Logistic Regression

Linear Regression

Linear Regression

How to create an approximated function?

Machine learning is the function approximation process

Hypothesis

$$h\colon \hat{f}(x;\theta) = \theta_0 + \sum_{i=1}^{n} \theta_i x_i = \sum_{i=0}^{n} \theta_i x_i$$

n is the number of the feature values

Two aspects: the linearly weight sum(Linear model), the parameter θ

How to find the better θ?

Finding θ in Linear Regression

$$h: \hat{f}(x;\theta) = \sum_{i=0}^{n} \theta_i x_i \rightarrow \hat{f}(x;\theta) = X\theta$$

$$X = \begin{pmatrix} 1 & \cdots & x_n^1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & x_n^D \end{pmatrix}, \theta = \begin{pmatrix} \theta_0 \\ \vdots \\ \theta_n \end{pmatrix}$$

But, the reality would be the noisy

$$f(x;\theta) = \sum_{i=0}^{n} \theta_i x_i + e = y \rightarrow f(x;\theta) = X\theta + e = Y$$

$$
\begin{aligned}
\hat{\theta} = argmin_{\theta}(f - \hat{f})^2 &= argmin_{\theta}(Y - X\theta)^2 \\
&= argmin_{\theta}(Y - X\theta)^T(Y - X\theta) \\
&= argmin_{\theta}(Y^T - \theta^T X^T)(Y - X\theta) \\
&= argmin_{\theta}(Y^T Y - Y^T X\theta - \theta^T X^T Y + \theta^T X^T X\theta) \\
&= argmin_{\theta}(Y^T Y - 2\theta^T X^T Y + \theta^T X^T X\theta) \\
&= argmin_{\theta}(\theta^T X^T X\theta - 2\theta^T X^T Y)
\end{aligned}
$$

Now, we need to optimize θ

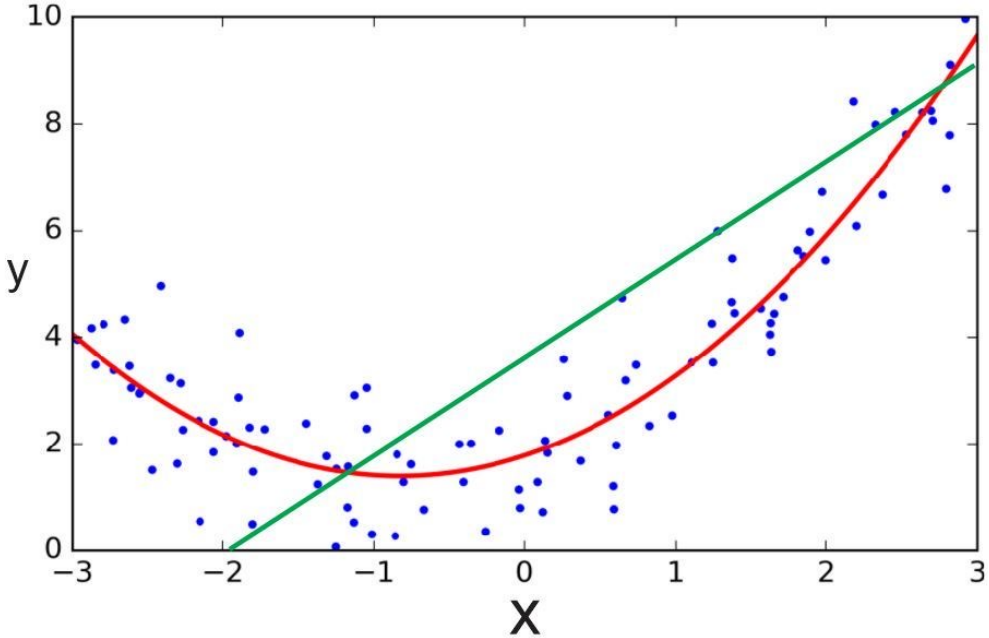
Optimized θ

$$\hat{\theta} = argmin_{\theta}(\theta^T X^T X\theta - 2\theta^T X^T Y)$$

$$\nabla_{\theta}\ (\theta^T X^T X\theta - 2\theta^T X^T Y) = 0$$

$$2X^T X\theta - 2X^T Y = 0$$

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



$$h: \hat{f}(x;\theta) = \sum_{i=0}^{n} \sum_{j=0}^{m} \theta_{i,j} \phi_j(x_i)$$

Simple Linear Regression

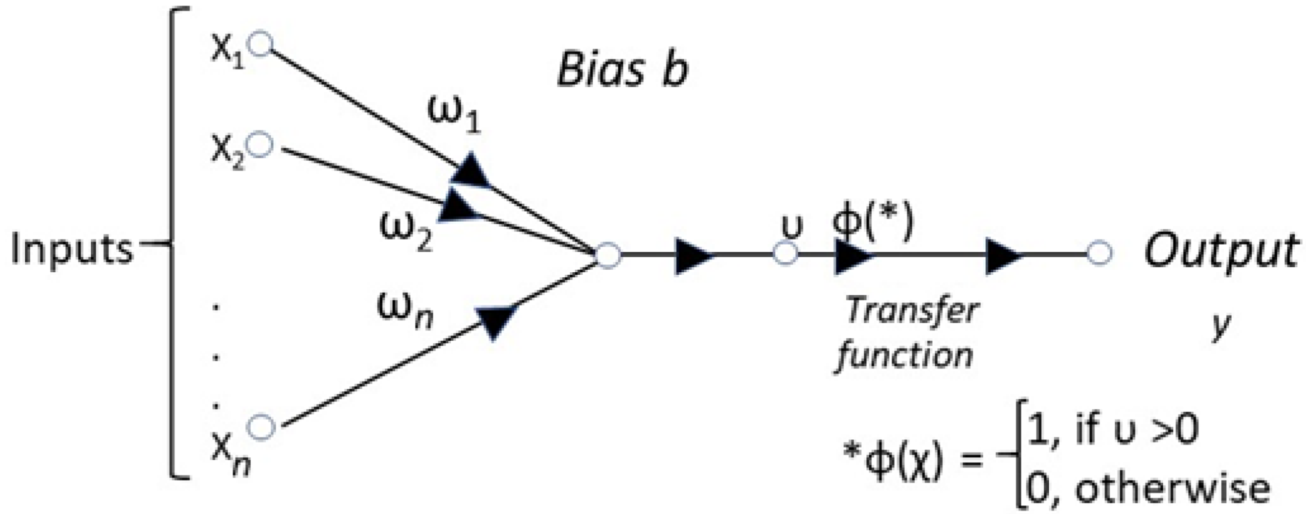
$$y = b_0 + b_1 x_1$$

Multiple Linear Regression

$$y = b_0 + b_1 x_1 + b_2 x_2 + \ldots + b_n x_n$$

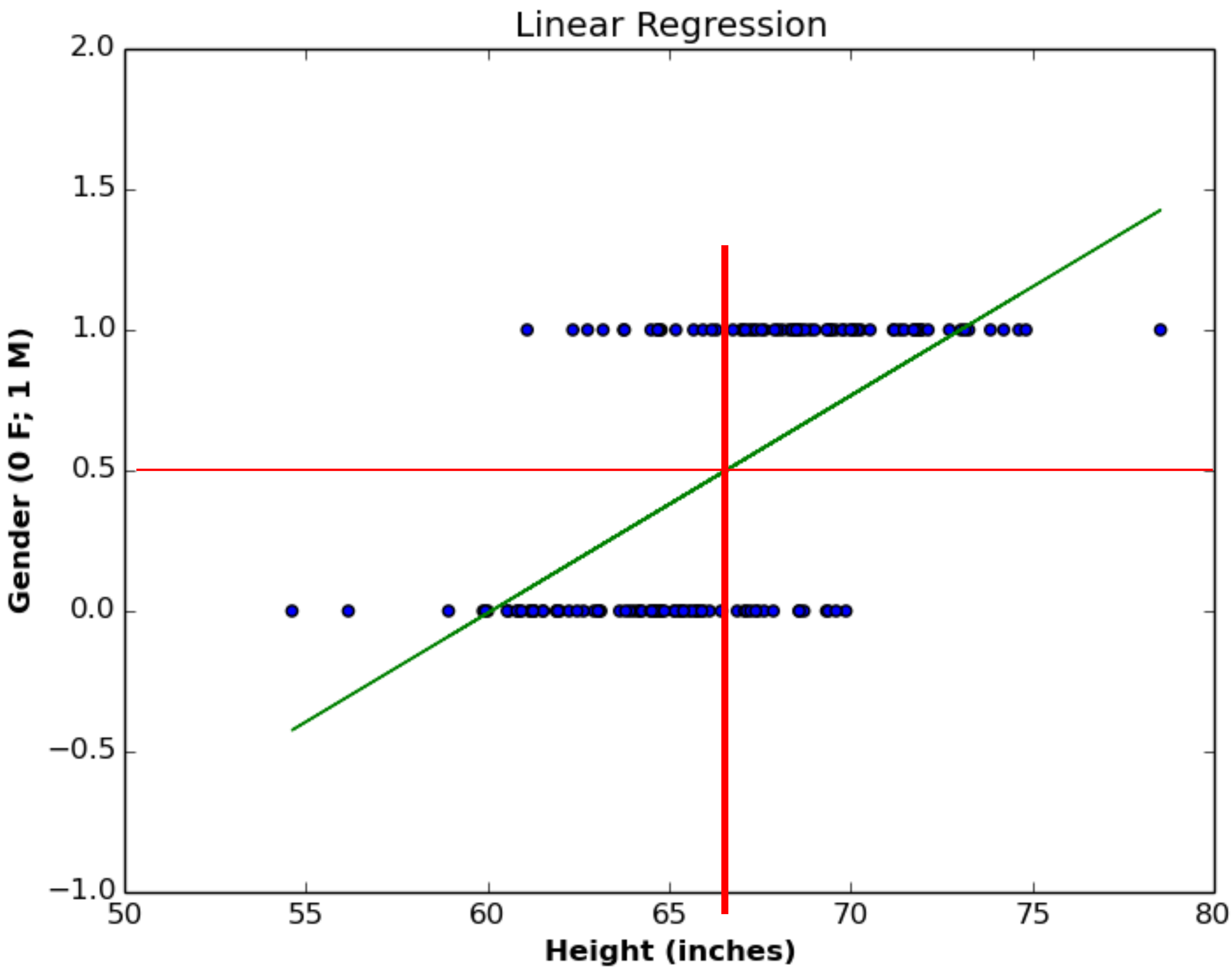
Polynomial Linear Regression

$$y = b_0 + b_1 x_1 + b_2 x_1^2 + \ldots + b_n x_1^n$$



$$X = \begin{pmatrix} x_0 \\ . \\ . \\ . \\ x_n \end{pmatrix} \quad W = \begin{pmatrix} \omega_0 \\ . \\ . \\ . \\ \omega_n \end{pmatrix} \quad \upsilon = \sum_{j=1}^{n} x_j \omega_j + b \quad = \quad \omega^T x$$

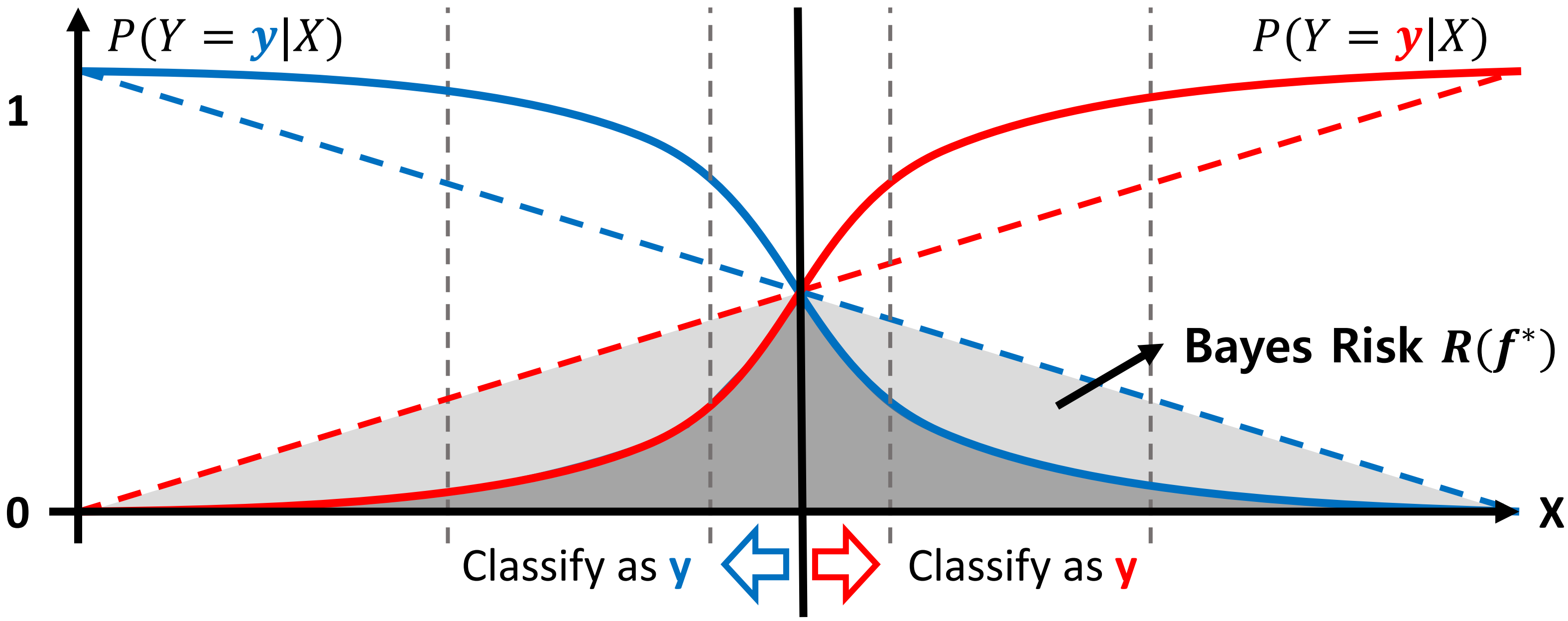
$$b = \omega x_0 \,, \; x_0 = 1$$



Linear Regression
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
50
55
60
65
70
75
80
Height (inches)
Gender (0 F; 1 M)

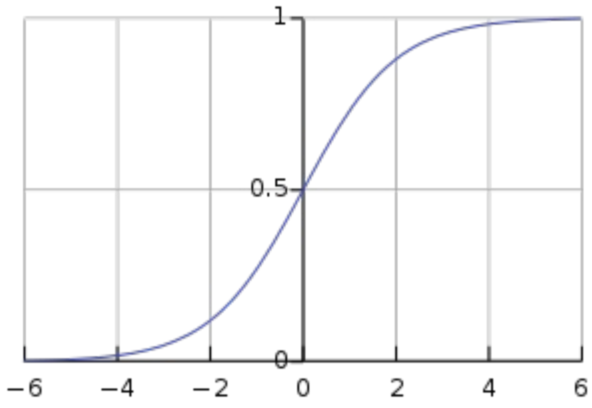
Logistic Regression

Optimal Classification and Bayes Risk

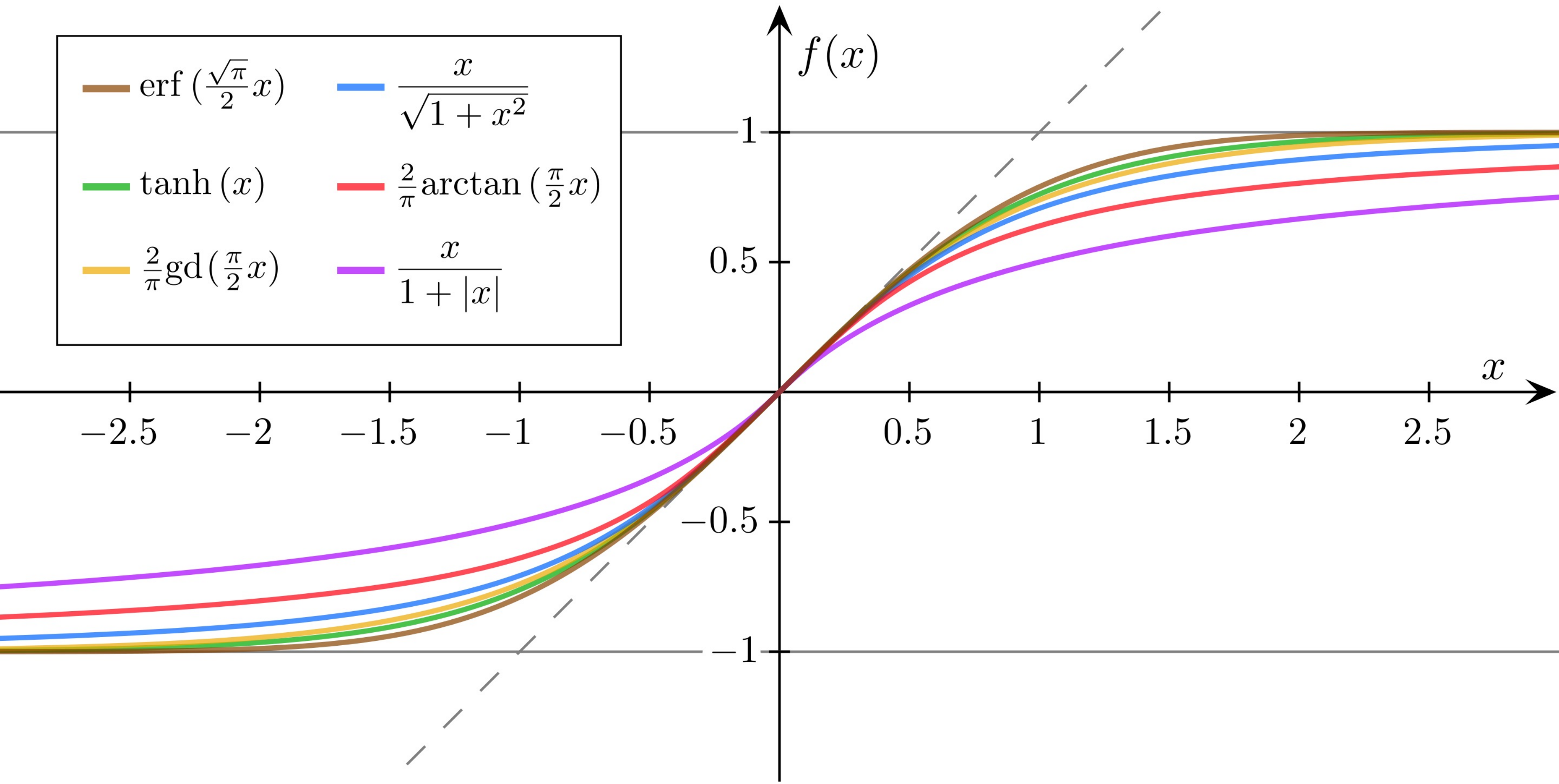


Which is better?

Linear function vs. Non-linear function of $P(Y|X)$



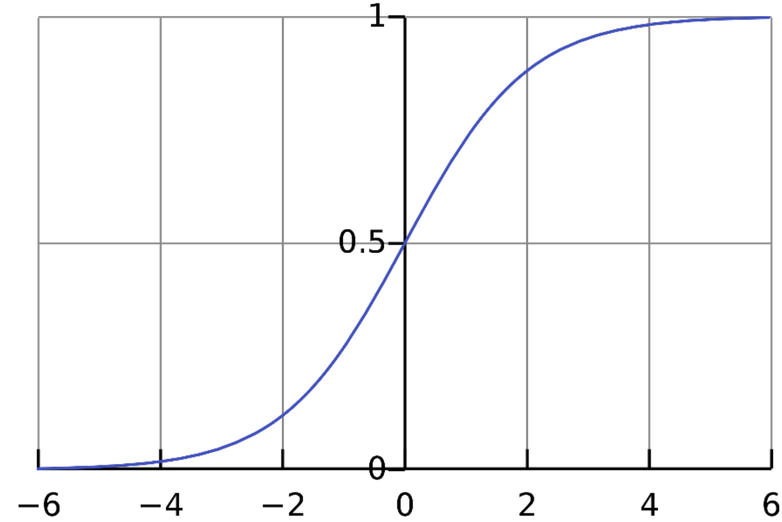
Sigmoid functions



Logistic Function

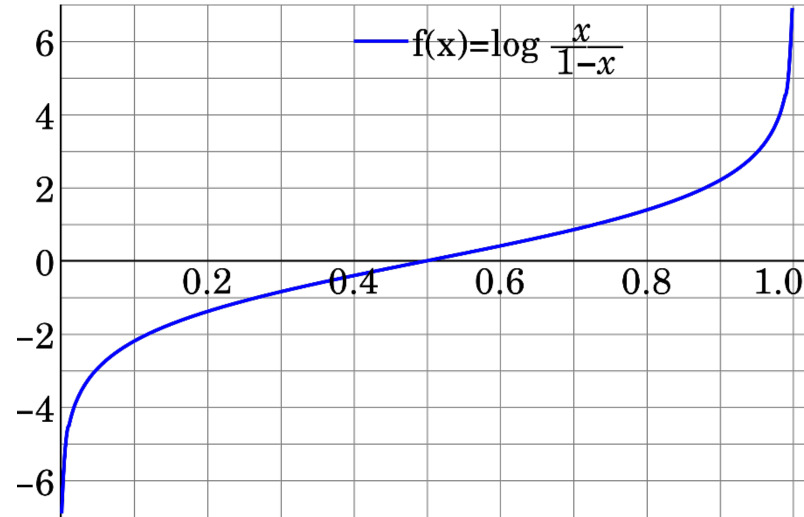
Sigmoid function is

- Bounded
- Differentiable
- Real function
- Defined for all real inputs
- With positive derivative



Logistic function is

$$f(x) = \frac{1}{1+e^{-x}}$$



Logistic Function Fitting

Logic to Logistic

Inverse of X and Y

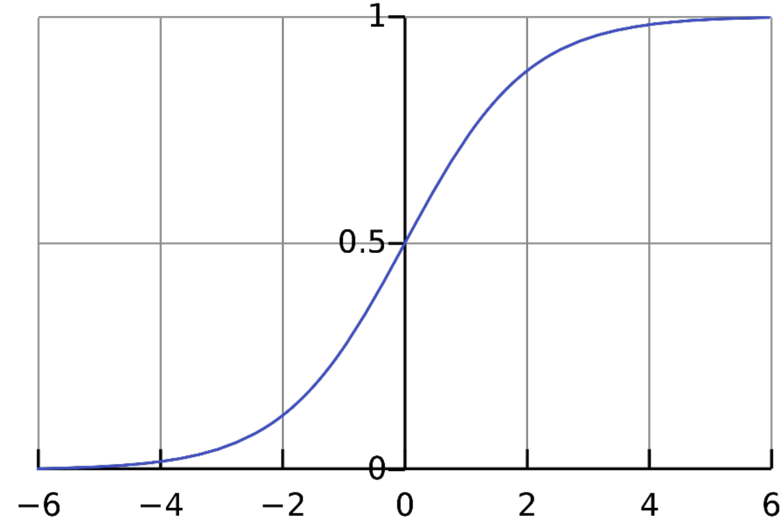
$$f(x) = \log\frac{x}{1-x} \to x = \log\frac{p}{1-p}$$

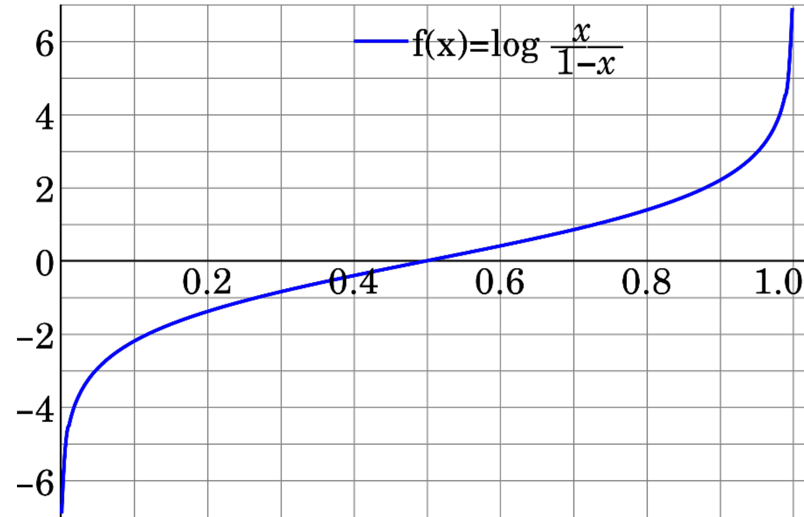
Linear function fitting

$$ax + b = \log\frac{p}{1-p} \to X\theta = \log\frac{p}{1-p}$$

Linear to Logistic

$$X\theta = P(Y|X) \to X\theta = \log\frac{P(Y|X)}{1-P(Y|X)}$$





Logistic Regression

Probabilistic classifier to predict the binomial or the multinomial outcome by fitting the conditional probability to the logistic function

Bernoulli experiments

$$P(y|x) = \mu(x)^y \left(1 - \mu(x)\right)^{1-y}$$

$$\mu(x) = \frac{1}{1 + e^{-\theta^T x}} = P(y = 1|x)$$

Here, $\mu(x)$ is the logistic function

$$X\theta = \log \frac{P(Y|X)}{1 - P(Y|X)} \rightarrow P(Y|X) = \frac{e^{X\theta}}{1 + e^{X\theta}}$$

$$f(x) = \frac{1}{1 + e^{-x}}$$

Finding the Parameter, θ

Maximum Likelihood Estimation(MLE) of θ

Choose θ that maximizes the probability of observed data

$$\hat{\theta} = argmax_{\theta} P(D|\theta)$$

Maximum Conditional Likelihood Estimation(MCLE)

$$\hat{\theta} = argmax_{\theta} P(D|\theta)$$

$$= argmax_{\theta} \prod_{1 \le i \le N} P(Y_i|X_i;\theta)$$

$$= argmax_{\theta} \log\left(\prod_{1 \le i \le N} P(Y_i|X_i;\theta)\right)$$

$$= argmax_{\theta} \sum_{1 \le i \le N} \log\big(P(Y_i|X_i;\theta)\big)$$

$$P(Y_i|X_i;\theta) = \mu(X_i)^{Y_i}\big(1-\mu(X_i)\big)^{1-Y_i}$$

$$\begin{aligned}
\log\big(P(Y_i|X_i;\theta)\big) &= Y_i\log\big(\mu(X_i)\big) + (1-Y_i)\log\big(1-\mu(X_i)\big) \\
&= Y_i\Big(\log\big(\mu(X_i)\big) - \log\big(1-\mu(X_i)\big)\Big) + \log\big(1-\mu(X_i)\big) \\
&= Y_i\log\left(\frac{\mu(X_i)}{1-\mu(X_i)}\right) + \log\big(1-\mu(X_i)\big) \\
&= Y_iX_i\theta + \log\big(1-\mu(X_i)\big) \\
&= Y_iX_i\theta - \log\big(1+e^{X_i\theta}\big)
\end{aligned}$$

$$X\theta = \log\frac{P(Y|X)}{1-P(Y|X)}$$

$$P(y=1|x) = \mu(x)$$

$$= \frac{1}{1+e^{-\theta^T x}} = \frac{e^{X\theta}}{1+e^{X\theta}}$$

$$\hat{\theta} = argmax_\theta \sum_{1 \le i \le N} \log\big(P(Y_i|X_i;\theta)\big)$$

$$= argmax_\theta \sum_{1 \le i \le N} Y_i X_i \theta - \log\big(1 + e^{X_i\theta}\big)$$

Now, we need to optimize θ

$$\frac{\partial}{\partial \theta_j} \sum_{1 \le i \le N} Y_i X_i \theta - \log\big(1 + e^{X_i\theta}\big)$$

$$= \sum_{1 \le i \le N} Y_i X_{i,j} + \sum_{1 \le i \le N} - \frac{1}{1 + e^{X_i\theta}} \times e^{X_i\theta} \times X_{i,j}$$

$$= \sum_{1 \le i \le N} X_{i,j} \left(Y_i - \frac{e^{X_i\theta}}{1 + e^{X_i\theta}} \right)$$

$$= \sum_{1 \le i \le N} X_{i,j} \big(Y_i - P(Y_i = 1|X_i;\theta) \big) = 0 \longleftarrow \text{Open form solution!}$$

$$\theta = (X^T X)^{-1} X^T Y \longleftarrow \text{Closed form solution!}$$

Gradient Descent

Taylor Expansion

Taylor series is a representation of a function

- A infinite sum of terms
- Calculated from the values of the function's derivatives at a fixed point

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + \frac{f''(a)}{2!}(x-a)^2 + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x-a)^n$$

- Here, a is a constant value

Taylor series is possible when

- Infinitely differentiable at a real or complex number of a

Gradient Descent/Ascent

Gradient descent/ascent method

Given a differentiable function of $f(x)$ and a initial parameter of x_1

Iteratively moving the parameter to the lower/higher value of $f(x)$

By taking the direction of the negative/positive gradient of $f(x)$

$$f(x) = f(a) + \frac{f'(a)}{1!}(x-a) + O(|x-a|^2) \qquad (a = x_1, x = x_1 + hu)$$

$$f(x_1 + hu) = f(x_1) + f'(x_1)(x_1 + hu - x_1) + O(|x_1 + hu - x_1|^2)$$

$$f(x_1 + hu) = f(x_1) + hf'(x_1)u + h^2 O(1)$$

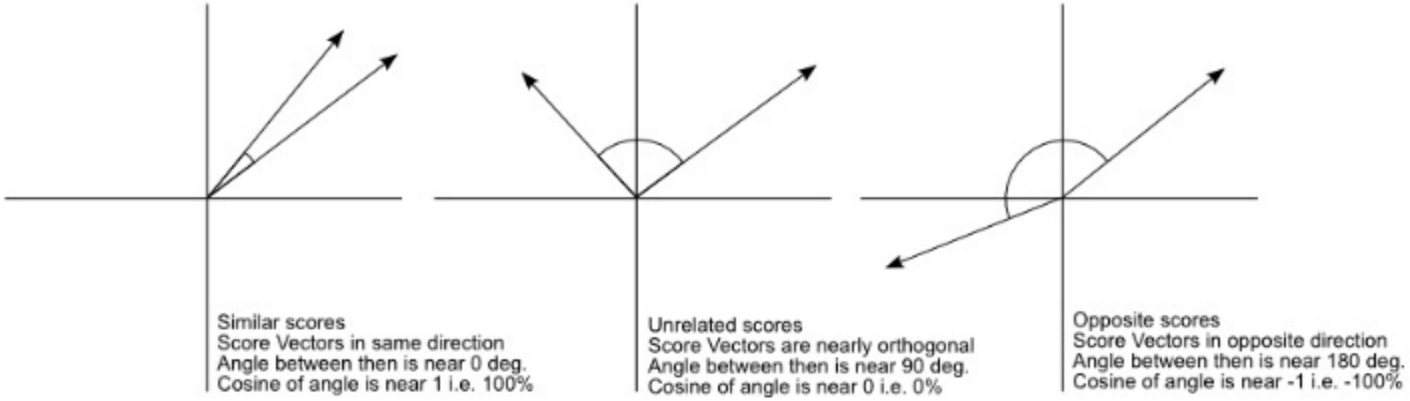
$$f(x_1 + hu) - f(x_1) \approx hf'(x_1)u$$

$$u^* = argmin_u f(x_1 + hu) - f(x_1)$$

$$= argmin_u h f'(x_1) u$$

$$= -\frac{f'(x_1)}{|f'(x_1)|} \qquad (\textit{Gradient Descent})$$

$$x_{t+1} \leftarrow x_t + hu^* = x_t - h\frac{f'(x_1)}{|f'(x_1)|}$$



The Cosine Similarity values for different documents, 1 (same direction), 0 (90 deg.), –1 (opposite directions).

Rosenbrock Function

$$f(x_1, x_2) = (1 - x_1)^2 + 100(x_2 - x_1^2)^2$$

$$\frac{\partial}{\partial x_1} f(x_1, x_2) = -2(1 - x_1) - 400x_1(x_2 - x_1^2)^2$$

$$\frac{\partial}{\partial x_2} f(x_1, x_2) = 200(x_2 - x_1^2)$$

Assume the initial point

$$x^0 = (x_1^0, x_2^0) = (-1.3, 0.9)$$

Partial derivative vector at the point

$$f'(x^0) = \left(\frac{\partial}{\partial x_1} f(x_1, x_2), \frac{\partial}{\partial x_2} f(x_1, x_2)\right) = (-415.4, -158.0)$$

$$x^1 \leftarrow x^0 - h\,\frac{f'(x^0)}{|f'(x^0)|}$$ (*Repeat updating until convergence*)

Logistic Regression

$$\hat{\theta} = argmax_{\theta} \sum_{1 \le i \le N} \log\big(P(Y_i|X_i;\theta)\big)$$ (*Gradient Ascent*)

$$f(\theta) = \sum_{1 \le i \le N} \log\big(P(Y_i|X_i;\theta)\big)$$ ($a = \theta_1, \theta = \theta_1 + hu$)

$$\theta_{t+1} \leftarrow \theta_t + hu^* = \theta_t + h\frac{f'(\theta_1)}{|f'(\theta_1)|}$$

Setup an initial parameter of θ_1

Iteratively moving θ_t to the higher value of $f(\theta_t)$

By taking the direction of the ***positive*** gradient of $f(\theta_t)$

$$f(\theta) = \sum_{1 \le i \le N} \log\big(P(Y_i | X_i; \theta)\big)$$

$$\frac{\partial}{\partial \theta_j} f(\theta) = \frac{\partial}{\partial \theta_j} \sum_{1 \le i \le N} \log\big(P(Y_i | X_i; \theta)\big)$$

$$= \frac{\partial}{\partial \theta_j} \sum_{1 \le i \le N} X_{i,j}\big(Y_i - P(Y_i = 1 | X_i; \theta)\big)$$

To utilize the gradient method

$$\theta_j^{t+1} = \theta_j^t + h \frac{\partial f(\theta^t)}{\partial \theta_j^t}$$

$$= \theta_j^t + h \left(\sum_{1 \le i \le N} X_{i,j}\big(Y_i - P(Y_i = 1 | X_i; \theta^t)\big) \right)$$

$$= \theta_j^t + \frac{h}{C} \left(\sum_{1 \le i \le N} X_{i,j} \left(Y_i - \frac{e^{X_i \theta^t}}{1 + e^{X_i \theta^t}} \right) \right)$$

Linear Regression

$$\hat{\theta} = argmin_{\theta}(f - \hat{f})^2 = argmin_{\theta}(Y - X\theta)^2$$

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

To utilize the gradient method

$$\hat{\theta} = argmin_{\theta}(f - \hat{f})^2 = argmin_{\theta}(Y - X\theta)^2$$

$$= \sum_{1 \le i \le N} (Y_i - \sum_{1 \le j \le d} X_j^i \theta_j)^2$$

$$\frac{\partial}{\partial \theta_k} \sum_{1 \le i \le N} (Y_i - \sum_{1 \le j \le d} X_j^i \theta_j)^2 = - \sum_{1 \le i \le N} 2 \left(Y_i - \sum_{1 \le j \le d} X_j^i \theta_j \right) X_k^i$$

$$\theta_k^{t+1} \leftarrow \theta_k^t - h \frac{\partial f(\theta^t)}{\partial \theta_k^t} = \theta_k^t + h \sum_{1 \le i \le N} 2 \left(Y_i - \sum_{1 \le j \le d} X_j^i \theta_j \right) X_k^i$$