Lecture 14
Linear Regression

Mahdi Roozbahani
Georgia Tech

These slides are adopted based on slides from Le Song, Chao Zhang, Yaser Abu-Mostafa, Andrew Zisserman.

Outline

- Supervised Learning
- Linear Regression
- Extension

Supervised Learning: Overview

Functions $\mathcal{F}$

$$f : \mathcal{X} \to \mathcal{Y}$$

Training data

$$\{(x_i, y_i) \in \mathcal{X} \times \mathcal{Y}\}$$

LEARNING

$$\boxed{\text{find } \hat{f} \in \mathcal{F} \quad \text{s.t. } y_i \approx \hat{f}(x_i)}$$

Learning machine

New data

PREDICTION

$$\boxed{y = \hat{f}(x)} \Leftarrow \boxed{x}$$

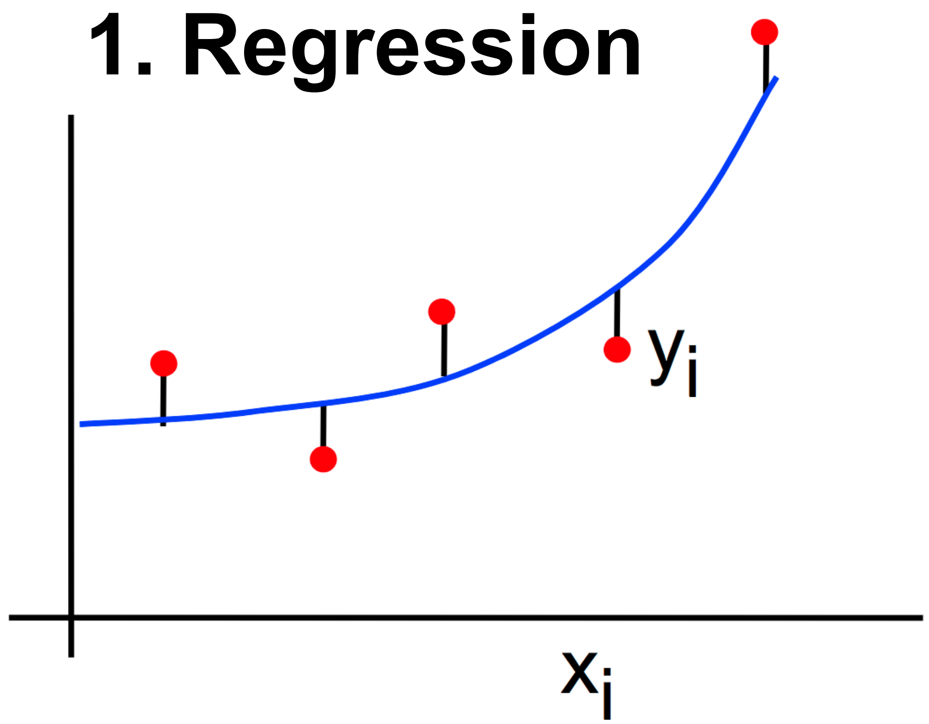
Supervised Learning: Two Types of Tasks

Given: training data $\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)\}$

Learn: a function $f(\mathbf{x}) : y = f(\mathbf{x})$

When y is continuous:

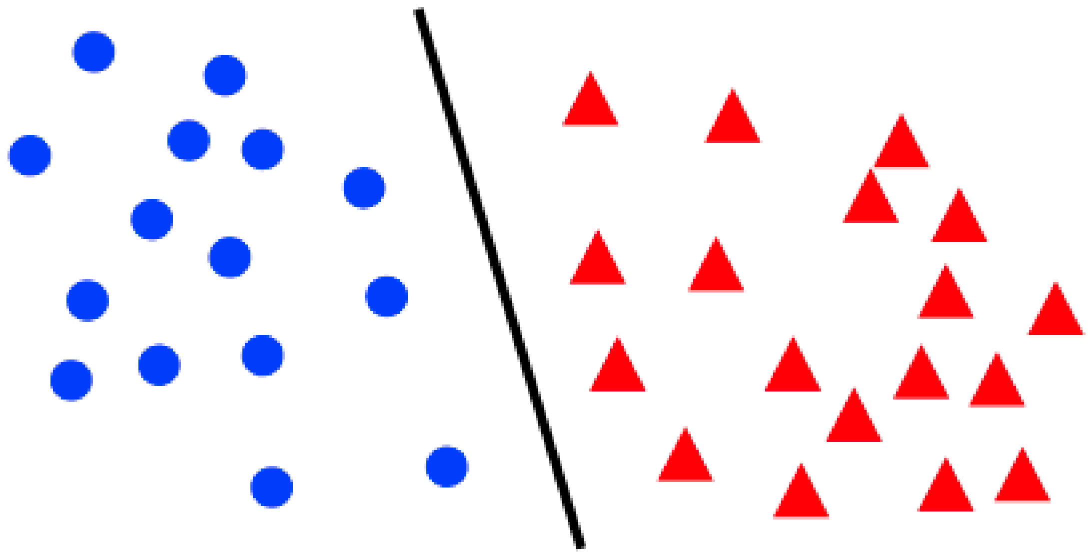
1. Regression



Curve fitting

When y is discrete:

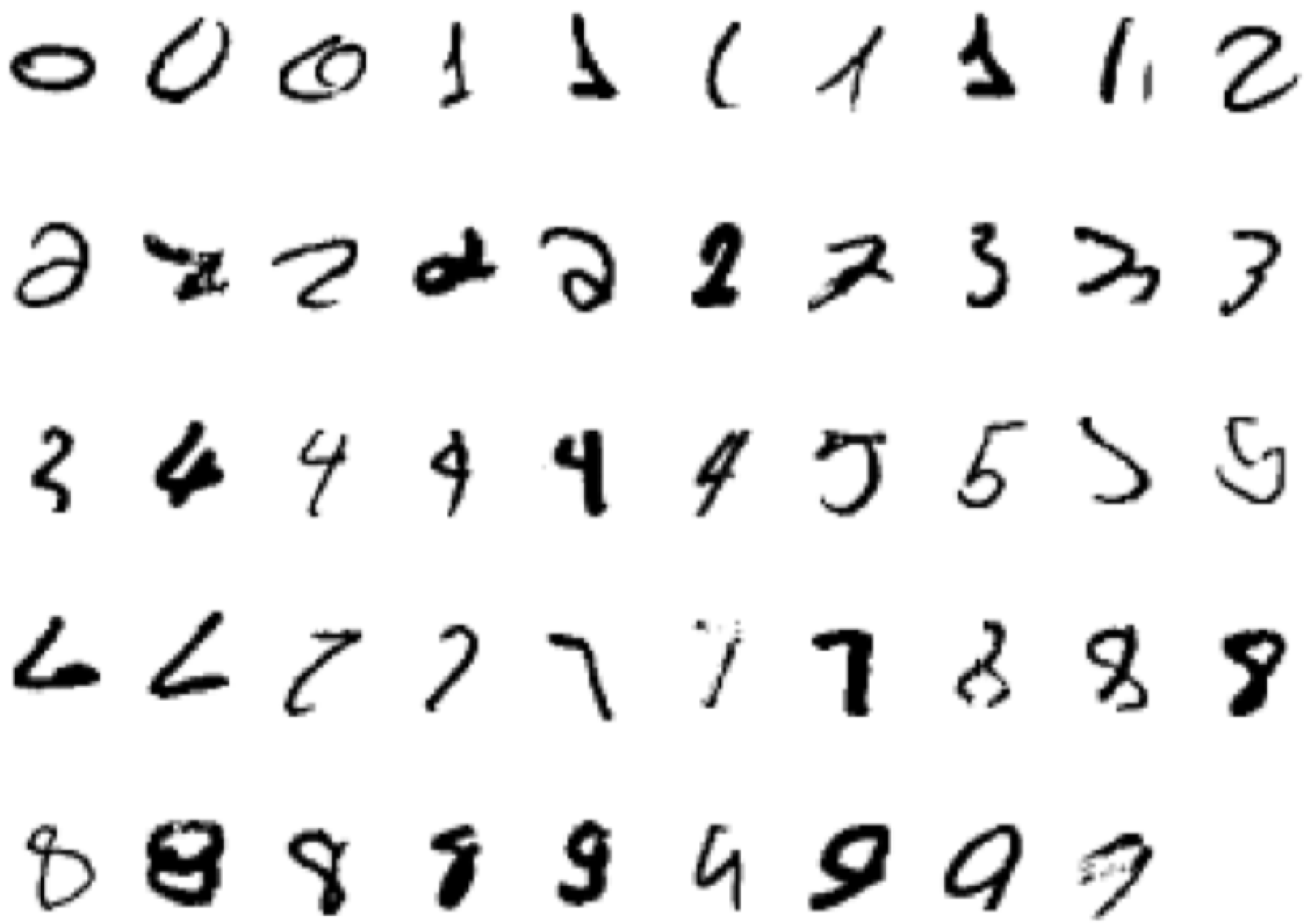
2. Classification



Class estimation

As a supervised classification problem

Start with training data, e.g. 6000 examples of each digit



- Can achieve testing error of 0.4%
- One of first commercial and widely used ML systems (for zip codes & checks)

Example 1: Apartment Rent Prediction

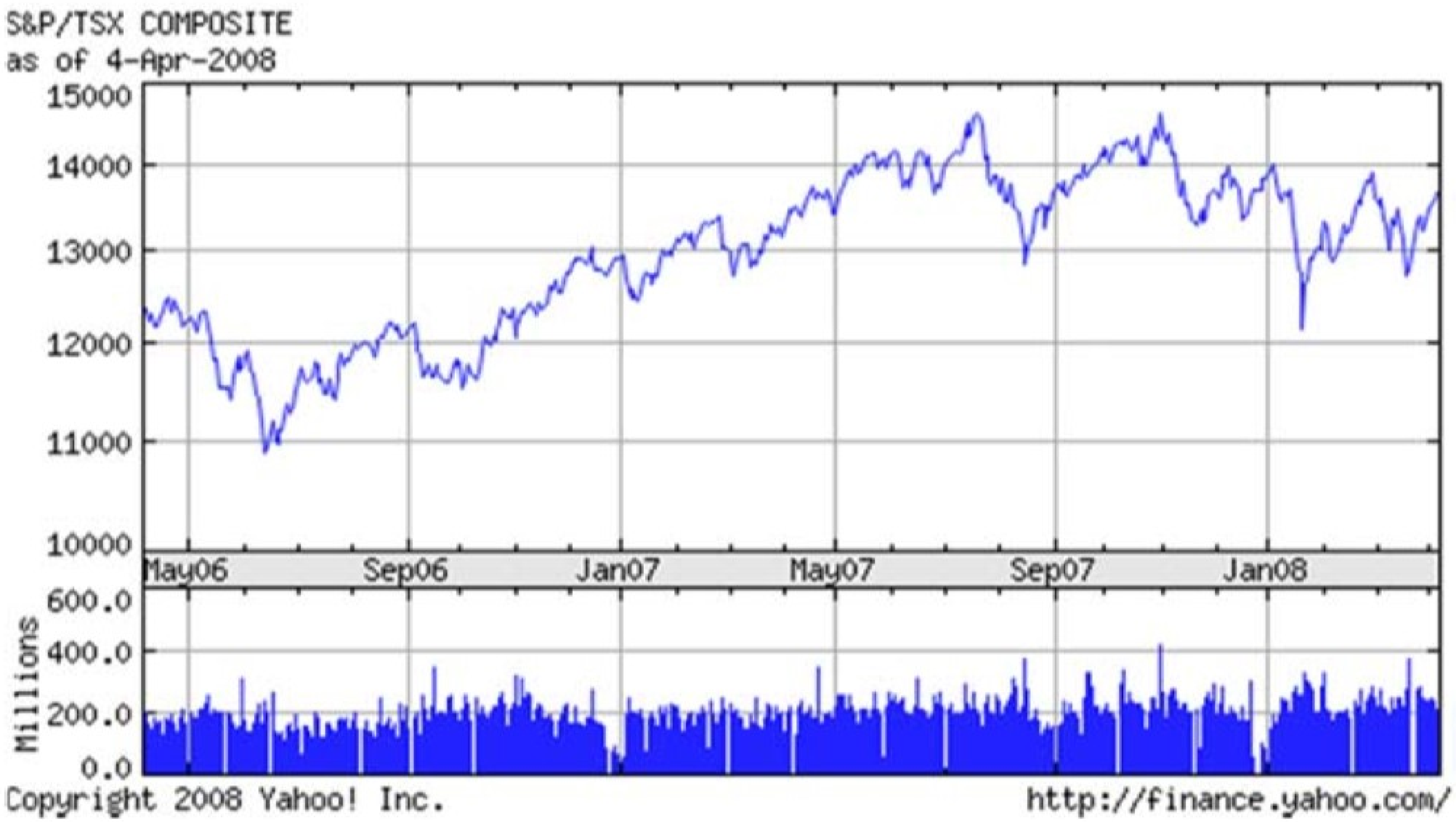
- Suppose you are to move to Atlanta
- And you want to find the **most reasonably priced** apartment satisfying your **needs:**

  square-ft., # of bedroom, distance to campus …

A regression problem

Living area (ft^2)	# bedroom	Rent ($)
230	1	600
506	2	1000
433	2	1100
109	1	500
…		
150	1	?
270	1.5	?

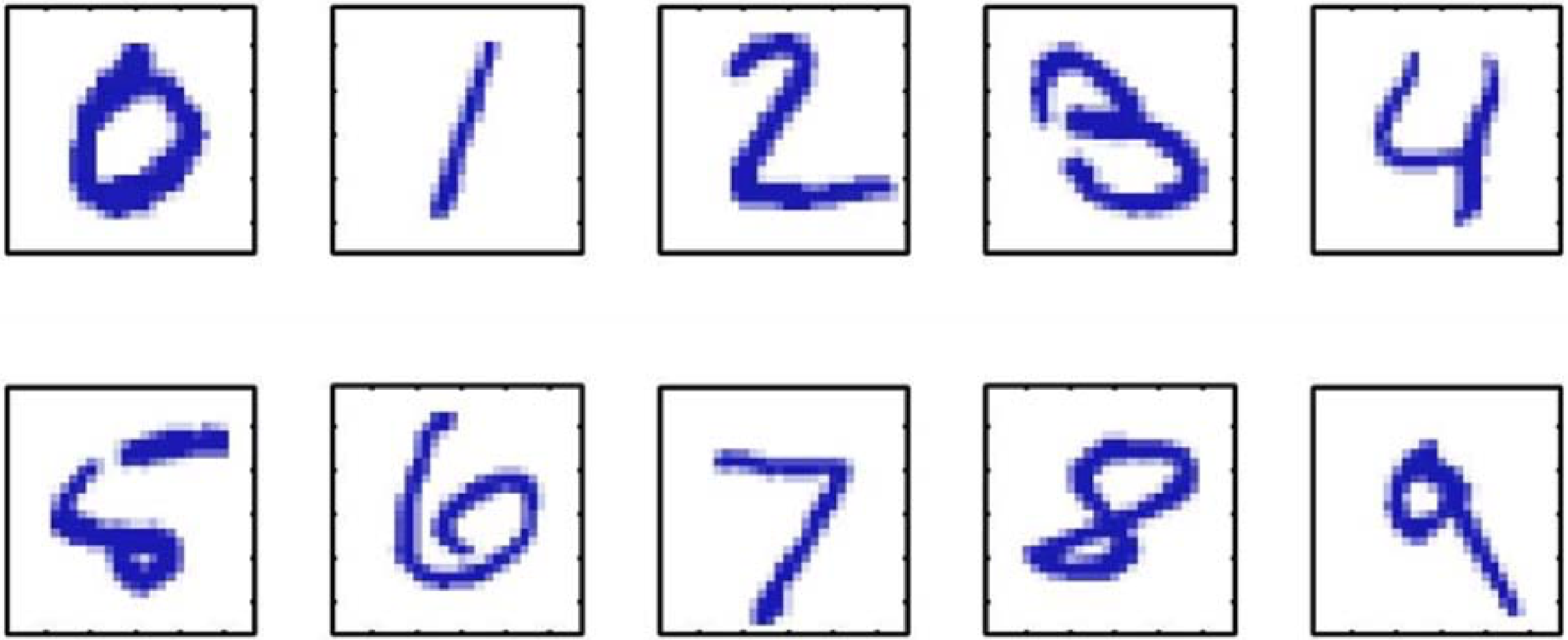
Example 2: Stock Price Prediction



- Task is to predict stock price at future date

A regression problem

Example 3: Hand-Written Digit Recognition



Images are 28 x 28 pixels

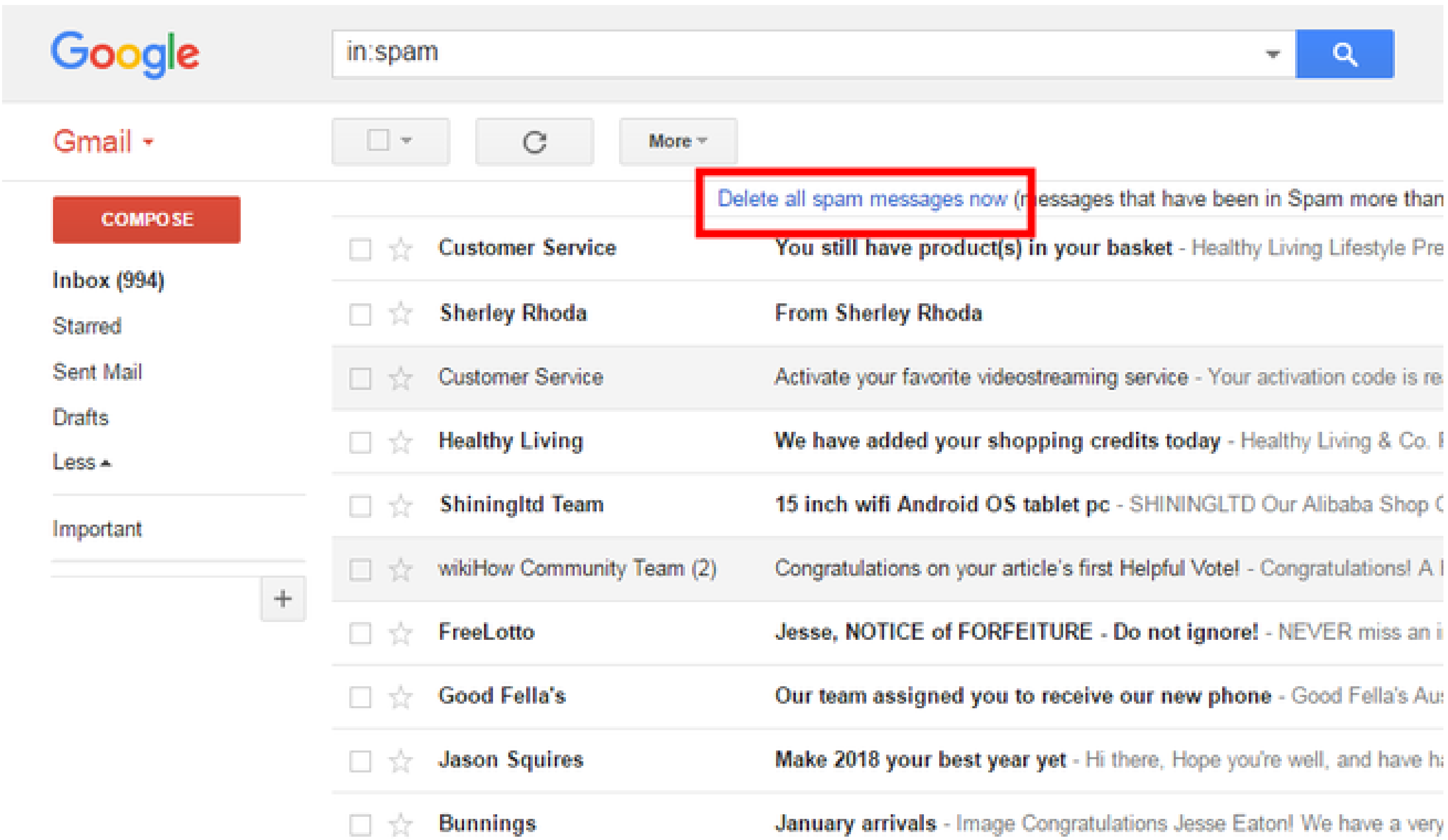
A classification problem

Represent input image as a vector $\mathbf{x} \in \mathbb{R}^{784}$

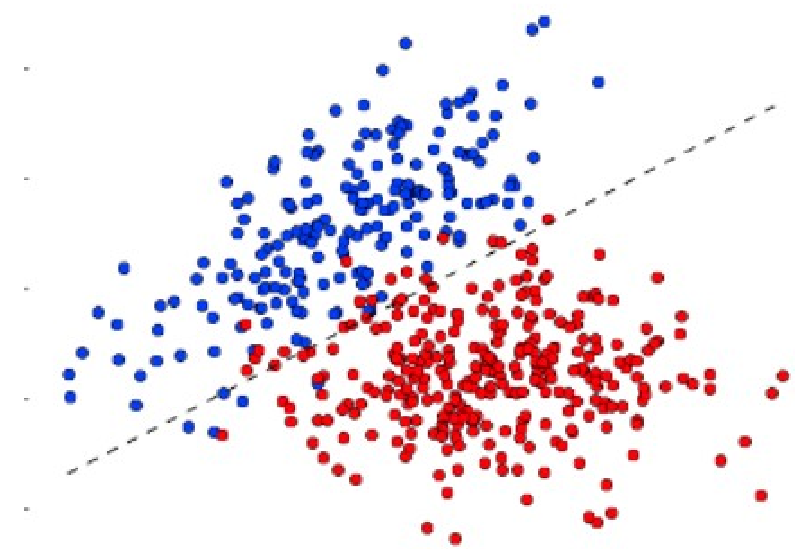
Learn a classifier $f(\mathbf{x})$ such that,

$$f : \mathbf{x} \to \{0, 1, 2, 3, 4, 5, 6, 7, 8, 9\}$$

Example 4: Spam Detection



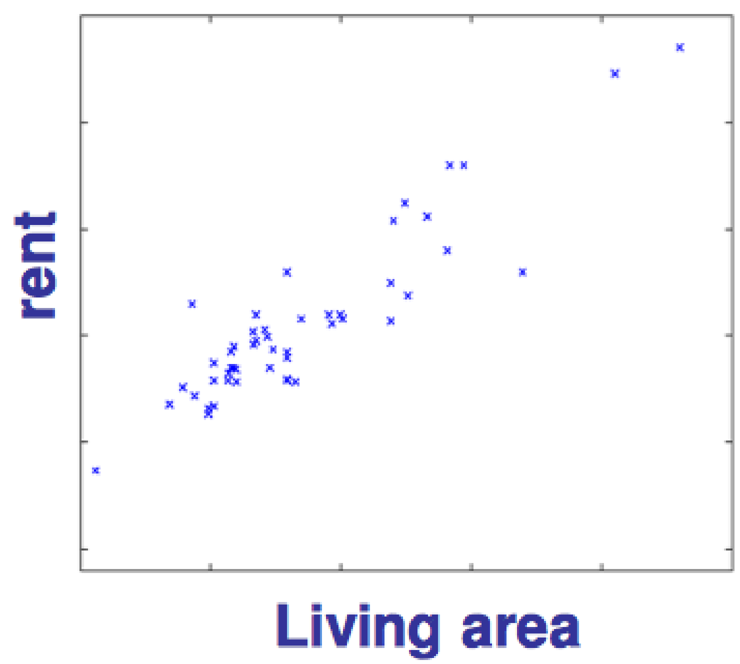
NOT SPAM

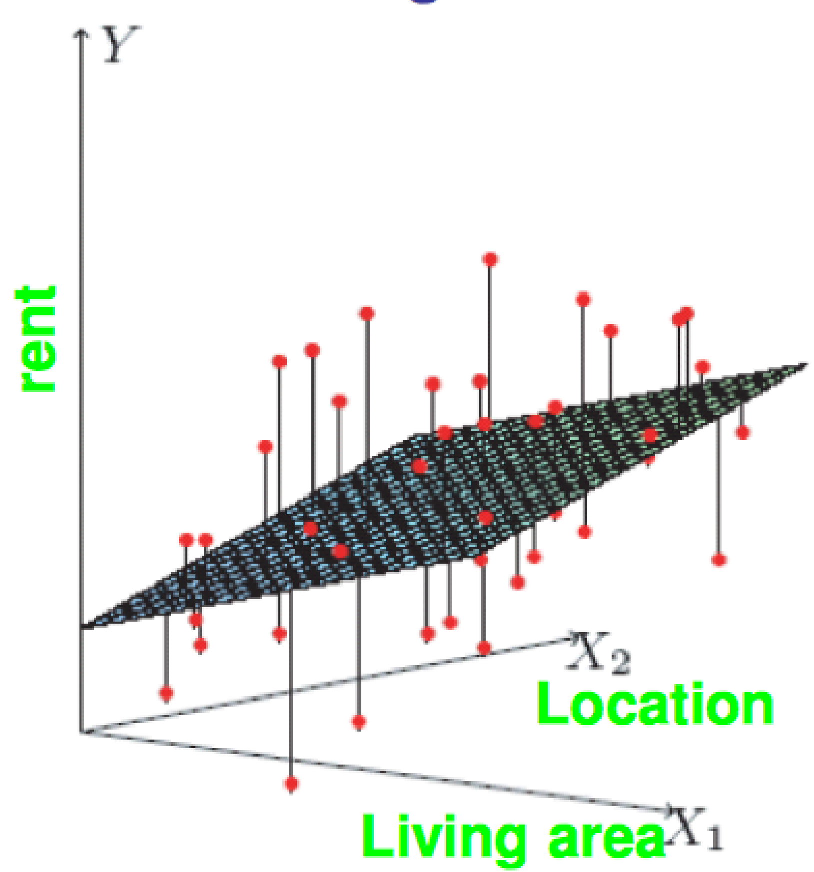


SPAM

A classification problem

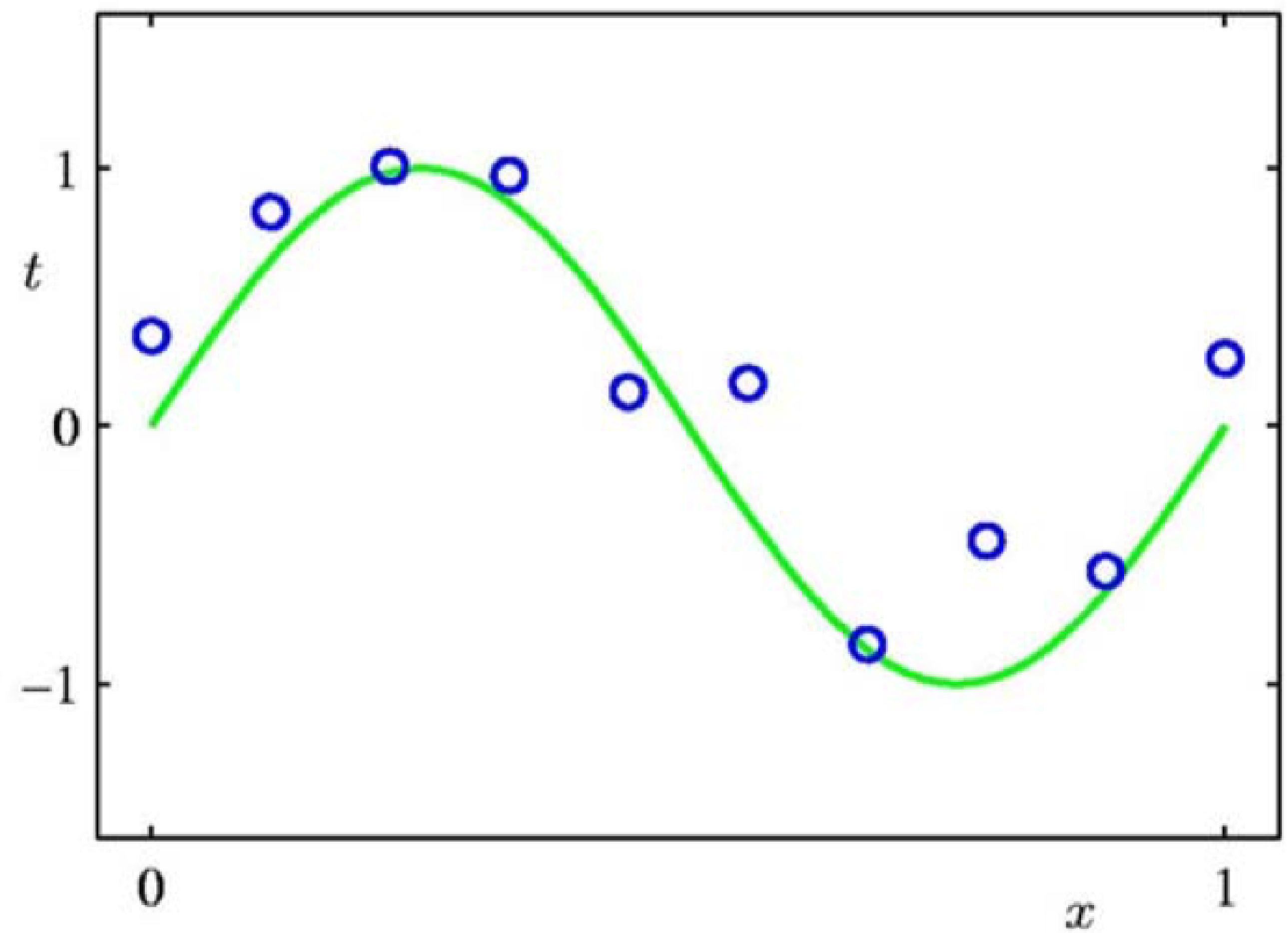
- This is a classification problem
- Task is to classify email into spam/non-spam
- Data x_i is word count
- Requires a learning system as “enemy” keeps innovating





- Features:
  - Living area, distance to campus, # bedroom …
  - Denote as $x = (x_1, x_2, \dots, x_d)$
- Target:
  - Rent
  - Denoted as y
- Training set:
  - $x = \{x_1, x_2, \dots, x_n\} \in R^d$
  - $y = \{y_1, y_2, \dots, y_n\}$

Regression: Problem Setup



- Suppose we are given a training set of N observations

$$(x_1, \ldots, x_N) \text{ and } (y_1, \ldots, y_N), x_i, y_i \in \mathbb{R}$$

- Regression problem is to estimate y(x) from this data

Outline

- Supervised Learning
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- Extension

Linear Regression

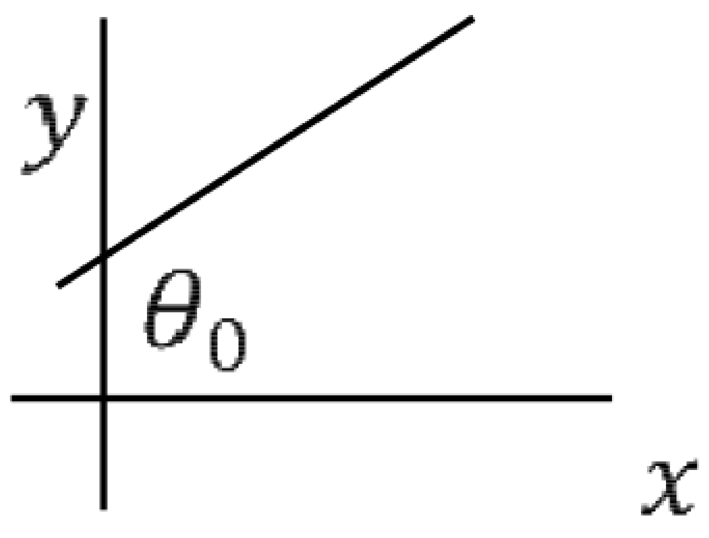
- Assume y is a linear function of x (features) plus noise ϵ

$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_d x_d + \epsilon$$

- where ϵ is an error term of unmodeled effects or random noise

- Let $\theta = (\theta_0, \theta_1, \ldots, \theta_d)^{\top}$, and augment data by one dimension

- Then $y = x\theta + \epsilon$



Least Mean Square Method

- Given n data points, find θ that minimizes the mean square error

Training $$\hat{\theta} = argmin_{\theta}\, L(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - x_i\theta)^2$$

- Our usual trick: set gradient to 0 and find parameter $\dfrac{\partial L(\theta)}{\partial \theta} = 0$

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\sum_{i=1}^{n} x_i^T(y_i - x_i\theta) = 0$$

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\sum_{i=1}^{n} x_i^T y_i + \frac{2}{n}\sum_{i=1}^{n} x_i^T x_i\theta = 0$$

Matrix form

$$x = \begin{bmatrix} 1 & x_1^{\{1\}} & \cdots & x_1^{\{d\}} \\ 1 & x_2^{\{1\}} & \ddots & x_2^{\{d\}} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n^{\{1\}} & \cdots & x_1^{\{d\}} \end{bmatrix}_{n \times (d+1)} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}_{n \times 1} \quad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}_{(d+1) \times 1}$$

$$MSE(\theta) = argmin_{\ \theta}\ L(\theta) = \frac{1}{n}(y - x\theta)^{\mathrm{T}}(\mathrm{y} - x\theta)$$

$$x\theta = \begin{bmatrix} \theta_0 + \theta_1 x_1^{\{1\}} + \theta_2 x_1^{\{2\}} + \cdots + \theta_d x_1^{\{d\}} \\ \theta_0 + \theta_1 x_2^{\{1\}} + \theta_2 x_2^{\{2\}} + \cdots + \theta_d x_2^{\{d\}} \\ \vdots \\ \theta_0 + \theta_1 x_n^{\{1\}} + \theta_2 x_n^{\{2\}} + \cdots + \theta_d x_n^{\{d\}} \end{bmatrix}_{n \times 1}$$

Matrix Version and Optimization

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\sum_{i=1}^{n} x_i^T y_i + \frac{2}{n}\sum_{i=1}^{n} x_i^T x_i \theta = 0$$

Let's rewrite it as:

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}(x_1, \dots, x_n)^T (y_1, \dots, y_n) + \frac{2}{n}(x_1, \dots, x_n)^T (x_1, \dots, x_n)\theta = 0$$

Define $\mathrm{X} = (x_1, \dots, x_n)$ and $\mathrm{y} = (y_1, \dots, y_n)$

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\mathrm{X}^{\mathrm{T}}\mathrm{y} + \frac{2}{n}X^T X\theta = 0$$

$\Rightarrow\ \theta = (X^T X)^{-1} X^T y = X^+ y$

X^+ is the **pseudo-inverse** of X

$X^T X X^+ = X^T$

$$\theta = (X^T X)^{-1} X^T y = X^+ y$$

$X_{n \times d}$ $\quad$ $n =$ instances $\quad$ $d =$ dimension

$$X^T X = \begin{bmatrix} & d \times n & \end{bmatrix} \begin{bmatrix} \\ n \times d \\ \\ \end{bmatrix} = \begin{bmatrix} d \times d \end{bmatrix}$$

Not a big matrix because $n \gg d$This matrix is invertible most of the times. If we are VERY unlucky and columns of $\mathbf{X^T}\boldsymbol{X}$ are not linearly independent (it's not a full rank matrix), then it is not invertible.

Alternative Way to Optimize

- The matrix inversion in $\theta = (X^T X)^{-1} X^T y$ can be very expensive to compute

- $$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\sum_{i=1}^{n} x_i^T (y_i - x_i\theta)$$

- Gradient descent

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^t + \frac{\alpha}{n}\sum_{i=1}^{n} x_i^T (y_i - x_i\theta)$$

- Stochastic gradient descent (use one data point at a time)

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^t + \beta_t \times x_i^T (y_i - x_i\theta)$$

Recap

- Stochastic gradient update rule

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^{t} + \beta_t \ \times x_i^T (y_i - x_i \theta)$$

  - Pros: on-line, low per-step cost
  - Cons: coordinate, maybe slow-converging
- Gradient descent

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^{t} \ + \frac{\alpha}{n} \sum_{i=1}^{n} x_i^T (y_i - x_i \theta)$$

  - Pros: fast-converging, easy to implement
  - Cons: need to read all data
- Solve normal equations

$$\theta = (X^T X)^{-1} X^T y$$

  - Pros: a single-shot algorithm! Easiest to implement.
  - Cons: need to compute inverse $(X^T X)^{-1}$, expensive, numerical issues (e.g., matrix is singular ..)

Linear regression for classification

Raw Input $x = (x_0, x_1, \ldots, x_{256})$

Linear model $(\theta_0, \theta_1, \ldots, \theta_{256})$

16

16

Extract useful information

$intensity\ and\ symmetry\ x = (x_0, x_1. x_2)$

$Sum\ up\ all\ the\ pixels = intensity$

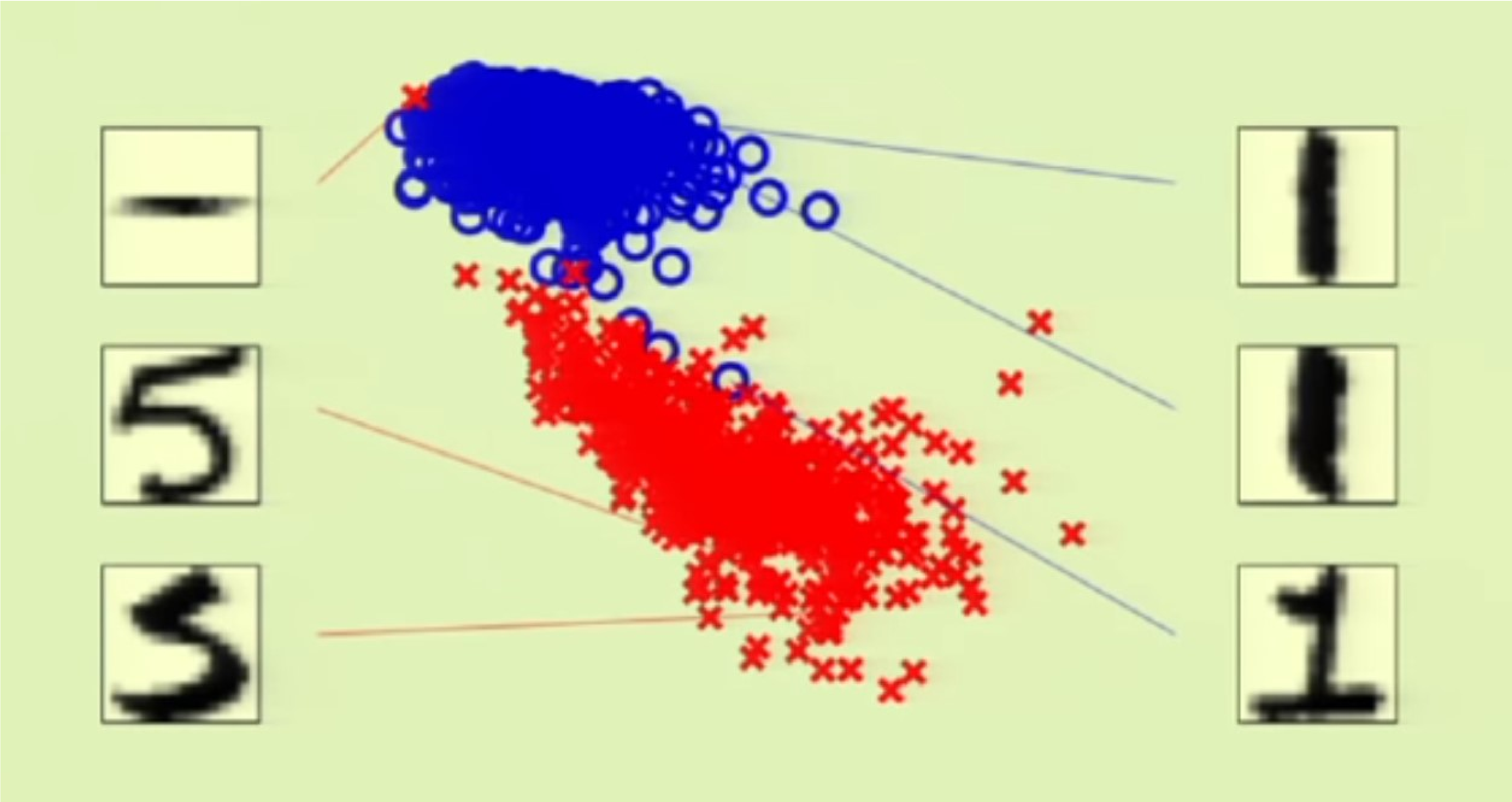
$Symmetry =$ -(*difference between flip version*)

$x = (x_0, x_1, x_2)$

$x_1 = intensity \; x_2 = symmetry$

It is almost linearly separable

$symmetry$



$intensity$

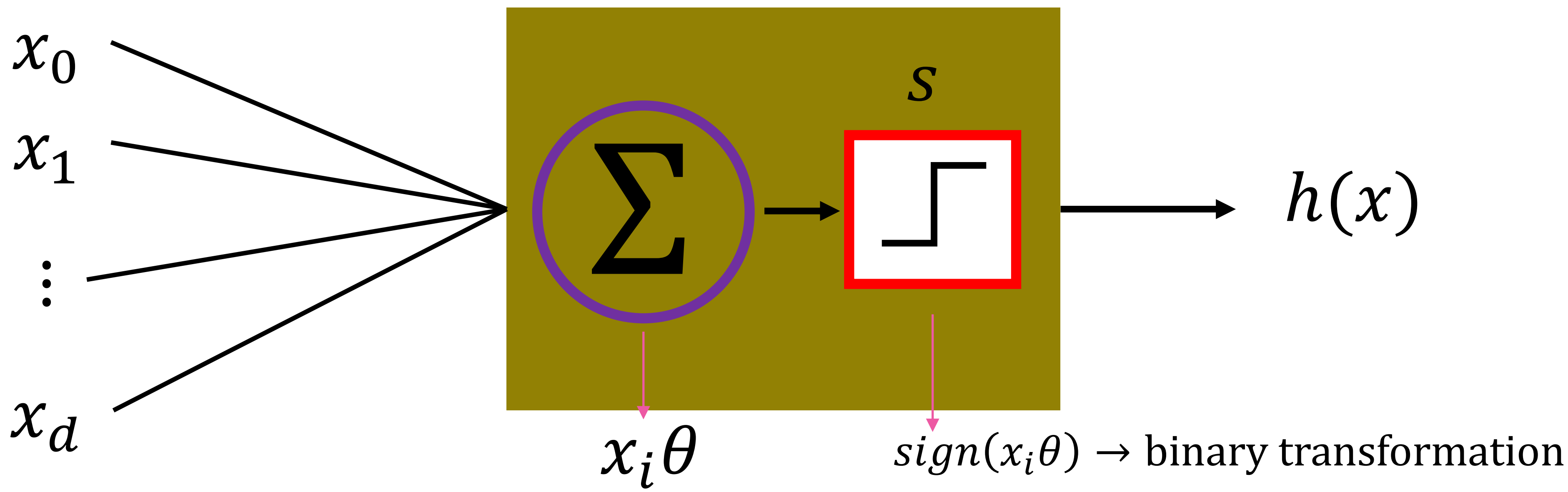
Linear regression for classification

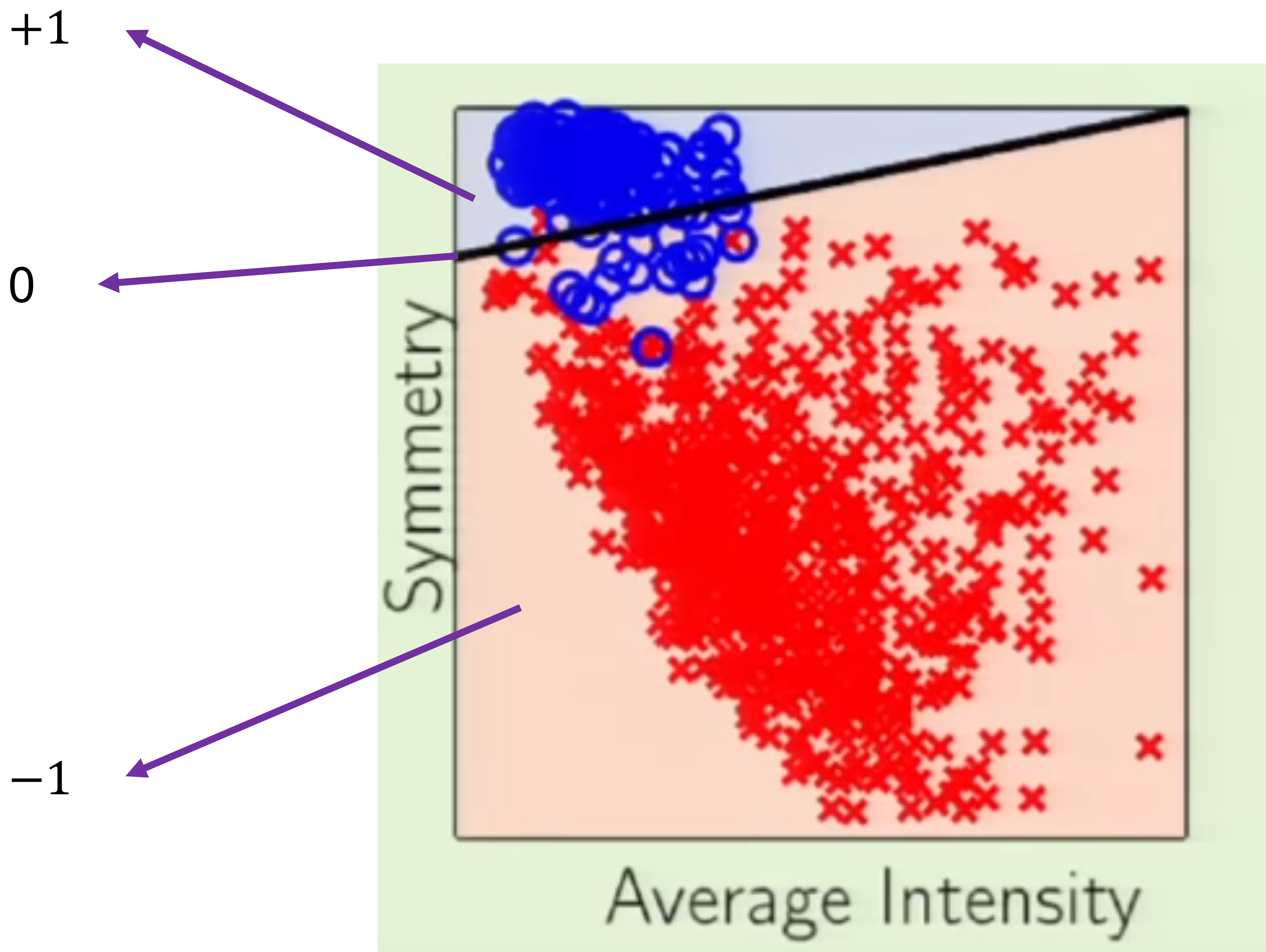
Binary-valued functions are also real-valued $\pm 1 \in R$

Use linear regression $x_i\theta \approx y_n = \pm 1$ $\quad$ i = index of a data-point

Let's calculate, $sign(x_i\theta) = \begin{cases} -1 & x_i\theta < 0 \\ 0 & x_i\theta = 0 \\ 1 & x_i\theta > 0 \end{cases}$

For one data point (data-point i) with **d** dimensions (instance):





Not really the best for classification, but t’s a good start

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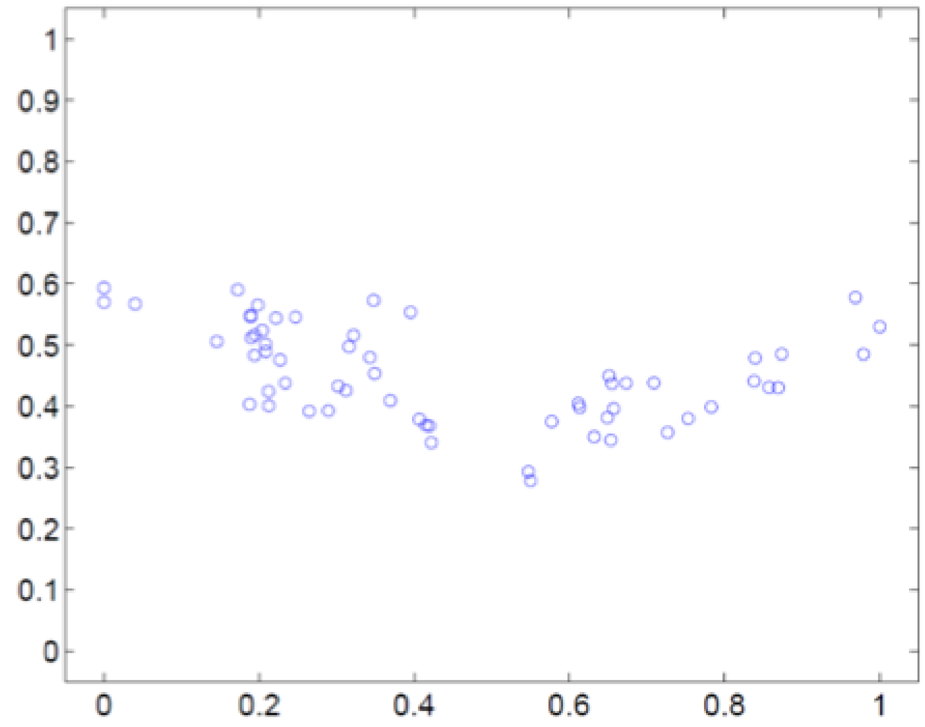
Extension to Higher-Order Regression



- Want to fit a polynomial regression model

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_{\mathrm{d}} x^{\mathrm{d}} + \epsilon$$

- $z = \{1, x, x^2, \ldots, x^d\} \in R^d$ and $\theta = (\theta_0, \theta_1, \theta_2, \ldots, \theta_{\mathrm{d}})^{\mathrm{T}}$

$$y = z\theta$$

Least Mean Square Still Works the Same

- Given n data points, find θ that minimizes the mean square error

$$\hat{\theta} = argmin_{\theta}\ L(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - z_i\theta)^2$$

- Our usual trick: set gradient to 0 and find parameter

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\sum_{i=1}^{n} z_i^T(y_i - z_i\theta) = 0$$

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\sum_{i=1}^{n} z_i^T y_i + \frac{2}{n}\sum_{i=1}^{n} z_i^T z_i\theta = 0$$

Matrix Version of the Gradient

$z = \{1, x, x^2, \dots, x^d\} \in R^d$ $\qquad$ $y = \{y_1, y_2, \dots, y_n\}$

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n} z^{\mathrm{T}} \mathrm{y} + \frac{2}{n} z^T z \theta = 0$$

$$\Rightarrow \ \theta = (z^T z)^{-1} z^T y = z^+ \, y$$

- If we choose a different maximal degree **d** for the polynomial, the solution will be different.

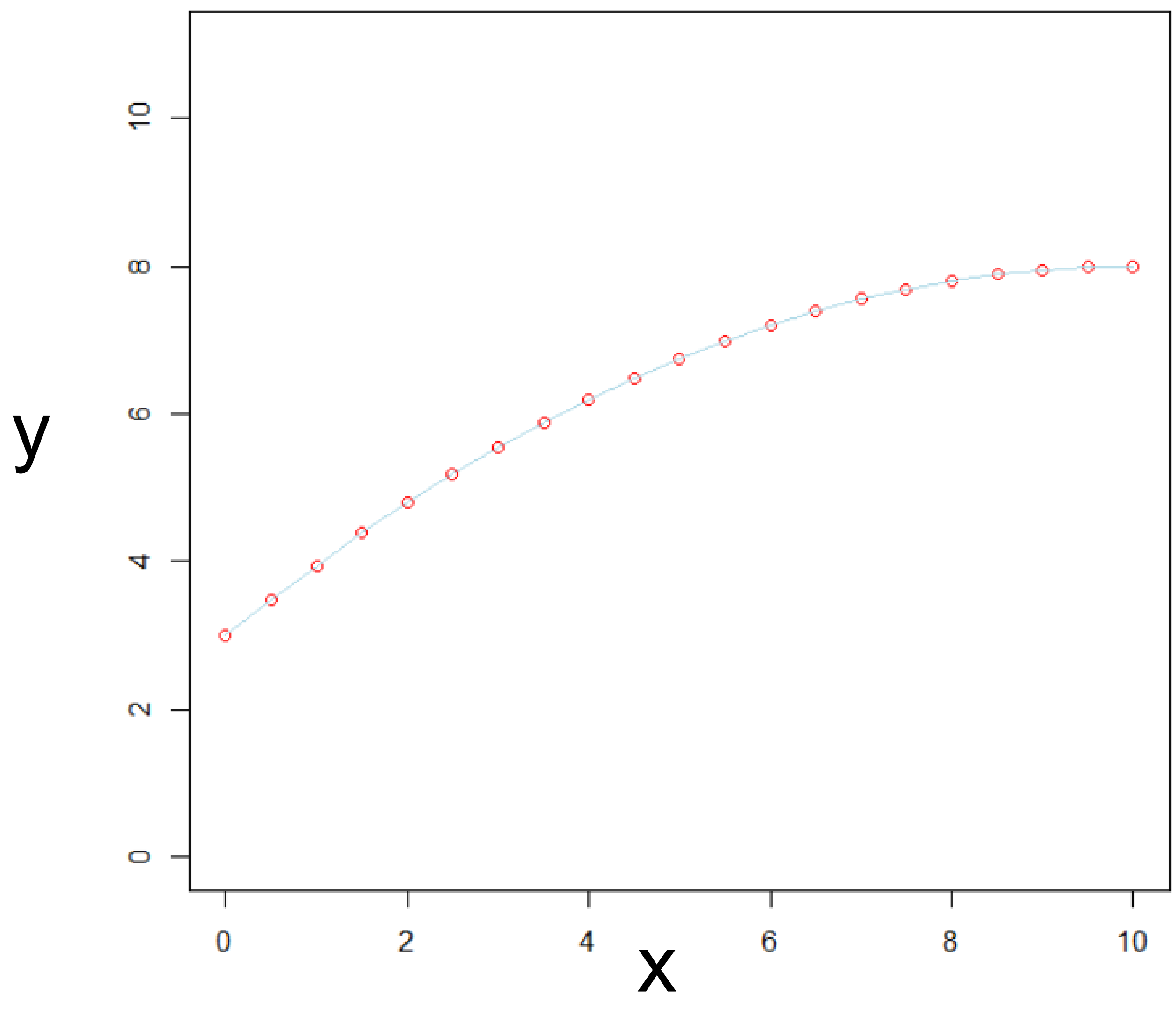
What is happening in polynomial regression?

$x = [0,0.5,1,\ldots,9.5,10]$

$y = [3,3.4875,3.95,\ldots,7.98,8]$

$f = \theta_0 + \theta_1 x + \theta_2 x^2$

$\theta_0 = 3; \theta_1 = 1; \theta_2 = -0.5$

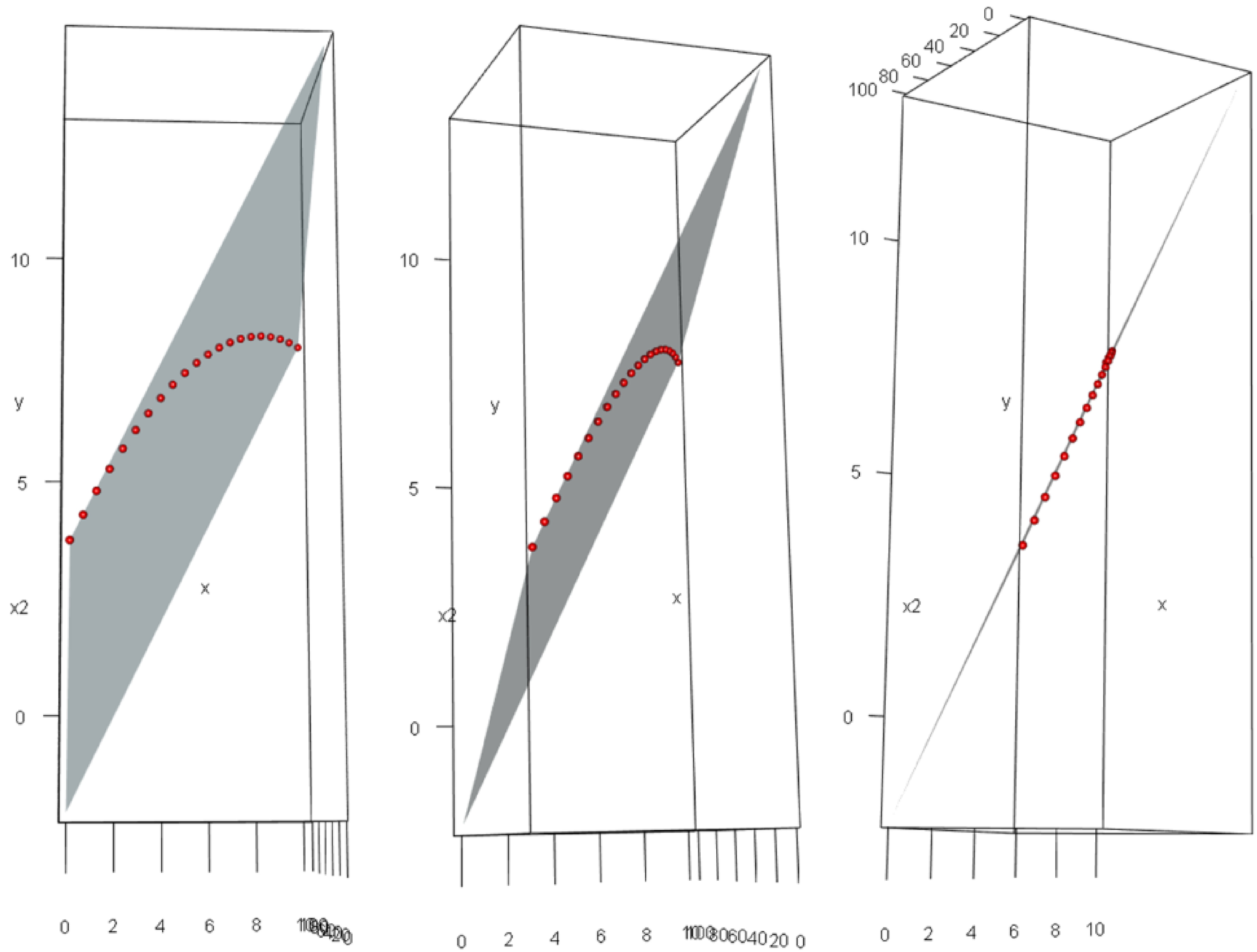


RMSE=0

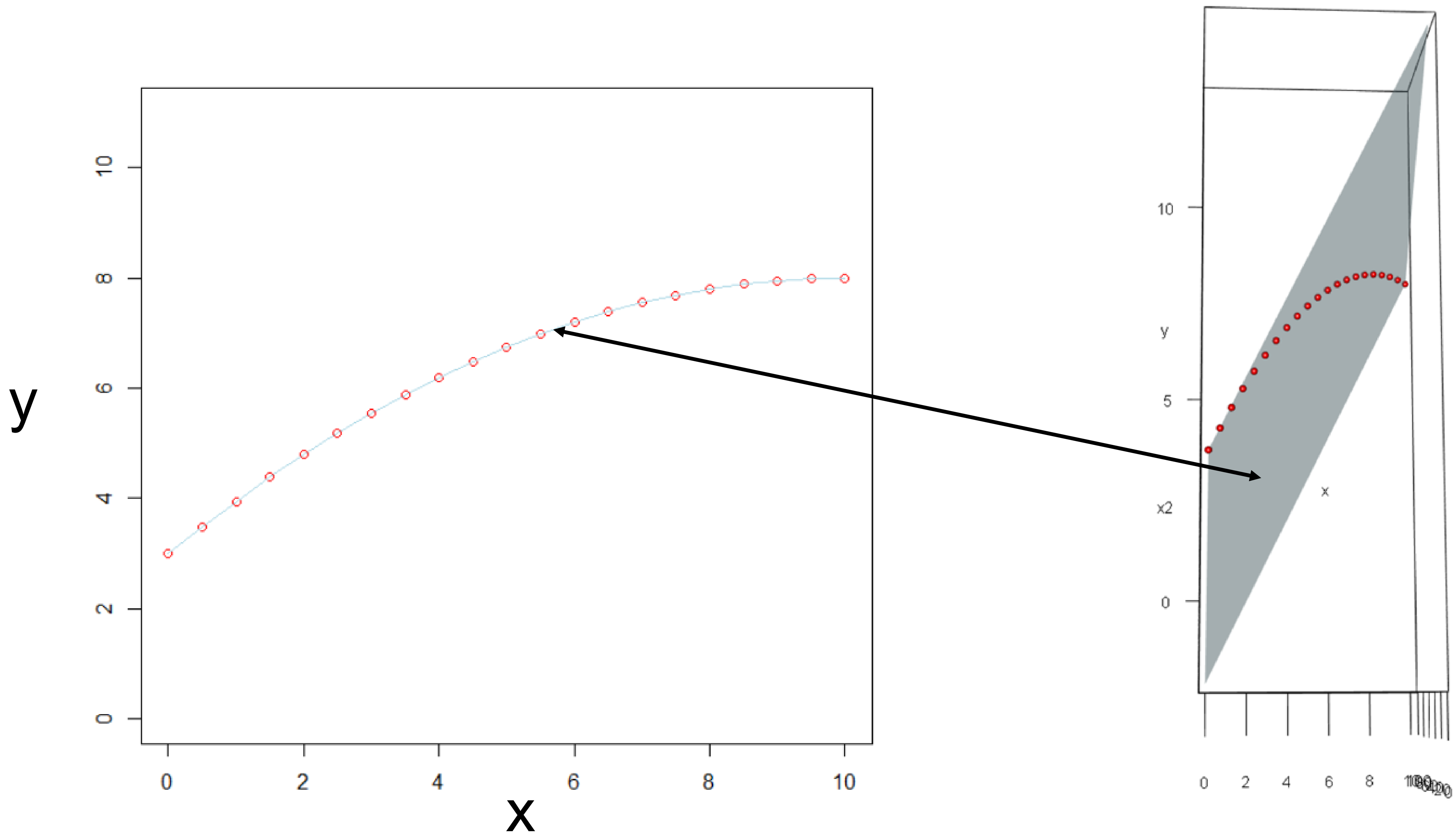
Let's add to the feature space

$x_1 = [0,0.5,1,\dots,9.5,10]$ $\quad x_2^2 = [0,0.25,1,\dots,90.25,100]$

$y = [3,3.4875,3.95,\dots,7.98,8]$

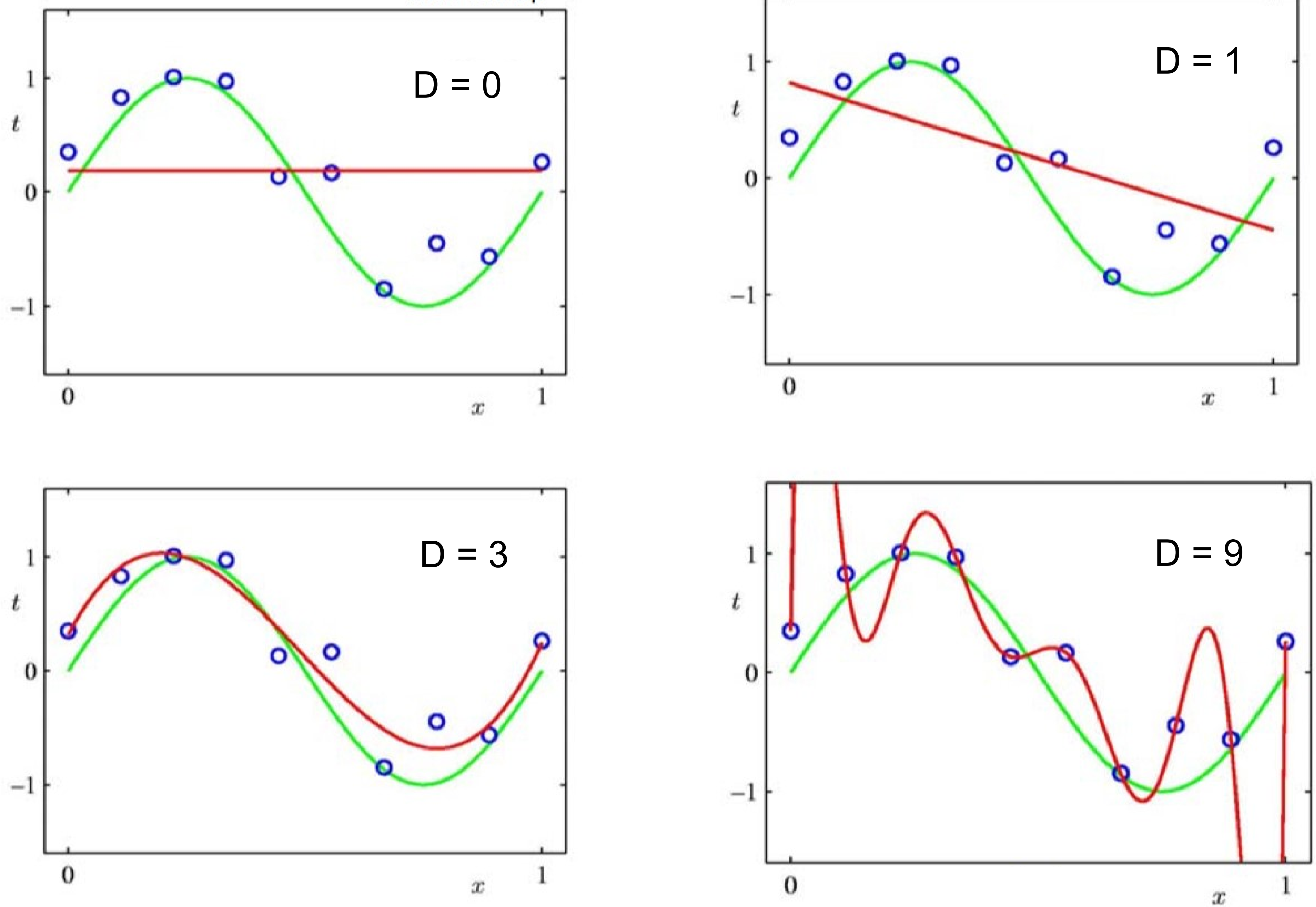


We are fitting a D-dimensional hyperplane in a D+1 dimensional hyperspace (in above example a 2D plane in a 3D space). That hyperplane really is 'flat' / 'linear' in 3D. It can be seen a non-linear regression (a curvy line) in our 2D example in fact it is a flat surface in 3D. So the fact that it is mentioned that the model is linear in parameters, it is shown here.

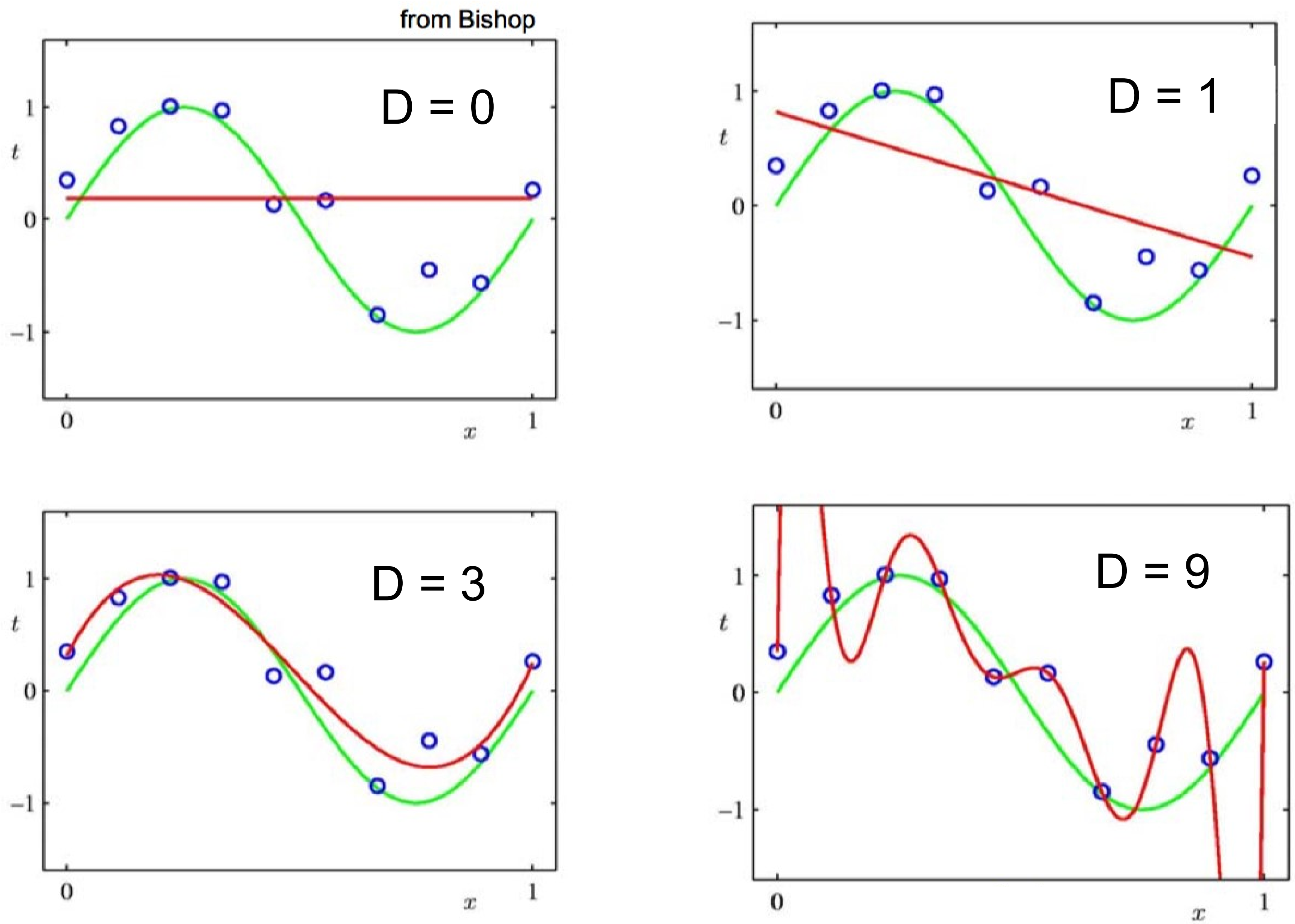


Increasing the Maximal Degree

from Bishop



Which One is Better?



- Can we increase the maximal polynomial degree to very large, such that the curve passes through all training points?

  - We will know the answer in next lecture.

Take-Home Messages

- Supervised learning paradigm
- Linear regression and least mean square
- Extension to high-order polynomials