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.

Announcements

- Chris ran the python introduction last week
- Project sign-ups have begun
- TA hours – Start assignments early

What is a line?

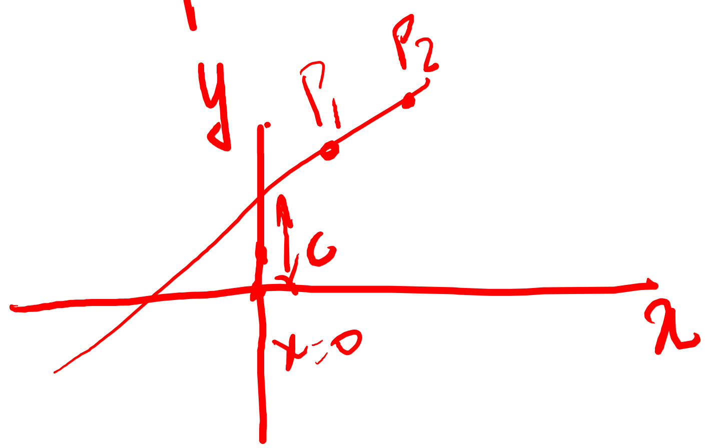
$$y = mx + c$$

$$P_1 = (x_1, y_1)$$

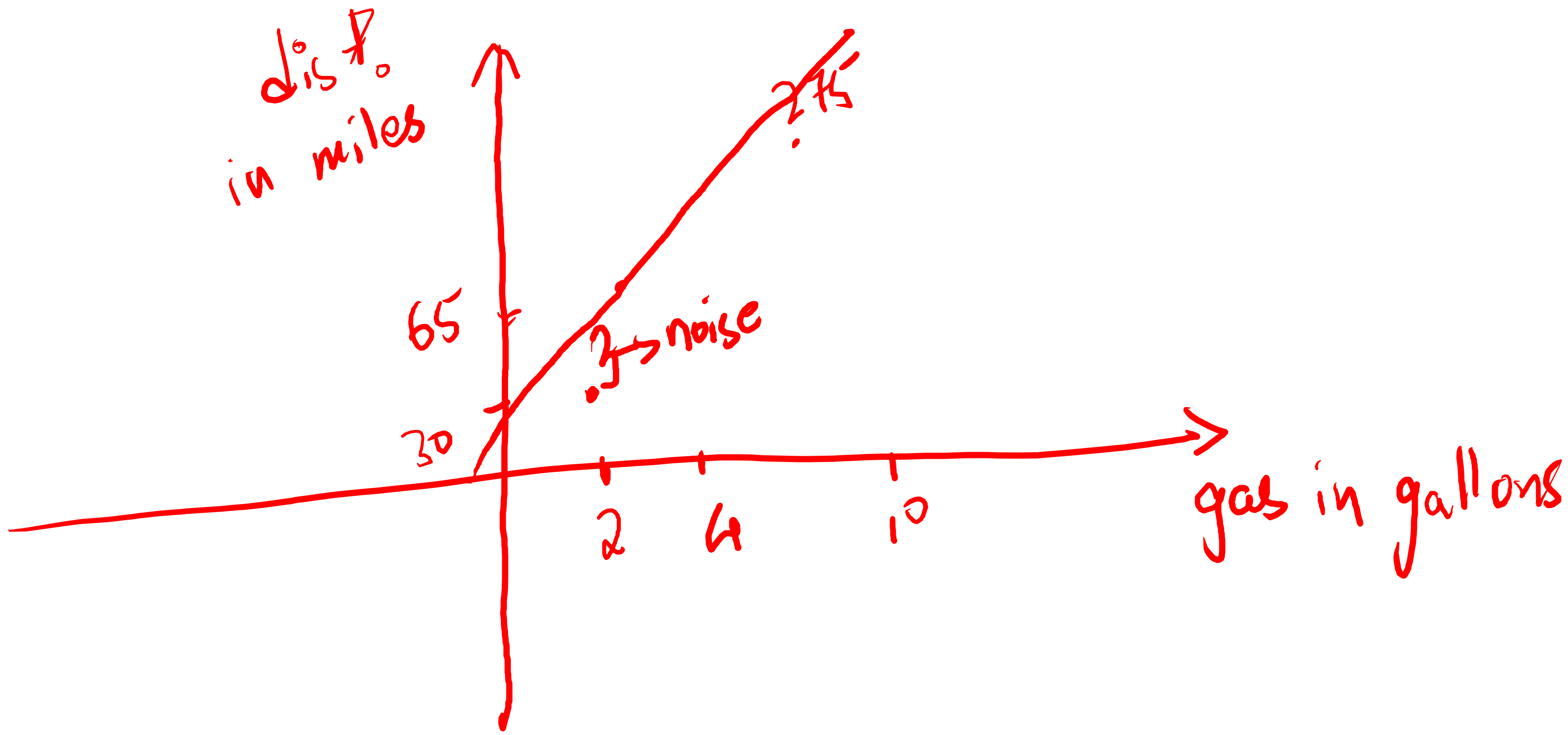
$$P_2 = (x_2, y_2)$$

$$m = \frac{y_1 - y_2}{x_1 - x_2}$$

$$c = y\big|_{x=0}$$



Are things linear?



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

PREDICTION

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

New data

x

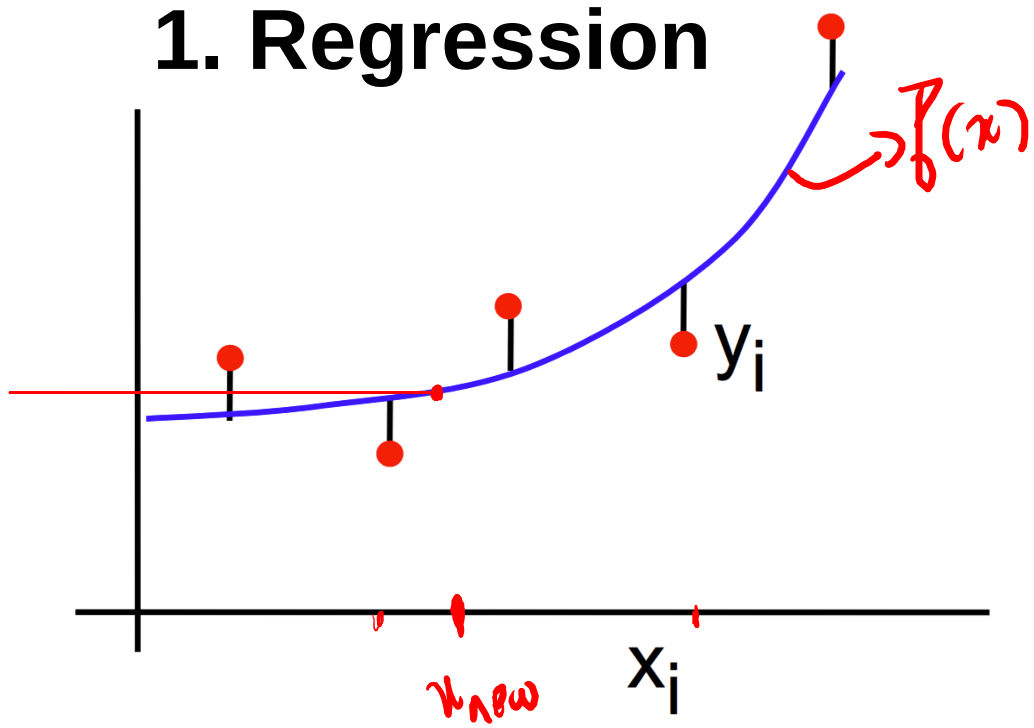
Supervised Learning: Two Types of Tasks

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:

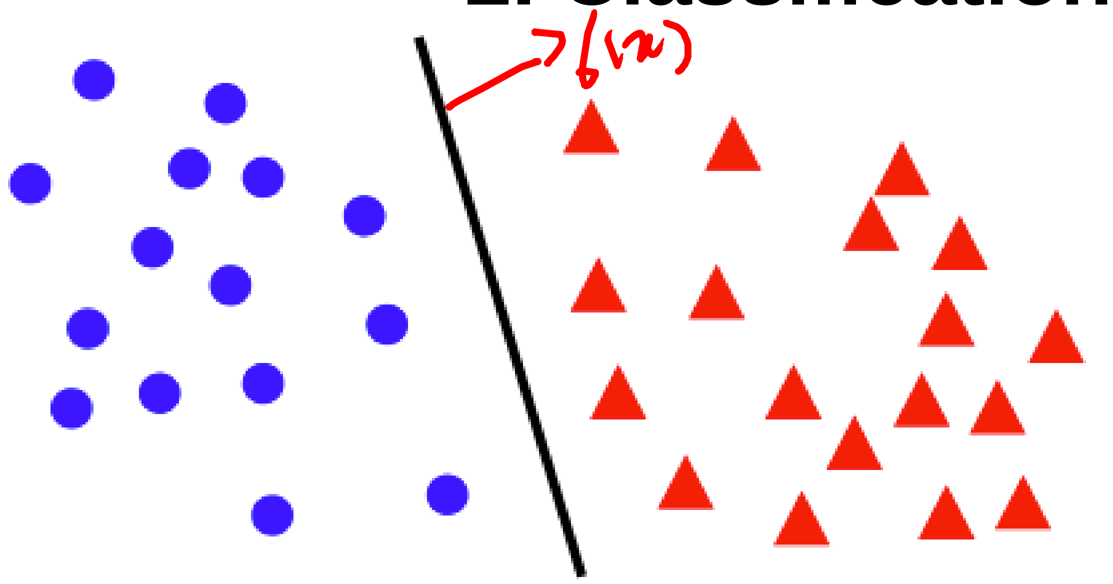
1. Regression



Curve fitting

When y is discrete:

2. Classification

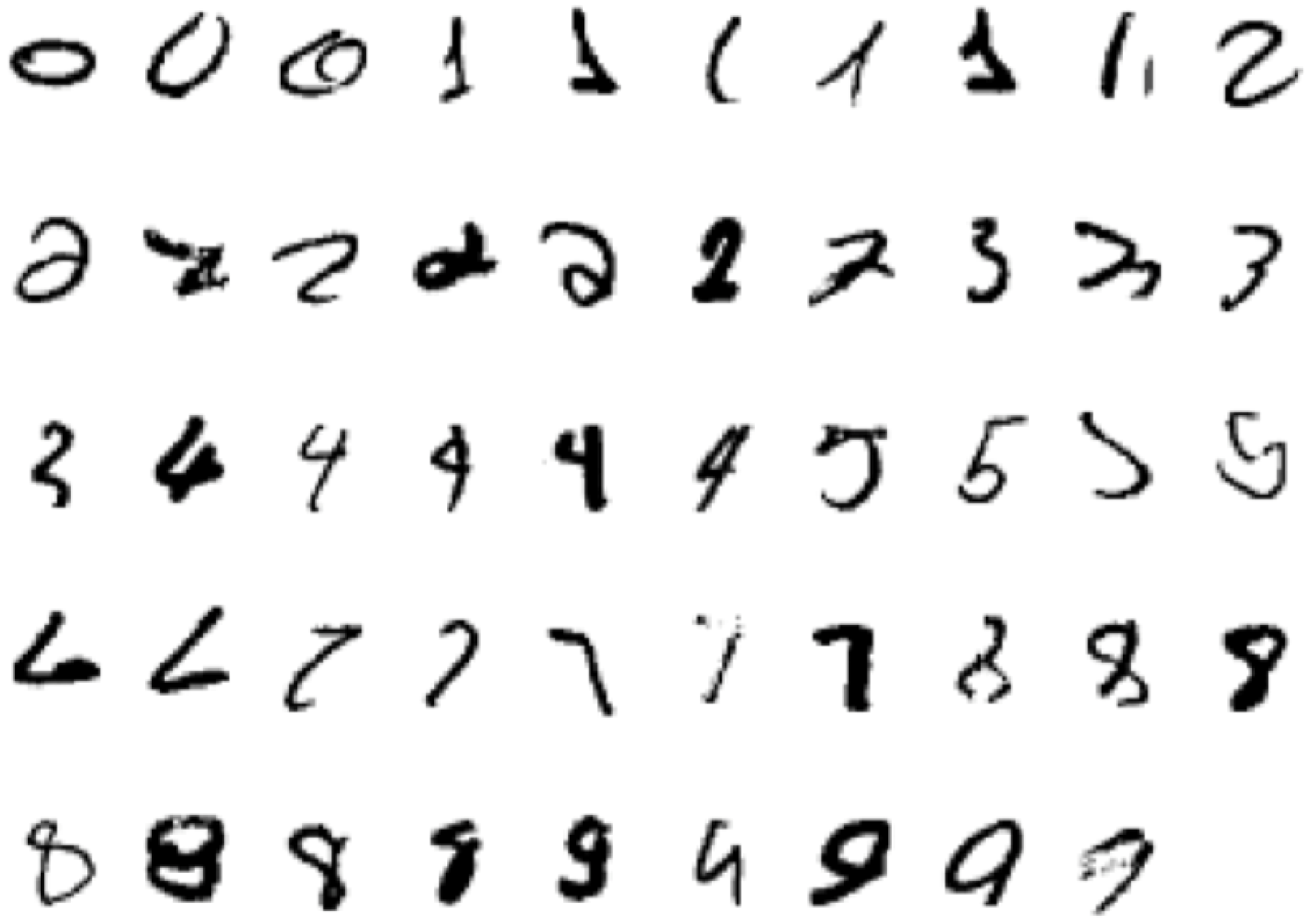


Class estimation

Classification Example 1: Handwritten digit recognition

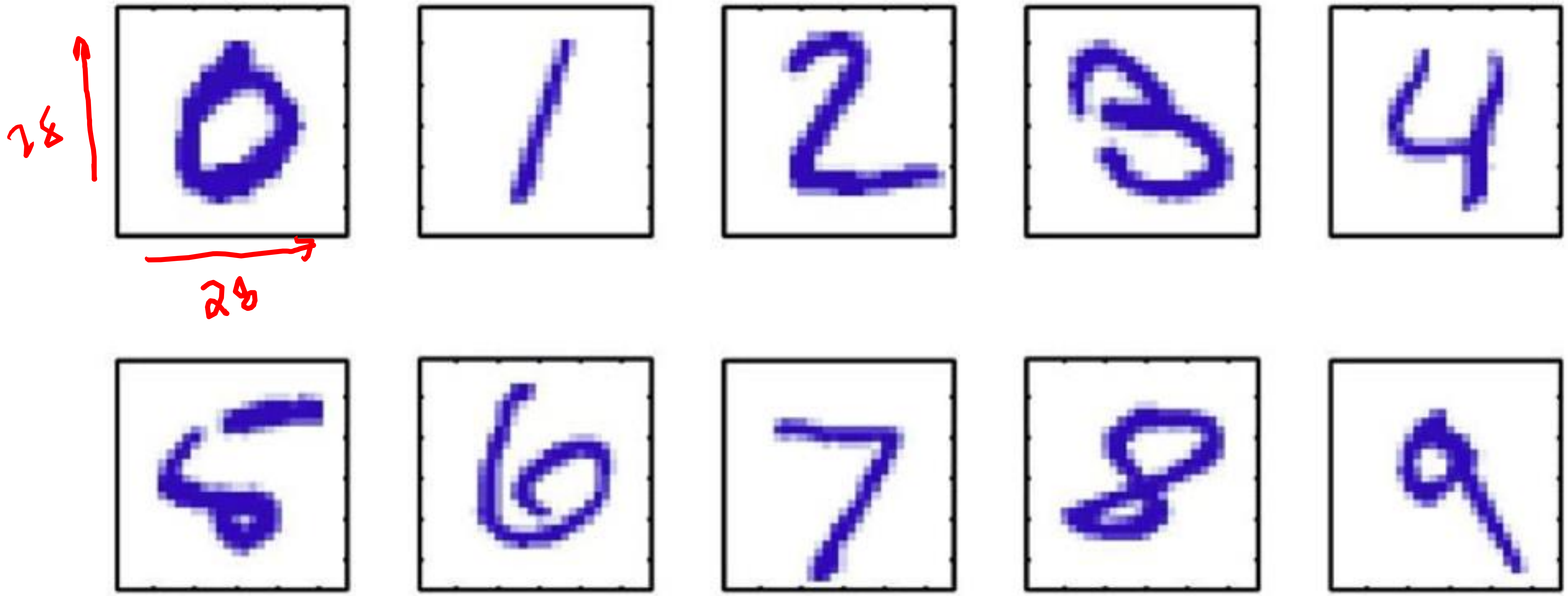
As a supervised classification problem

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

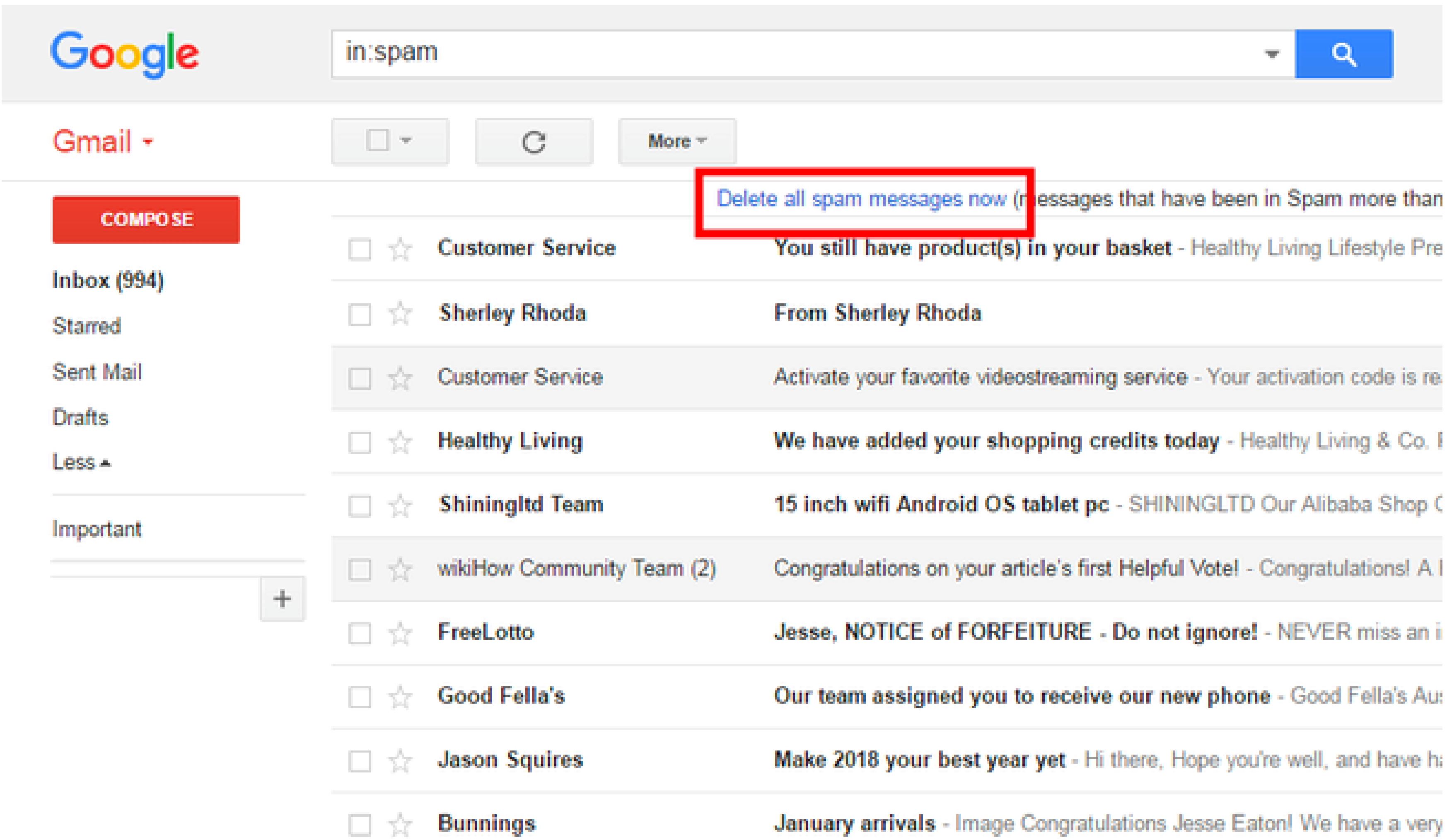
A classification problem

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

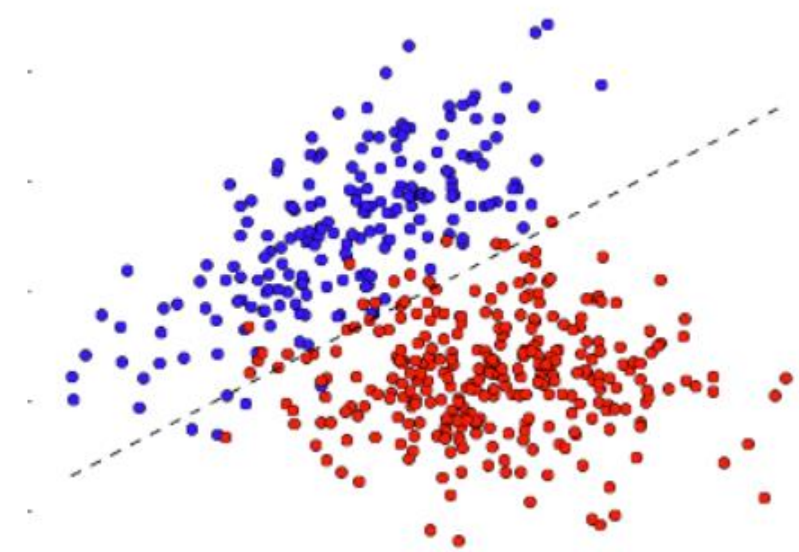
Learn a classifier $f(\mathbf{x})$ such that,

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

Classification Example 2: Spam Detection



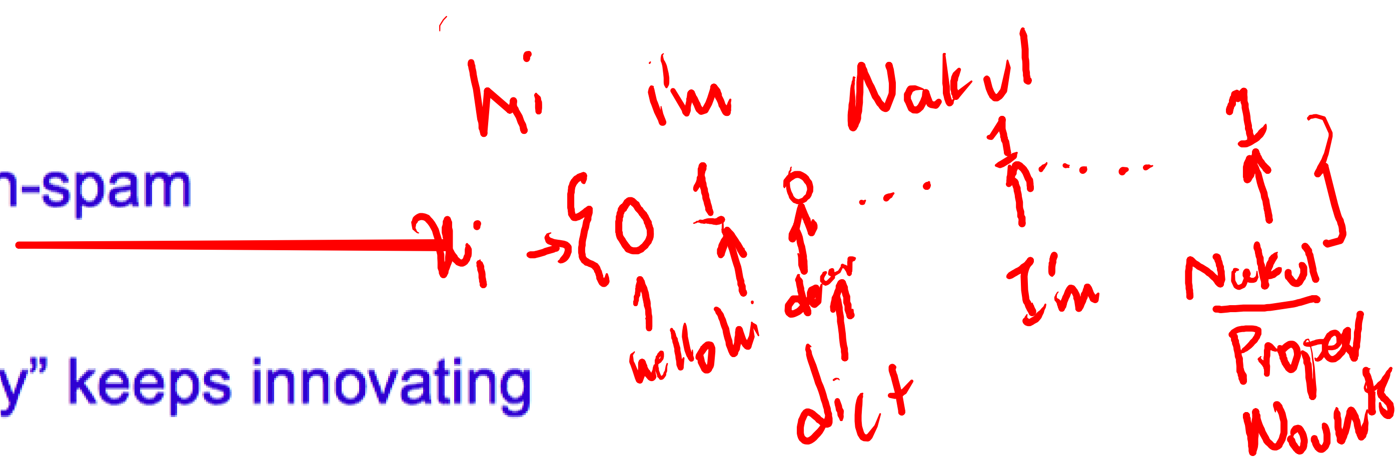
NOT SPAM



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



Regression Example 1: Apartment Rent Prediction

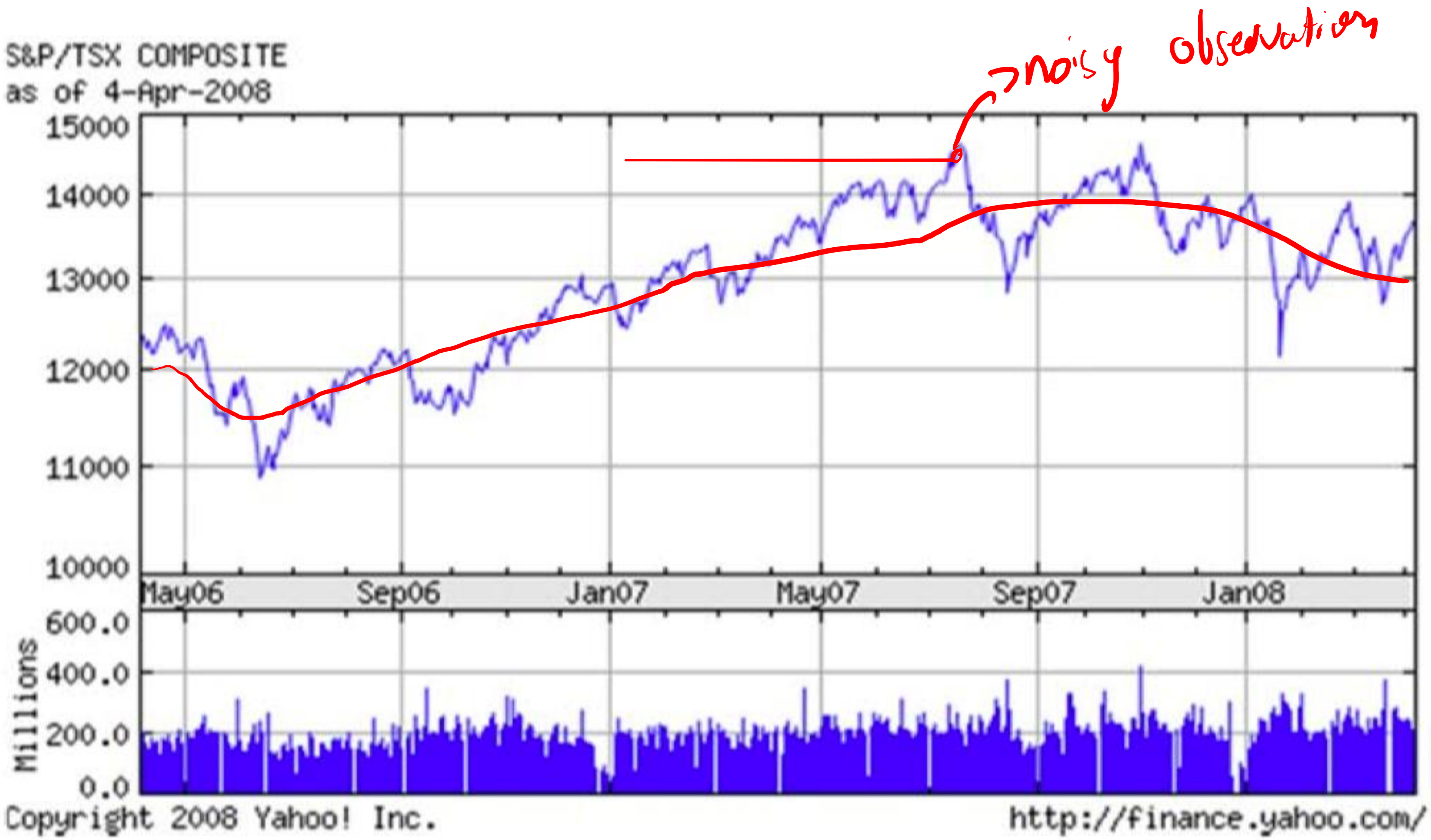
- Suppose you are to move to Atlanta
- And you want to find the **most reasonably priced** apartment satisfying your **needs:**

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

A regression problem

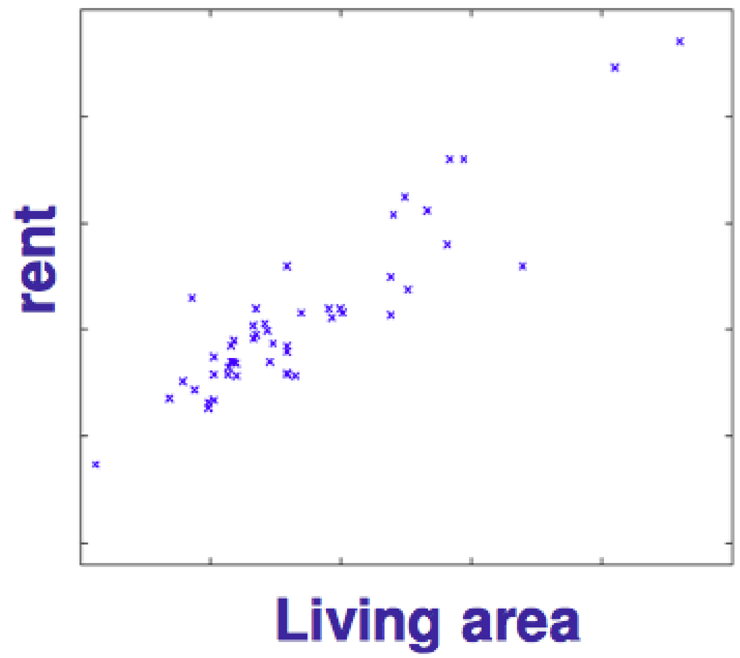
Living area (ft^2)	# bedroom	Rent ($)
230	1	600
506	2	1000
433	2	1100
109	1	500
…		
150	1	?
270	1.5	?

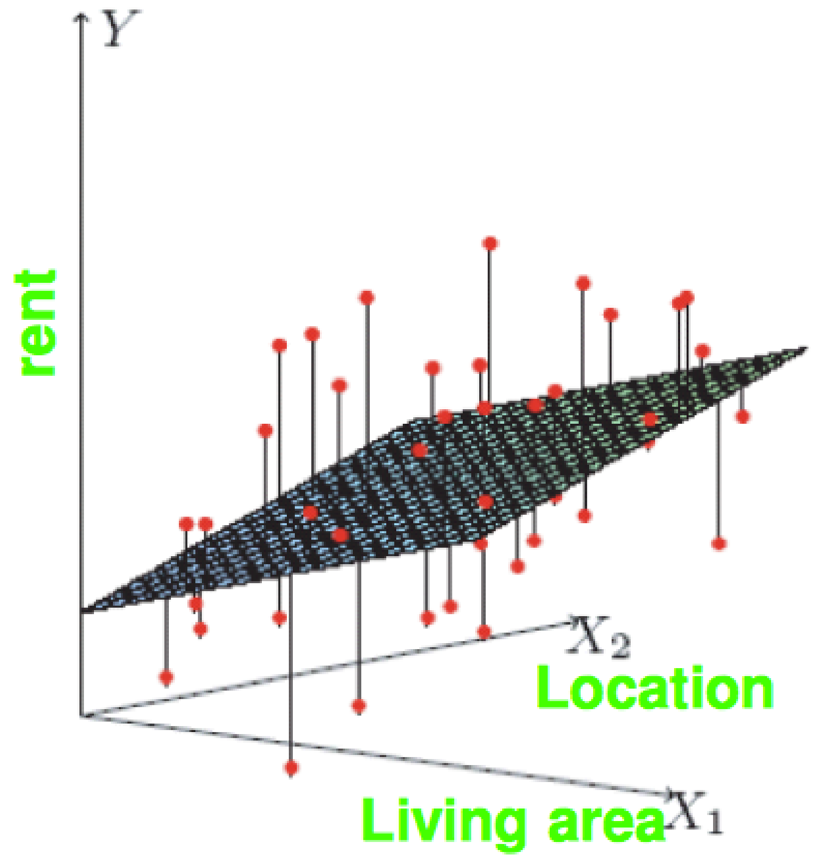
Regression Example 2: Stock Price Prediction



- Task is to predict stock price at future date

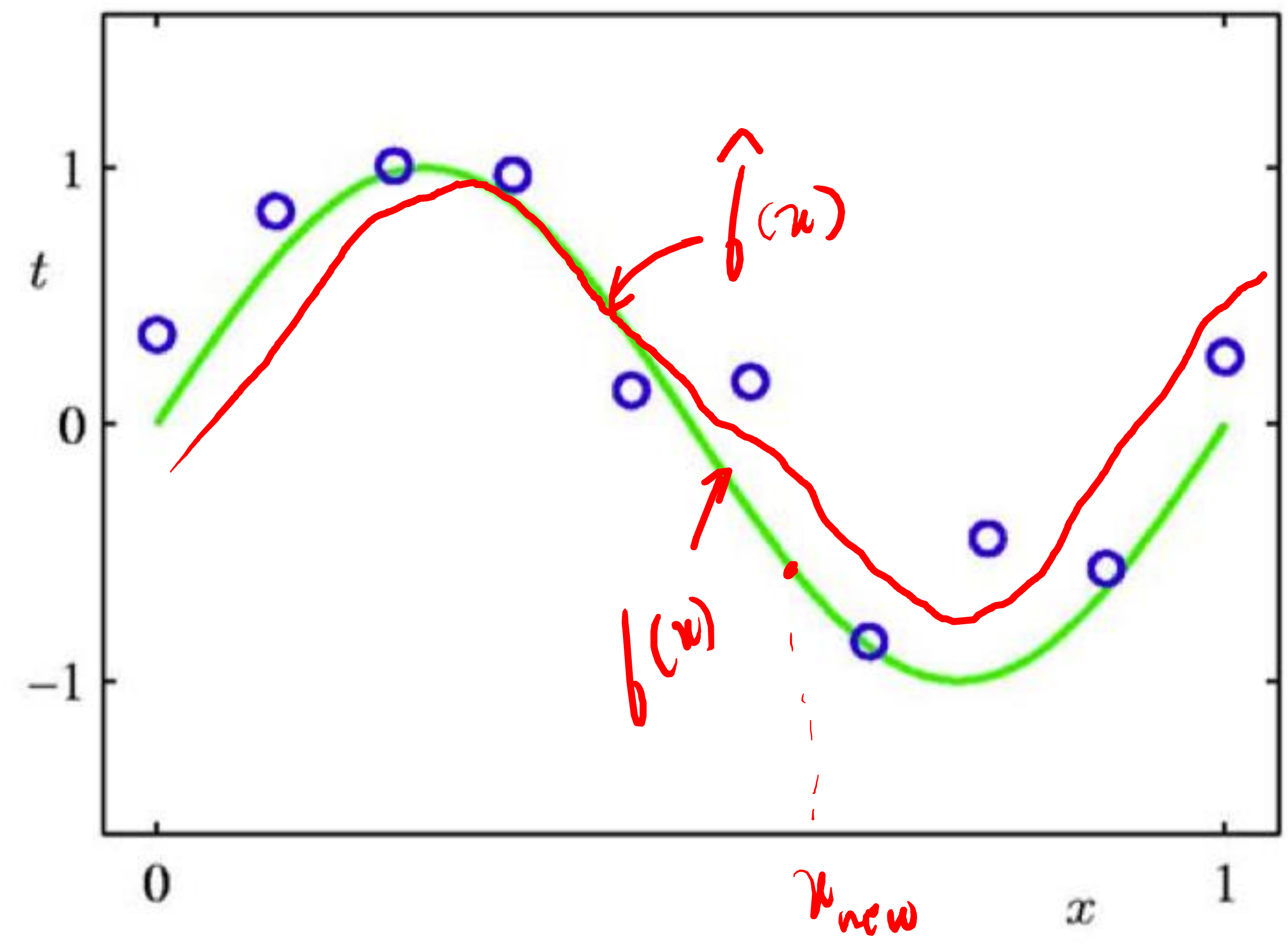
A regression problem





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

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

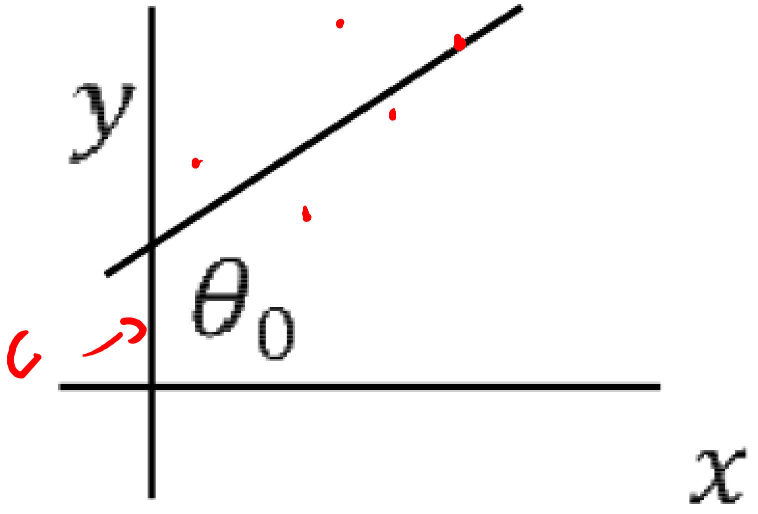
- Assume y is a linear function of x (features) plus noise ϵ

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

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

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

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



Least Mean Square Method

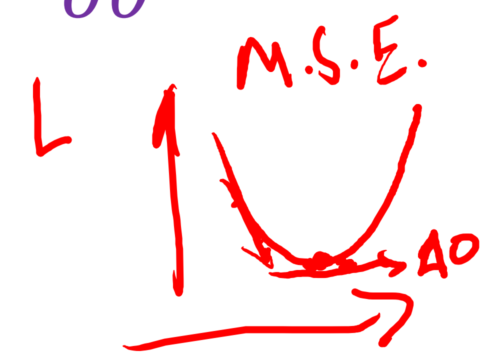
- Given n data points, find θ that minimizes the mean square error

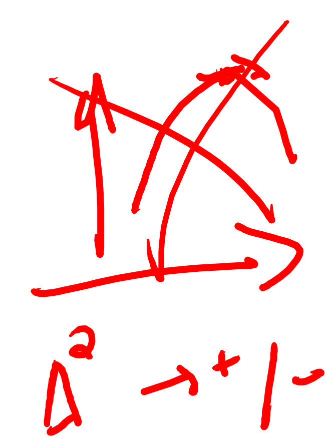
Training $$\hat{\theta} = argmin_{\,\theta}\, L(\theta) = \frac{1}{n}\sum_{i=1}^{n}(y_i - x_i\theta)^2$$

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

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

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





Matrix form

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

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

$$x\theta = \begin{bmatrix} \theta_0 + \theta_1 x_1^{\{1\}} + \theta_2 x_1^{\{2\}} + \cdots + \theta_d x_1^{\{d\}} \\ \theta_0 + \theta_1 x_2^{\{1\}} + \theta_2 x_2^{\{2\}} + \cdots + \theta_d x_2^{\{d\}} \\ \vdots \\ \theta_0 + \theta_1 x_n^{\{1\}} + \theta_2 x_n^{\{2\}} + \cdots + \theta_d x_n^{\{d\}} \end{bmatrix}_{n \times 1} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

$y \quad n \times 1$

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

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

Real inv.

X^{-1}

$X X^{-1} = I$

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

$X^T X \theta = X^T y$

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

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

$X_{n\times d}$ $\quad$ 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 $\mathbf{X^T X}$ 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

1 million × 1 million

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

- Gradient descent

learning rate

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

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

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

data point

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 ..)

Batch gradient descent

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

$m << n$

batch size

Linear regression for classification

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

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

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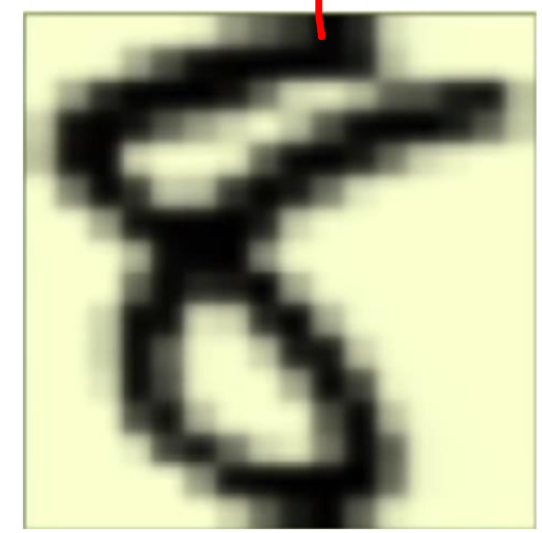

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Extract useful information

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

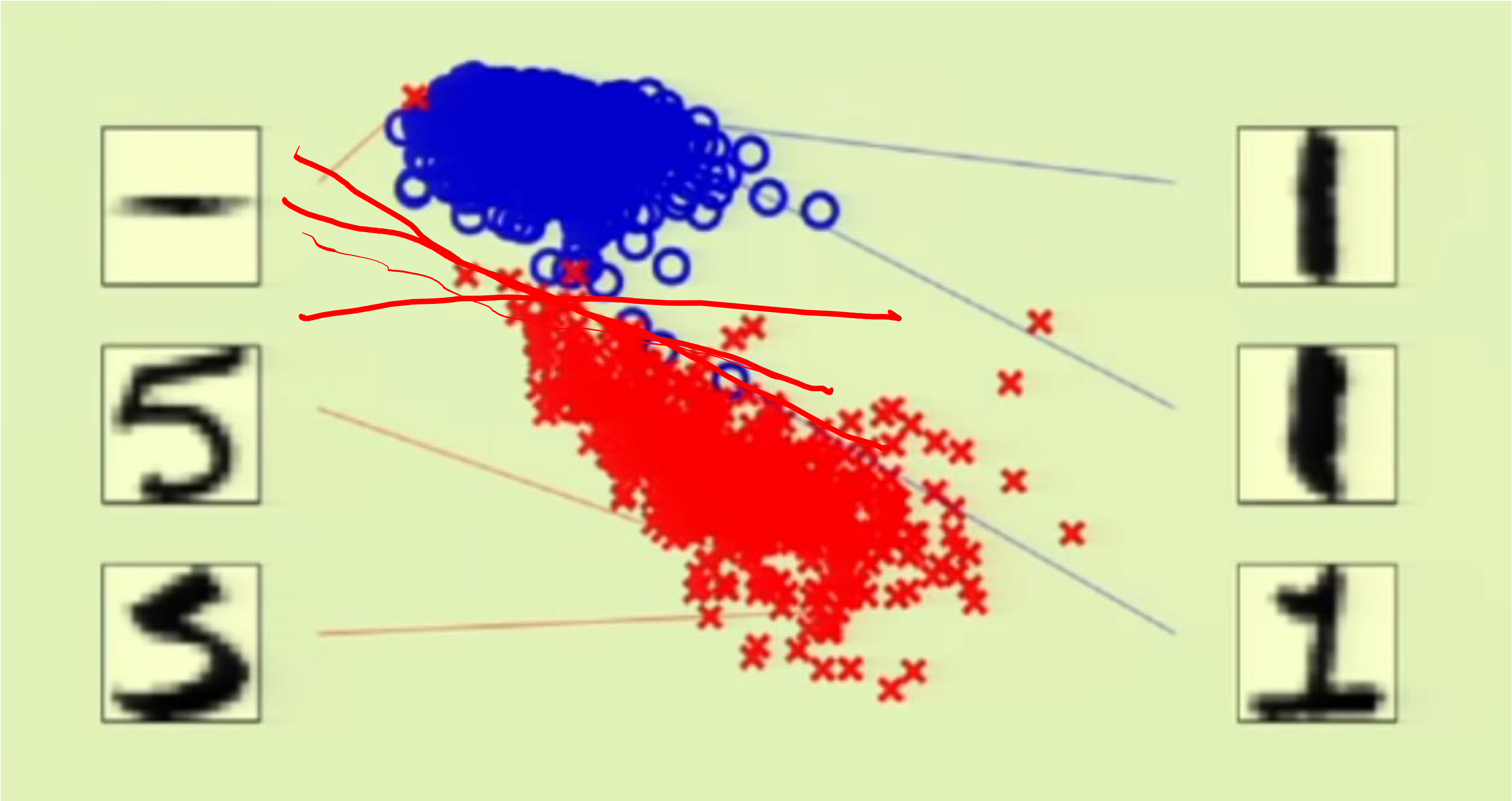
Sum up all the pixels = intensity

Symmetry = -(difference between flip version)

$x = (x_0, x_1, x_2)$

$x_1 = intensity \; x_2 = symmetry$

It is almost linearly separable



symmetry

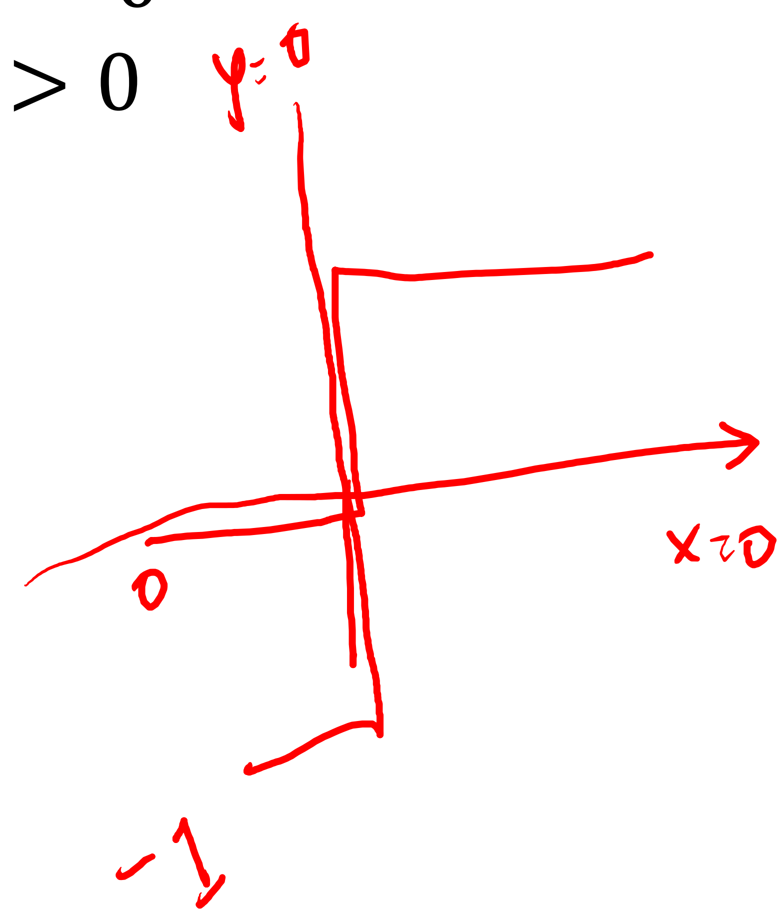
intensity

Linear regression for classification

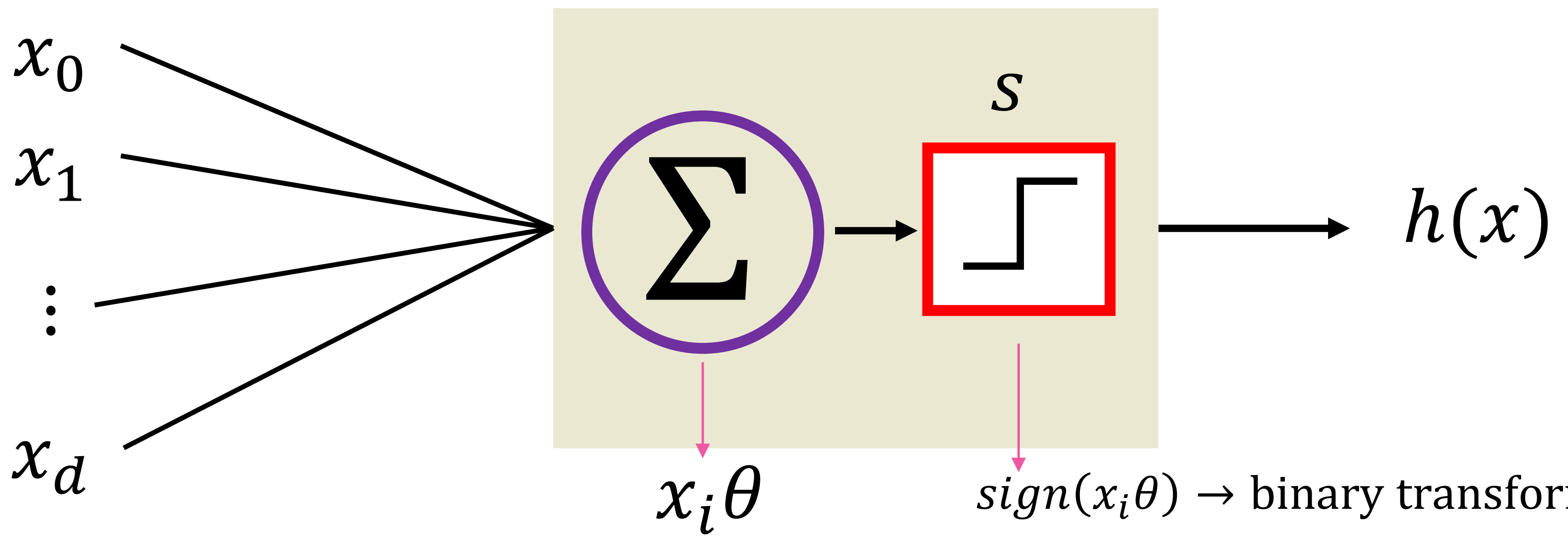
Binary-valued functions are also real-valued $\pm 1 \in R$

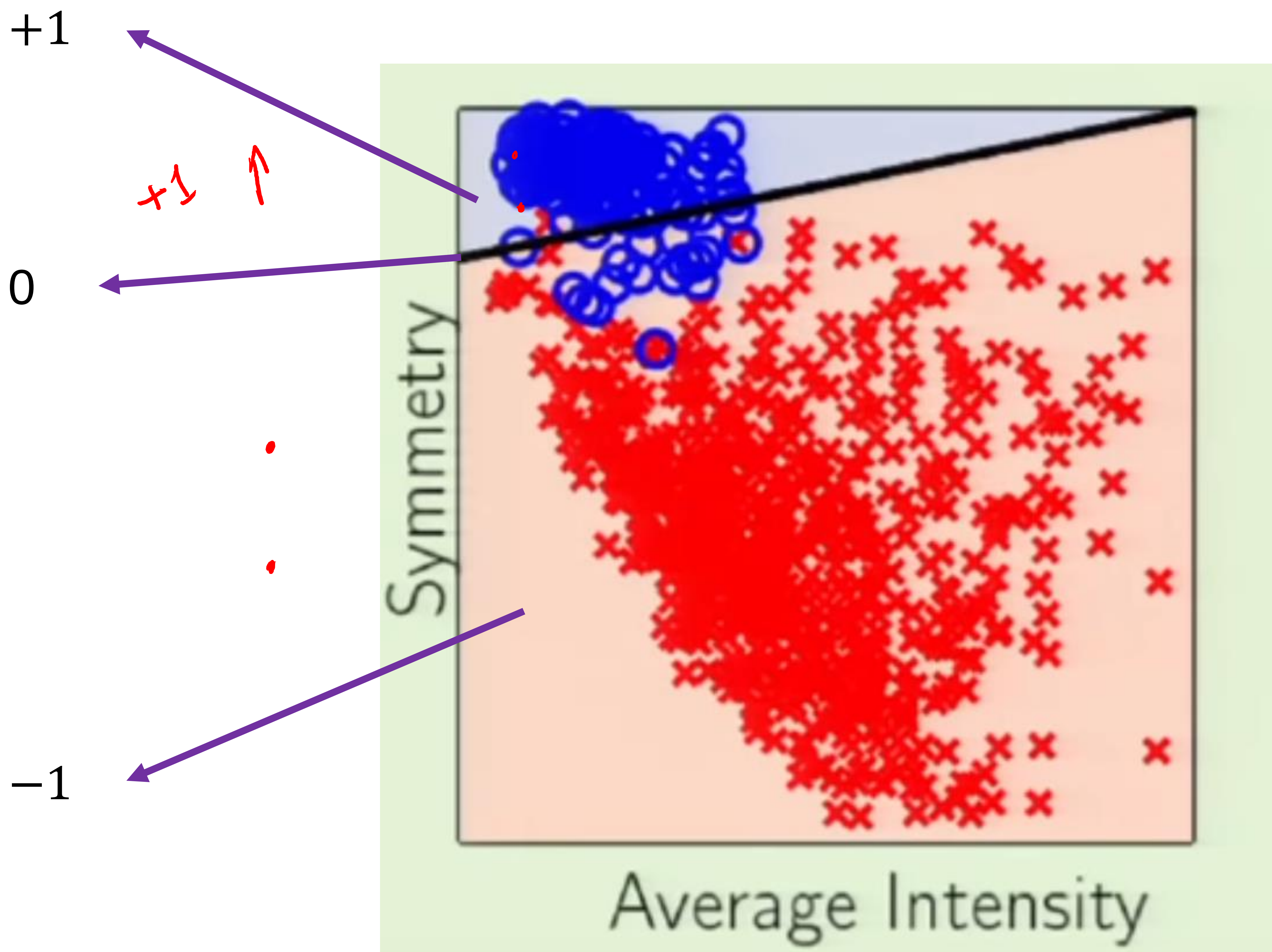
Use linear regression $x_i\theta \approx y_n = \pm 1$ i = index of a data-point

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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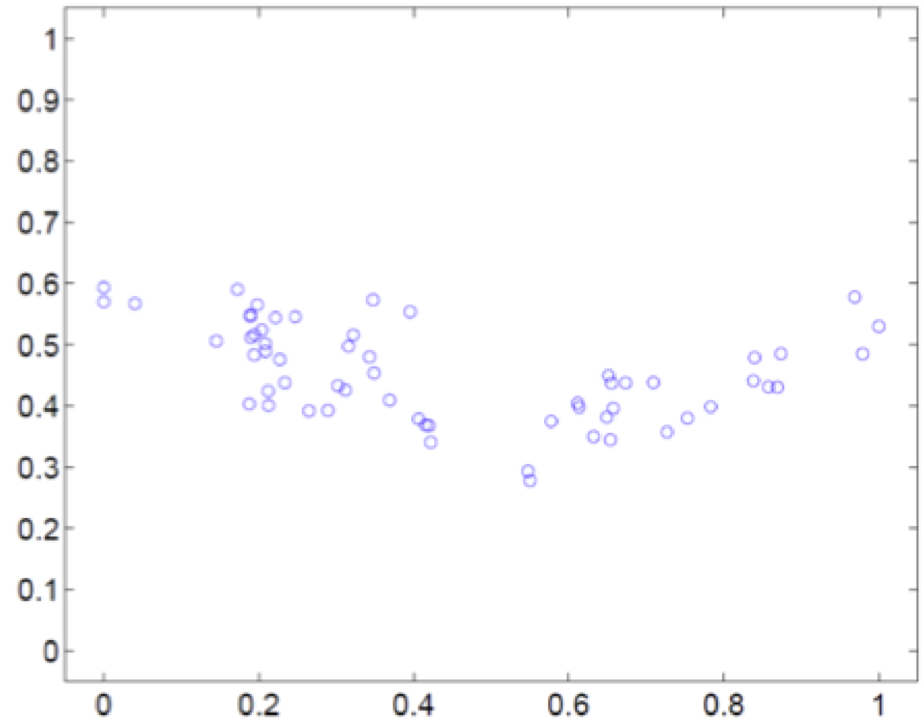
Extension to Higher-Order Regression



- Want to fit a polynomial regression model

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

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

$$y = z\theta$$

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

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

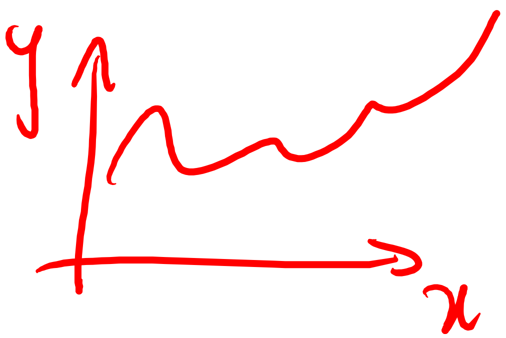
$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\sum_{i=1}^{n} z_i^T y_i + \frac{2}{n}\sum_{i=1}^{n} z_i^T z_i\theta = 0$$

Matrix Version of the Gradient

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

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

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



$\theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4 + \theta_5 x^5$

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

Poll

Can every non-linear problem be separated by a linear boundary?

- Yes → non-linear → linear problem
- No

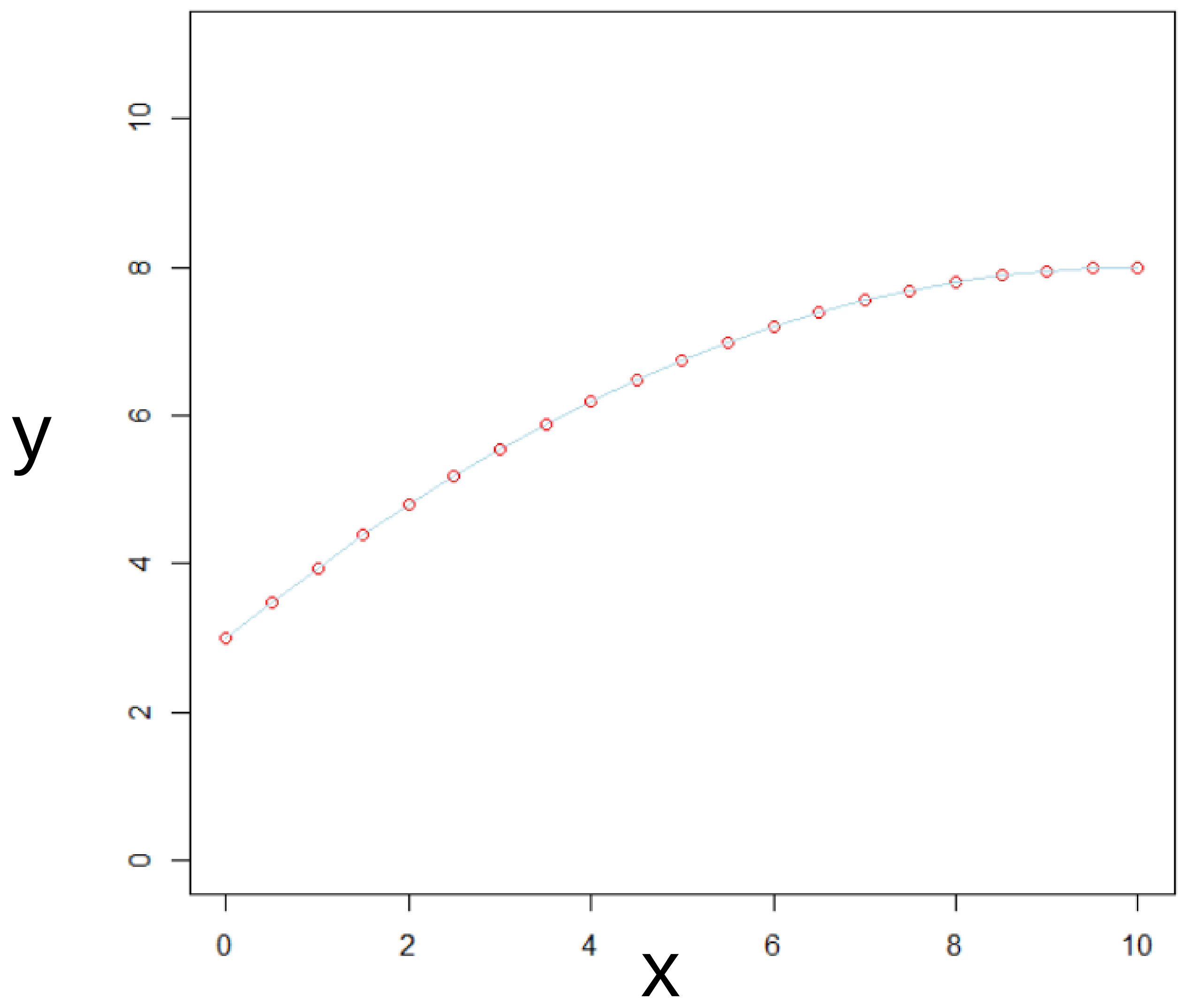
What is happening in polynomial regression?

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

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

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

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

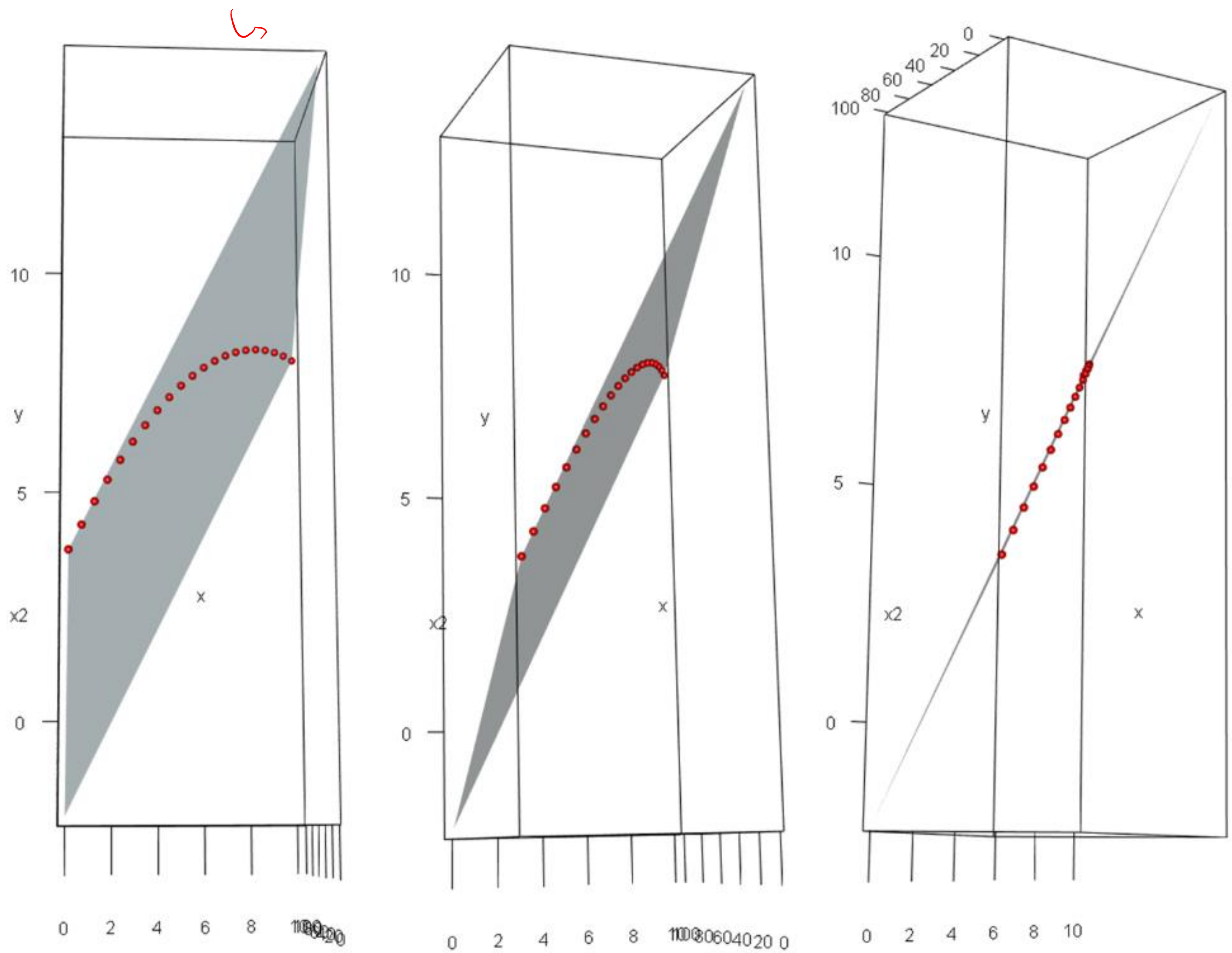


RMSE=0

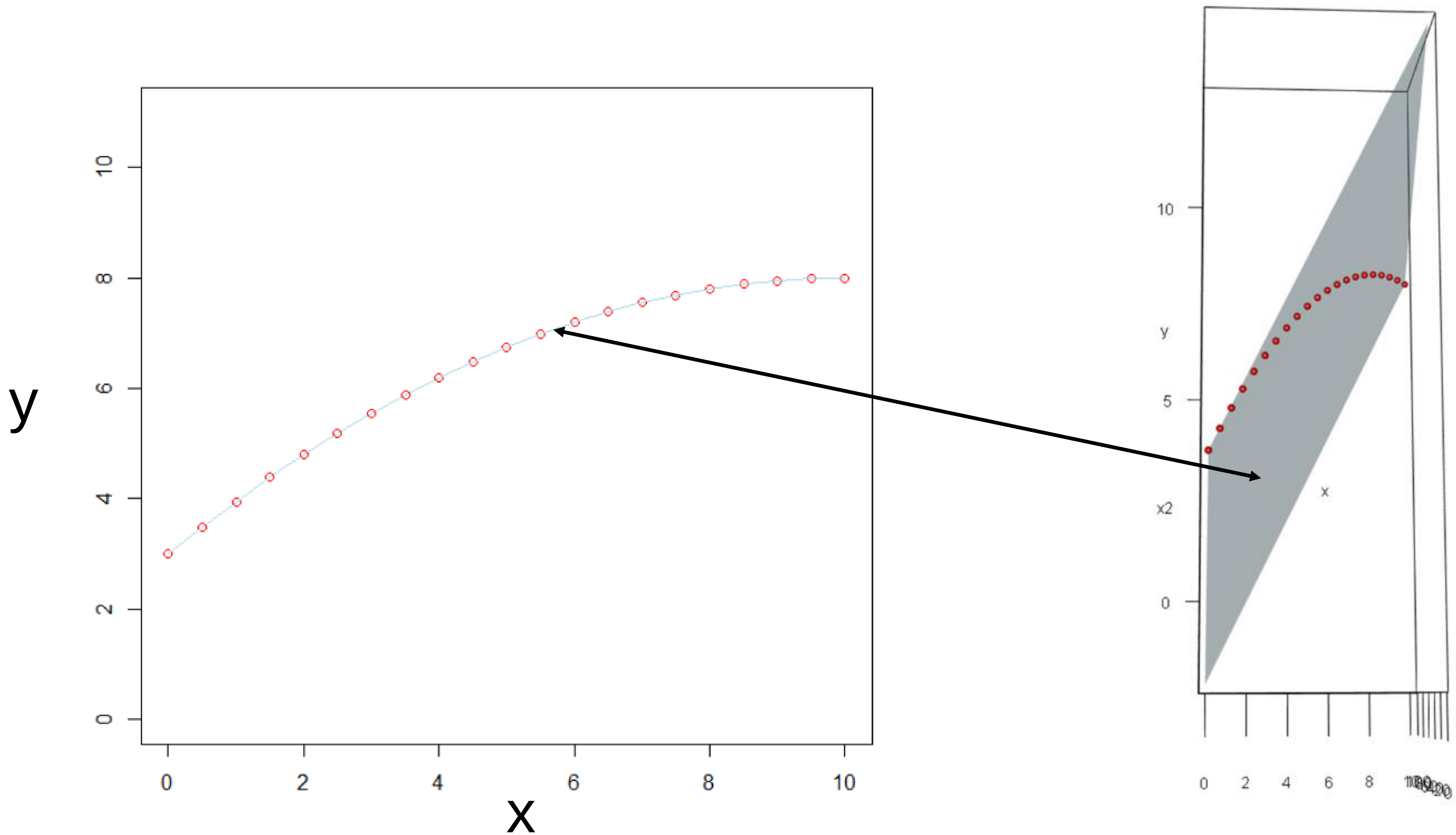
Let's add to the feature space

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

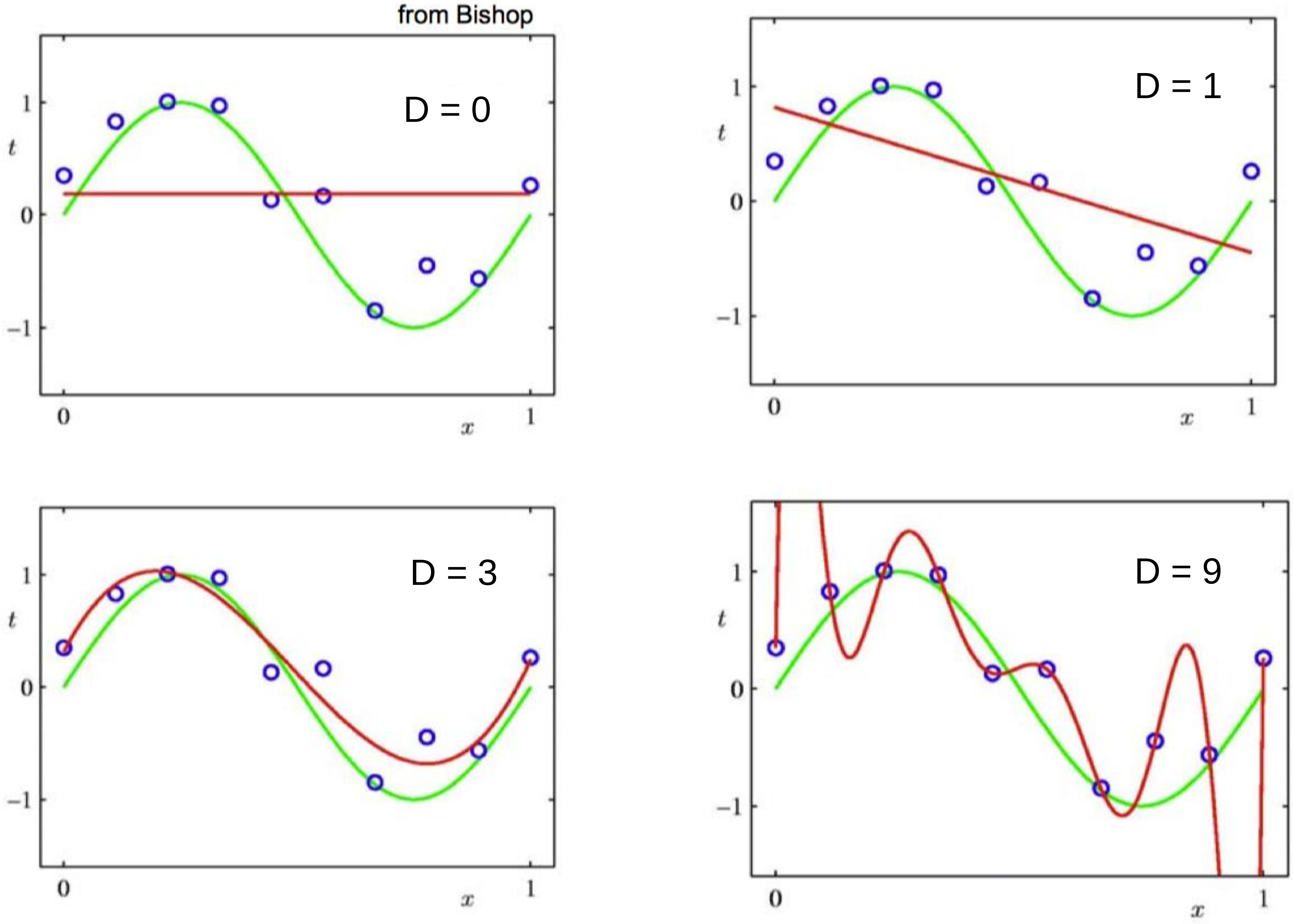
$y = [3, 3.4875, 3.95, \ldots, 7.98, 8]$



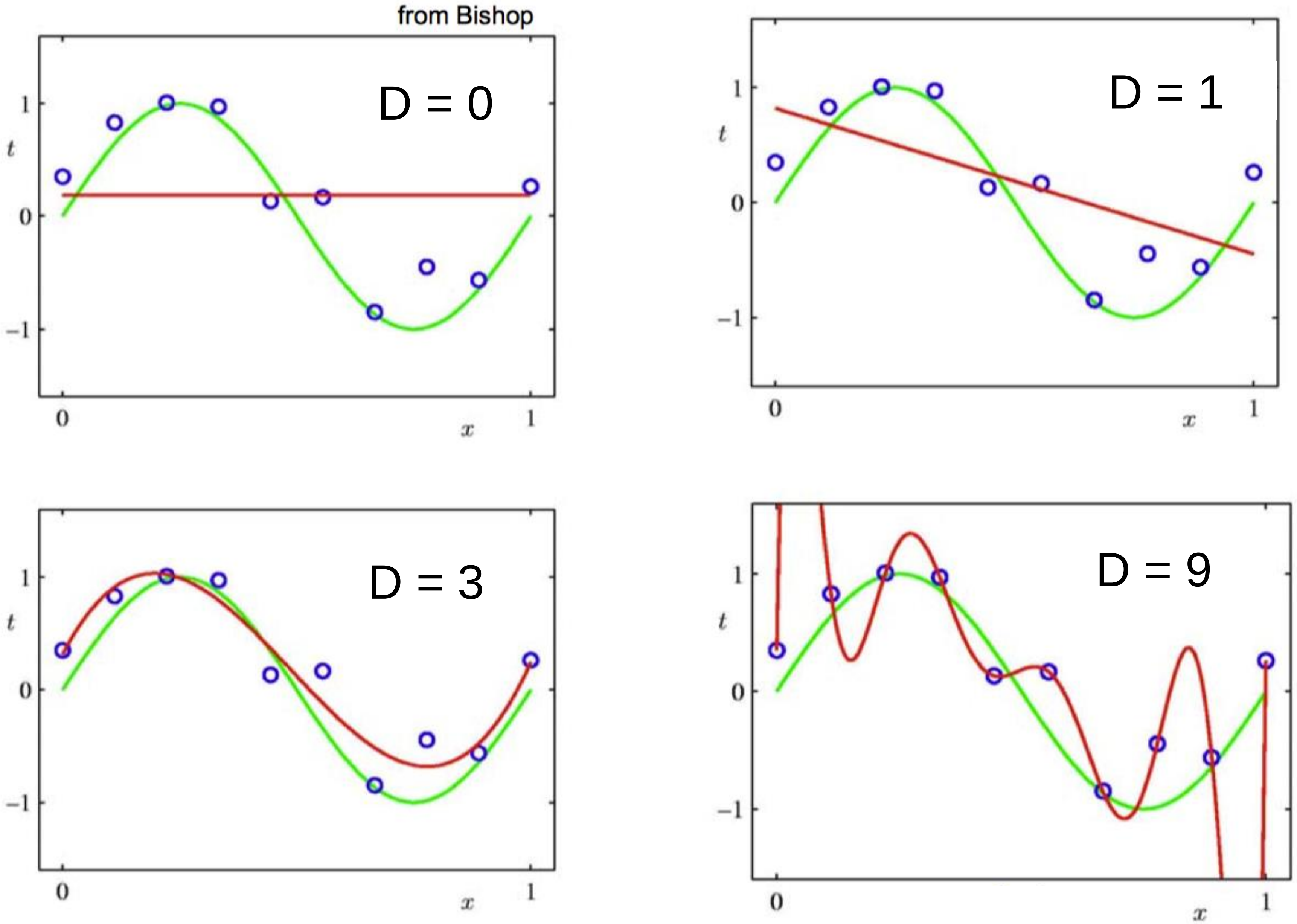
We are fitting a D-dimensional hyperplane in a D+1 dimensional hyperspace (in above example a 2D plane in a 3D space). That hyperplane really is 'flat' / 'linear' in 3D. It can be seen a non-linear regression (a curvy line) in our 2D example in fact it is a flat surface in 3D. So the fact that it is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