

Linear and Logistic Regression

David I. Inouye

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Outline

- ▶ Linear regression
 - ▶ Formalization
 - ▶ Intuitions
 - ▶ Solution in closed-form

- ▶ Logistic regression
 - ▶ Intuitions
 - ▶ Formalization
 - ▶ Solution requires numerical algorithms

The linear regression model is defined by the coefficients (or parameters) for each feature

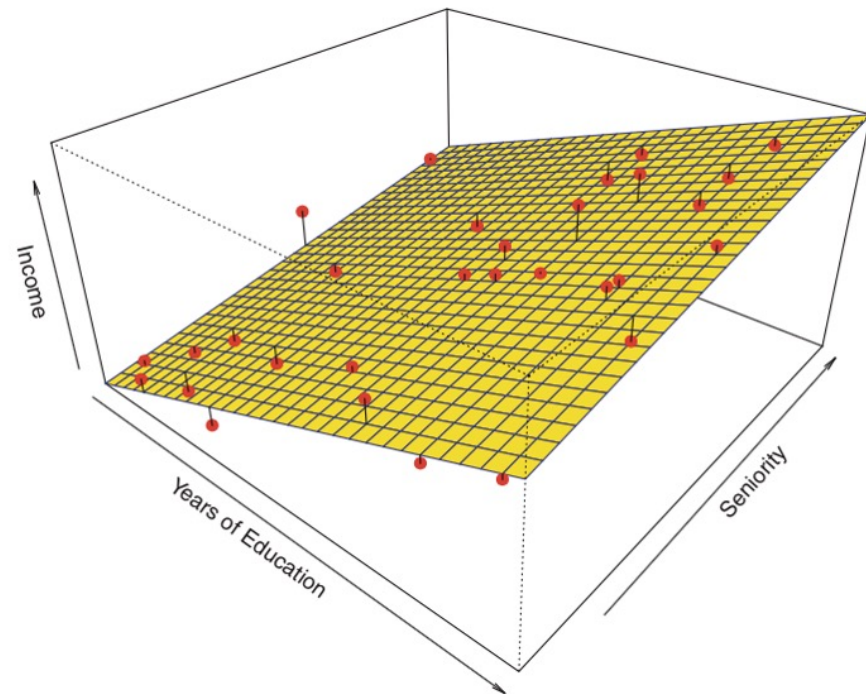
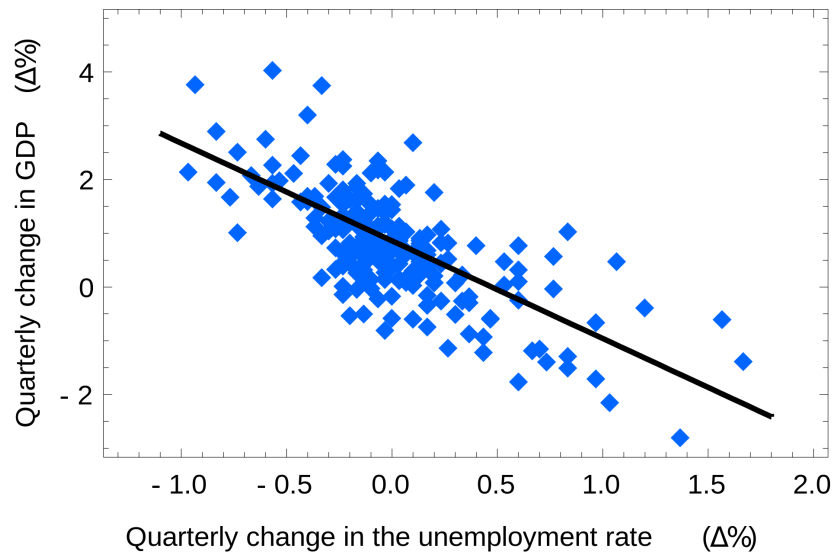
- ▶ A simple linear combination where θ are the parameters

$$f_{\theta}(x) = \theta_1 x_1 + \theta_2 x_2 + \dots + \theta_d x_d + \theta_{d+1}$$

- ▶ Letting $\mathbf{x} = [x_1, x_2, \dots, x_d, \mathbf{1}]$, we can write as
$$f_{\theta}(x) = \theta^T \mathbf{x}$$

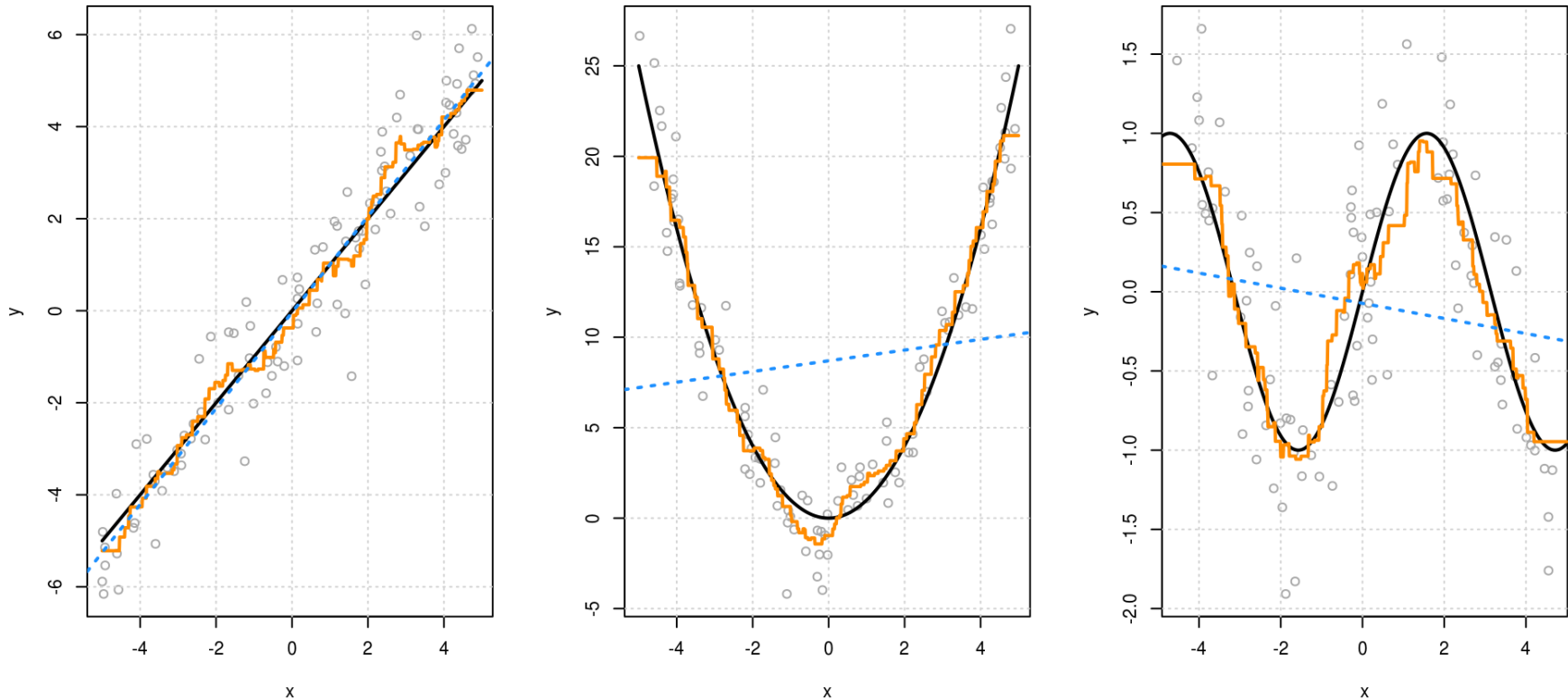
- ▶ This is known as a parametric model

Linear regression models the output as a line (1D) or hyperplane (>1D)



<https://towardsdatascience.com/linear-regression-detailed-view-ea73175f6e86>

How does this compare to KNN regression? Linear regression is a much simpler function



If true phenomena is linear (i.e., *assumption matches reality*), linear regression will do the best (left). However, if true phenomena is not linear, KNN regression will perform better. (Black line is true function, dotted blue line is best linear approximation, and orange line is KNN regression.)

<https://davidalpiaz.github.io/r4sl/knn-reg.html>

The goal of linear regression is to find the parameters θ that minimize the prediction error

- ▶ Using mean squared error (MSE) this means:

$$\theta^* = \arg \min_{\theta} \frac{1}{n} \sum_{i=1}^n (y_i - f_{\theta}(\mathbf{x}_i))^2$$

- ▶ Or equivalently

$$\theta^* = \arg \min_{\theta} \sum_{i=1}^n (y_i - \theta^T \mathbf{x}_i)^2$$

- ▶ Or in matrix form

$$\theta^* = \arg \min_{\theta} \|\mathbf{y} - X\theta\|_2^2$$

- ▶ Known as **Ordinary Least Squares (OLS)**

The solution for OLS
can be computed in closed form

- ▶ How do you find maximum or minimum in calculus?
- ▶ Calculate gradient

$$\begin{aligned} & \nabla_{\theta} \|\mathbf{y} - X\theta\|_2^2 \\ &= \left(2(\mathbf{y} - X\theta)^T (-X) \right)^T \\ &= \left(2(-X^T)(\mathbf{y} - X\theta) \right) \\ &= 2(-X^T \mathbf{y} + X^T X\theta) \end{aligned}$$

- ▶ Set equal to zero and solve

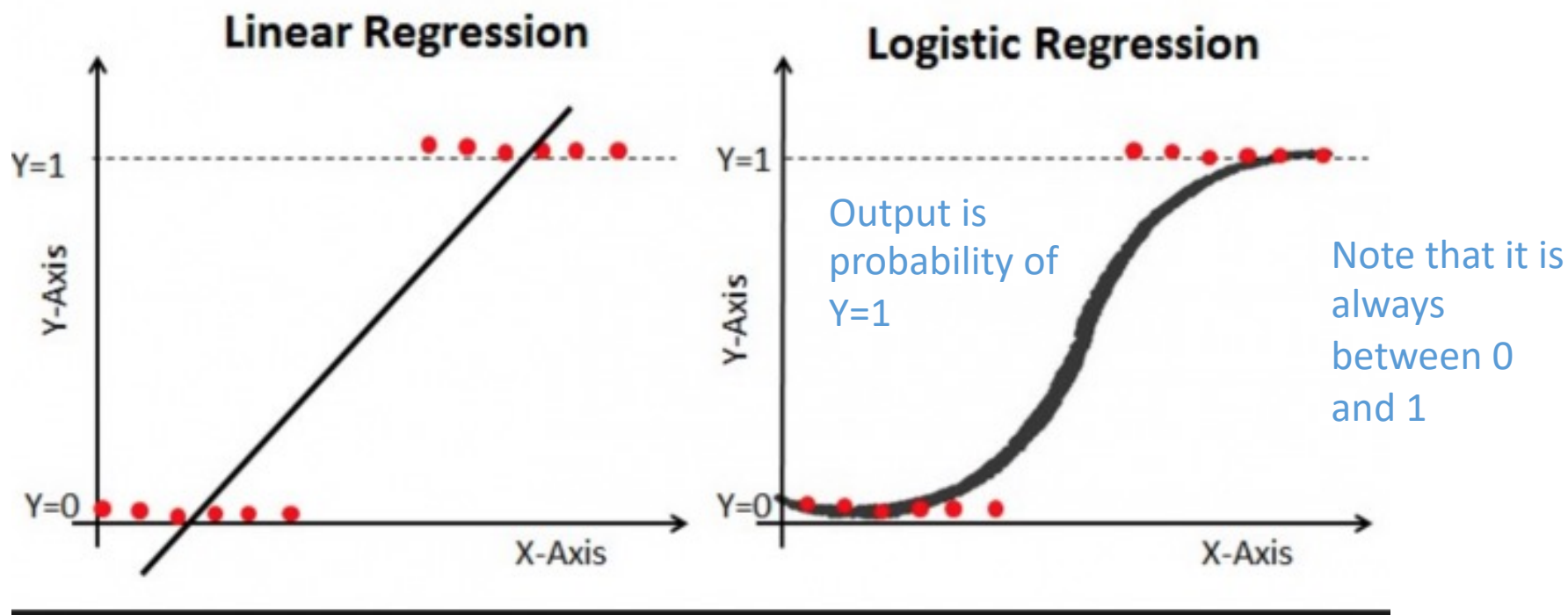
$$\begin{aligned} -2(X^T \mathbf{y} + X^T X\theta) &= 0 \\ X^T X\theta &= X^T \mathbf{y} \\ \theta^* &= (X^T X)^{-1} X^T \mathbf{y} \end{aligned}$$

Derivation hints:
Use equivalence
of $\|\mathbf{v}\|_2^2 = \mathbf{v}^T \mathbf{v}$.
Then use [matrix
calculus \(wikipedia
reference\)](#).

Known as **normal
equations**

https://en.wikipedia.org/wiki/Ordinary_least_squares

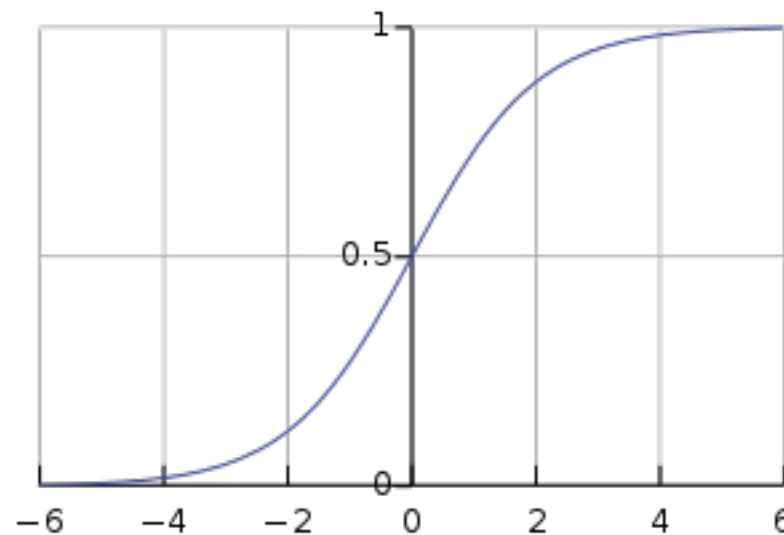
Logistic regression *generalizes* linear regression to the classification setting (*despite the name*)



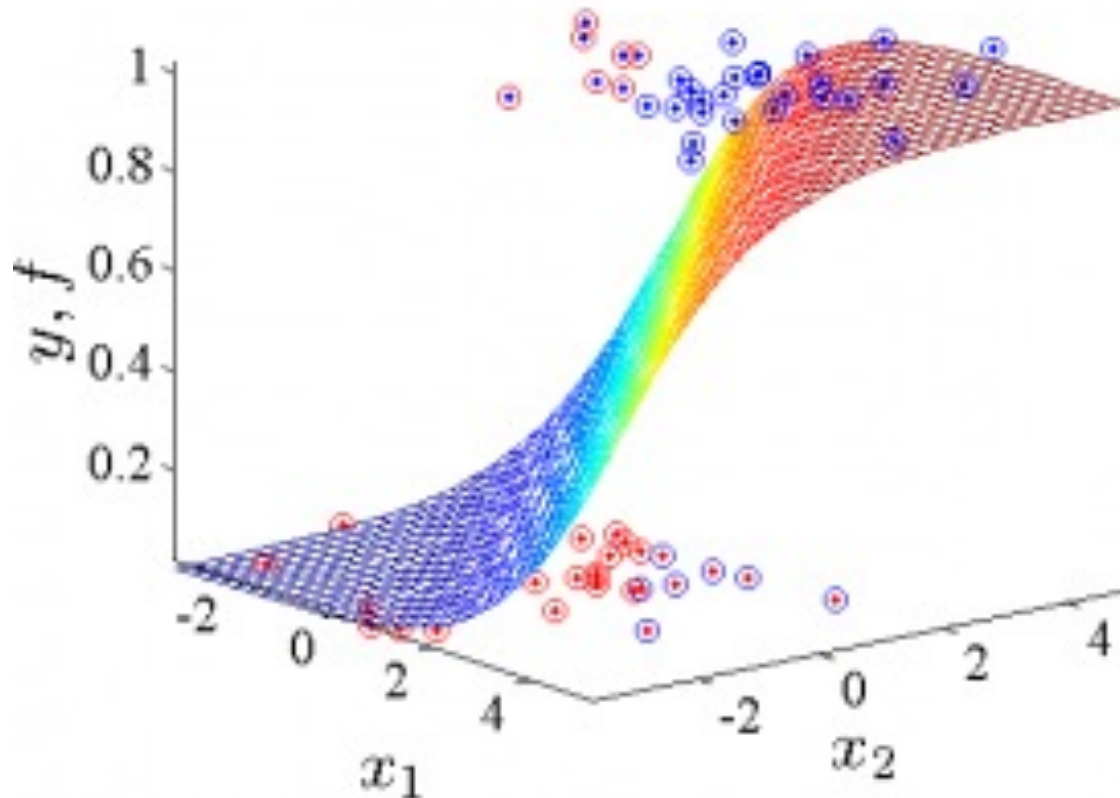
<https://medium.com/@ODSC/logistic-regression-with-python-ed39f8573c7>

The logistic function is a sigmoid curve with a simple form

- ▶ $\sigma(a) = \frac{1}{1+e^{-a}}$
- ▶ Equivalently
$$\sigma(a) = \frac{e^a}{e^a + 1}$$
- ▶ Bounds
 - ▶ $a \rightarrow \infty, \sigma(a) \rightarrow 1$
 - ▶ $a \rightarrow -\infty, \sigma(a) \rightarrow 0$
- ▶ 1D logistic model
$$f_{\theta}(x) = \sigma(\theta_1 x + \theta_2)$$



Logistic regression in higher dimensions is just the logistic curve along a single direction



Multivariate logistic regression merely applies a logistic function to the output of a linear function

- ▶ The multivariate logistic regression model is

$$f_{\theta}(\mathbf{x}) = \sigma(\theta^T \mathbf{x})$$

- ▶ Notice similarity to linear regression model

- ▶ However, we can *interpret* $f_{\theta}(x)$ as the **probability** of $y = 1$ instead of predicting y directly

- ▶ Thresholding this probability allows us to predict the class

$$\hat{y} = \begin{cases} 1, & \text{if } f_{\theta}(x) \geq 0.5 \\ 0, & \text{otherwise} \end{cases}$$

The logistic regression optimization minimizes the log likelihood of the training data

- ▶ In theory, we could use MSE:

$$\theta^* = \arg \min_{\theta} \|\mathbf{y} - \sigma(X\theta)\|_2^2$$

- ▶ However, the true output y is always 0 or 1
- ▶ Instead we maximize the **log likelihood** (which is equal to the log probability of the data)

$$\theta^* = \arg \max_{\theta} \sum_{i=1}^n y_i \log \Pr(y_i = 1 | x_i) + (1 - y_i) \log \Pr(y_i = 0 | x_i)$$

- ▶ Equivalently

$$\theta^* = \arg \max_{\theta} \sum_{i=1}^n y_i \log \sigma(\theta^T \mathbf{x}_i) + (1 - y_i) \log(1 - \sigma(\theta^T \mathbf{x}_i))$$

Logistic regression does not have a closed-form solution!

- ▶ Must resort to numerical optimization
- ▶ Examples: Gradient descent, Newton's method

