UNIVERSITÀ
DEGLI STUDI
DI BERGAMO

Dipartimento
di Ingegneria Gestionale,
dell'Informazione e della Produzione

Lesson 2.

Linear regression

DATA SCIENCE AND
AUTOMATION COURSE

MASTER DEGREE SMART
TECHNOLOGY ENGINEERING

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Outline

1. Components of learning
2. Linear regression
3. Least squares
4. Gradient descent

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1. **Components of learning**

2. Linear regression

3. Least squares

4. Gradient descent

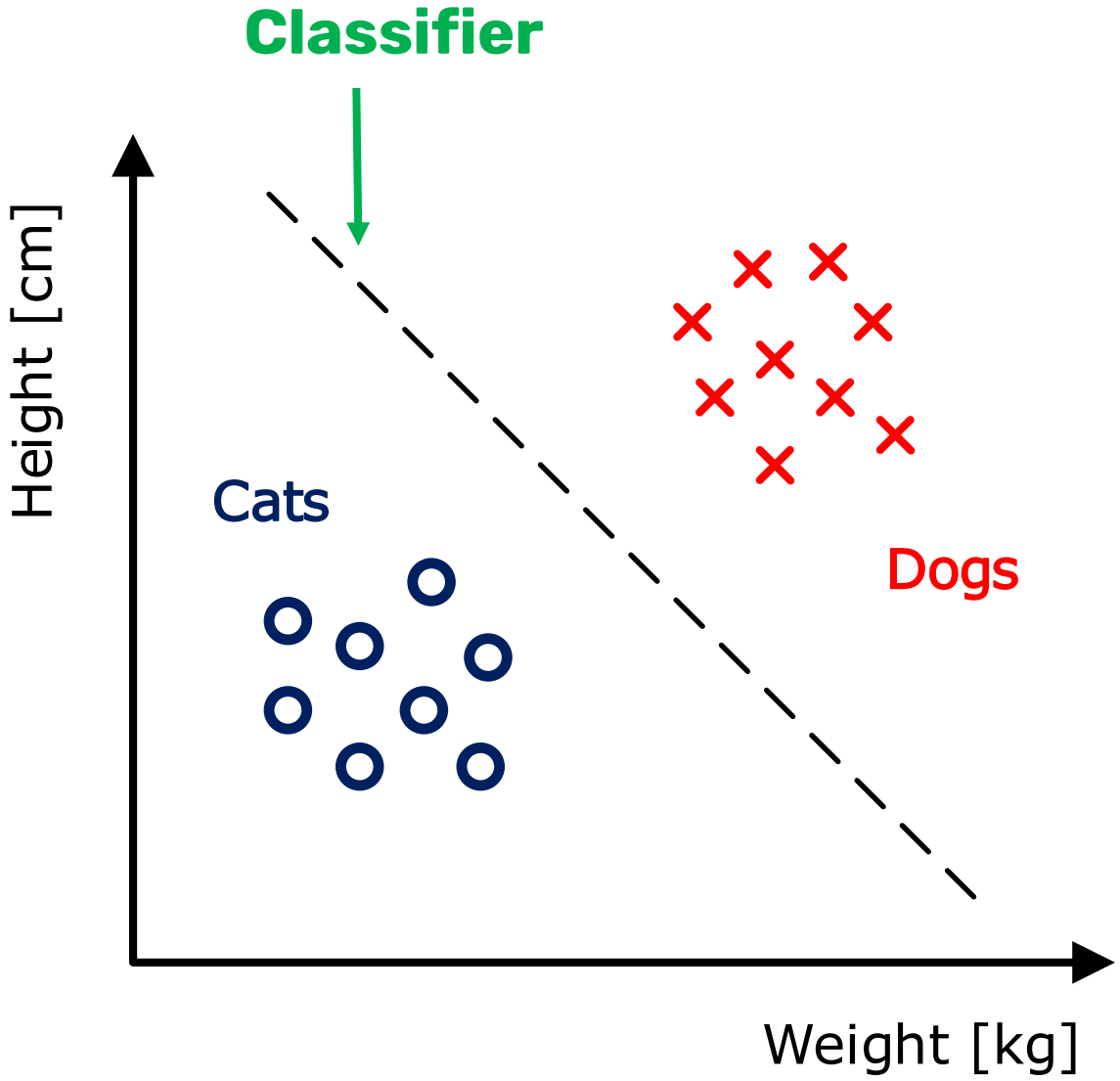
Components of learning (in general)

- Input: $\boldsymbol{x}$ (e-mail textual content) → each dimension is some e-mail attribute
- Output: y (spam / not spam?) → the decision that we have to take in the end
- Target function: $f: \mathcal{X} \to \mathcal{Y}$ (Ideal spam filter formula) → unknown, we have to learn it
- Data: $\mathcal{D} = \{(\boldsymbol{x}(1), y(1)), \ldots, (\boldsymbol{x}(N), y(N))\}$ (historical records of e-mail examples)
  - ✓ Each **feature vector** $\boldsymbol{x}$ consists of different **regressors** or **features**, i.e. information used to predict the output variable
- Hypothesis: $g: \mathcal{X} \to \mathcal{Y}, g \in \mathcal{H}$ (formula to be used) → g is an **approximation** of f

$\mathcal{H}$ is called the **Hypothesis space**. This, together with the **Learning algorithm**, form the **learning model**

Supervised learning

- The “correct answer” (output label) y is given
- Predict y from a set of inputs $\boldsymbol{x} \in \mathbb{R}^{d \times 1}$
- **Regression:** predict a continuous output $y \in \mathbb{R}$ **(real value)**
- **Classification:** predict a discrete categorical output $y \in \{1,2,\dots,C\}$ **(class)**



Example: house prices regression

- Suppose we want to find a linear function which relates the **measured** regressors x_1, x_2, x_3, x_4 with the **observed** output y

Single feature x_3

Output variable y

Number of observations N

Size $[\text{feet}^2]$	Number of bedrooms	Number of floors	Age of home [year]	Price [$]
2104	5	1	45	$4.60 \cdot 10^5$
1416	3	2	40	$2.32 \cdot 10^5$
1534	2	1	30	$3.15 \cdot 10^5$
⋮	⋮	⋮	⋮	⋮
↓	↓	↓	↓	↓
x_1	x_2	x_3	x_4	y

Single observation (feature vector) x

- The number of rows is the number of data points (also known as number of observations) N
- The i-th observation is the vector $\boldsymbol{x}(i) = [x_1(i) \;\; x_2(i) \;\; x_3(i) \;\; x_4(i)]^T \in \mathbb{R}^{4x1}$
- Each feature vector $\boldsymbol{x}$ has associated a response $y \in \mathbb{R}$ that we want to predict for new observations $\boldsymbol{x}^*$

Example: house prices classification

- The components of the features vector are the same. The difference lies in the response variable, which now is a **class** (categorical data type) and not a real value

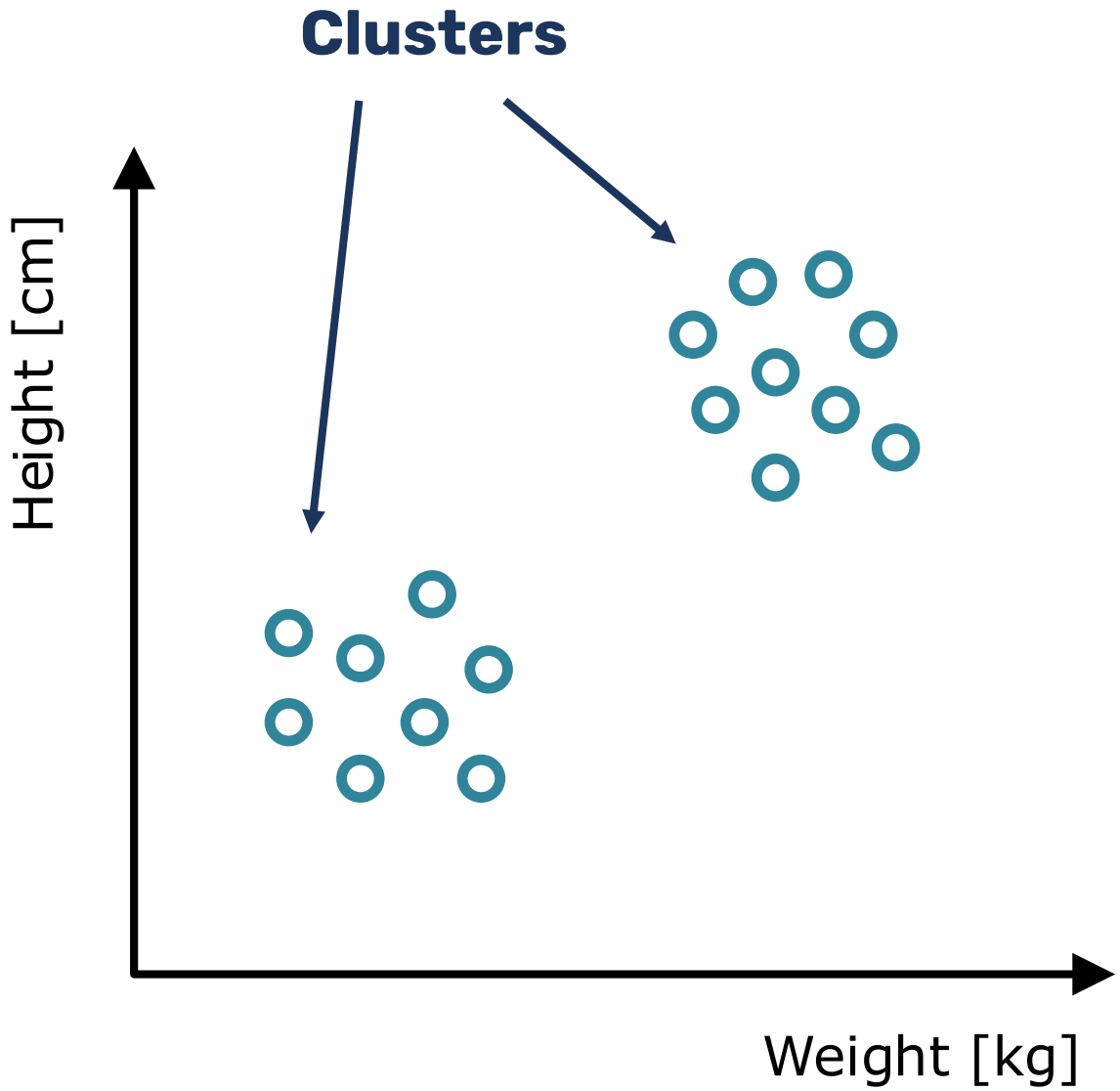
- Suppose that instead of the price value in dollars, we want to classify houses as **expensive** *(class* $y = 1$*)* or **cheap** *(class* $y = 0$*)*

Size $[\text{feet}^2]$	Number of bedrooms	Number of floors	Age of home [year]	Price [class]
2104	5	1	45	1
1416	3	2	40	0
1534	2	1	30	1
⋮	⋮	⋮	⋮	⋮
↓	↓	↓	↓	↓
x_1	x_2	x_3	x_4	y

- The point $\boldsymbol{x}$ could be classified to class $y = 1$ if *the probability of* $\boldsymbol{x}$ *to belong to class 1 is* ≥ 0.5

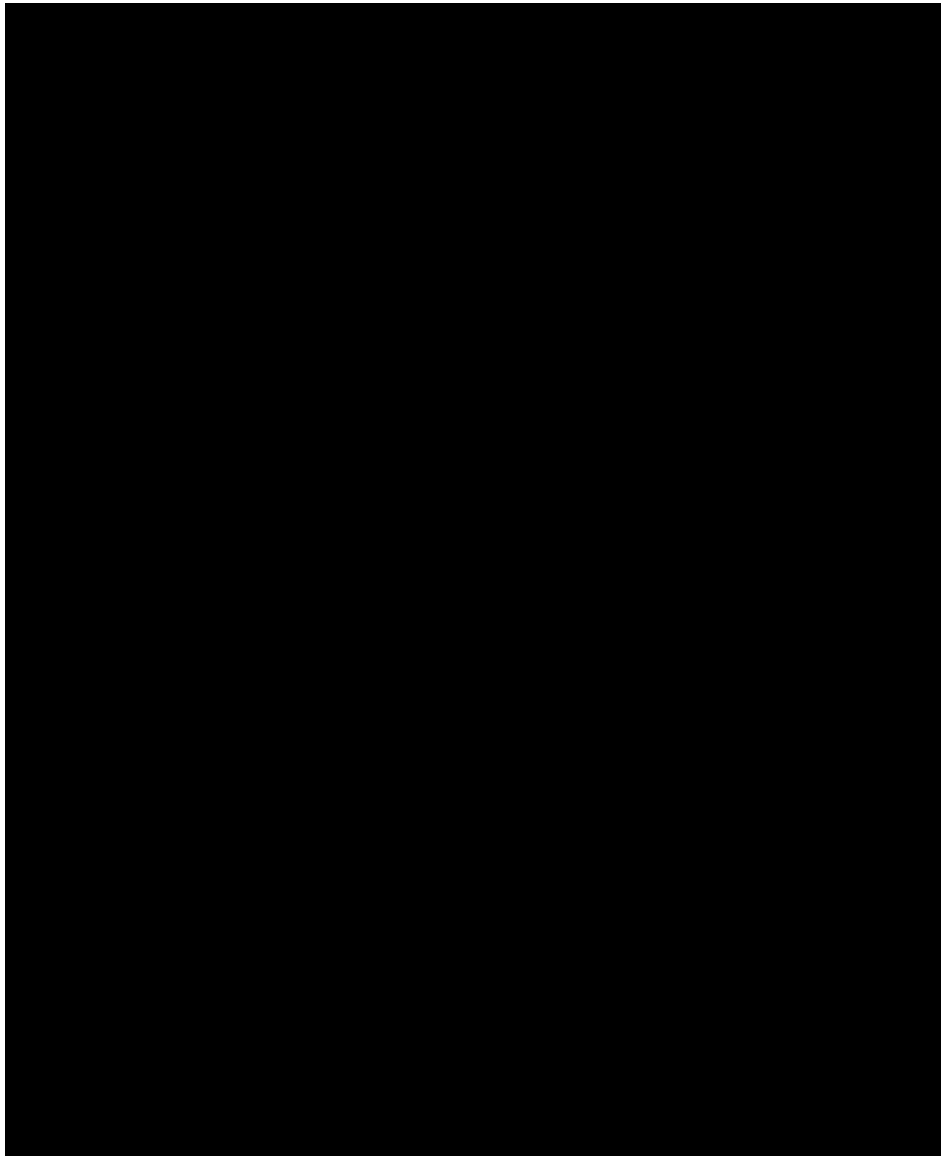
Unsupervised learning

- Instead of **(input, output)** we get **(input, ?)**
- Here there is no a function f to learn
- Find properties of the inputs $\boldsymbol{x} \in \mathbb{R}^{d \times 1}$
- High-level representation of the input
- Elements into the same cluster have similar properties



Reinforcement learning

- Instead of **(input, output)** we get **(input, output, reward)**
- The algorithm tries to learn what action to take, in order to maximize the reward
- This is called a policy
- Applications in control, robotics, A/B testing



Business problems as data science examples - revisited

Supervised

- Spam e-mail detection system **Classification**
- Credit approval **Classification**
- Recognize objects in images **Classification**
- Find the relation between house prices and house sizes **Regression**
- Predict the stock market **Regression**

Unsupervised

- Market segmentation **Clustering**
- Market basket analysis **Co-occurence grouping**
- Language models (word2vec) **Similarity matching**
- Social network analysis **Link prediction**
- Low-order data representations **Data reduction**

- Movies recommendation **Similaritiy matching**

Supervised or unsupervised

Supervised learning: problem statement

The aim is to **learn an unknown function** f given a dataset $\mathcal{D}$

- The function is searched in the hypothesis space $\mathcal{H}$, where $h \in \mathcal{H}$ is a specific function
- We want to find a function h that approximates f well, on the **whole domain** $\mathcal{X}$

What does $h \approx f$ mean?

- We need to define an **error measure**
- Almost always this is a **pointwise** definition: $e\big(f(\boldsymbol{x}), h(\boldsymbol{x})\big)$

Cost functions

Pointwise error examples

- *Squared error:* $e\big(f(\boldsymbol{x}), h(\boldsymbol{x})\big) = \big(f(\boldsymbol{x}) - h(\boldsymbol{x})\big)^2$ → used for regression
- *Binary error:* $e\big(f(\boldsymbol{x}), h(\boldsymbol{x})\big) = \mathbb{I}[f(\boldsymbol{x}) \neq h(\boldsymbol{x})]$ → used for classification

It is interesting to look at the **overall error**, which considers all N examples:

Overall error examples

- *In-sample error:* $E_{in} = \frac{1}{N}\sum_{i=1}^{N} e\big(f(\boldsymbol{x}), h(\boldsymbol{x})\big)$ → error on data that I actually have
- *Out-of-sample error:* $E_{out} = \mathbb{E}_{\boldsymbol{x}}\big[e\big(f(\boldsymbol{x}), h(\boldsymbol{x})\big)\big]$ → error on data I could possibly observe

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Linear regression

Aim: Suppose to have at disposal a dataset $\mathcal{D} = \{(\boldsymbol{x}(1), y(1)), \dots, (\boldsymbol{x}(N), y(N))\}$. Find the relation between a set of input variables $\boldsymbol{x} \in \mathbb{R}^{(d-1)\times 1}$ and an output variable $y \in \mathbb{R}$, using a **linear model:**

$$y(i) = \theta_0 + \theta_1 x_1(i) + \cdots + \theta_{d-1} x_{d-1}(i) + \epsilon(i) = \sum_{j=0}^{d-1} \theta_j \, x_j(i) + \epsilon(i)$$

$$= \underset{1\times d}{\boldsymbol{x}(i)^T} \underset{d\times 1}{\boldsymbol{\theta}} + \underset{1\times 1}{\epsilon(i)}$$

$$\begin{bmatrix} \cdots \end{bmatrix} \begin{bmatrix} \vdots \end{bmatrix}$$

i −th observation

- $x_0 = 1$
- $\boldsymbol{x} = [x_0, x_1, \dots, x_{d-1}]^T \in \mathbb{R}^{d\times 1}$
- $\boldsymbol{\theta} = [\theta_0, \theta_1, \dots, \theta_{d-1}]^T \in \mathbb{R}^{d\times 1}$

Hypothesis $h(\boldsymbol{\theta})$: linear model with parameters $\boldsymbol{\theta}$

Hypothesis space $\mathcal{H}$: set of all linear models

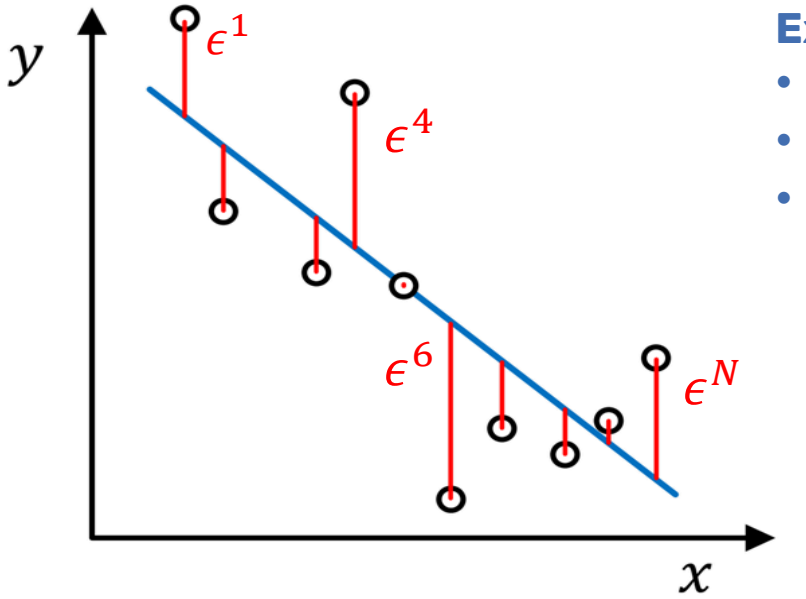
- The vector $\boldsymbol{\theta}$ is called **parameters vector** → to be found by minimizing a cost function
- The vector $\boldsymbol{x}(i)$ is called **features vector** for i-th observation → attributes of individuals
- The quantity $\epsilon(i)$ is the error due not perfect explanation of the $y(i)$ using $\boldsymbol{x}(i)$

Geometrical interpretation

One-variable case

In this case, there is only **one feature** x_1 and **two parameters** θ_0, θ_1

$$y(i) = \theta_0 + \theta_1 x_1(i) + \epsilon(i)$$



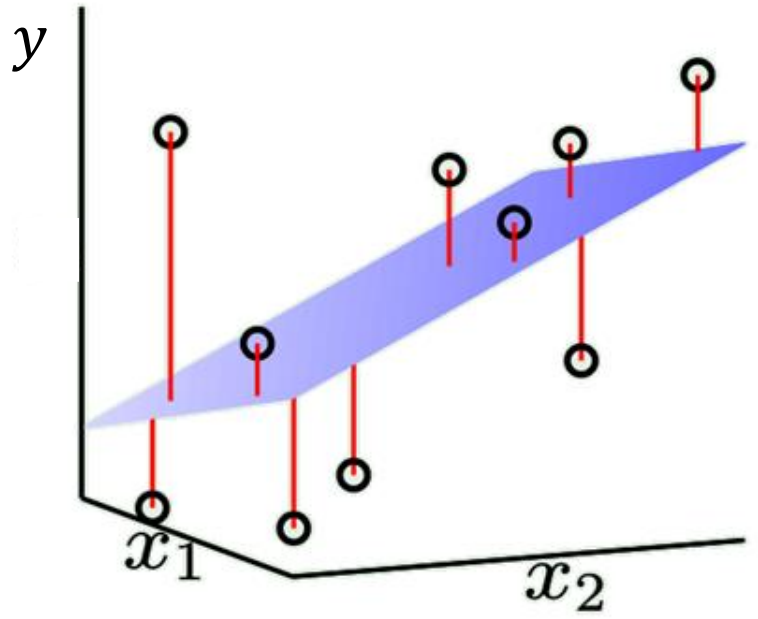
Example

- y: weight [kg]
- x_1: height [m]
- x_2: sex [M/F]

Two-variables case

In this case, there are **two features** x_1, x_2 and **three parameters** $\theta_0, \theta_1, \theta_2$

$$y(i) = \theta_0 + \theta_1 x_1(i) + \theta_2 x_2 + \epsilon(i)$$



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Least squares cost function

How well does $h(\boldsymbol{x}) = \boldsymbol{x}^T\boldsymbol{\theta}$ approximates $f(\boldsymbol{x})$?

- Linear regression estimates the parameters $\boldsymbol{\theta}$ using the **least squares method**, i.e. by minimizing the **squared error** between **observed** and **predicted** output

Cost function

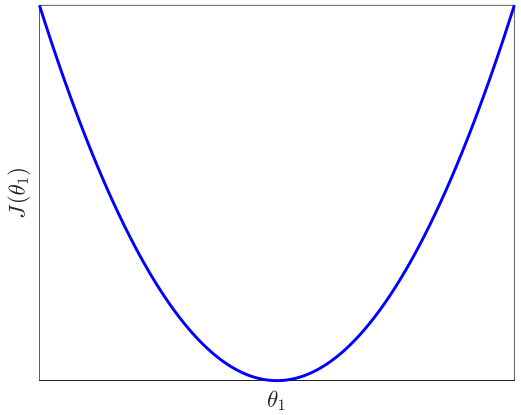
$$\hat{\boldsymbol{\theta}} = \arg\min_{\theta} J(\boldsymbol{\theta}) \qquad J(\boldsymbol{\theta}) = E_{in}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}(y(i) - \boldsymbol{x}(i)^T\boldsymbol{\theta})^2 = \frac{1}{N}\sum_{i=1}^{N}\big(\epsilon(i)\big)^2$$

$\boldsymbol{x}(i)^T$: $\begin{bmatrix} \cdots \end{bmatrix}$ $\boldsymbol{\theta}$: $\begin{bmatrix} \vdots \end{bmatrix}$

One-variable case

with $\theta_0 = 0$

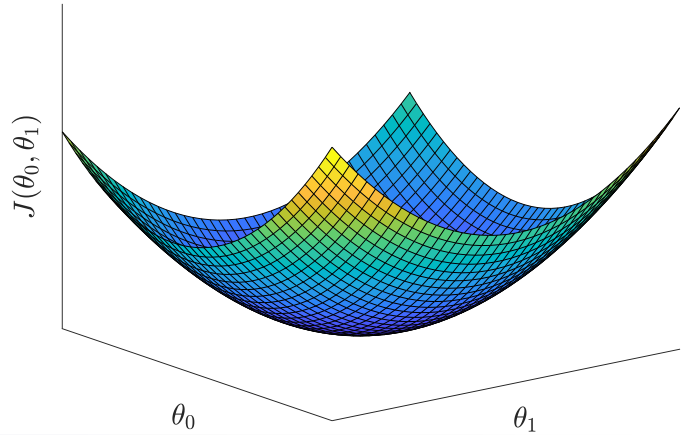
$$y(i) = \theta_1 x_1(i) + \epsilon(i)$$



One-variable case

with $\theta_0 \neq 0$

$$y(i) = \theta_0 + \theta_1 x_1(i) + \epsilon(i)$$



Cost function - minimization

$$J(\boldsymbol{\theta}) = E_{in}(\boldsymbol{\theta}) = \frac{1}{N}\sum_{i=1}^{N}(y(i) - \boldsymbol{x}(i)^T\boldsymbol{\theta})^2$$

$$\nabla J(\boldsymbol{\theta}) = \frac{\partial J(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = \mathbf{0} \Rightarrow \frac{2}{N}\sum_{i=1}^{N} \boldsymbol{x}(i) \cdot (y(i) - \boldsymbol{x}(i)^T\boldsymbol{\theta}) = \mathbf{0} \Rightarrow \sum_{i=1}^{N} \boldsymbol{x}(i)y(i) - \sum_{i=1}^{N} \boldsymbol{x}(i)\boldsymbol{x}(i)^T\boldsymbol{\theta} = \mathbf{0}$$

$$\Rightarrow \left[\sum_{i=1}^{N} \boldsymbol{x}(i)\boldsymbol{x}(i)^T\right]\boldsymbol{\theta} = \sum_{i=1}^{N} \boldsymbol{x}(i)y(i)$$

$$\Rightarrow \widehat{\boldsymbol{\theta}} = \left[\sum_{i=1}^{N} \boldsymbol{x}(i)\boldsymbol{x}(i)^T\right]^{-1} \cdot \left[\sum_{i=1}^{N} \boldsymbol{x}(i)y(i)\right]$$

- Since the model is **linear in the parameters** and the error measure is **quadratic**, the cost function is **convex** → it admits a **unique** (global) minimum
- In this case the minimum can be found in **closed-form**

Least squares cost function – matrix form

We can express the linear regression problem using matrices

Features vector $\boldsymbol{x}^T(i)$

$$\underset{N\times d}{X} = \begin{bmatrix} 1 & x_1(1) & x_2(1) & \cdots & x_{d-1}(1) \\ 1 & x_1(2) & x_2(2) & & x_{d-1}(2) \\ \vdots & \vdots & & \ddots & \vdots \\ 1 & x_1(N) & x_2(N) & \cdots & x_{d-1}(N) \end{bmatrix} \quad \underset{d\times 1}{\boldsymbol{\theta}} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_{d-1} \end{bmatrix} \quad \underset{N\times 1}{Y} = \begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ y(N) \end{bmatrix} \quad \underset{N\times 1}{E} = \begin{bmatrix} \epsilon(1) \\ \epsilon(2) \\ \vdots \\ \epsilon(N) \end{bmatrix}$$

$$\underset{N\times d}{X} = \begin{bmatrix} \boldsymbol{x}^T(1) \\ \boldsymbol{x}^T(2) \\ \vdots \\ \boldsymbol{x}^T(N) \end{bmatrix}$$

$$Y = X\boldsymbol{\theta} + E \Rightarrow \boxed{J(\boldsymbol{\theta}) = \frac{1}{N}\|Y - X\boldsymbol{\theta}\|_2^2 = \frac{1}{N}\underset{1\times N}{(Y - X\boldsymbol{\theta})^T}\underset{N\times 1}{(Y - X\boldsymbol{\theta})}}$$

IN-DEPTH ANALYSIS

Least squares cost function – matrix form

It is useful to remember these matrix derivation properties:

$$\underset{1\times d}{\nabla_{\boldsymbol{x}}}\left(\underset{1\times d}{\boldsymbol{x}^T}\cdot\underset{d\times d}{A}\cdot\underset{d\times 1}{\boldsymbol{x}}\right)=\underset{d\times d}{(A+A^T)}\cdot\underset{d\times 1}{\boldsymbol{x}} \qquad \underset{1\times d}{\nabla_{\boldsymbol{x}}}\left(\underset{1\times d}{\boldsymbol{x}^T}\cdot\underset{d\times 1}{\boldsymbol{b}}\right)=\underset{d\times 1}{\boldsymbol{b}}$$

$$J(\boldsymbol{\theta})=\frac{1}{N}(Y-X\boldsymbol{\theta})^T(Y-X\boldsymbol{\theta})=\frac{1}{N}(Y^TY-\underset{1\times N\ N\times d\ d\times 1}{Y^TX\cdot\boldsymbol{\theta}}-\underset{1\times d\ d\times N\ N\times 1}{\boldsymbol{\theta}^T\cdot X^T\,Y}+\boldsymbol{\theta}^T\cdot X^T\,X\cdot\boldsymbol{\theta})$$

$$=\frac{1}{N}(Y^TY-\ 2\cdot\boldsymbol{\theta}^T\cdot X^T\,Y\ +\ \boldsymbol{\theta}^T\cdot X^T\,X\cdot\boldsymbol{\theta})$$

$$\nabla J(\boldsymbol{\theta})=\mathbf{0}\Rightarrow\frac{1}{N}(-2X^TY+2X^TX\boldsymbol{\theta})=\mathbf{0}\Rightarrow \qquad \underset{d\times 1}{\widehat{\boldsymbol{\theta}}}=\underset{d\times d}{(X^TX)^{-1}}\underset{d\times N\ N\times 1}{X^TY}$$

Normal equations

$$\widehat{\boldsymbol{\theta}} = (X^T X)^{-1} X^T Y$$

Normal equations

What if the matrix $X^T X$ is **not invertible**? → Use **pseudo-inverse**. In MatLab:

```
theta_hat = pinv(X'*X)*X*y
```

- Redundant features (linearly dependent)
  - ✓ $x_1 = \text{height in m}^2$
  - ✓ $x_2 = \text{height in feet}^2$
- Too many features (ex. $N \leq d$)
  - ✓ Delete some feature
  - ✓ Use regularization (later in the course)

- The method of normal equations is **slow** if d is very large
  - ✓ To solve this, iterative methods using **gradient descent** can be used

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Gradient descent

- The **gradient descent** is a general iterative method for minimizing differentiable functions

- The value of the parameters at iteration $t + 1$ is (given a random initial point $\widehat{\boldsymbol{\theta}}(0)$)

$$\underset{d \times 1}{\widehat{\boldsymbol{\theta}}(t+1)} = \underset{d \times 1}{\widehat{\boldsymbol{\theta}}(t)} - \underset{1 \times 1}{\alpha} \cdot \underset{d \times 1}{\nabla J(\boldsymbol{\theta})} \Big|_{\boldsymbol{\theta}=\widehat{\boldsymbol{\theta}}(t)}$$

$\alpha \in \mathbb{R}_{>0}$: learning rate

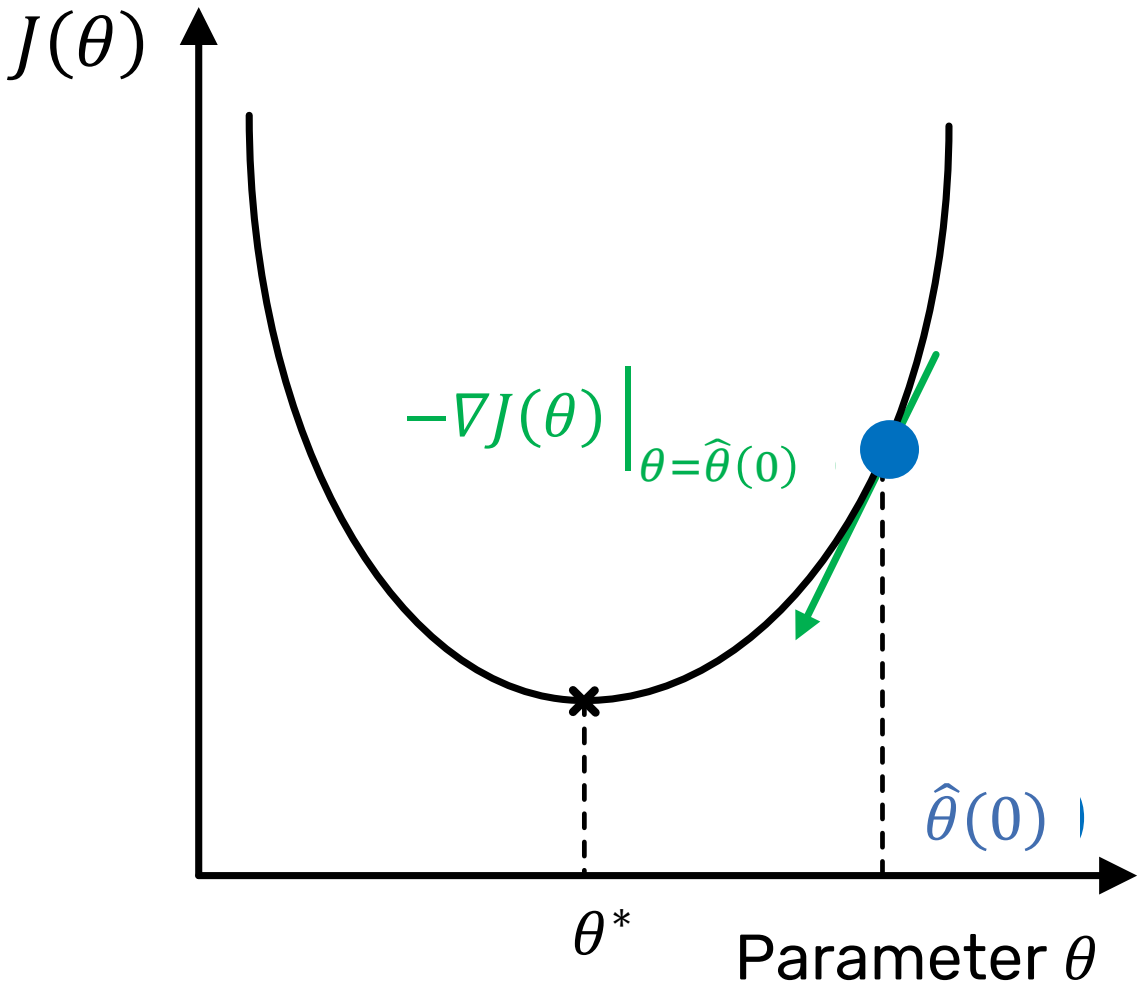
Gradient descent

Consider the **scalar** case where $\theta \in \mathbb{R}$

$$\hat{\theta}(t+1) = \hat{\theta}(t) - \alpha \nabla J(\theta)\Big|_{\theta=\hat{\theta}(t)}$$

- $\nabla J(\theta)|_{\theta=\hat{\theta}(t)} > 0 \Rightarrow \hat{\theta}(t+1) < \hat{\theta}(t)$

The new estimate is closer to the optimal value θ^*



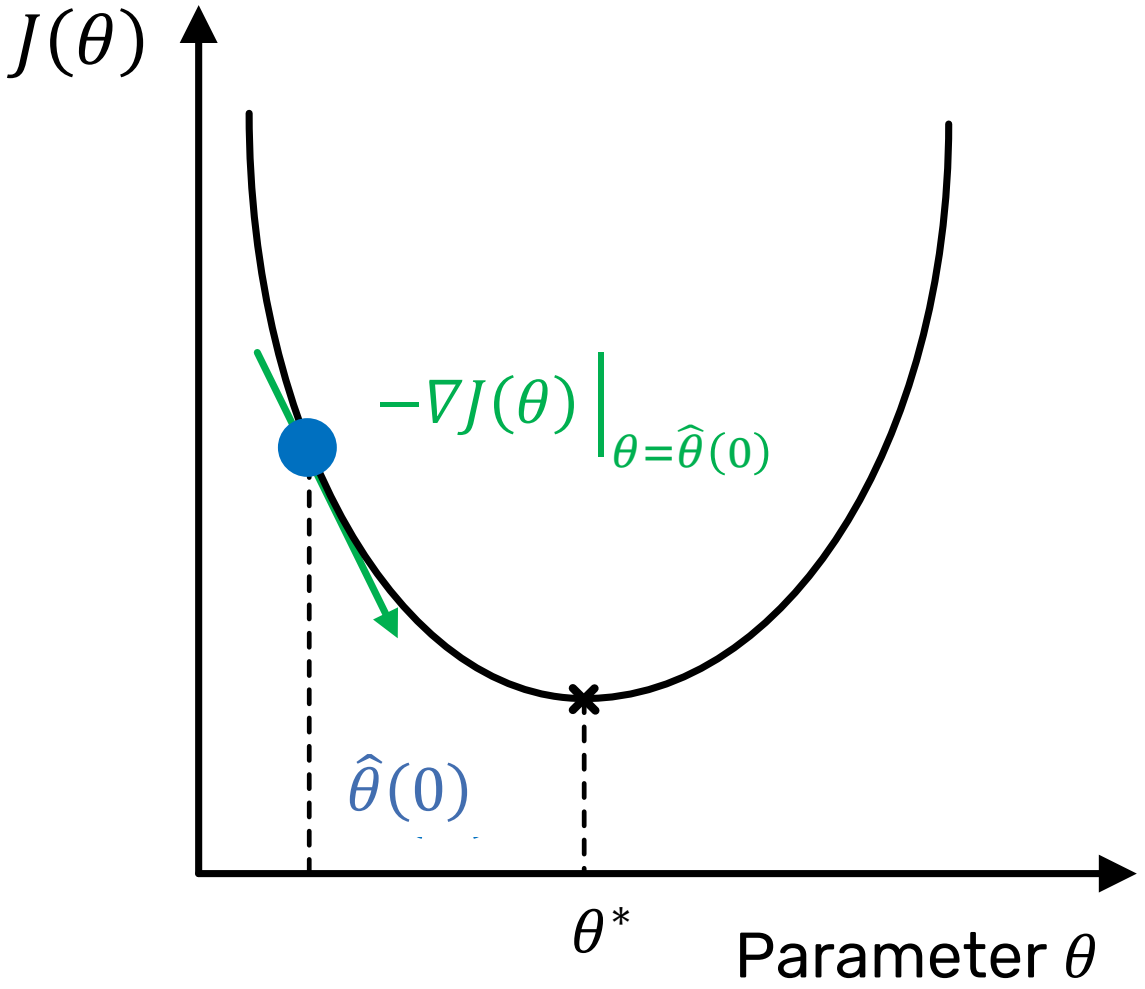
Gradient descent

Consider the **scalar** case where $\theta \in \mathbb{R}$

$$\hat{\theta}(t+1) = \hat{\theta}(t) - \alpha \nabla J(\theta)\Big|_{\theta=\hat{\theta}(t)}$$

- $\nabla J(\theta)|_{\theta=\hat{\theta}(t)} < 0 \Rightarrow \hat{\theta}(t+1) > \hat{\theta}(t)$

The new estimate is closer to the optimal value θ^*



Linear regression laboratory: predict house prices

We want to **predict the price** of the houses in Portland, Oregon

- Each house is described by the following features
  - ✓ x_1: Number of **bedrooms**
  - ✓ x_2: **Size** [feet^2]
- The **training set** consists of $N = 47$ houses with $x_1(i), x_2(i)$ and $y(i)$, for $i = 1, \dots, N$

$$y(i) = \boldsymbol{x}(i)^T \boldsymbol{\theta} + \epsilon(i) \qquad \underset{3 \times 1}{\boldsymbol{x}(i)} = [1 \quad x_1(i) \quad x_2(i)]^T$$

$$\underset{47 \times 3}{X} = \begin{bmatrix} \boldsymbol{x}^T(1) \\ \boldsymbol{x}^T(2) \\ \vdots \\ \boldsymbol{x}^T(N) \end{bmatrix} \qquad \underset{3 \times 1}{\boldsymbol{\theta}} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} \qquad \underset{47 \times 1}{Y} = \begin{bmatrix} y(1) \\ y(2) \\ \vdots \\ y(47) \end{bmatrix}$$

```
% Read data from file
data = csvread('housedata.txt');
X = data(:, 1:2); % Features
y = data(:, 3); % Price
N = length(y); % Number of data

% Add intercept term to X
X = [ones(N, 1) X];

% Calculate the parameters from
the normal equation
theta_hat = pinv(X'*X)*X'*y;
```

```
% Estimate the price of a 1650
sq-ft, 3 br house
price_hat = [1 3 1650]*theta_hat;
```

Point not seen during training (i.e. estimation of θ)