Linear and Logistic Regression

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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

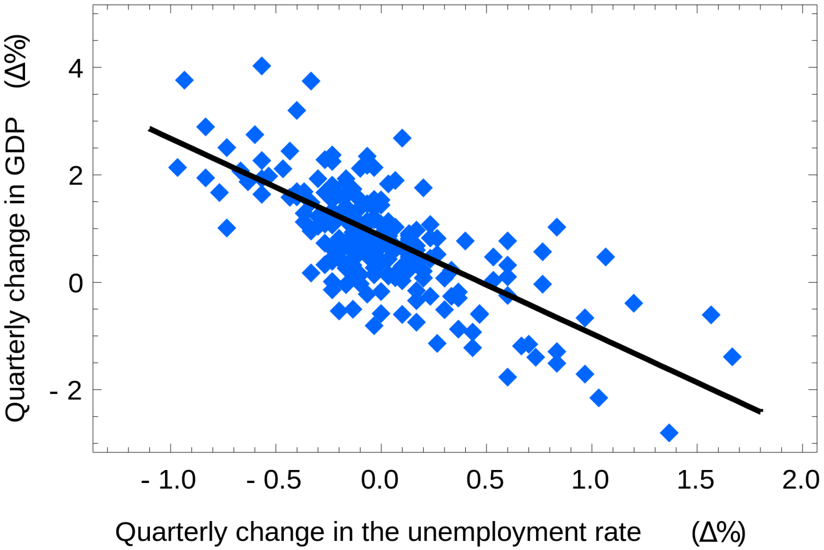
$$f_\theta(x) = \theta_1 x_1 + \theta_2 x_2 + \cdots + \theta_d x_d + \theta_{d+1}$$

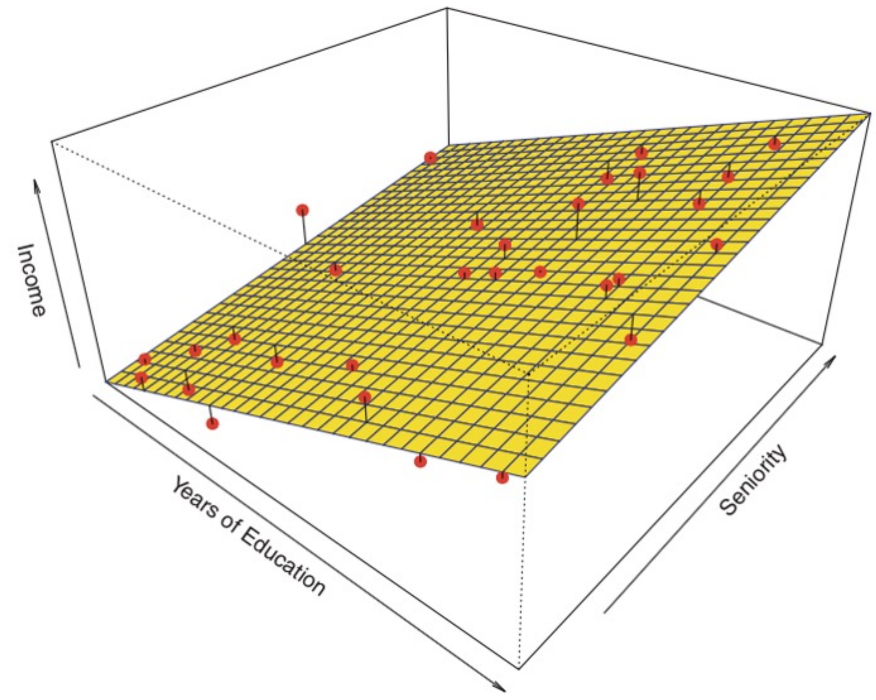
- Letting $\boldsymbol{x} = [x_1, x_2, \dots, x_d, 1]$, we can write as

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

- This is known as a **parametric model**

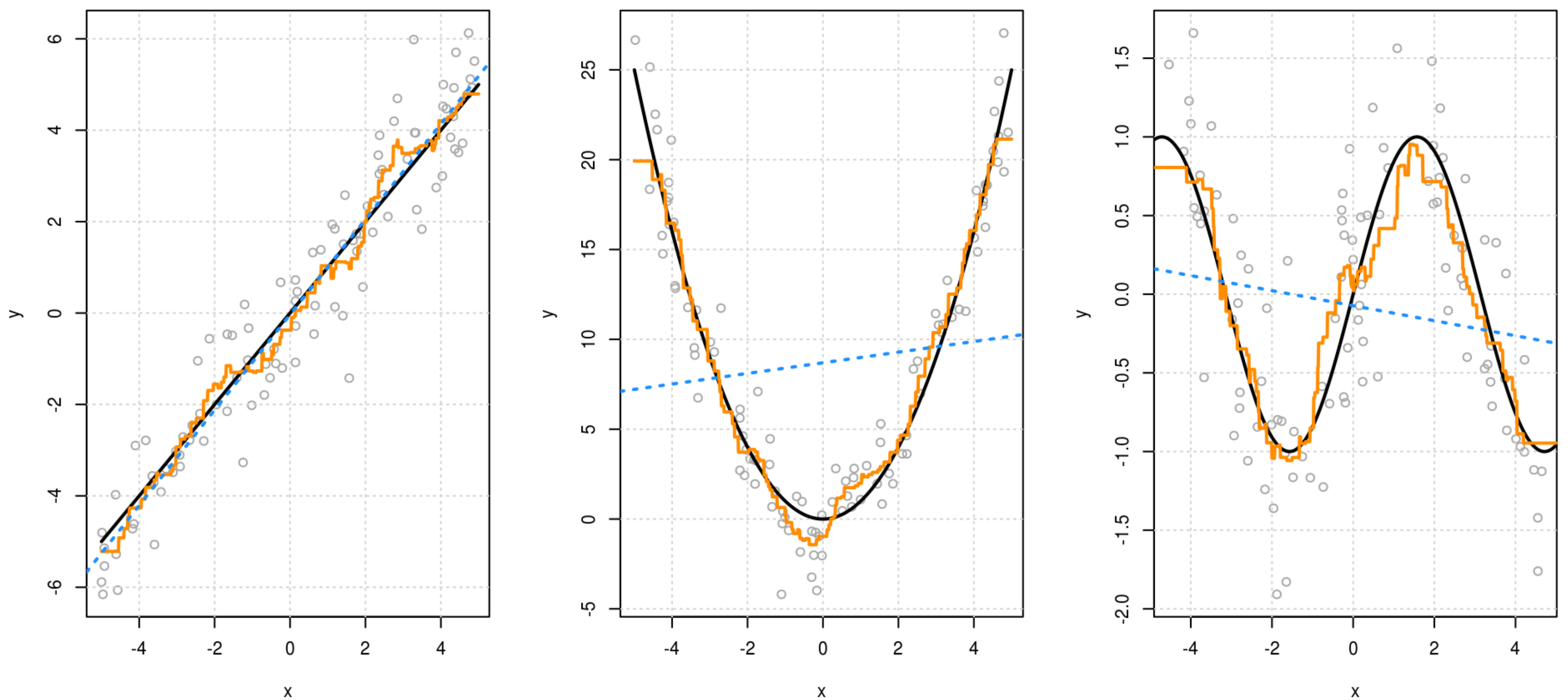
Linear regression models the output as a line (1D) or hyperplane (>1D)





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://daviddalpiaz.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:

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

- Or equivalently

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

- Or in matrix form

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

- Known as **<u>Ordinary Least Squares (OLS)</u>**

The solution for OLS can be computed in closed form

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

$$\nabla_\theta \|\boldsymbol{y} - X\theta\|_2^2$$
$$= \left(2(\boldsymbol{y} - X\theta)^T(-X)\right)^T$$
$$= \left(2(-X^T)(\boldsymbol{y} - X\theta)\right)$$
$$= 2(-X^T\boldsymbol{y} + X^T X\theta)$$

- Set equal to zero and solve

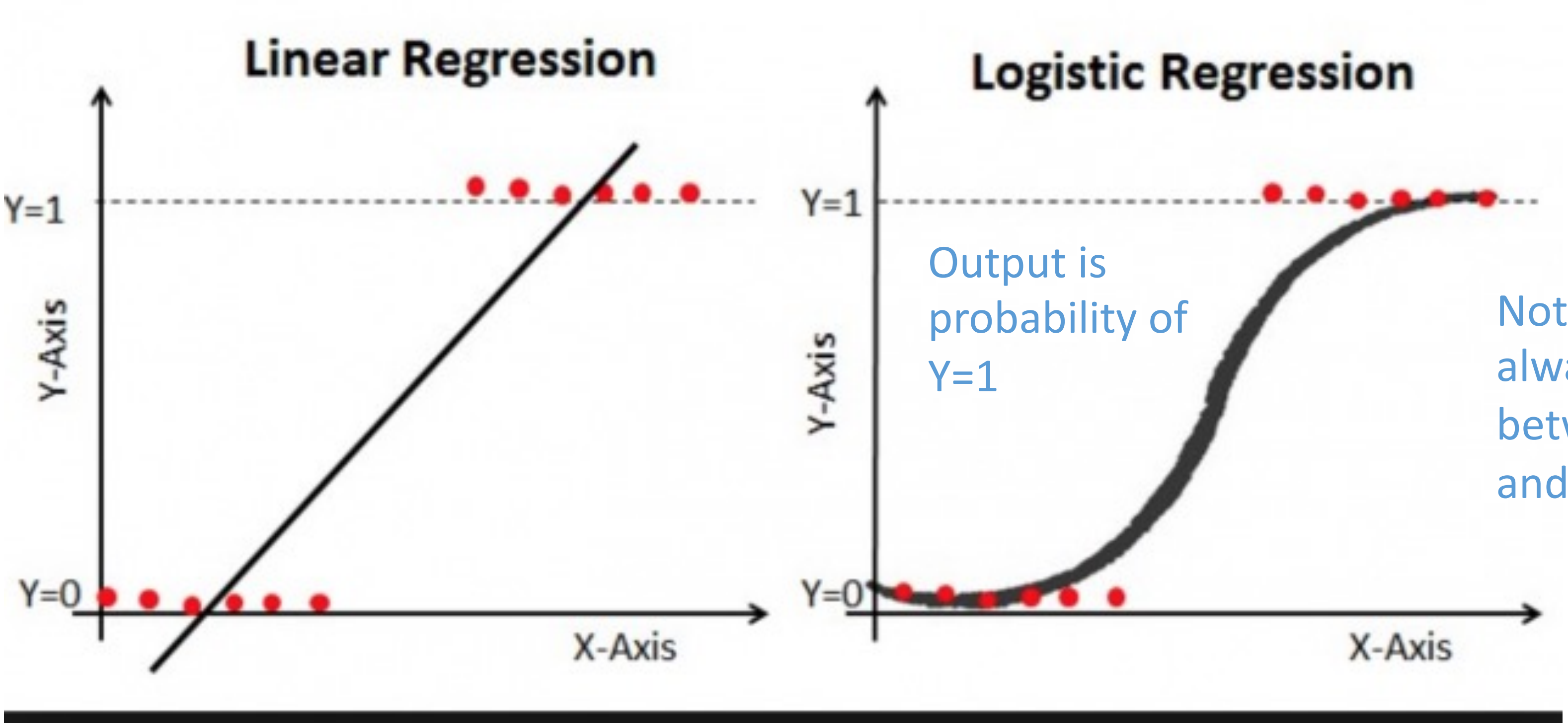
$$-2(X^T y + X^T X\theta) = 0$$
$$X^T X\theta = X^T\boldsymbol{y}$$
$$\theta^* = (X^T X)^{-1}X^T\boldsymbol{y}$$

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

Known as **normal equations**

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

<u>Logistic regression</u> *generalizes* linear regression to the classification setting (*despite the name*)



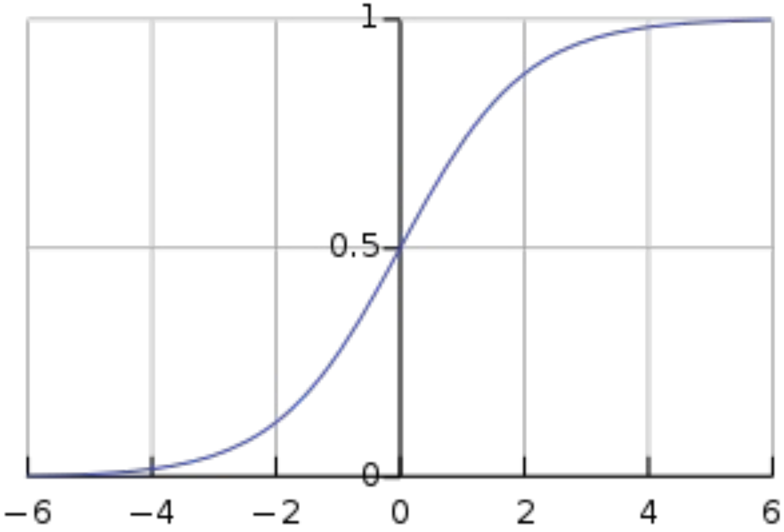
Output is probability of Y=1

Note that it is always between 0 and 1

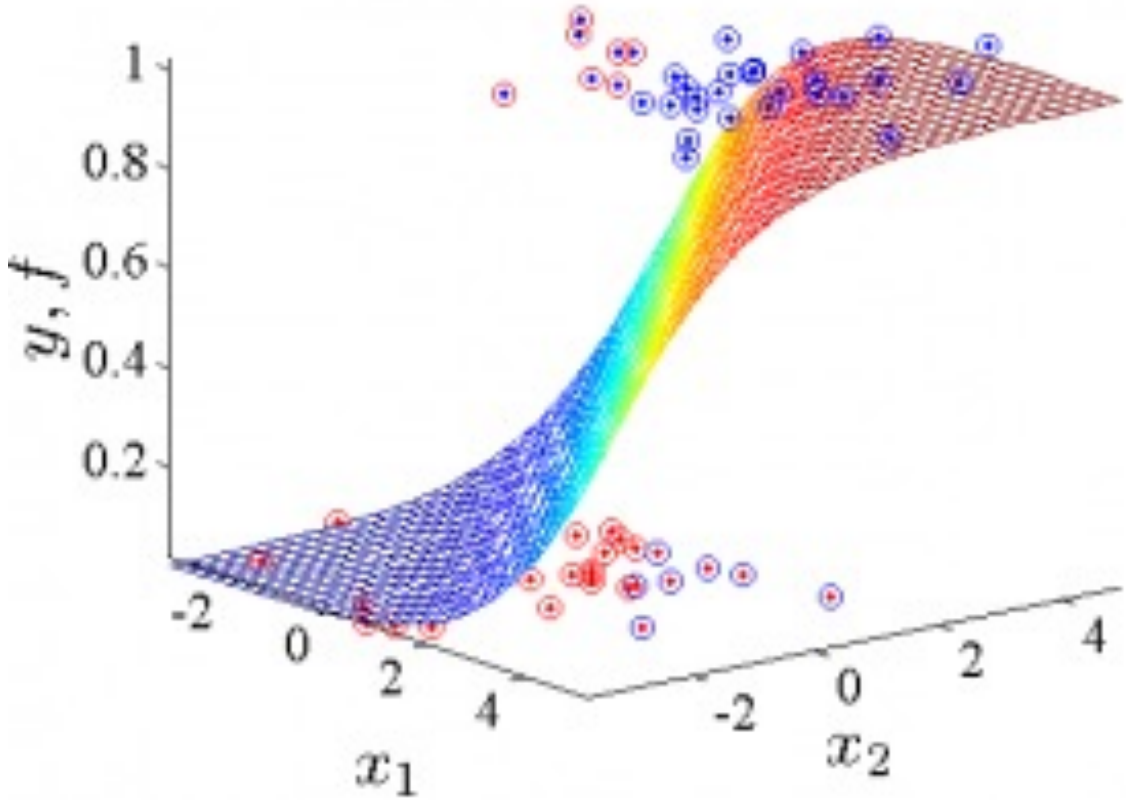
https://medium.com/@ODSC/logistic-regression-with-python-ede39f8573c7

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
  - $a \to \infty, \sigma(a) \to 1$
  - $a \to -\infty, \sigma(a) \to 0$
- 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
$$f_\theta(\boldsymbol{x}) = \sigma(\theta^T \boldsymbol{x})$$
- 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 maximizes the log likelihood of the training data

- In theory, we could use MSE:

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

- However, the true output y is always 0 or 1
- Instead we maximize the **<u>log likelihood</u>** (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

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

Logistic regression does **not** have a closed-form solution!

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