Linear Regression

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These slides are inspired 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

find $\hat{f} \in \mathcal{F}$

s.t. $y_a \approx f(x^{\{i\}})$

Learning machine

PREDICTION

$\hat{y}_p = f(x^{\{i\}})$

New data

x

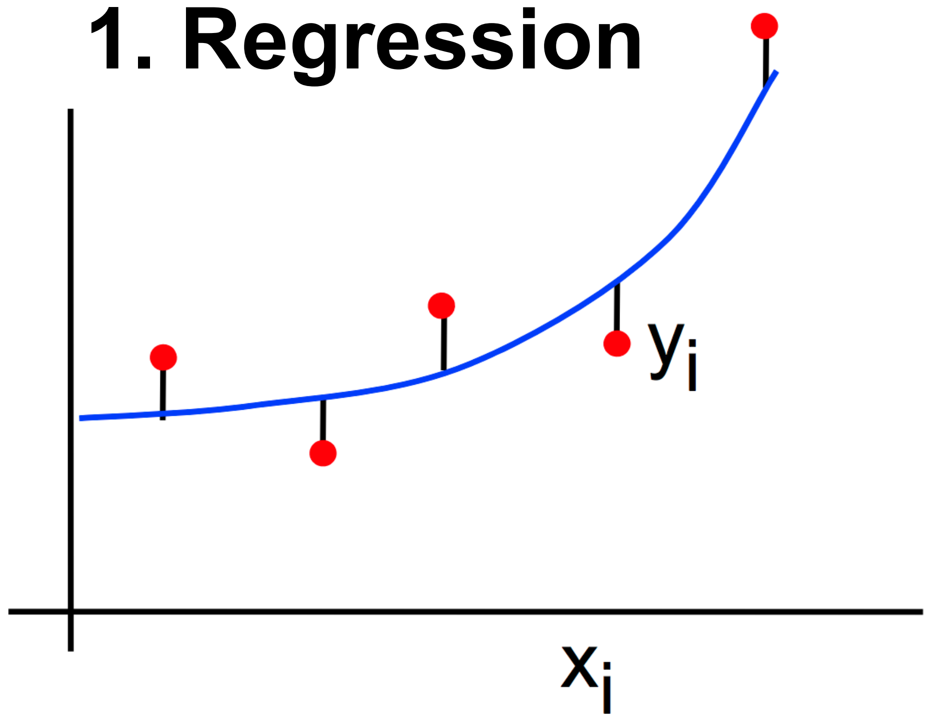
Supervised Learning: Two Types of Tasks

Given: training data $\{(x^{\{1\}}, y^{\{1\}}), (x^{\{2\}}, y^{\{2\}}), \ldots, (x^{\{n\}}, y^{\{n\}})\}$

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

When y is continuous:

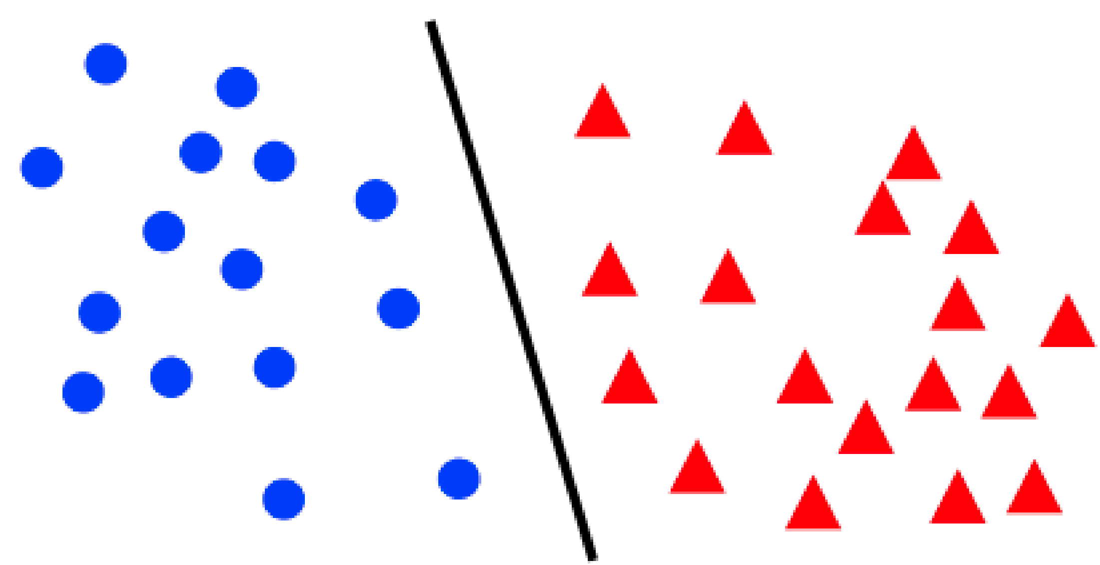
1. Regression



Curve fitting

When y is discrete:

2. Classification

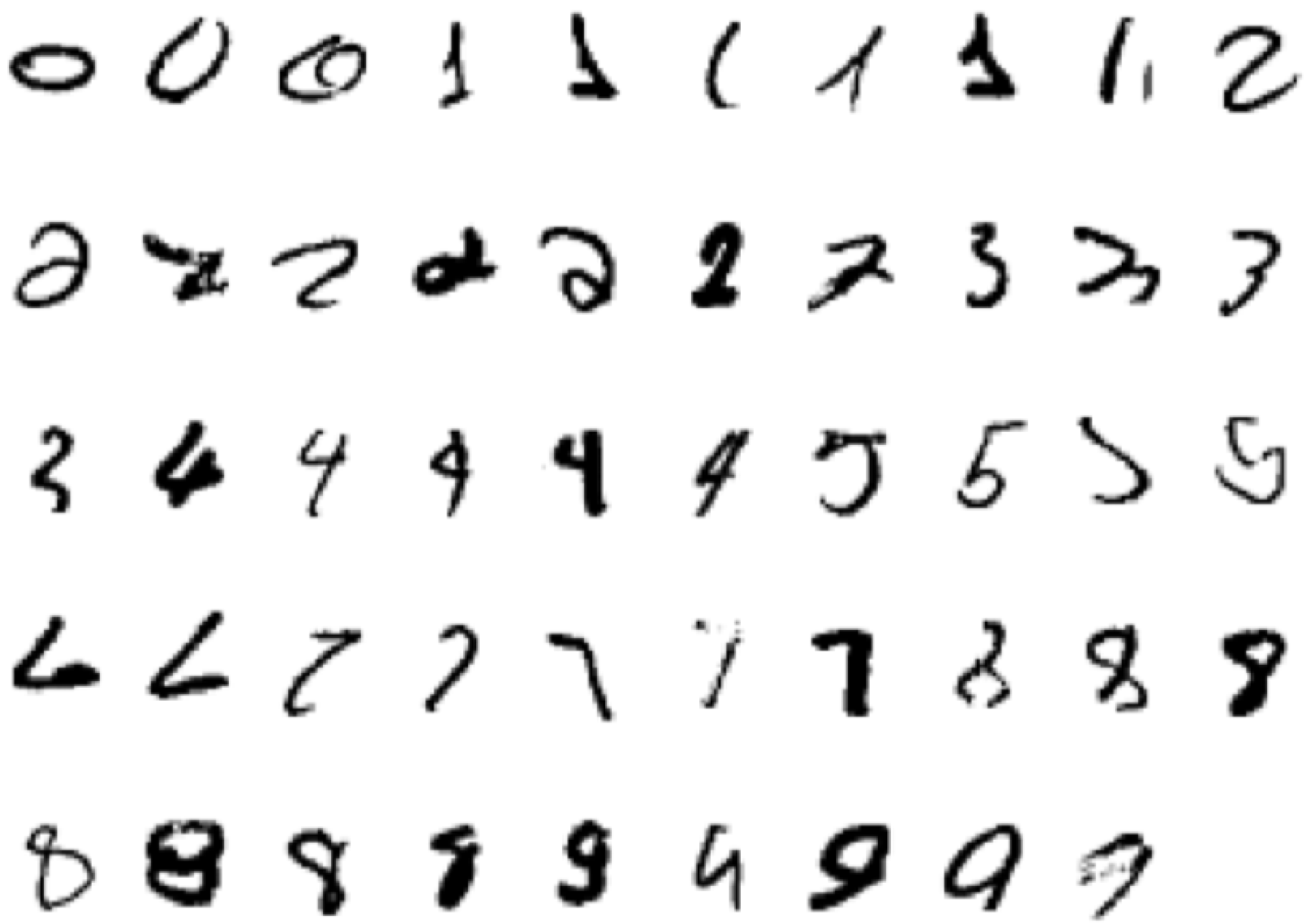


Class estimation

Classification Example 1: Handwritten digit recognition

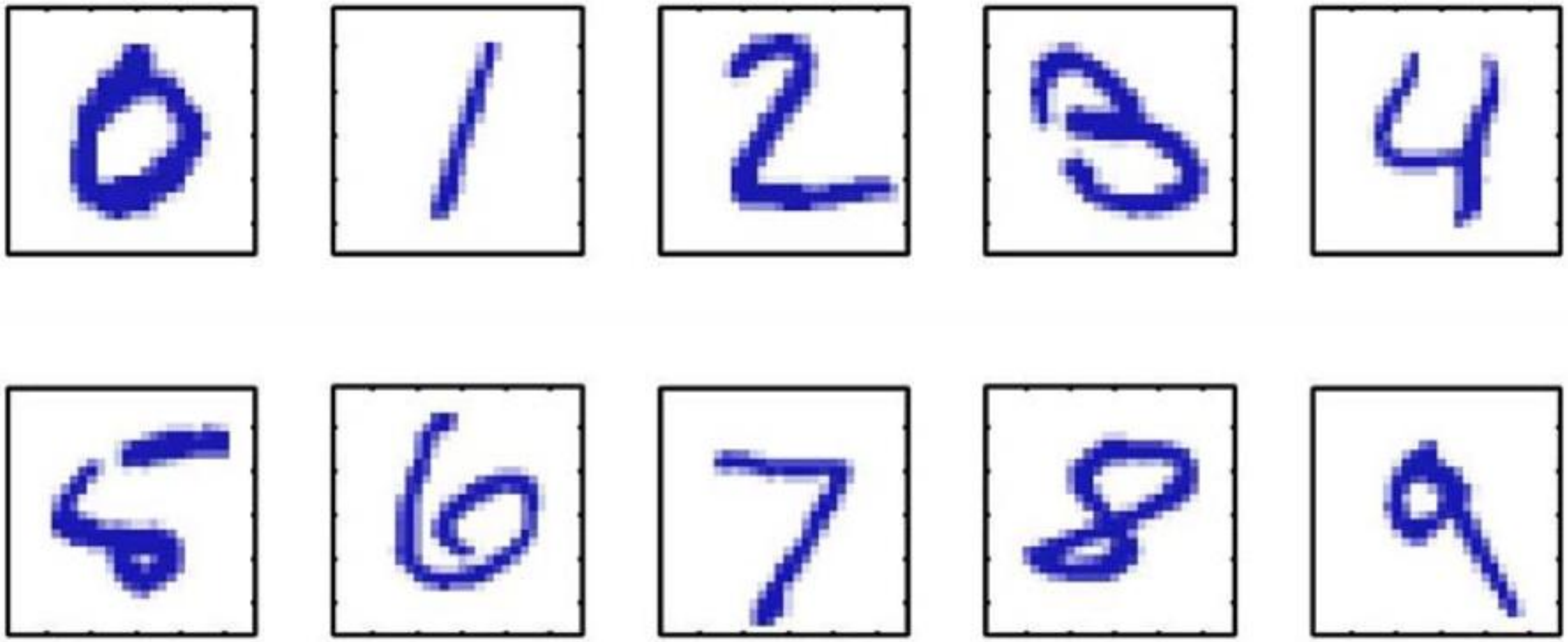
As a supervised classification problem

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

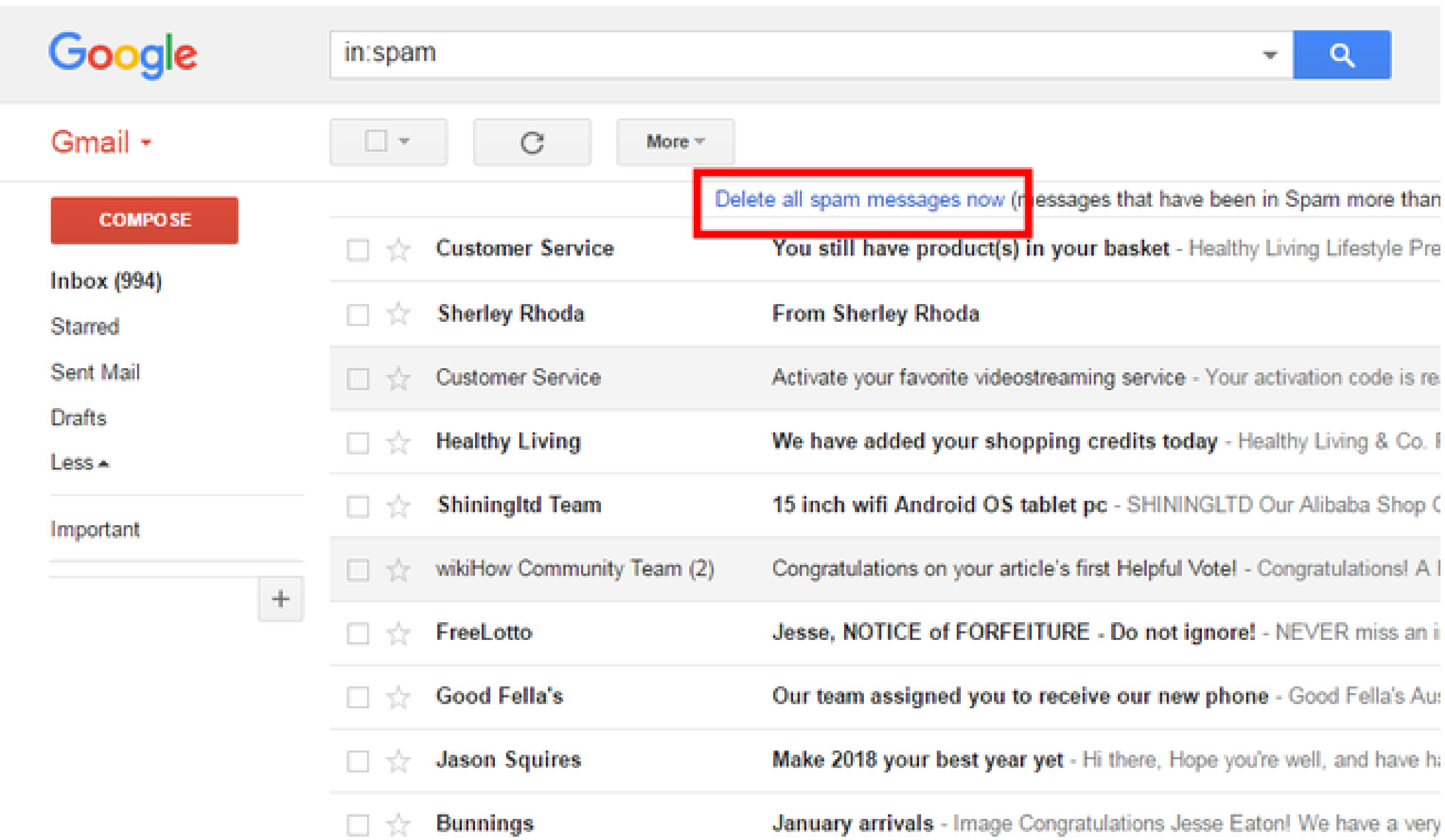
A classification problem

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

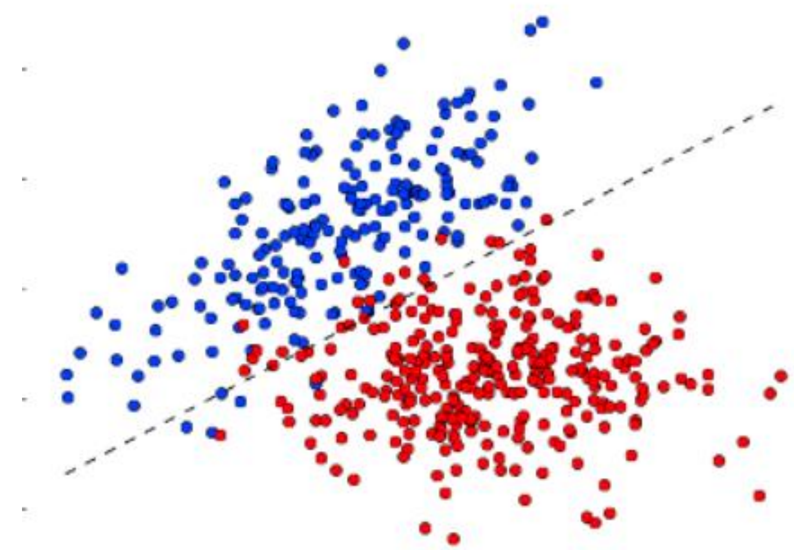
Learn a classifier $f(\mathbf{x})$ such that,

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

Classification Example 2: Spam Detection



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

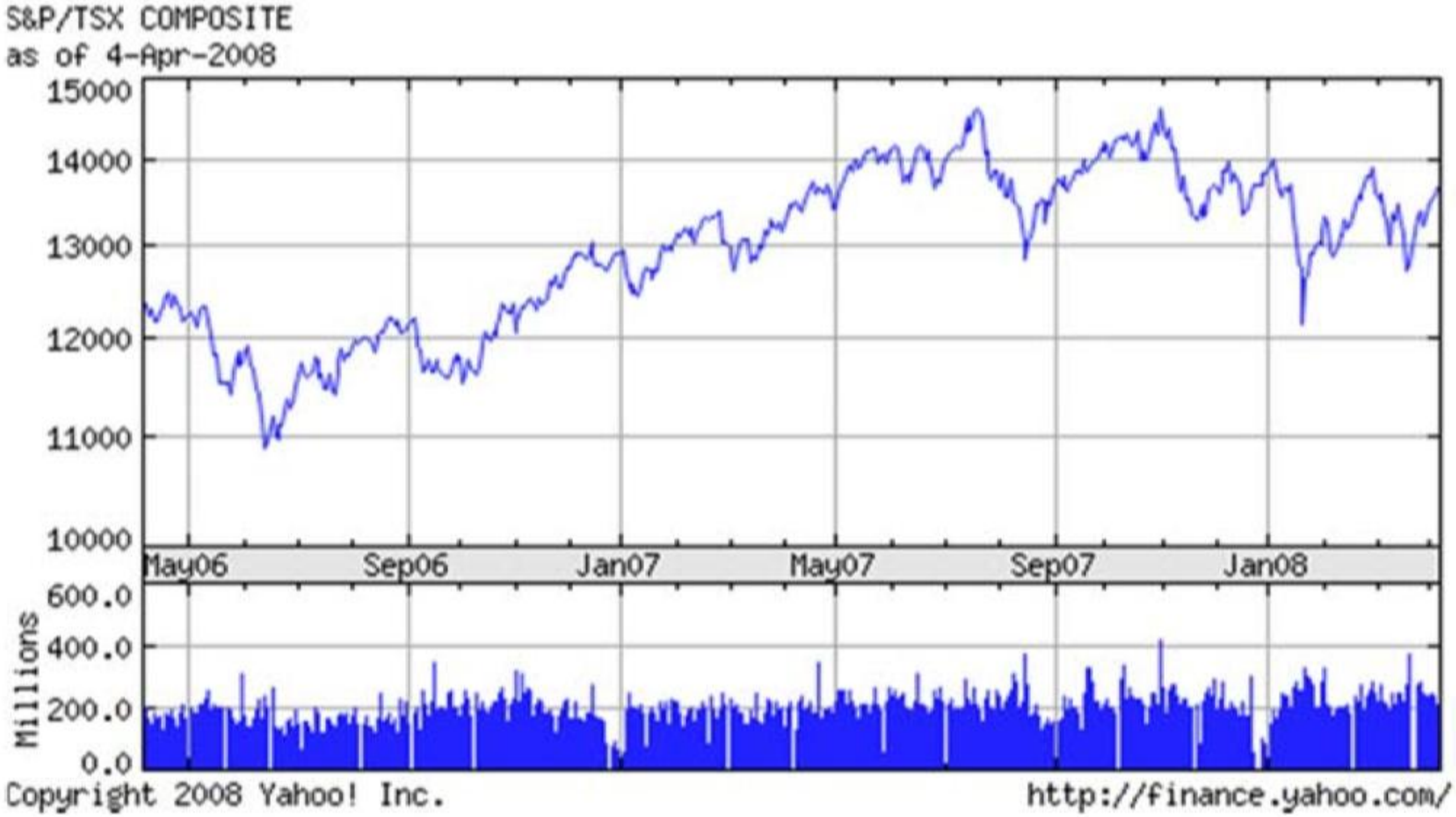
- Suppose you are to move to Atlanta
- And you want to find the **most reasonably priced** apartment satisfying your **needs:**

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

A regression problem

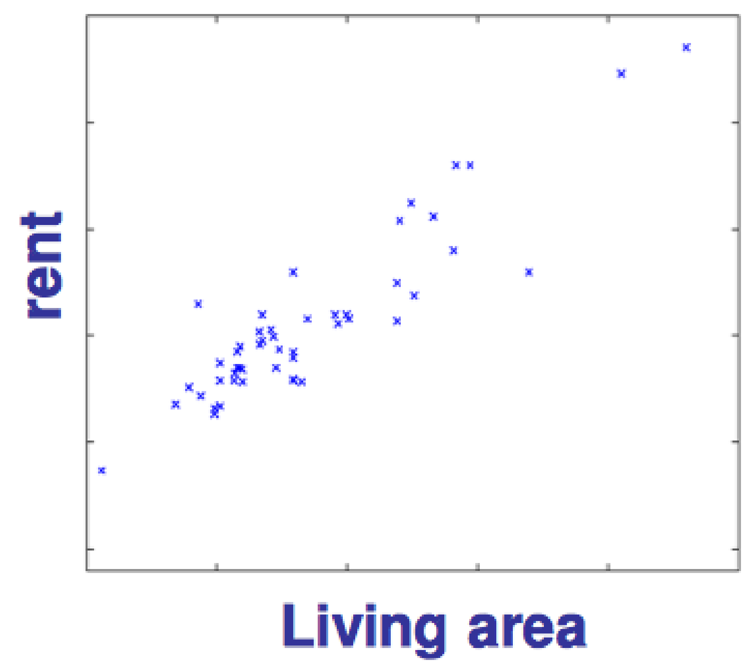
Living area (ft^2)	# bedroom	Rent ($)
230	1	600
506	2	1000
433	2	1100
109	1	500
…		
150	1	?
270	1.5	?

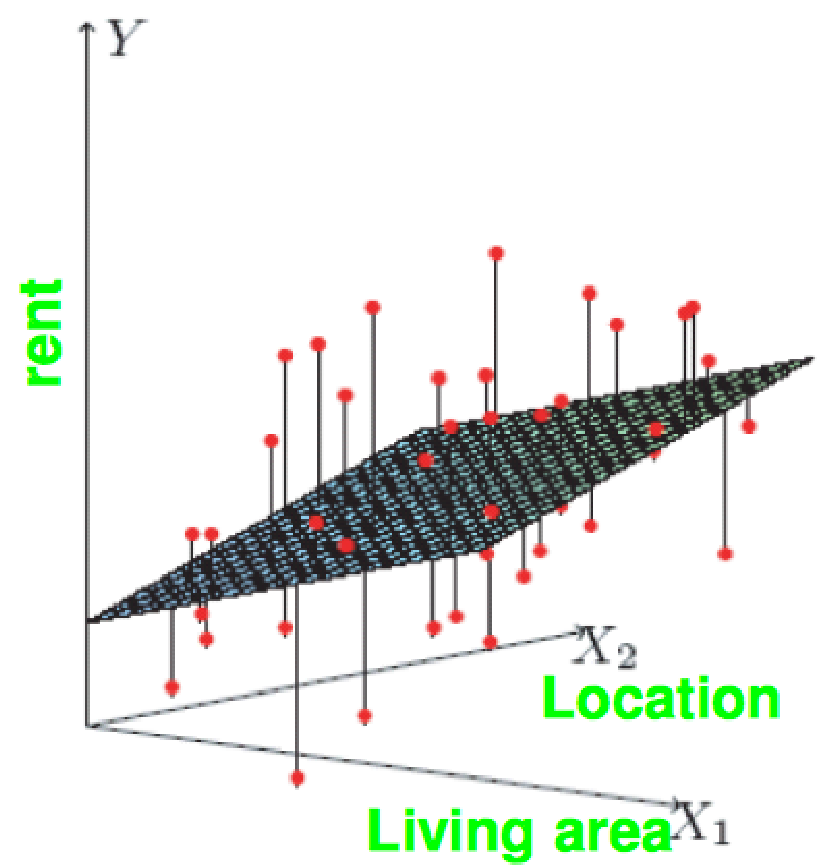
Regression Example 2: Stock Price Prediction



- Task is to predict stock price at future date

A regression problem



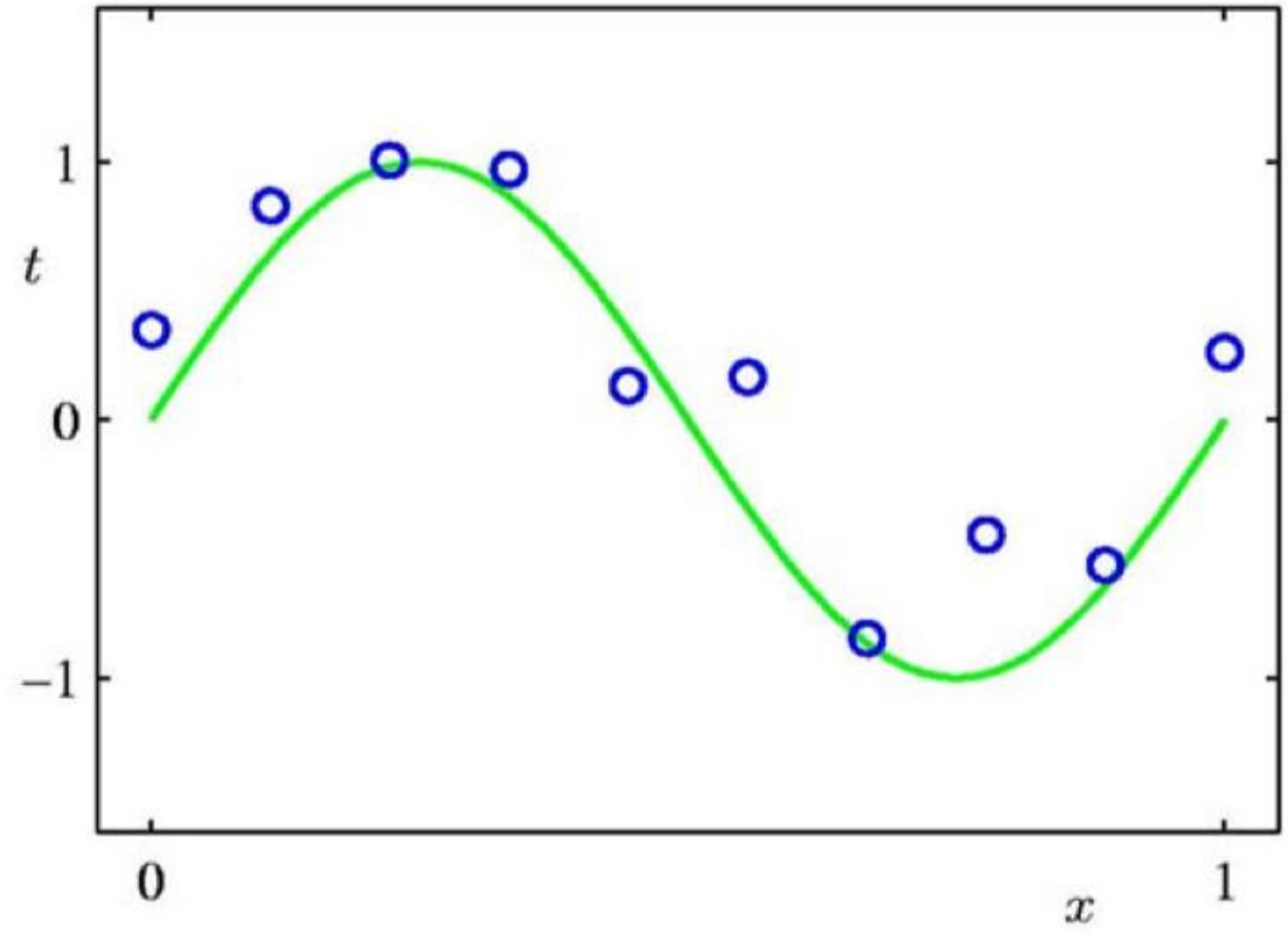


- Features:
  - Living area, distance to campus, # bedroom …
  - Denote as $x = (x_1, x_2, \dots, x_d)$
- Target:
  - Rent
  - Denoted as y
- Training set:

$$x = \{x^{\{1\}}, x^{\{2\}}, \dots, x^{\{n\}}\} \in R^d$$

$$y = \{y^{\{1\}}, y^{\{2\}}, \dots, y^{\{n\}}\}$$

Regression: Problem Setup



- Suppose we are given a training set of N observations

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

Outline

- Supervised Learning
- Linear Regression ⬅
- Extension

Linear Regression

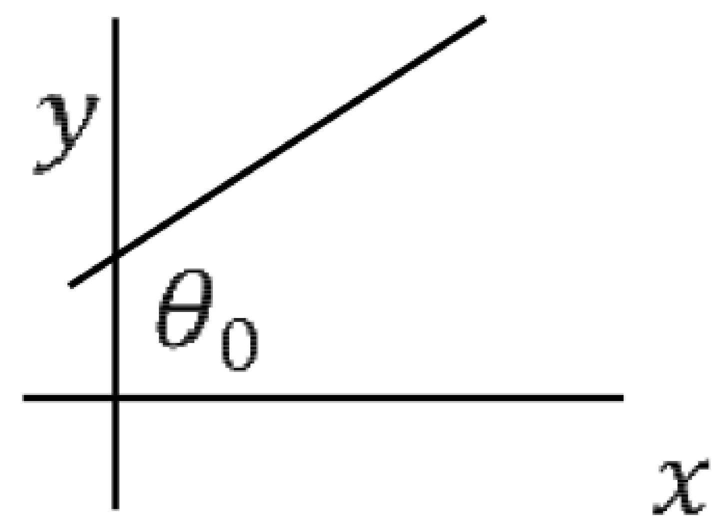
- Assume y is a linear function of x (features) plus noise ϵ

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

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

- Let $\theta = (\theta_0, \theta_1, \ldots, \theta_d)^\top$, 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 $\hat{\theta} = argmin_{\theta}\, L(\theta) = \frac{1}{n}\sum_{i=1}^{N}\left(y^{\{i\}} - x^{\{i\}}\theta\right)^2$

- 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

$$x = \begin{bmatrix} 1 & x_1^{\{1\}} & \cdots & x_d^{\{1\}} \\ 1 & x_1^{\{2\}} & \ddots & x_d^{\{2\}} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_1^{\{n\}} & \cdots & x_d^{\{n\}} \end{bmatrix}_{n \times (d+1)} \quad y = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}_{n \times 1} \quad \theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix}_{(d+1) \times 1}$$

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

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

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:

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{n}\left(x^{\{1\}}, \dots, x^{\{n\}}\right)^T\left(y^{\{1\}}, \dots, y^{\{n\}}\right) + \frac{2}{n}\left(x^{\{1\}}, \dots, x^{\{n\}}\right)^T\left(x^{\{1\}}, \dots, x^{\{n\}}\right)\theta = 0$$

Define $\mathrm{X} = \left(x^{\{1\}}, \dots, x^{\{n\}}\right)$ and $\mathrm{y} = \left(y^{\{1\}}, \dots, y^{\{n\}}\right)$

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

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

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

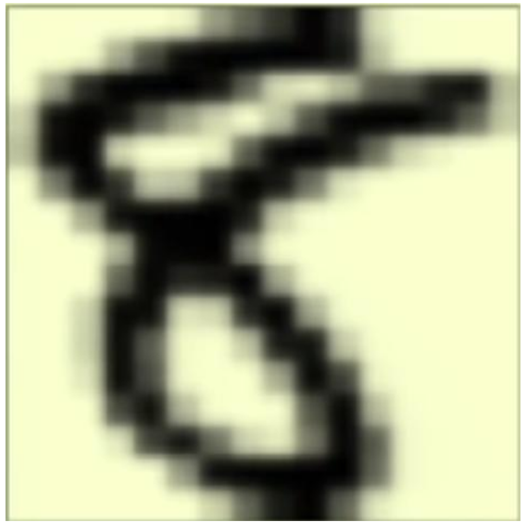
$$\theta = (X^T X)^{-1} X^T y$$

  - 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 $x = (1, x_1, \ldots, x_{256})$

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



Extract useful information

$intensity\ and\ symmetry\ x = (1, x_1, x_2)$

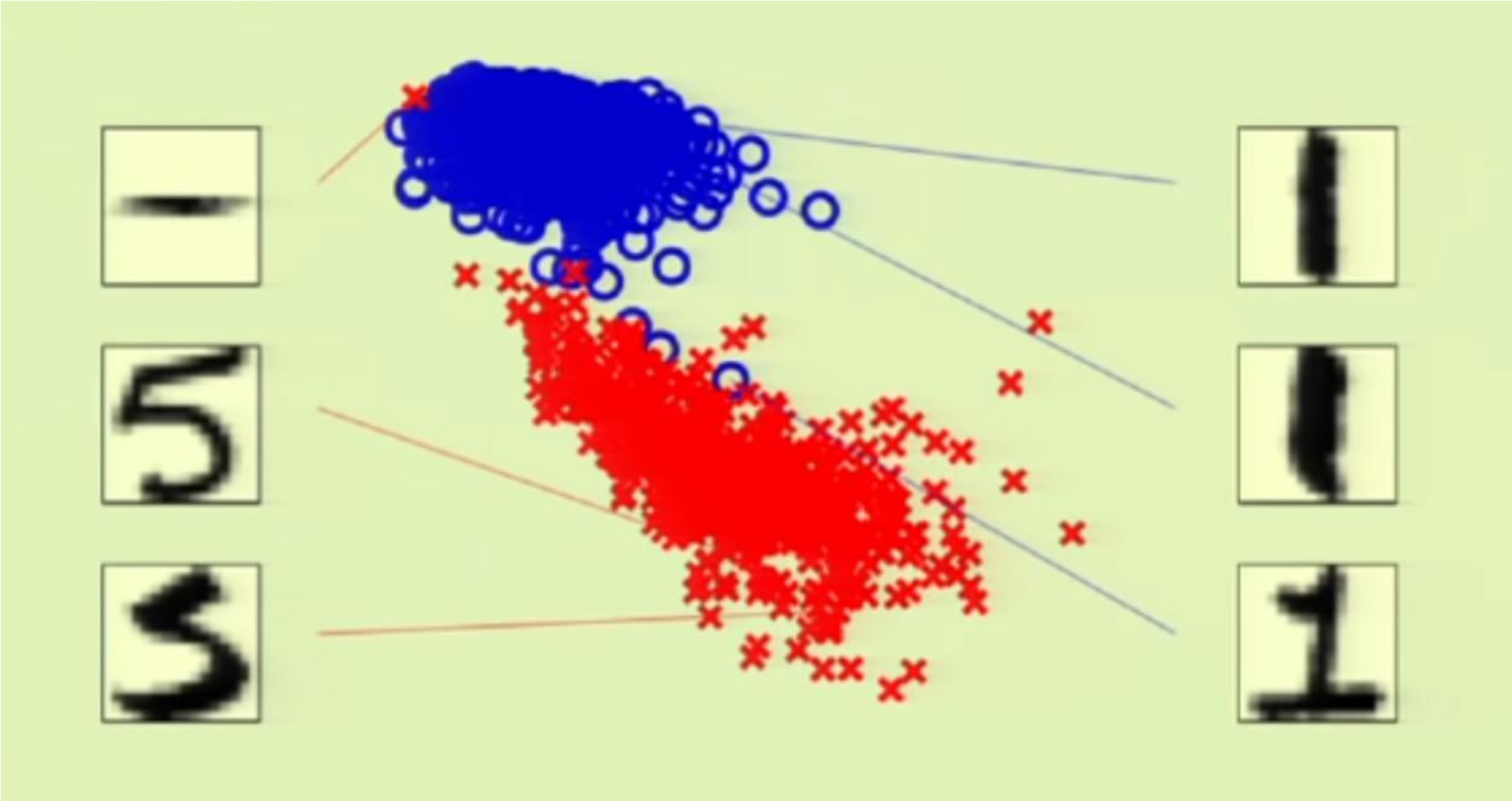
Sum up all the pixels = intensity
Symmetry = -(difference between flip version)

$x = (1, x_1, x_2)$

$x_1 = intensity \; x_2 = symmetry$

It is almost linearly separable

symmetry



intensity

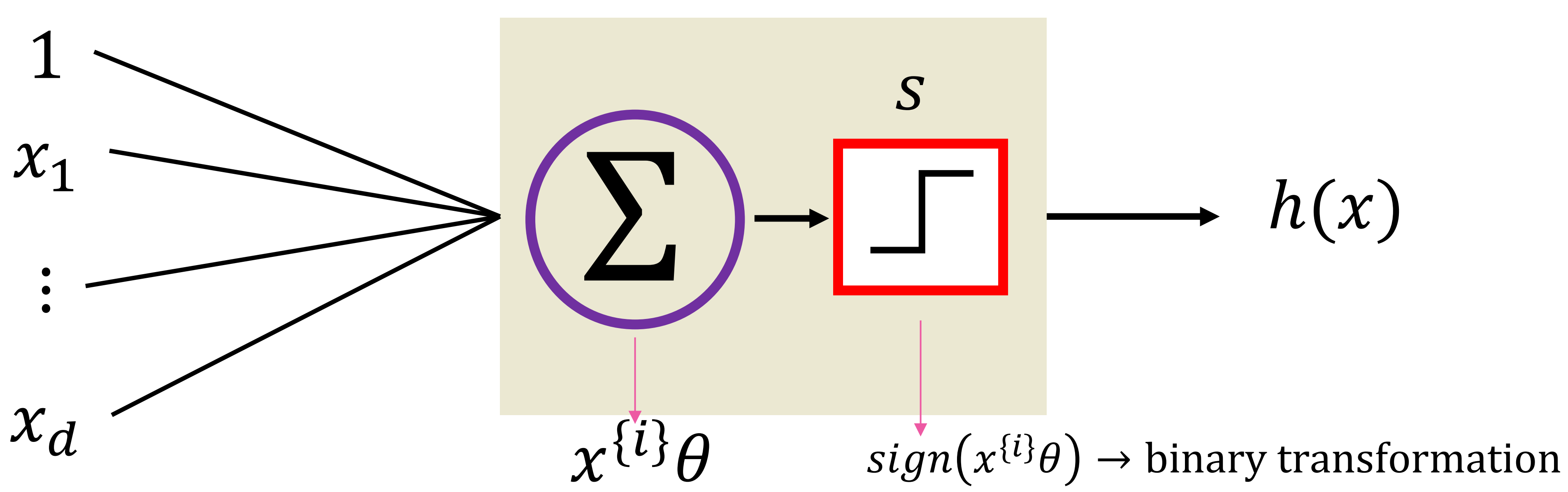
Linear regression for classification

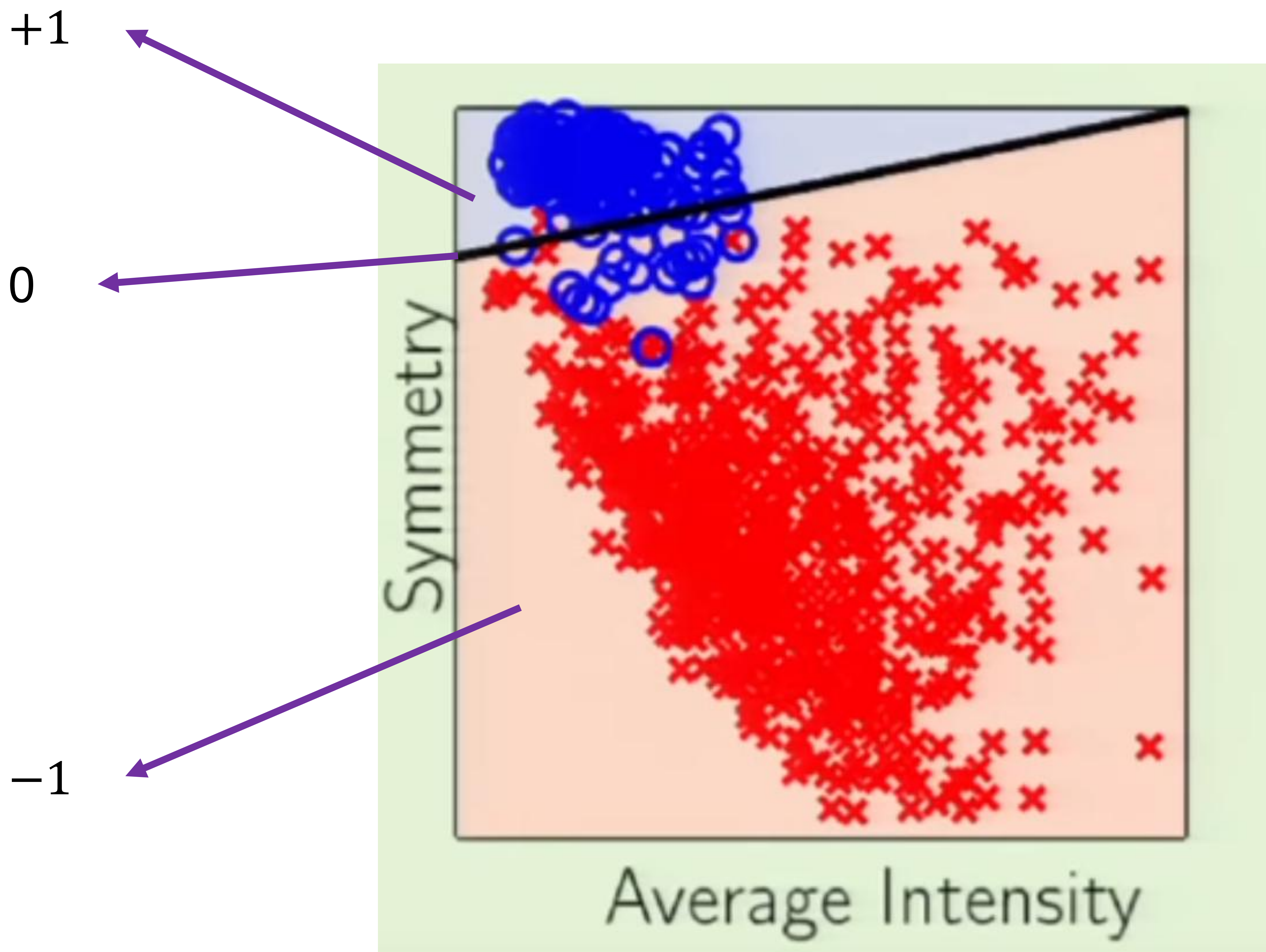
Binary-valued functions are also real-valued $\pm 1 \in R$

Use linear regression $x^{\{i\}}\theta \approx y^{\{i\}} = \pm 1$ i = index of a data-point

Let's calculate, $sign\left(x^{\{i\}}\theta\right) = \begin{cases} -1 & x^{\{i\}}\theta < 0 \\ 0 & x^{\{i\}}\theta = 0 \\ 1 & x^{\{i\}}\theta > 0 \end{cases}$

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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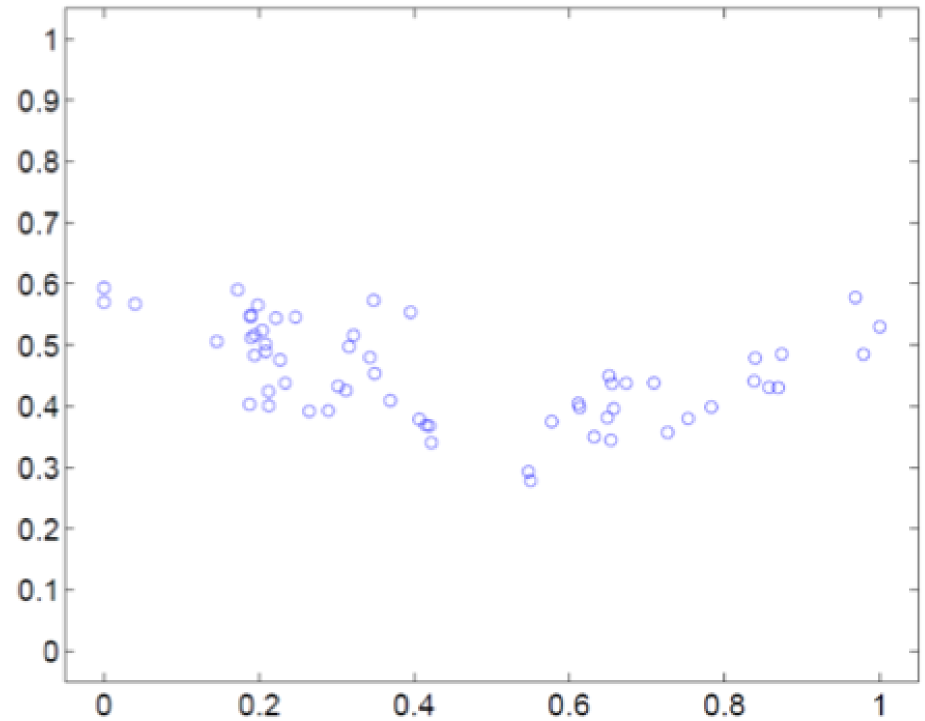
Extension to Higher-Order Regression



- Want to fit a polynomial regression model

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

- $z = \{1, x, x^2, \ldots, x^d\} \in R^d$ 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

$$\hat{\theta} = argmin_{\theta}\, L(\theta) = \frac{1}{n}\sum_{i=1}^{N}\left(y^{\{i\}} - z^{\{i\}}\theta\right)^2$$

- 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

$z = \{1, x, x^2, \ldots, x^d\} \in R^d \qquad y = \left\{y^{\{1\}}, y^{\{2\}}, \ldots, y^{\{n\}}\right\}$

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

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

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

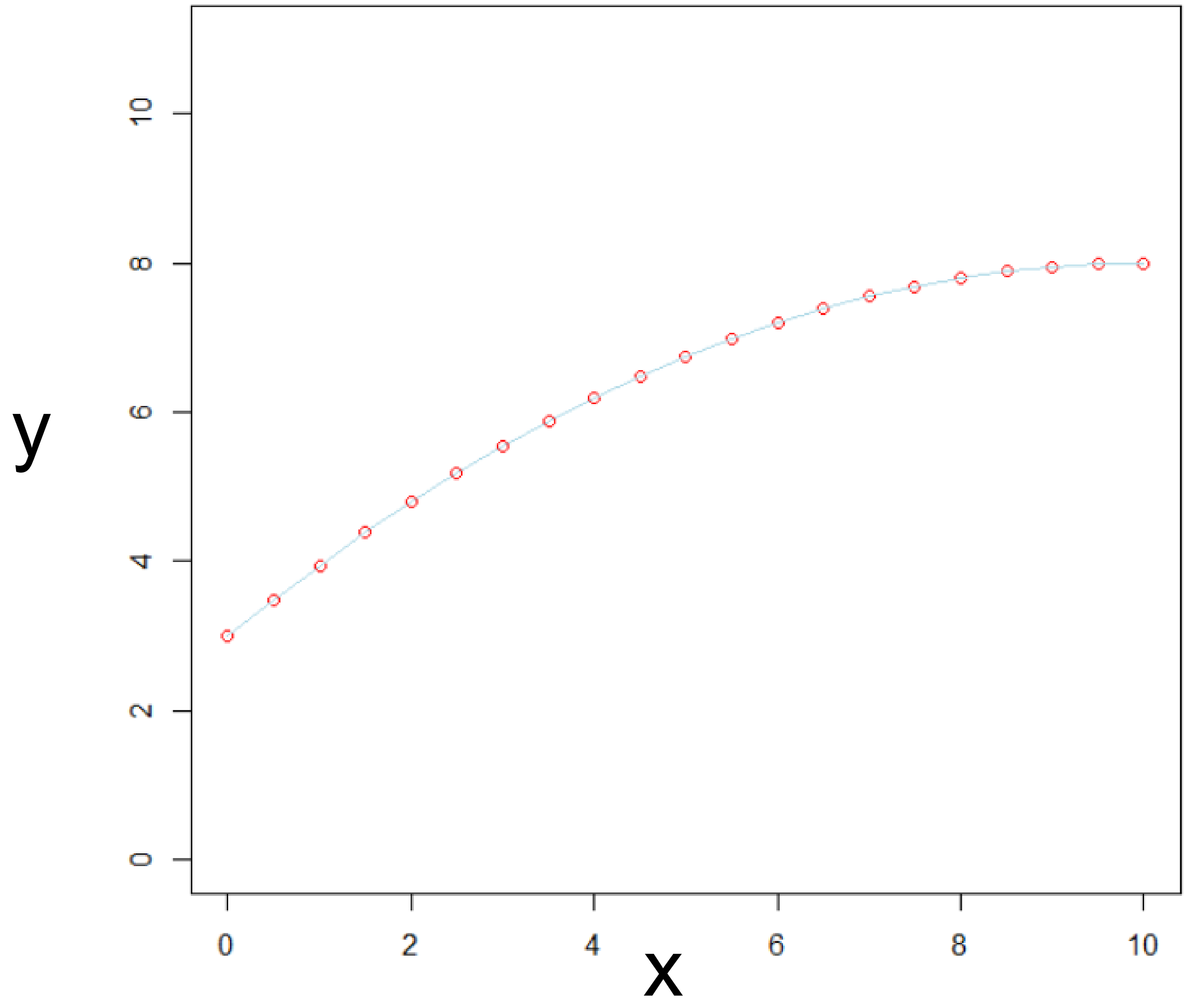
What is happening in polynomial regression?

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

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

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

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

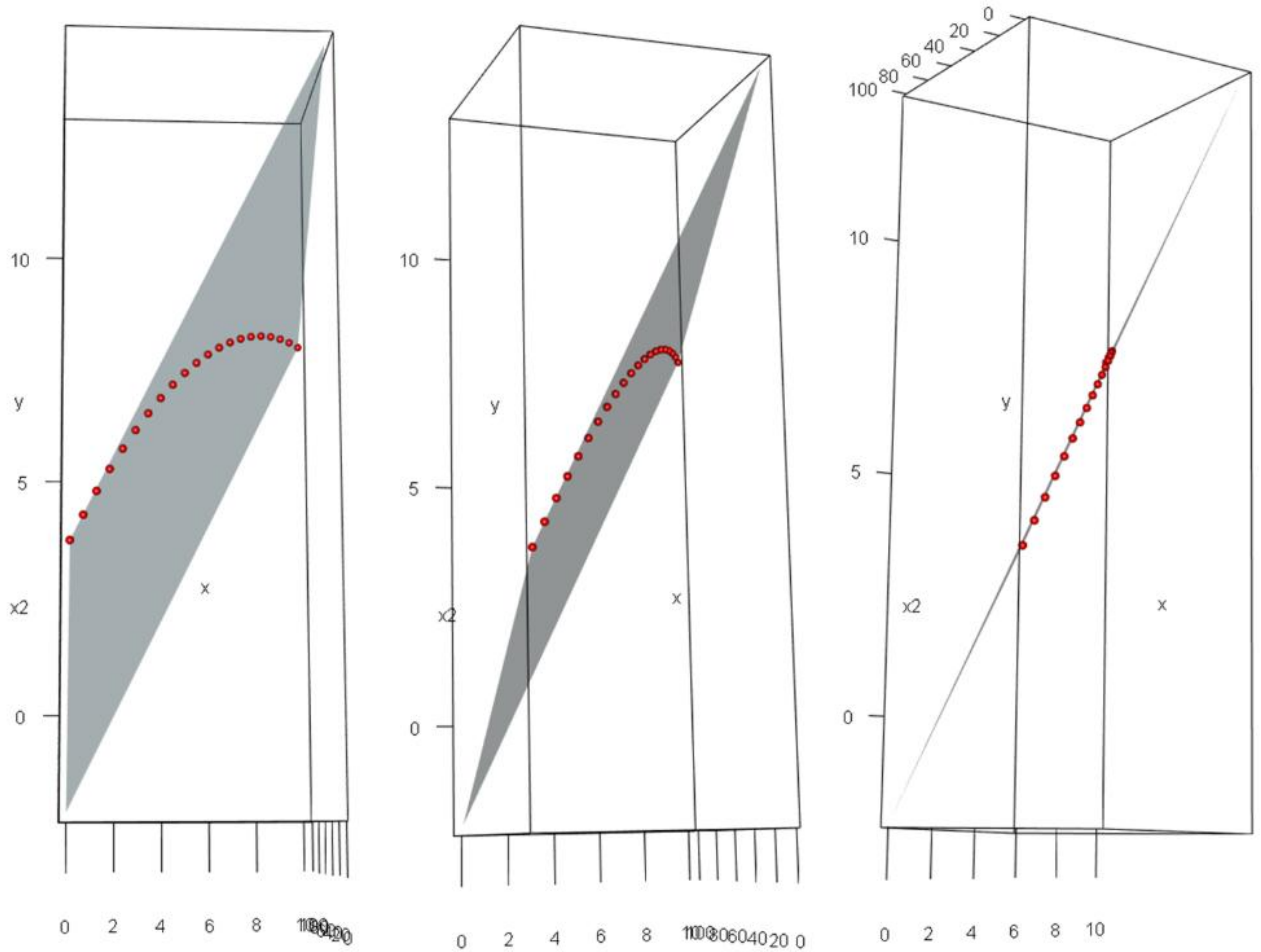


RMSE=0

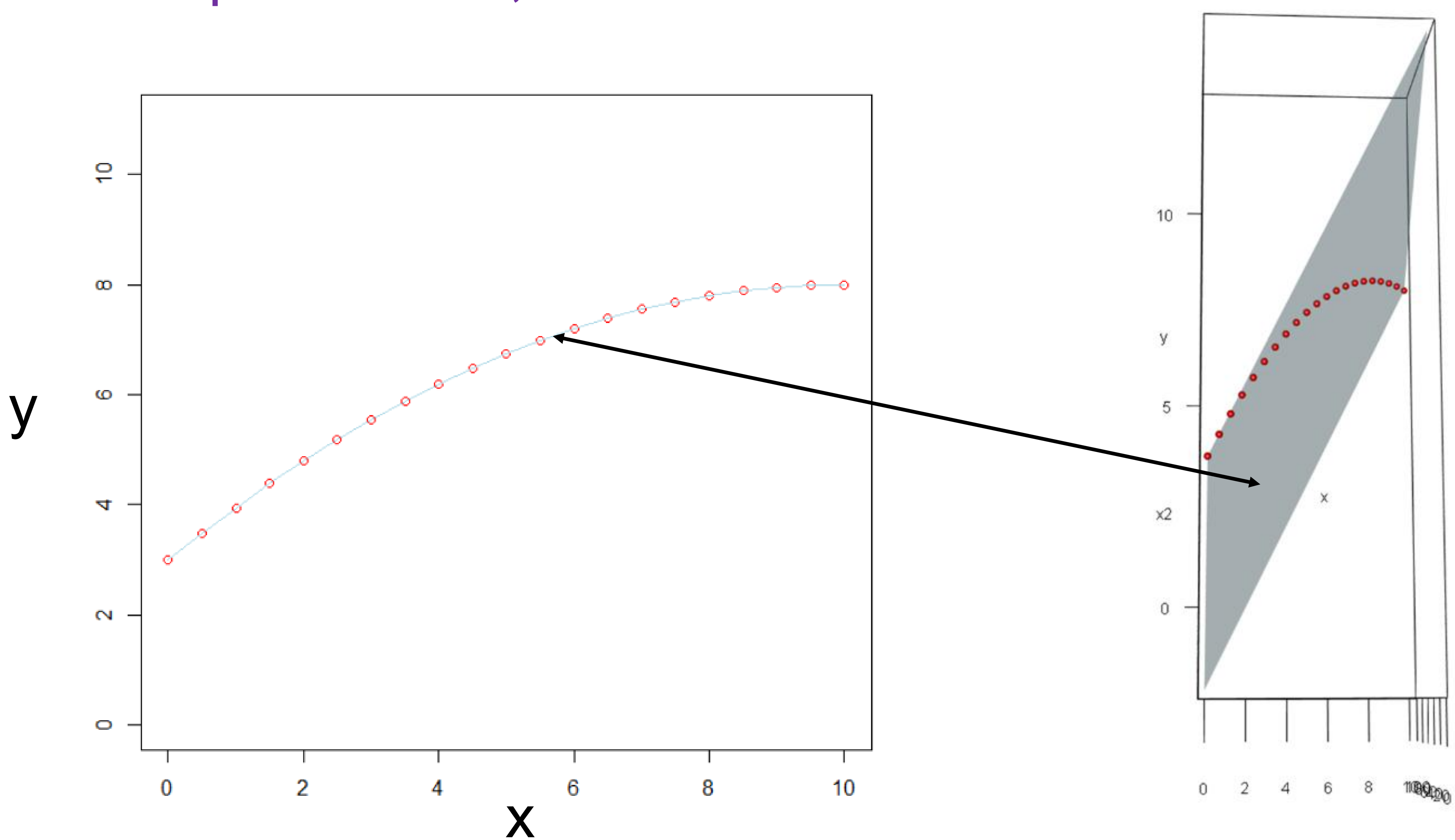
Let’s add to the feature space

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

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

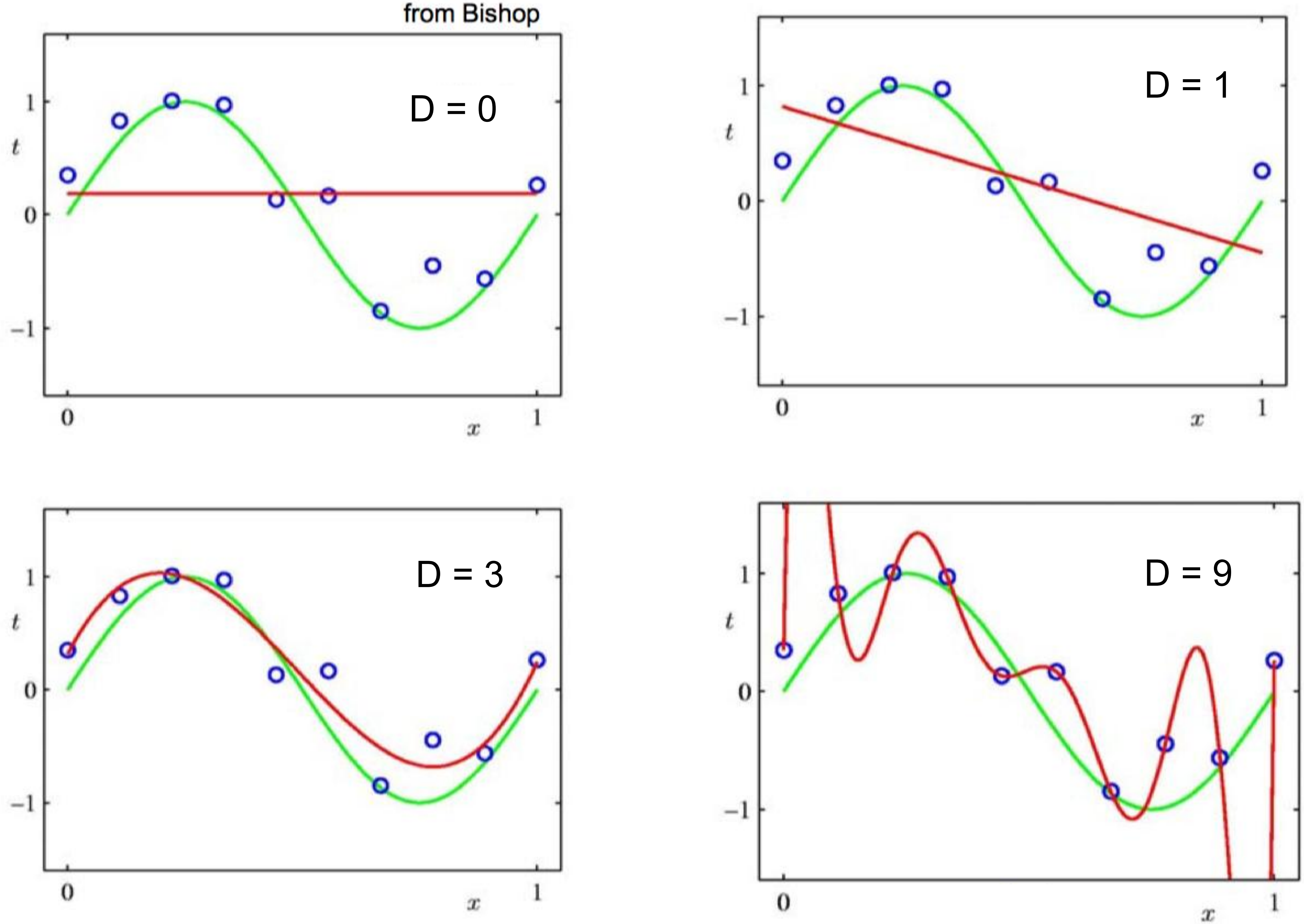


We are fitting a D-dimensional hyperplane in a D+1 dimensional hyperspace (in above example a 2D plane in a 3D space). That hyperplane really is 'flat' / 'linear' in 3D. It can be seen a non-linear regression (a curvy line) in our 2D example in fact it is a flat surface in 3D. So the fact that it is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



Increasing the Maximal Degree

from Bishop



Bias-Variance Trade off

Animation

We will have multiple prediction values (i.e. through Cross validation) $E\left[y_p\right]$

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{N}\left(y^{\{i\}} - x^{\{i\}}\theta\right)^2 = E\left[\left(\mathrm{y_a} - \mathrm{y_p}\right)^2\right]$$

$$\left(\mathrm{y_a} - \mathrm{y_p}\right)^2 = \left(y_a - E\left[y_p\right] + E\left[y_p\right] - y_p\right)^2$$

$$= \left(y_a - E\left[y_p\right]\right)^2 + \left(E\left[y_p\right] - y_p\right)^2 + 2\left(y_a - E\left[y_p\right]\right)\left(E\left[y_p\right] - y_p\right)$$

Bias-Variance Trade off

Animation

We will have multiple prediction values (i.e. through Cross validation) $E\left[y_p\right]$

$$L(\theta) = \frac{1}{n}\sum_{i=1}^{N}\left(y^{\{i\}} - x^{\{i\}}\theta\right)^2 = E\left[\left(\mathrm{y_a} - \mathrm{y_p}\right)^2\right]$$

$$\left(\mathrm{y_a} - \mathrm{y_p}\right)^2 = \left(y_a - E\left[y_p\right] + E\left[y_p\right] - y_p\right)^2$$

$$= \left(y_a - E\left[y_p\right]\right)^2 + \left(E\left[y_p\right] - y_p\right)^2 + 2\left(y_a - E\left[y_p\right]\right)\left(E\left[y_p\right] - y_p\right)$$

$$\mathbf{E}\left[\left(\boldsymbol{y_a} - \boldsymbol{y_p}\right)^{\mathbf{2}}\right] = \left(y_a - E\left[y_p\right]\right)^2 + E\left[\left(E\left[y_p\right] - y_p\right)^2\right]$$

$$= [Bias]^2 + Variance$$

$$= [true\ value - mean(predictions)]^2 - mean[(mean(prediction) - prediction)^2\ ]$$

Why $E[2(y_a - E[y_p])(E[y_p] - y_p)] = 0$?

$y_a - E[y_p]$ is a scalar, therefore $E\left[y_a - E[y_p]\right] = y_a - E[y_p]$

$$E[2(y_a - E[y_p])(E[y_p] - y_p)]$$

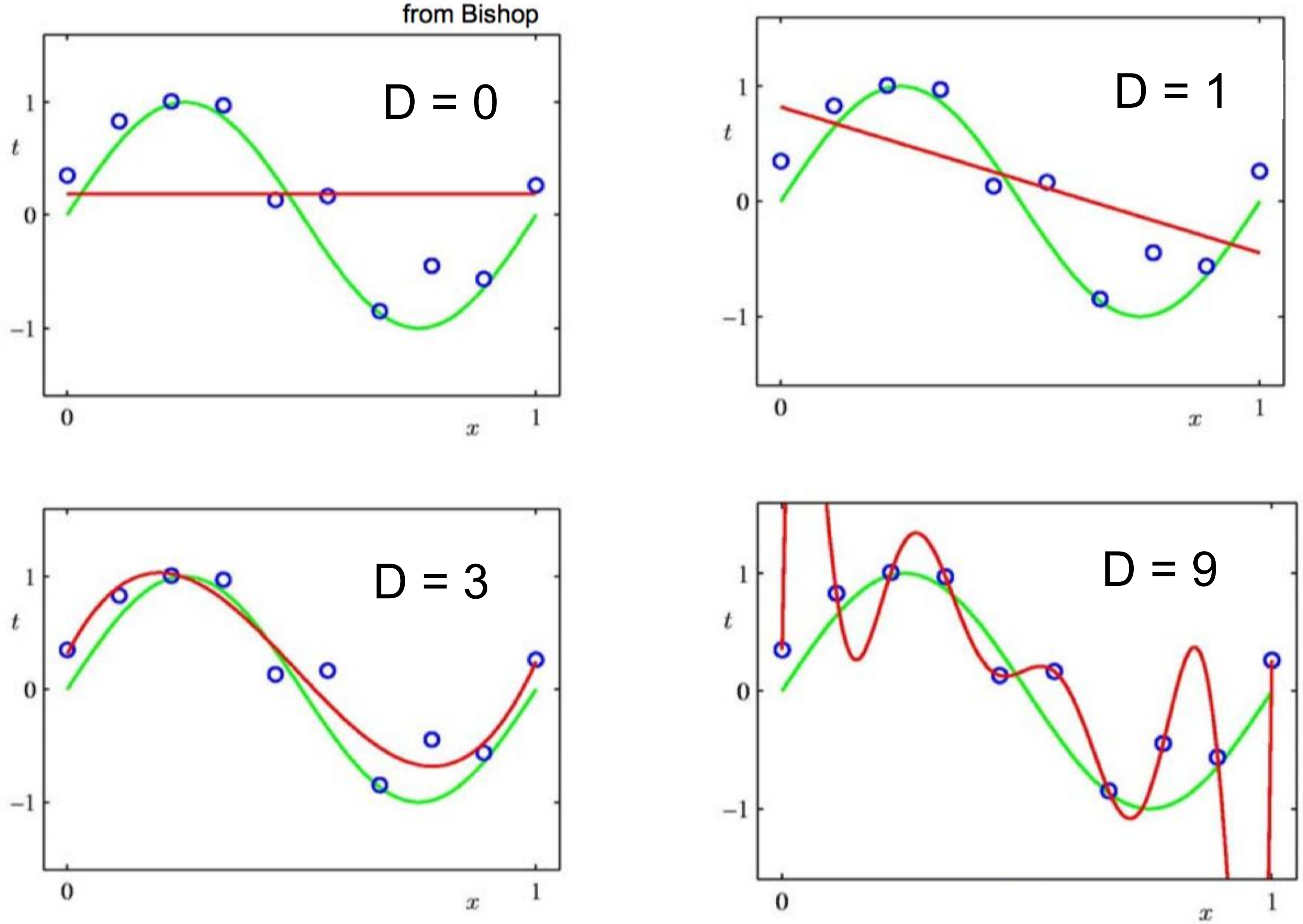
$$= 2(y_a - E[y_p])E[E[y_p] - y_p]$$

$$= 2(y_a - E[y_p])\left(E\left[E[y_p]\right] - E[y_p]\right)$$

$$= 2(y_a - E[y_p])(E[y_p] - E[y_p]) = 0$$

Which One is Better?

from Bishop



- 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