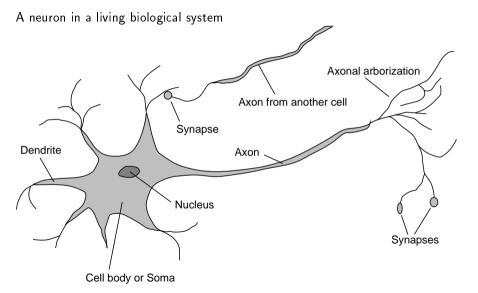
1. Machine Learning

2. Linear Regression Basics Extensions

#### 3. Artificial Neural Networks

Single-layer Networks Multi-layer Networks

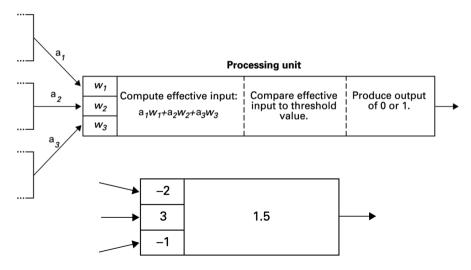
### The Biological Neuron



35

### McCulloch-Pitts "unit" (1943)

#### Activities within a processing unit



# Artificial Neural Networks

Basic idea:

- Artificial Neuron
  - Each input is multiplied by a weighting factor.
  - Output is 1 if sum of weighted inputs exceeds the threshold value; 0 otherwise.
- Network is programmed by adjusting weights using feedback from examples.

"**The** neural network" does not exist. There are different paradigms for neural networks, how they are trained and where they are used.

#### Generalization of McCulloch-Pitts unit

1.5

Machine Learning Linear Regression Artificial Neural Networks

Let  $a_j$  be the *j*th input to a node: Then, the output of the unit is 1 when:

 $-2a_1 + 3a_2 - 1a_3 \ge 1.5$ 

or equivalently when:

 $-1.5 - 2a_1 + 3a_2 - 1a_3 \ge 0$ 

and, defining  $a_0 = -1$ , when:

$$1.5a_0 - 2a_1 + 3a_2 - 1a_3 \ge 0$$

In general, for a neuron i and weights  $w_{ii}$  on arcs ji, the neuron outputs 1 when:

 $\sum_{j=0}^p w_{ji}a_j \ge 0,$ 

-2

3

-1

and 0 otherwise. (We will assume the zeroth input  $a_0$  to always be -1.)

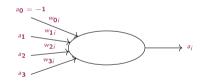
#### Machine Learning Linear Regression Artificial Neural Networks

# Generalization of McCulloch-Pitts unit

Hence, we can draw the artificial neuron unit *i*:



also in the following way:



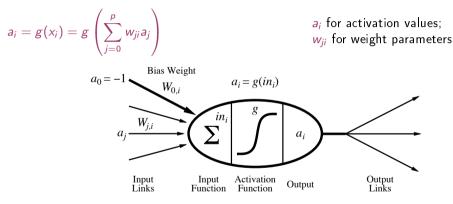
where now the output  $a_i$  is 1 when the linear combination of the inputs:

$$x_i = \sum_{j=0}^p w_{ji}a_j = \vec{w}_i \cdot \vec{a} \qquad \qquad \vec{a} = \begin{bmatrix} -1 & a_1 & a_2 & \cdots & a_p \end{bmatrix}$$

is > 0.

# Generalization of McCulloch-Pitts unit

Output is a function of weighted inputs. At unit *i* 



Changing the weight  $w_{0i}$  moves the threshold location

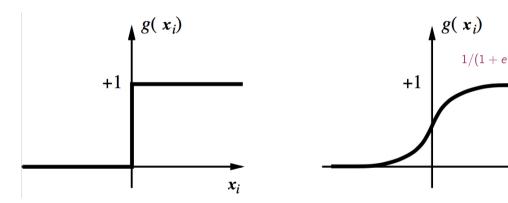
A gross oversimplification of real neurons, but its purpose is to develop understanding of what networks of simple units can do Machine Learning Linear Regression Artificial Neural Networks

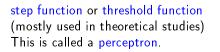
#### **Activation functions**

#### Non linear activation functions

Machine Learning Linear Regression Artificial Neural Networks

 $x_i$ 





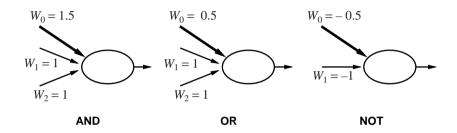
continuous activation function, e.g., sigmoid function  $1/(1 + e^{-x_i})$ This is called a sigmoid neuron.

#### Machine Learning Linear Regression Artificial Neural Networks

# **Activation functions**

Nane	Plot	Equation	Derivative
Identity	/	f(x) = x	f'(x) = 1
Binary step		$f(x) = \begin{cases} 0 & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x \neq 0 \\ ? & \text{for } x = 0 \end{cases}$
Logistic (a.k.a Soft step)		$f(x) = \frac{1}{1 + e^{-x}}$	f'(x) = f(x)(1 - f(x))
l'anH	$\square$	$f(x) = \tanh(x) = \frac{2}{1 + e^{-2x}} - 1$	$f'(x) = 1 - f(x)^2$
ArcTan		$f(x) = \tan^{-1}(x)$	$f'(x) = \frac{1}{x^2 + 1}$
Rectified Linear Unit (ReLU) -		$f(x) = \begin{cases} 0 & \text{for } x < 0 \\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} 0 & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
Parameteric Rectified Linear Unit (PReLU) <sup>[2]</sup>		$f(x) = \begin{cases} \alpha x & \text{for } x < 0\\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} \alpha & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
Exponential Linear Unit (ELU) <sup>[3]</sup>	/	$f(x) = \begin{cases} \alpha(e^x - 1) & \text{for } x < 0\\ x & \text{for } x \ge 0 \end{cases}$	$f'(x) = \begin{cases} f(x) + \alpha & \text{for } x < 0\\ 1 & \text{for } x \ge 0 \end{cases}$
SoftPlus		$f(x) = \log_e(1 + e^x)$	$f'(x) = \frac{1}{1 + e^{-x}}$

# Implementing logical functions



But not every Booelan function can be implemented by a single perceptron. Exclusive-or circuit cannot be processed (see next slide).

McCulloch and Pitts (1943) first mathematical model of neurons. Every Boolean function can be implemented by combining this type of units.

Rosenblatt (1958) showed how to learn the parameters of a perceptron. Minsky and Papert (1969) lamented the lack of a mathematical rigor in learning in multilayer networks.

# Expressiveness of single perceptrons

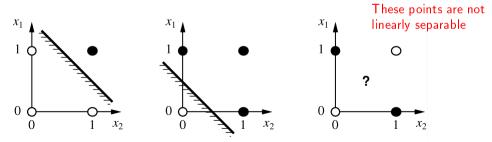
Machine Learning Linear Regression Artificial Neural Networks

Consider a perceptron with g step function At unit i the output is 1 when:

$$\sum_{j=0}^{p} w_{ji} x_j > 0$$
 or  $ec{w}_i \cdot ec{x} > 0$ 

Hence, it represents a linear separator in input space:

- line in 2 dimensions
- plane in 3 dimensions
- hyperplane in multidimensional space



## Network structures

Structure (or architecture): definition of number of nodes, interconnections and activation functions g (but not weights).

• Feed-forward networks:

no cycles in the connection graph

- single-layer networks (no hidden layer)
- multi-layer networks (one or more hidden layer)

Feed-forward networks implement functions, have no internal state

• Recurrent networks:

connections between units form a directed cycle.

- internal state of the network exhibit dynamic temporal behavior (memory, apriori knowledge)
- Hopfield networks for associative memory

#### Feed-Forward Networks – Use

Machine Learning Linear Regression Artificial Neural Networks

Neural Networks are used in classification and regression

- Boolean classification:
  - value over 0.5 one class
  - value below 0.5 other class
- *k*-way classification
  - divide single output into k portions
  - k separate output units
- continuous output
  - identity or linear activation function in output unit

Outline

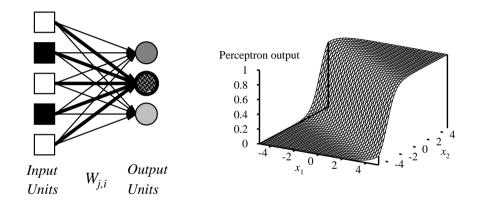
Machine Learning Linear Regression Artificial Neural Networks

1. Machine Learning

2. Linear Regression Basics Extensions

3. Artificial Neural Networks Single-layer Networks Multi-layer Networks

#### Single-layer NN



Output units all operate separately—no shared weights Adjusting weights moves the location, orientation, and steepness of cliff Outline

Machine Learning Linear Regression Artificial Neural Networks

1. Machine Learning

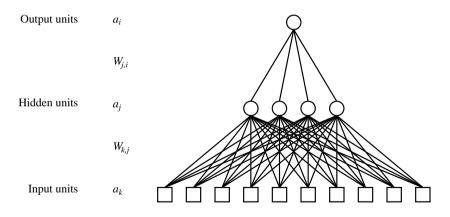
2. Linear Regression Basics Extensions

3. Artificial Neural Networks Single-layer Networks Multi-layer Networks

#### Machine Learning Linear Regression Artificial Neural Networks

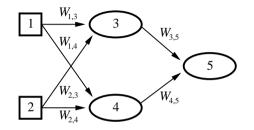
## **Multilayer Networks**

Layers are usually fully connected; number of hidden units typically chosen by hand



(a for activation values; W for weight parameters)

#### Multilayer Feed-forward



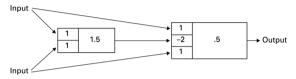
Feed-forward network = a parametrized family of nonlinear functions:

$$\begin{aligned} a_5 &= g(w_{3,5} \cdot a_3 + w_{4,5} \cdot a_4) \\ &= g(w_{3,5} \cdot g(w_{1,3} \cdot a_1 + w_{2,3} \cdot a_2) + w_{4,5} \cdot g(w_{1,4} \cdot a_1 + w_{2,4} \cdot a_2) \end{aligned}$$

Adjusting weights changes the function: do learning this way! Most methods are based on the "gradient descent" technique, which uses differentiation of cost functions to find weight adjustements, which improve the output.

#### Neural Network with two layers

What is the output of this two-layer network on the input  $a_1 = 1$ ,  $a_2 = 0$  using step-functions as activation functions?



The input of the first neuron (node 3) is:

$$\sum_{j} w_{j3} a_{j} = w_{13} \cdot a_{1} + w_{23} \cdot a_{2} = 1 \cdot 1 + 1 \cdot 0 = 1$$

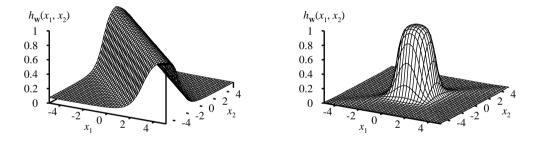
which is < 1.5, hence the output of node 3 is  $a_3 = g(\sum_j w_{j3}a_j) = 0$ . The input to the second neuron (node 4) is:

$$\sum_{j} w_{j4} a_{j} = w_{14} \cdot a_{1} + w_{34} \cdot a_{3} + w_{24} \cdot a_{24} = 1 \cdot 1 - 2 \cdot 0 + 1 \cdot 0 = 1$$

which is > 0.5, hence the output of the node 4 is  $a_3 = g(\sum_i w_{j4}a_j) = 1$ .

#### Expressiveness of MLPs

#### All continuous functions with 2 layers, all functions with 3 layers



Combine two opposite-facing threshold functions to make a ridge Combine two perpendicular ridges to make a bump Add bumps of various sizes and locations to fit any surface Proof requires exponentially many hidden units (Minsky & Papert, 1969)

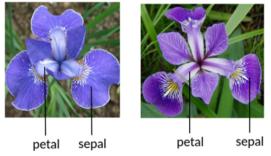
#### Numerical Example

The Fisher's iris flower data set: data to quantify the morphologic variation of Iris flowers of two related species.

50 samples from each of two species of Iris (Iris setosa and Iris versicolor). Four features were measured from each sample: the length and the width of the petals and sepals, in centimeters.

iris setosa

#### iris versicolor

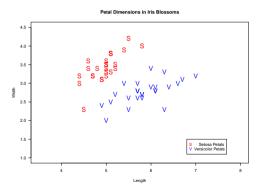


Source: Medium

#### Numerical Example

#### **Binary Classification**

In this case, preliminary observations show that two features, namely width and length of the petals, can be enough for the task of classifying: iris setosa and iris versicolor.



#### iris.data:

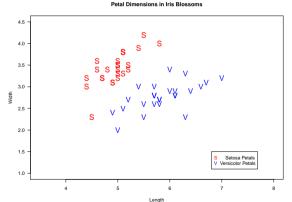
Petal.Length	Petal.Width	Species	id
4.9	3.1	setosa	0
5.5	2.6	versicolor	1
5.4	3.0	versicolor	1
6.0	3.4	versicolor	1
5.2	3.4	setosa	0
5.8	2.7	versicolor	1

#### Two classes encoded as 0/1

#### **Perceptron Learning**

Machine Learning Linear Regression Artificial Neural Networks

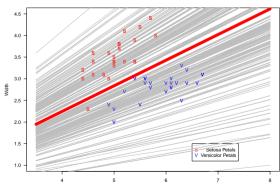
In 2D, the decision surface of a linear combination of inputs gives:  $\vec{w} \cdot \vec{x} = \text{constant}$ , a line! Training the perceptron  $\equiv$  searching the line that separates the points at best.



engtn

#### **Perceptron Learning**

We try different weight values moving towards the values that minimize the misprediction of the training data: the red line. (Gradient descent algorithm) (Rosenblatt, 1958: the algorithm converges)



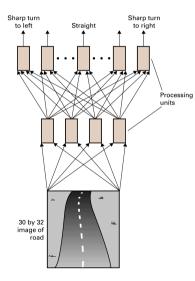
I onnt

grey lines: lines tried during the gradient descent algorithm red line: the final line indicated by the gradient descent algorithm

Petal Dimensions in Iris Blossoms

Machine Learning Linear Regression Artificial Neural Networks

# A Practical Example



# Deep learning $\equiv$ convolutional neural networks $\equiv$ multilayer neural network with structure on the arcs

Example: one layer only for image recognition, another for action decision.

The image can be subdivided in regions and each region linked only to a subset of nodes of the first layer.

# Summary

1. Machine Learning

2. Linear Regression Basics Extensions

3. Artificial Neural Networks

Single-layer Networks Multi-layer Networks Machine Learning Linear Regression Artificial Neural Networks

Deep learning has repeatedly demonstrated its superior performance with respect to classical ML on a wide variety of tasks including speech, natural language, vision, and playing games

