# Linear Regression

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

# Outline

- Supervised Learning ←
- Linear Regression
- Extension

# Supervised Learning: Overview

Functions $\mathcal{F}$

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

Training data

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

LEARNING

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

Learning machine

New data

$x$

PREDICTION

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

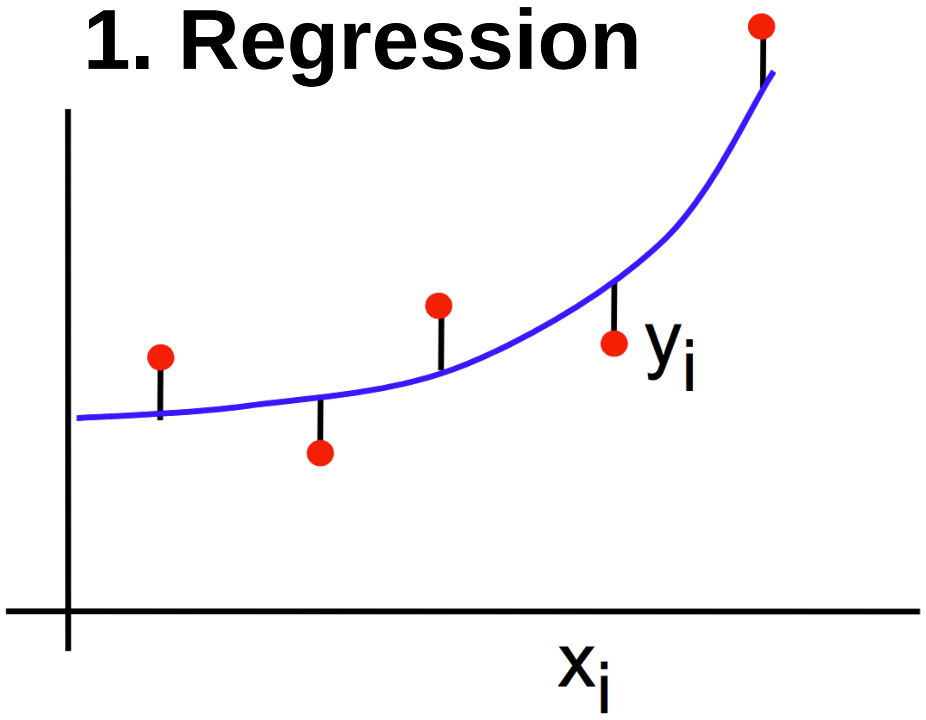
# Supervised Learning: Two Types of Tasks

**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:*

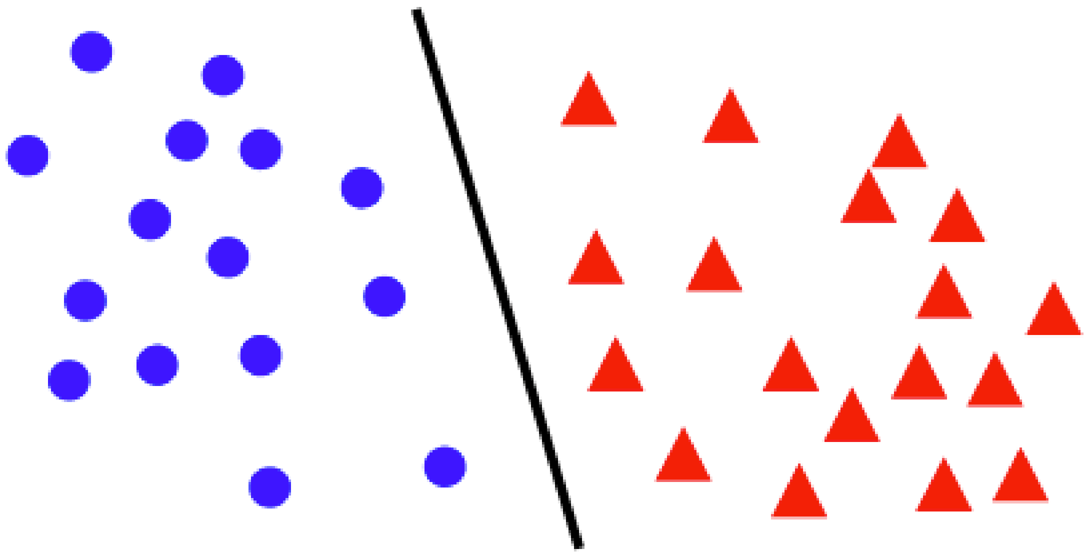
**1. Regression**




Curve fitting

*When y is discrete:*

**2. Classification**

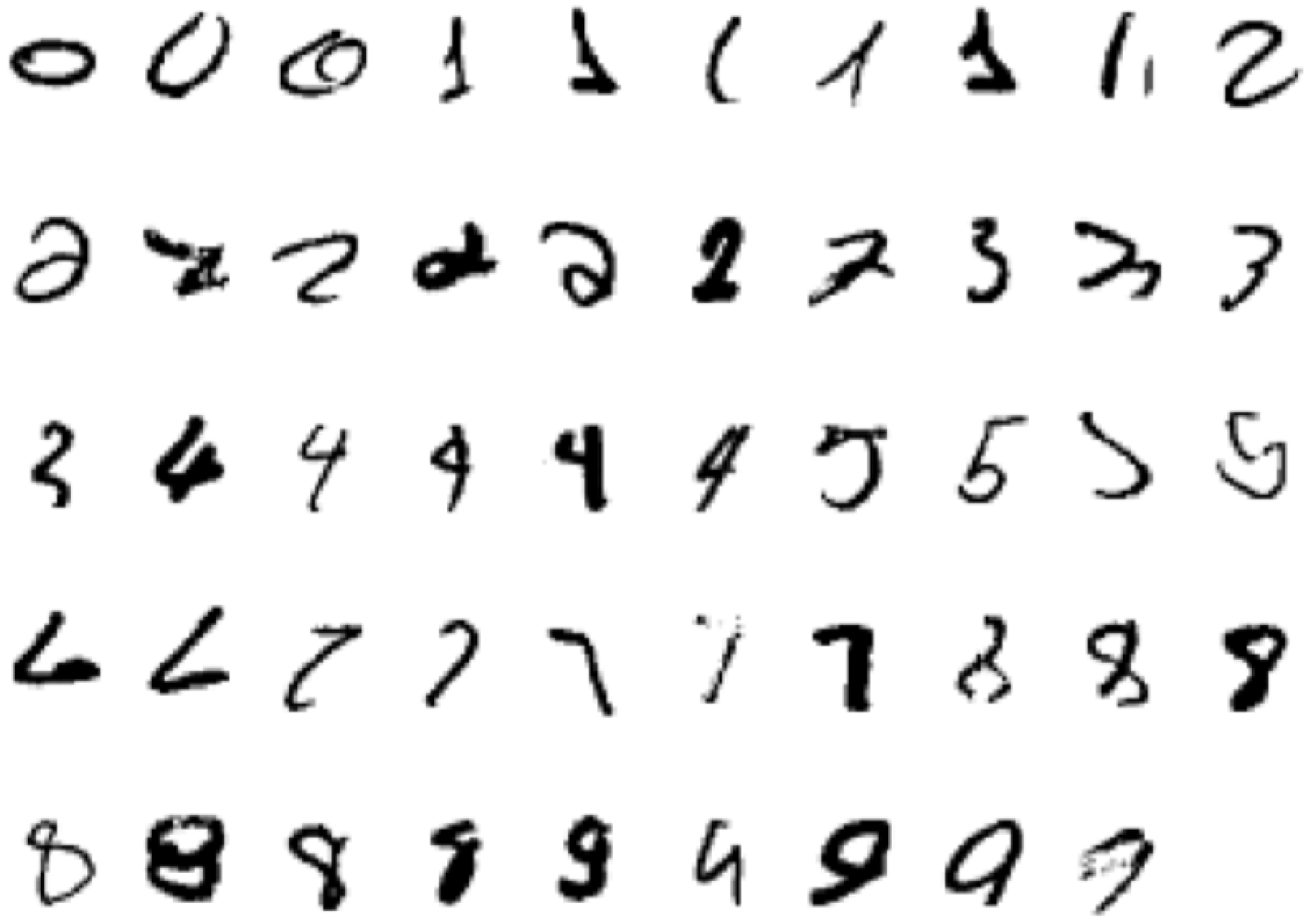


Class estimation

# Classification Example 1: Handwritten digit recognition

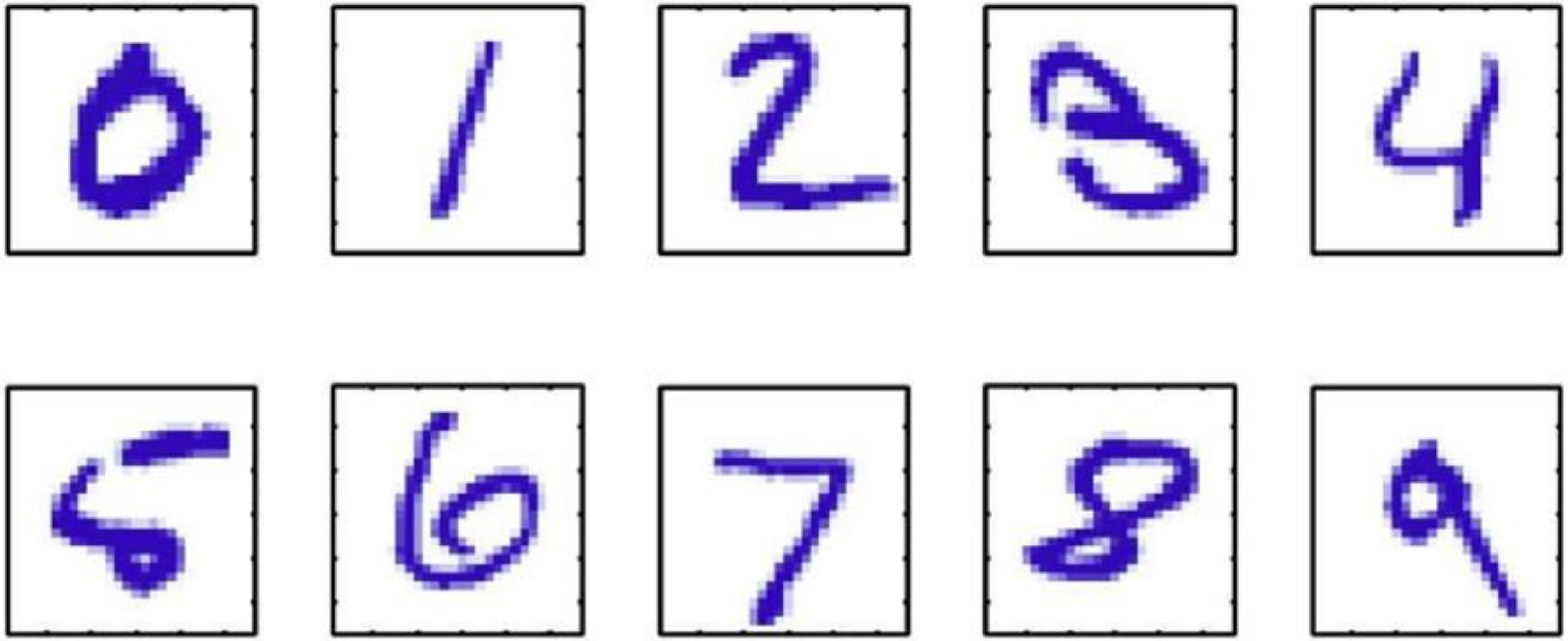
As a supervised classification problem

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)

# Classification Example 1: Hand-Written Digit Recognition



Images are 28 x 28 pixels

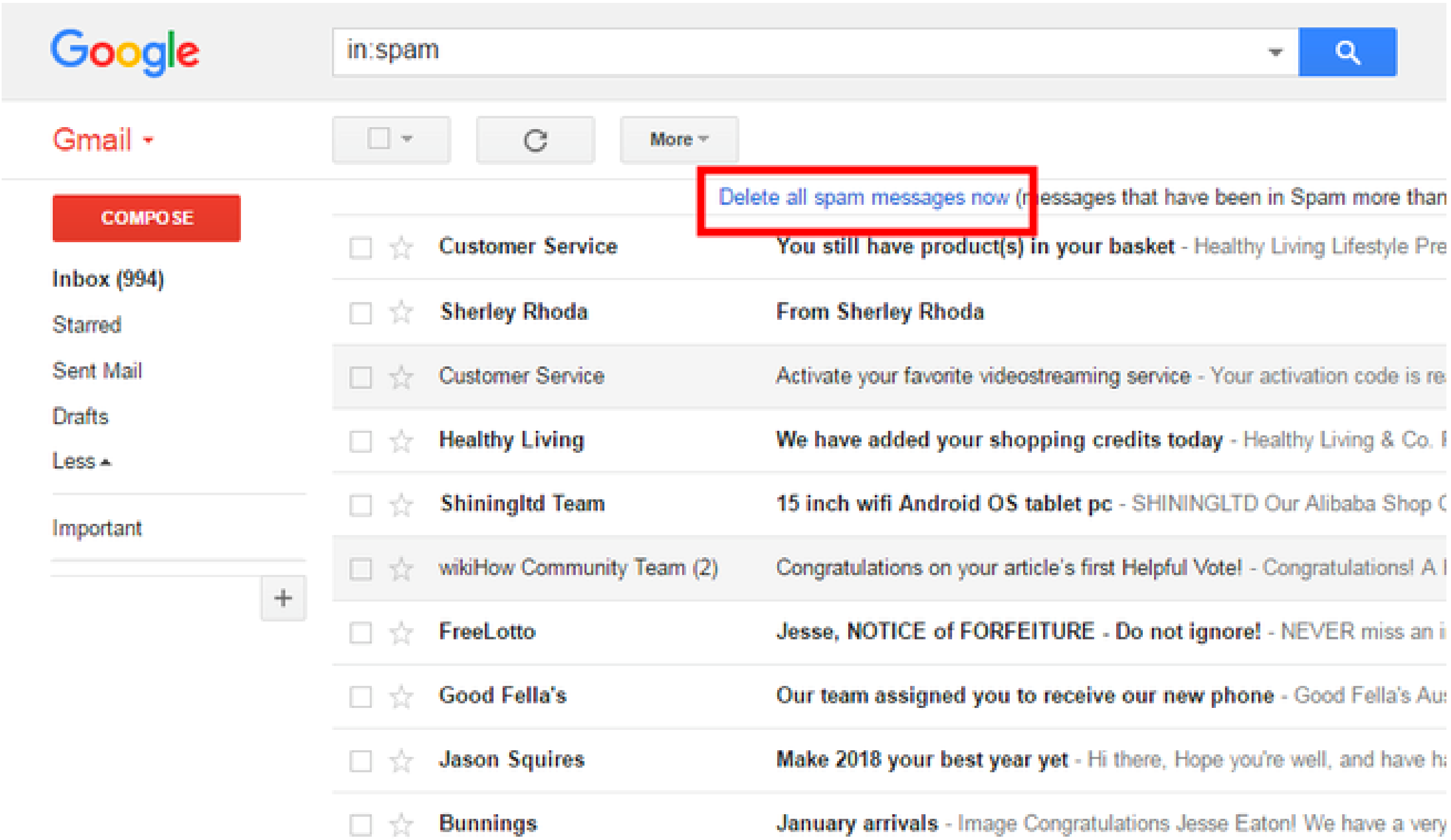
**A classification problem**

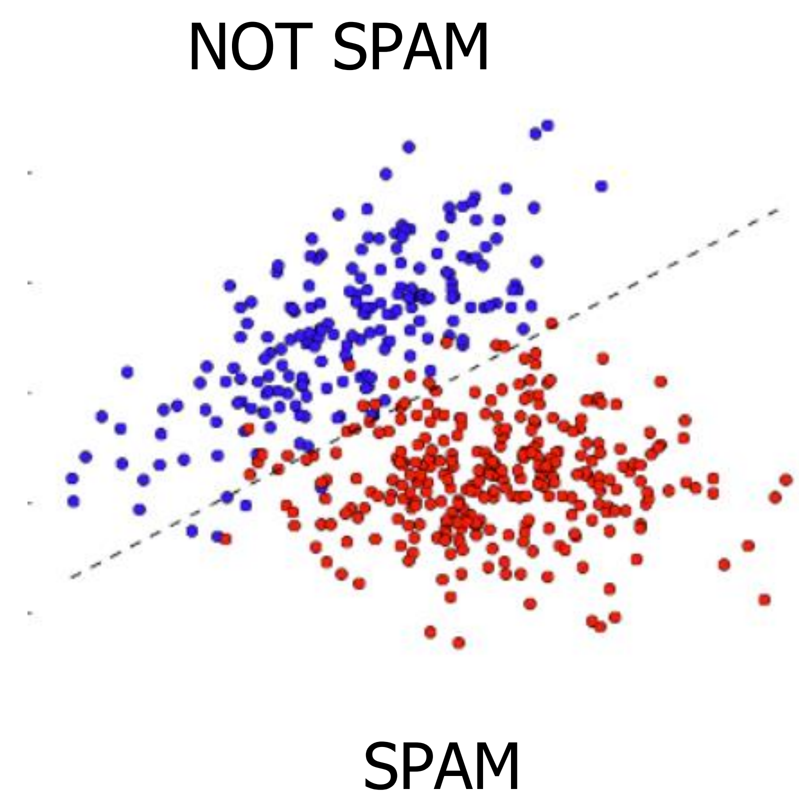
Represent input image as a vector $\mathbf{x} \in \mathbb{R}^{784}$

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

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

# Classification Example 2: Spam Detection




## 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

# Regression Example 1: Apartment Rent Prediction

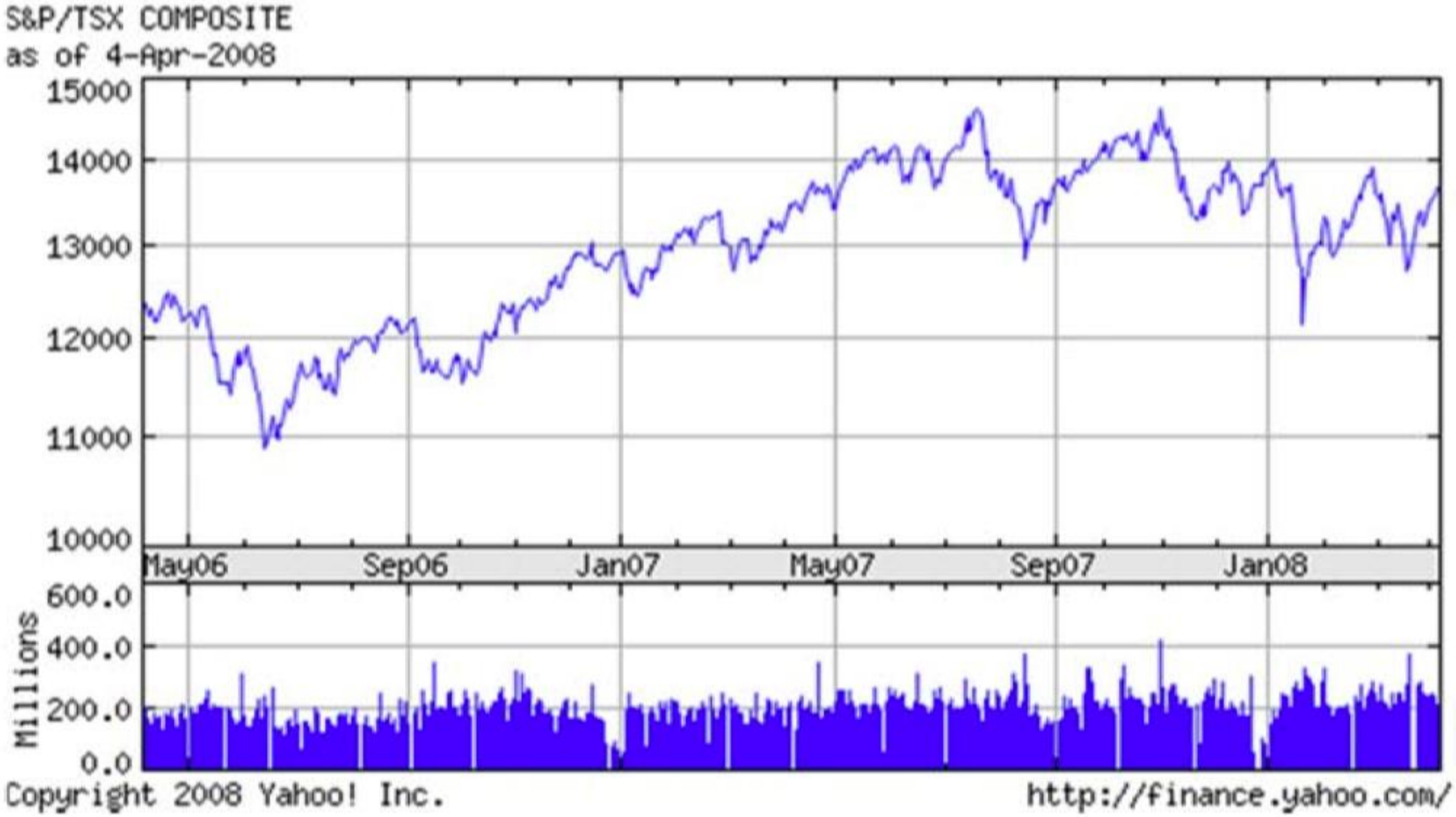
- Suppose you are to move to Atlanta
- And you want to find the **most reasonably priced** apartment satisfying your **needs:**

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

**A regression problem**

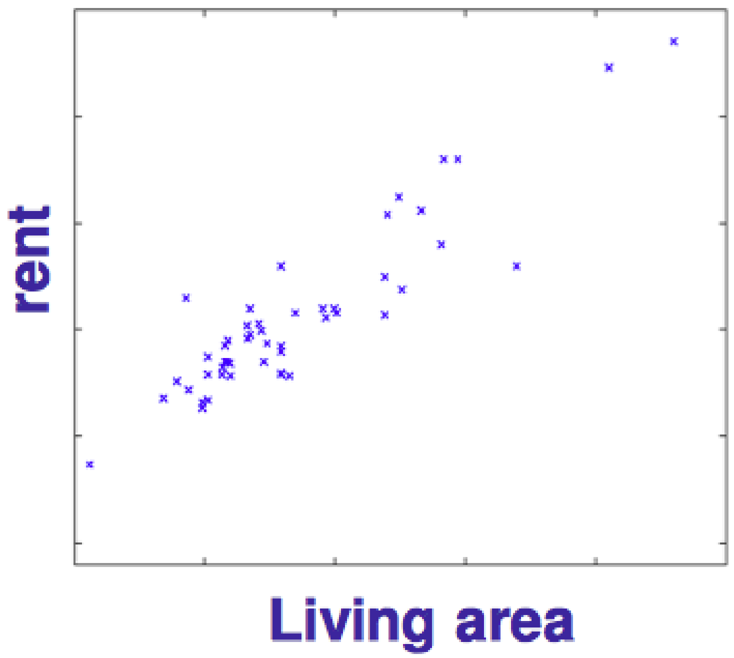
| Living area ($ft^2$) | # bedroom | Rent ($) |
|---|---|---|
| 230 | 1 | 600 |
| 506 | 2 | 1000 |
| 433 | 2 | 1100 |
| 109 | 1 | 500 |
| … | | |
| 150 | 1 | ? |
| 270 | 1.5 | ? |

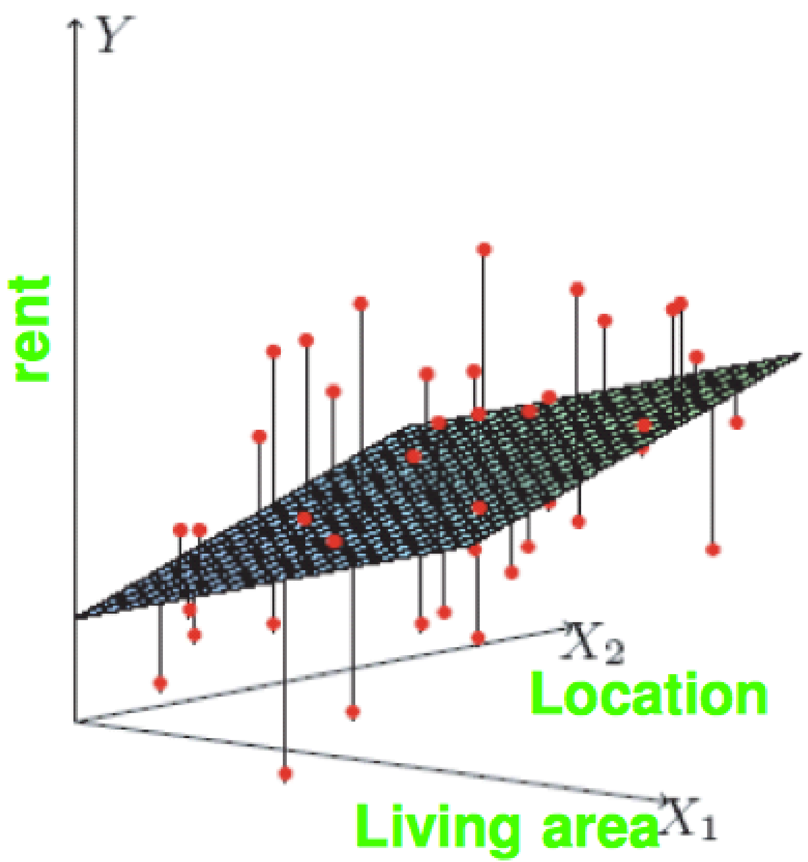
# Regression Example 2: Stock Price Prediction




- Task is to predict stock price at future date

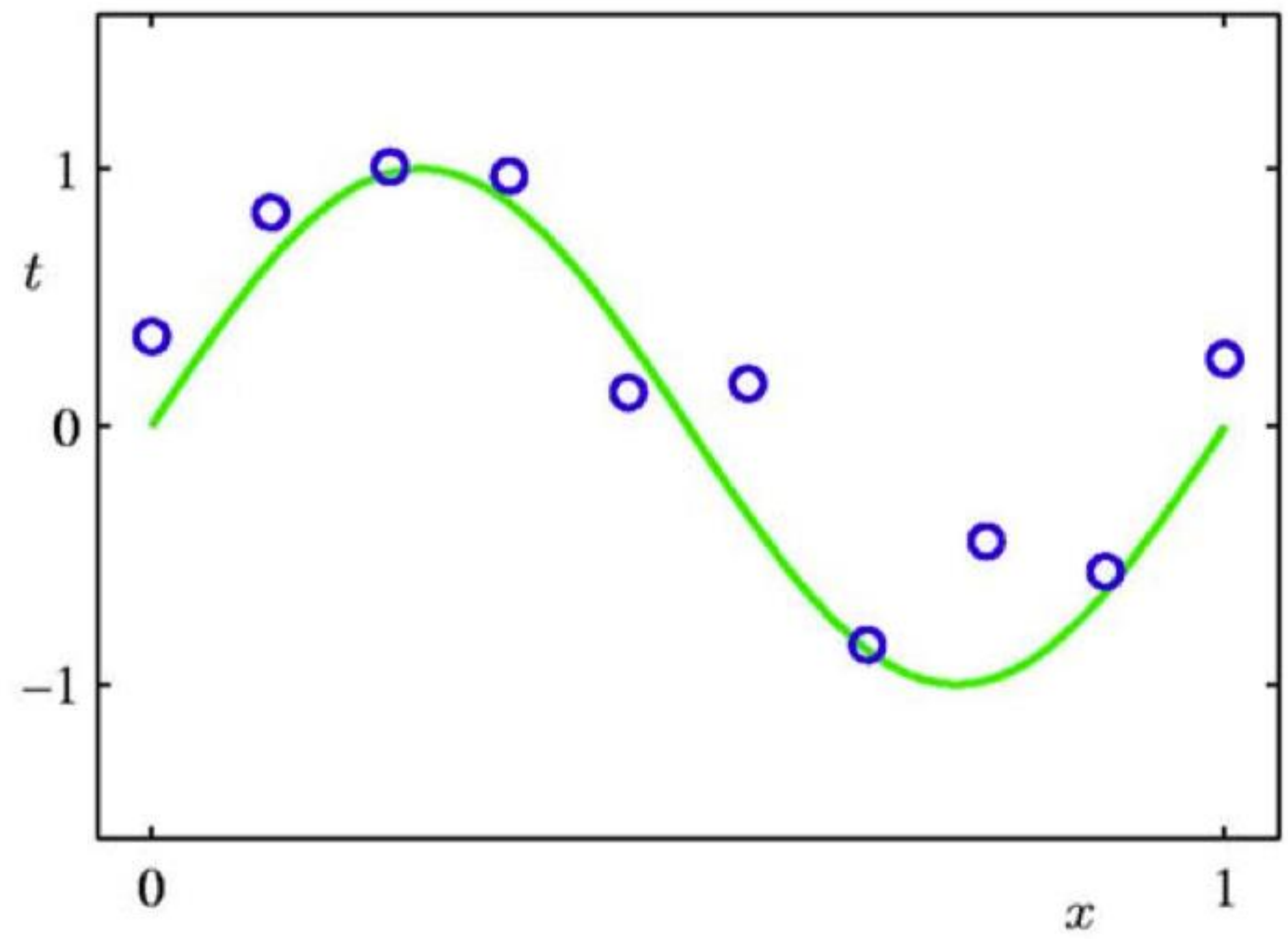
**A regression problem**




- 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
- Linear Regression ←
- Extension

# Linear Regression

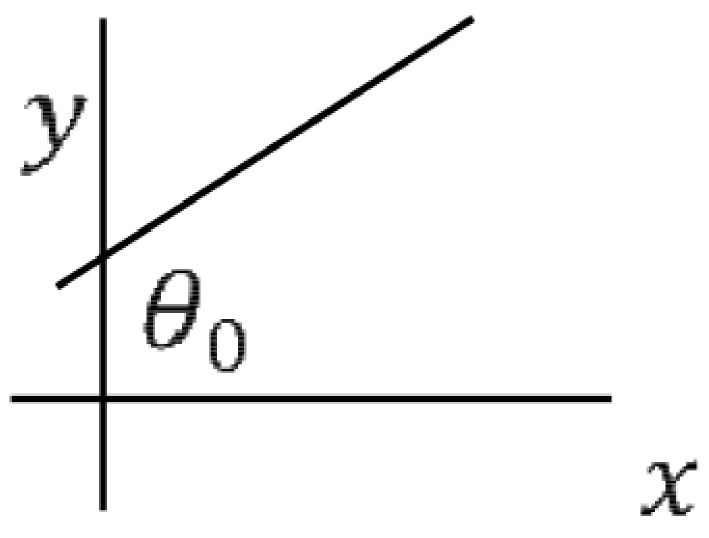
- Assume $y$ is a linear function of $x$ (features) plus noise $\epsilon$

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

- where $\epsilon$ is an error term of unmodeled effects or random noise

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

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



# Least Mean Square Method

- Given n data points, find $\theta$ 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 $\frac{\partial L(\theta)}{\partial \theta} = 0$

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

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

# Matrix form

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

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

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

# 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 $\mathbf{X}^{\mathbf{T}}\boldsymbol{X}$ 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)

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

# Methods to optimize

- 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

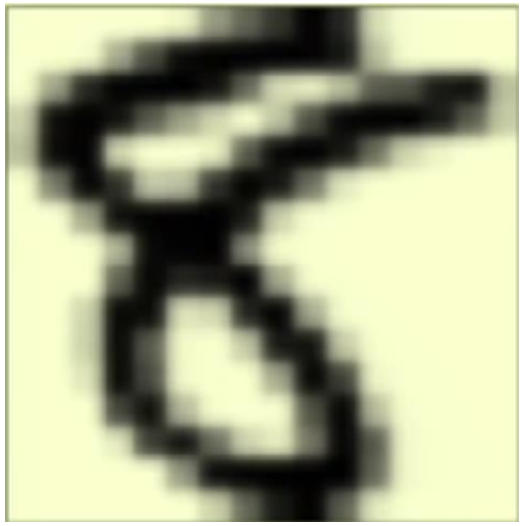
$$\theta = (X^T X)^{-1} X^T y$$

  - 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 $x = (x_0, x_1, \ldots, x_{255})$

Linear model $(\theta_0, \theta_1, \ldots, \theta_{255})$




Extract useful information

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

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

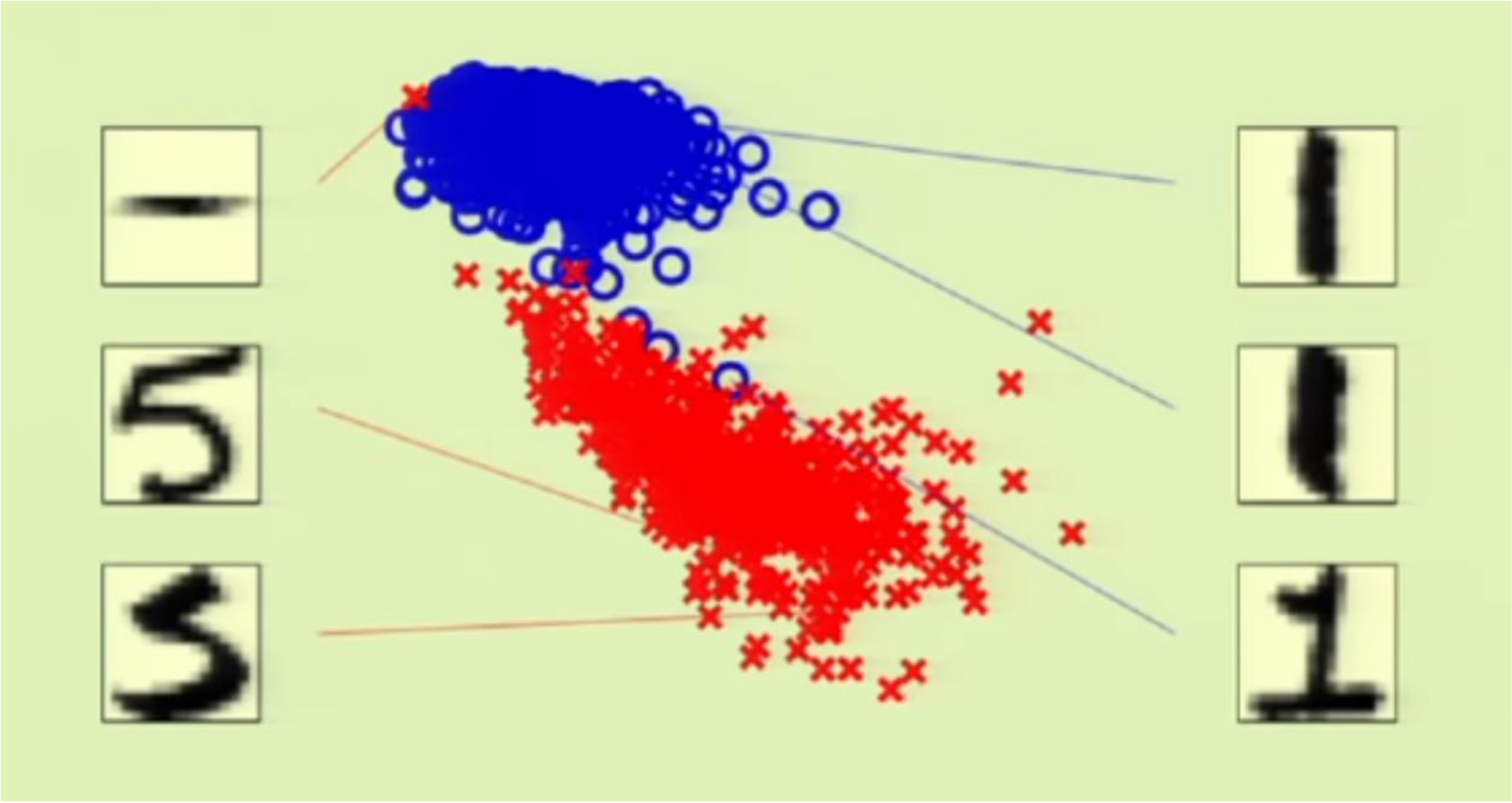
*Symmetry = -(difference between flip version)*

$x = (x_0, x_1, x_2)$

$x_1 = intensity \ x_2 = symmetry$

It is almost linearly separable

*symmetry*



*intensity*

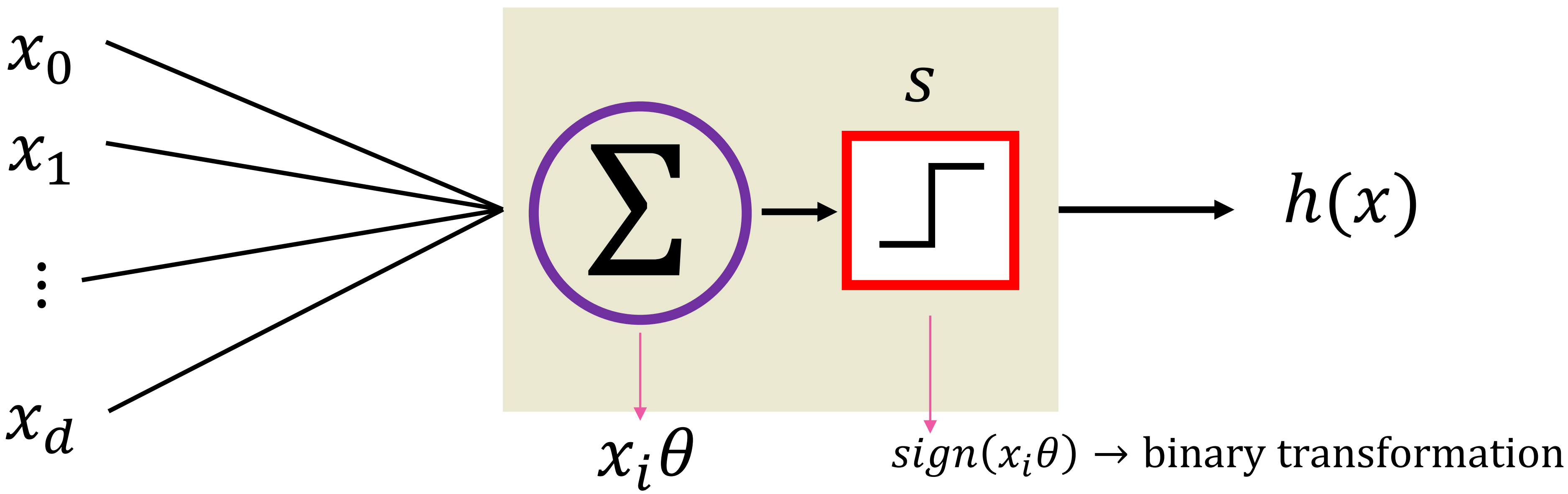
# Linear regression for classification

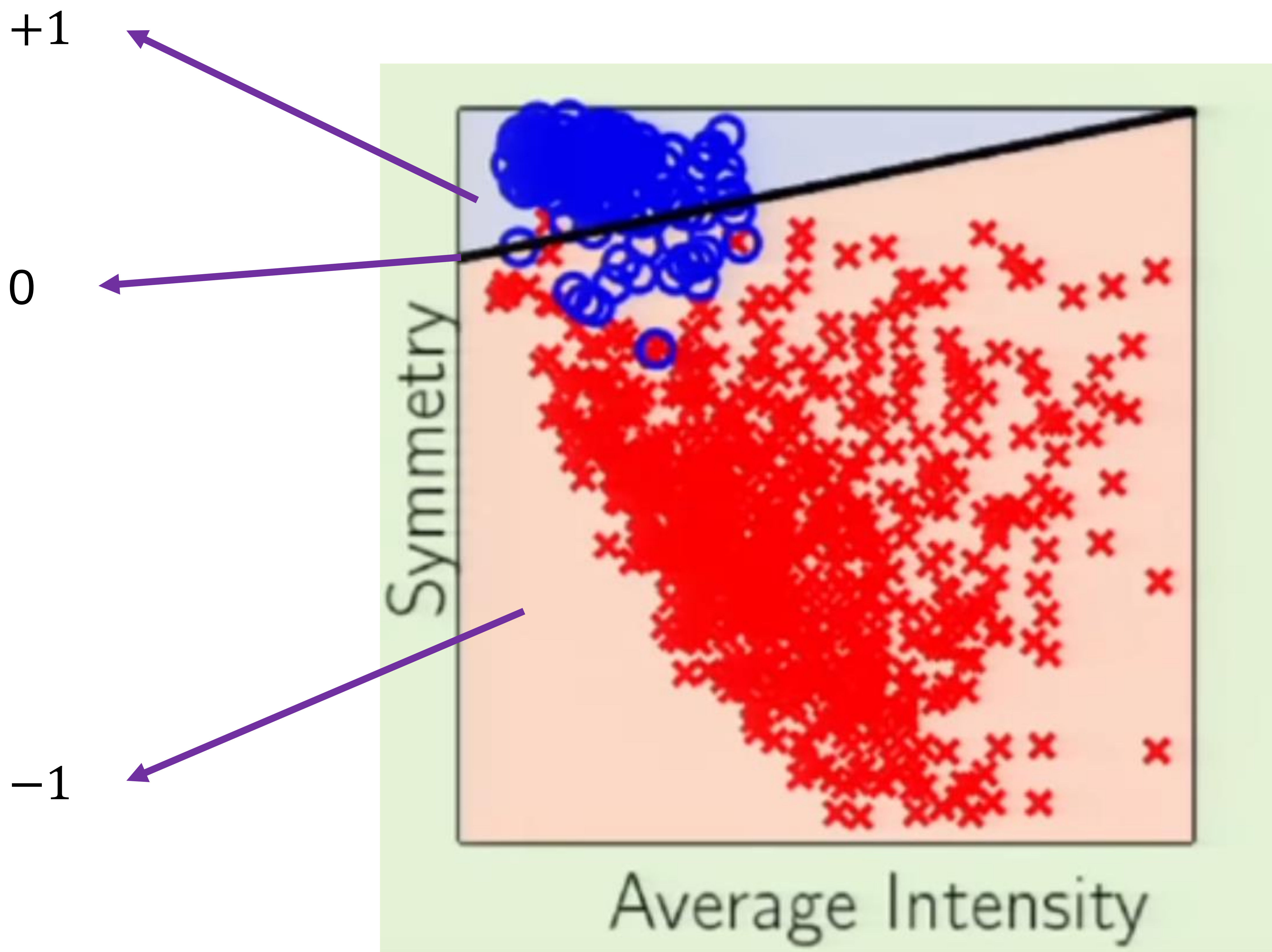
Binary-valued functions are also real-valued $\pm 1 \in R$

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

# Outline

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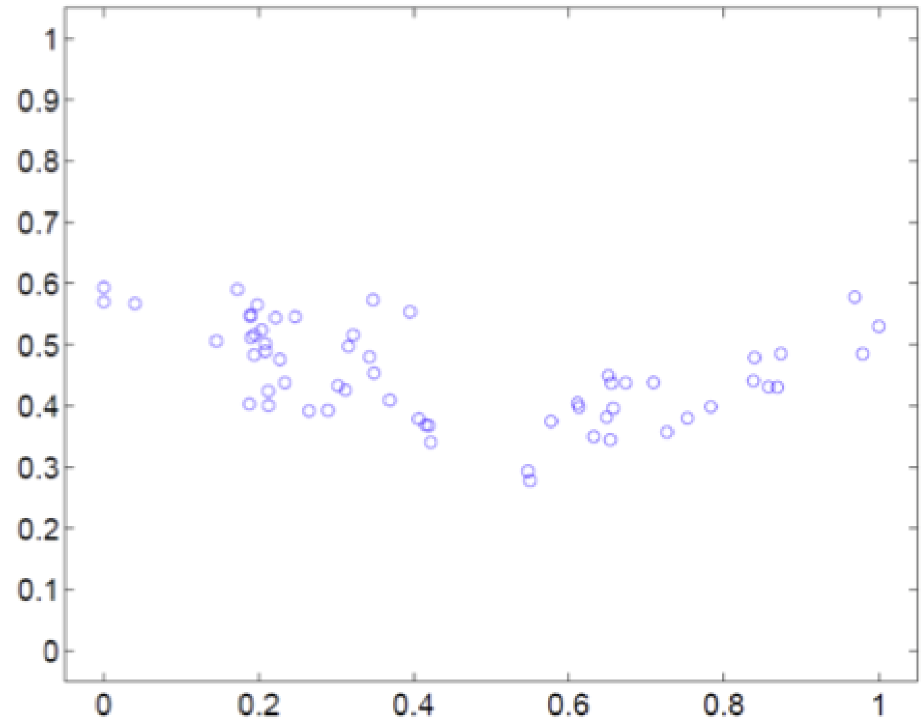
# Extension to Higher-Order Regression



- Want to fit a polynomial regression model

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_d x^d + \epsilon$$

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

$$y = z\theta$$

# Least Mean Square Still Works the Same

- Given n data points, find $\theta$ 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

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

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

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

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

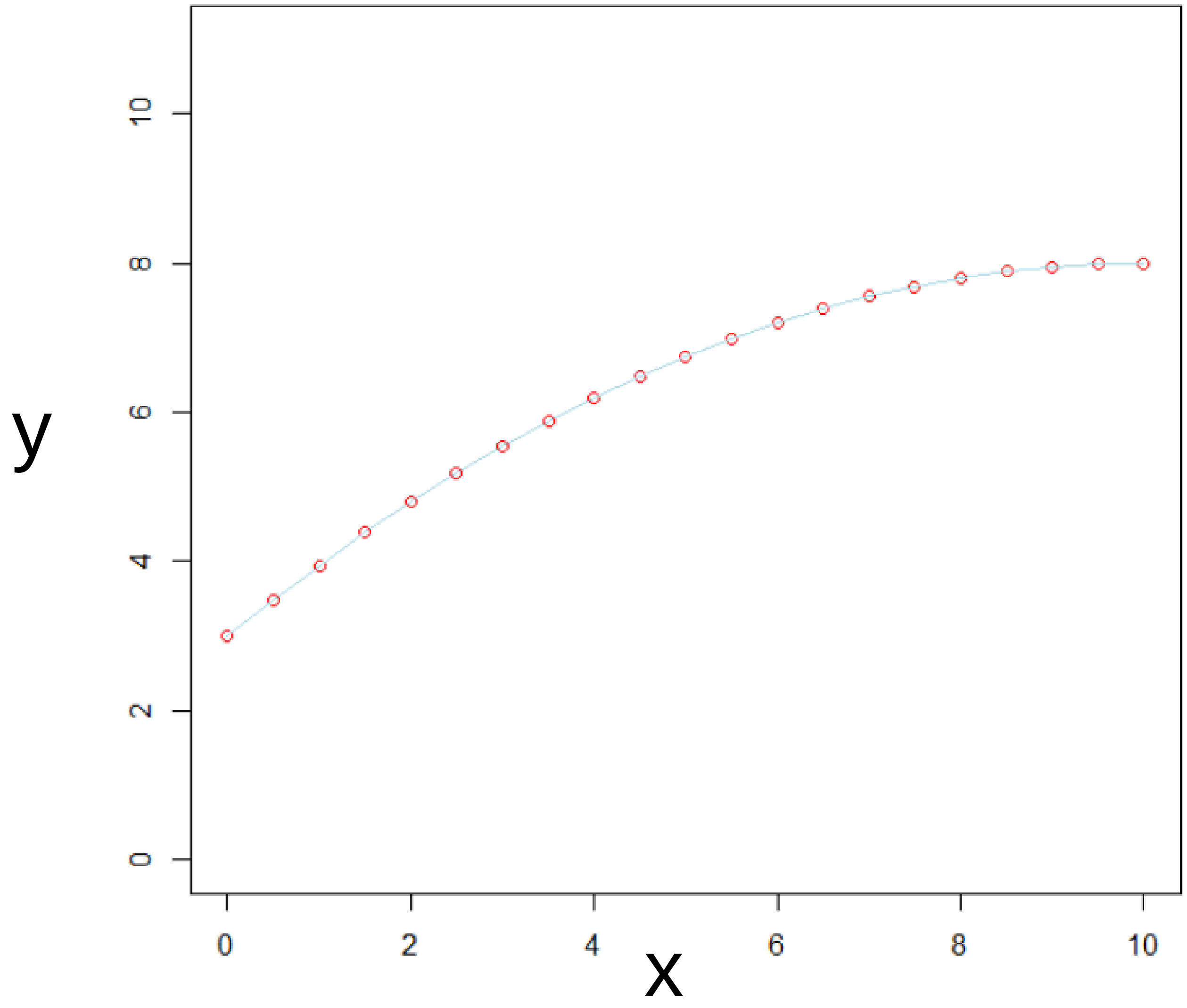
# What is happening in polynomial regression?

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

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

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

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

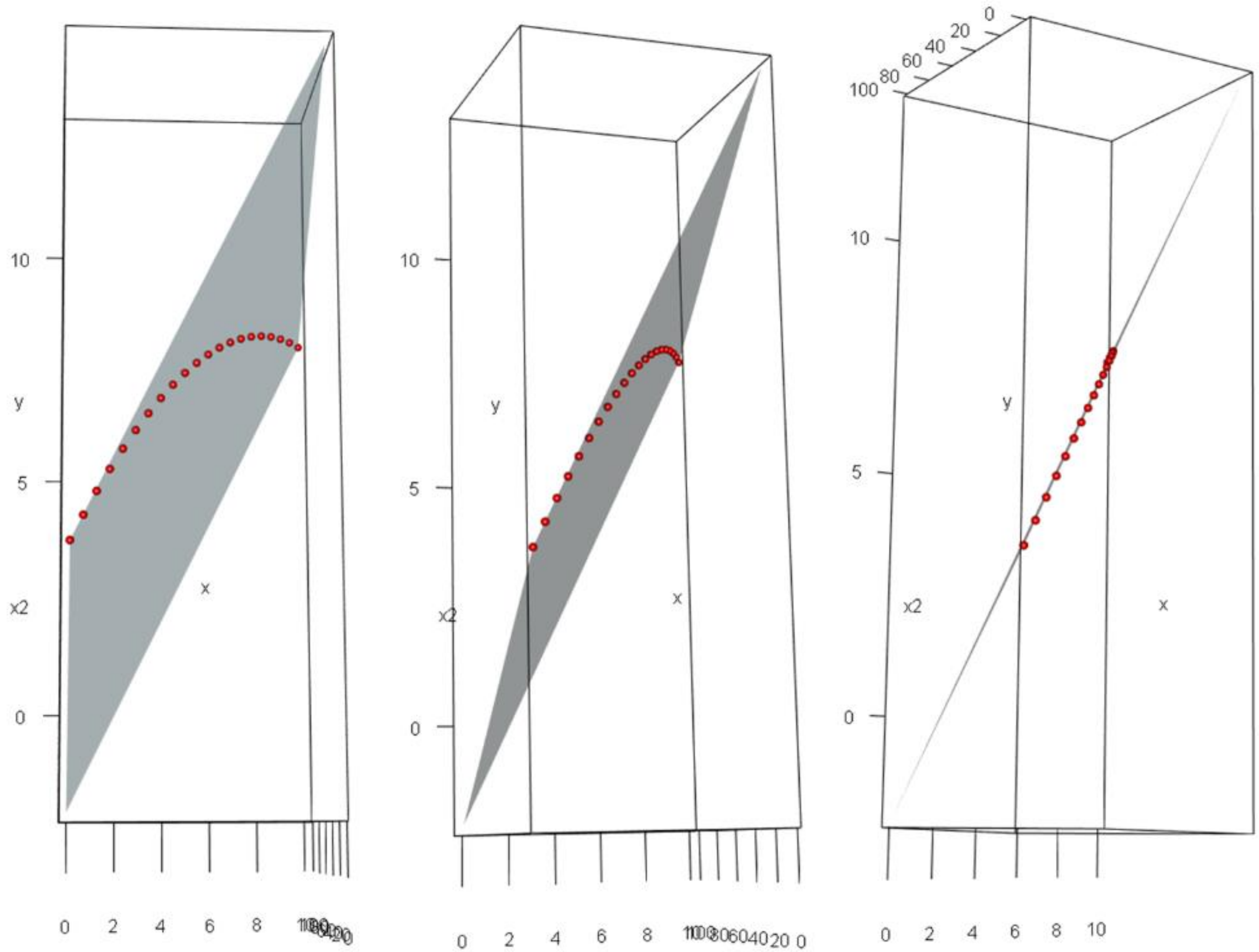



RMSE=0

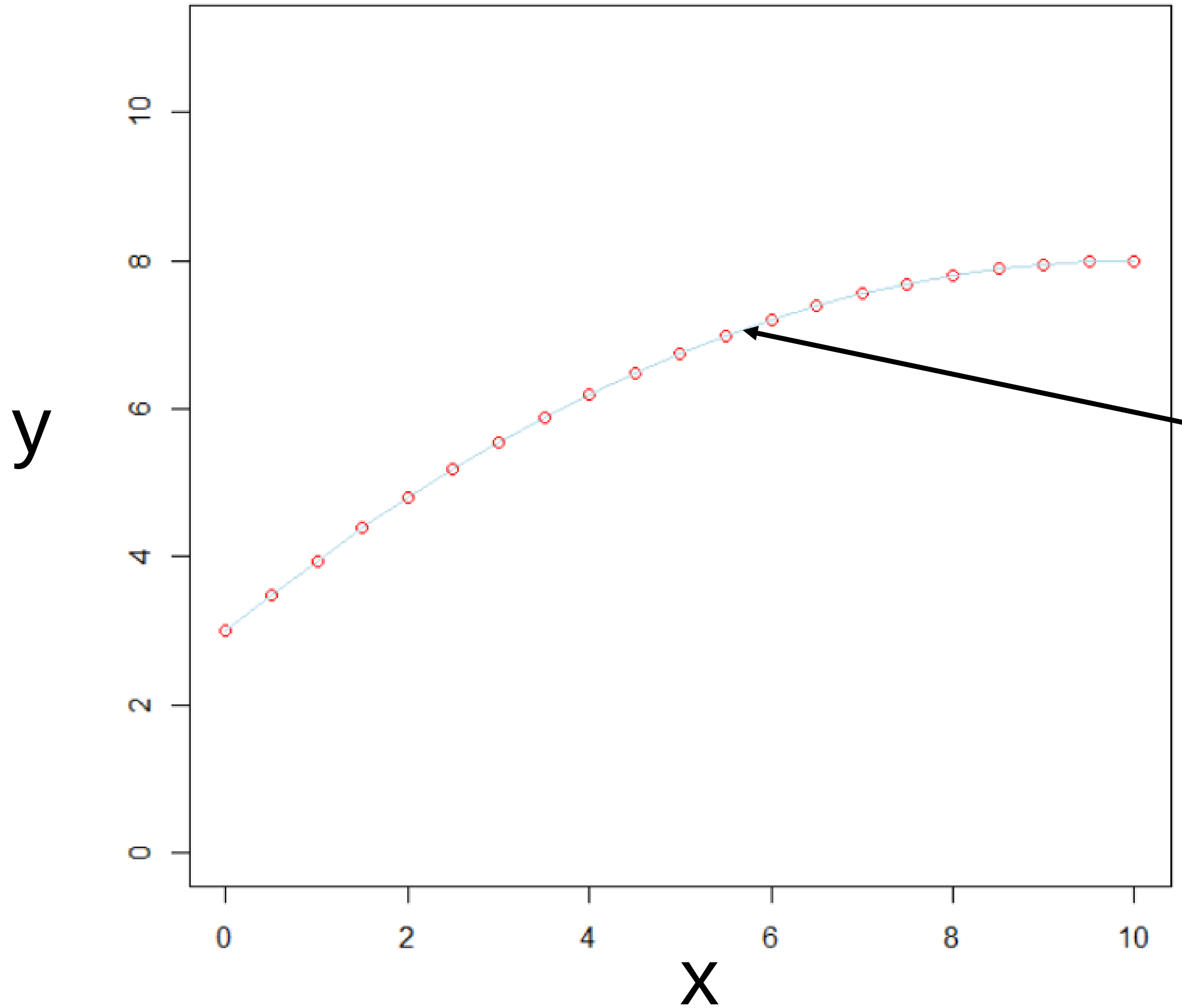
# Let's add to the feature space

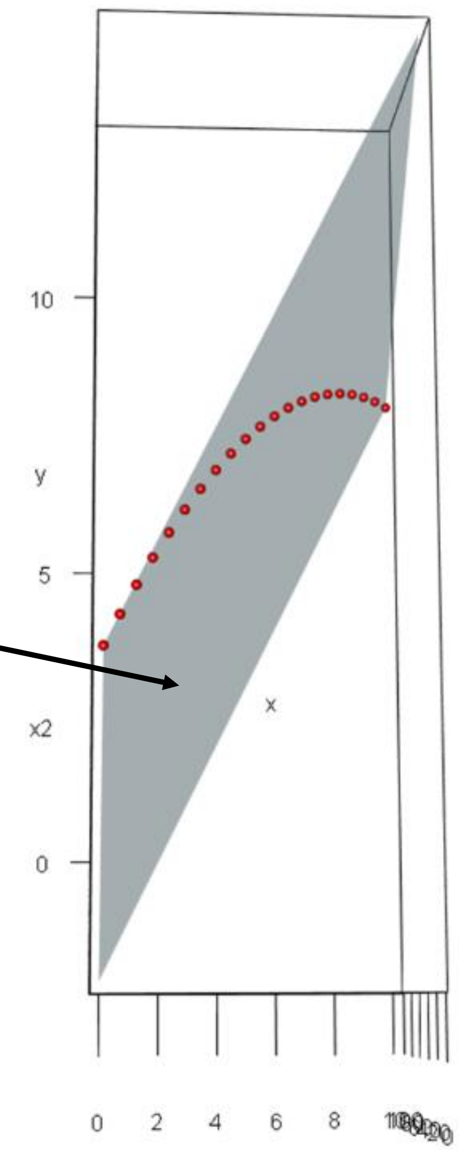
$x_1 = [0, 0.5, 1, \ldots, 9.5, 10]$ $\qquad$ $x_2^2 = [0, 0.25, 1, \ldots, 90.25, 100]$

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

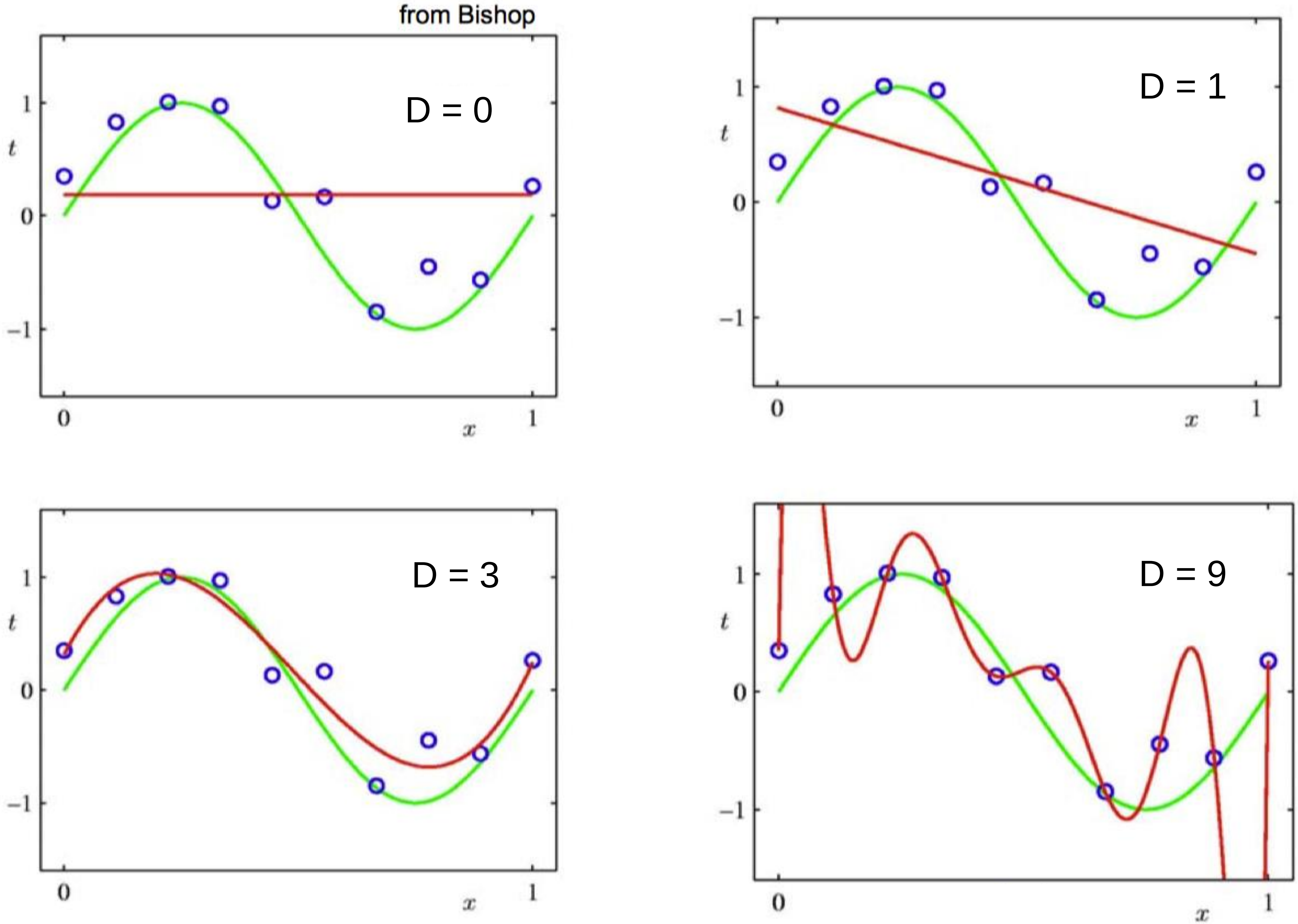


We are fitting a D-dimensional hyperplane in a D+1 dimensional hyperspace (in above example a 2D plane in a 3D space). That hyperplane really is 'flat' / 'linear' in 3D. It can be seen a non-linear regression (a curvy line) in our 2D example in fact it is a flat surface in 3D. So the fact that it is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

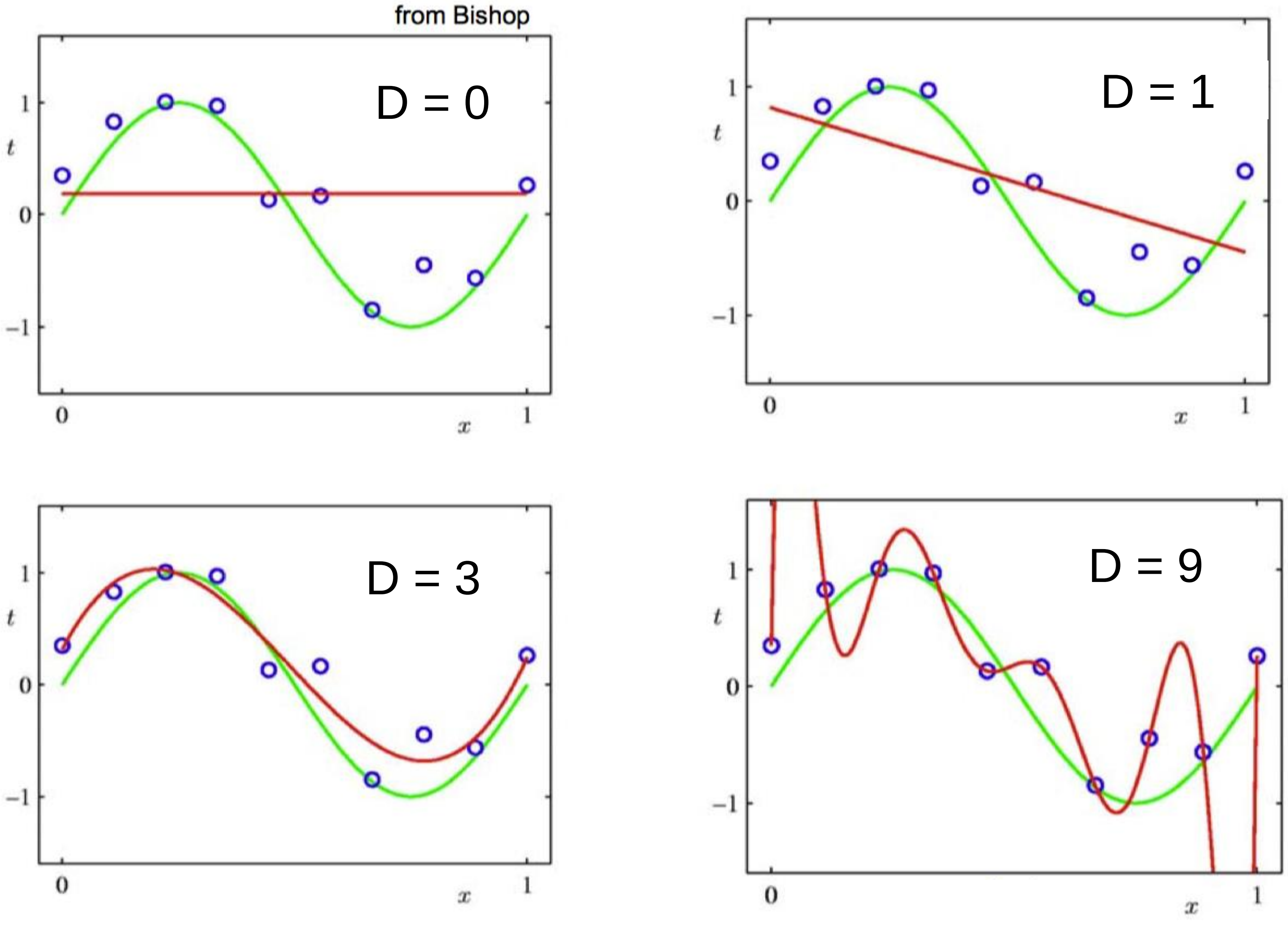


# Increasing the Maximal Degree



# 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