#### Lecture 8: 1 February, 2024

Madhavan Mukund https://www.cmi.ac.in/~madhavan

Data Mining and Machine Learning January–April 2024

- Regression line
- Set a threshold
- Classifier
  - Output below threshold : 0 (No)
  - Output above threshold : 1 (Yes)
- Classifier output is a step function



Sigmoid function

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

Input z is output of our regression

 $\sigma(z) = \frac{1}{1 + e^{-(\theta_0 + \theta_1 x_1 + \dots + \theta_k x_k)}}$ 

 Adjust parameters to fix horizontal position and steepness of step



# Logistic regression

- Compute the coefficients?
- Solve by gradient descent
- Need derivatives to exist
  - Hence smooth sigmoid, not step function
  - $\sigma'(z) = \sigma(z)(1 \sigma(z))$
- Need a cost function to minimize



#### Loss function for logistic regression

Goal is to maximize log likelihood

• Let 
$$h_{\theta}(x_i) = \sigma(z_i)$$
. So,  $P(y_i = 1 \mid x_i; \theta) = h_{\theta}(x_i)$ ,  
 $P(y_i = 0 \mid x_i; \theta) = 1 - h_{\theta}(x_i)$ 

• Combine as  $P(y_i \mid x_i; \theta) = h_{\theta}(x_i)^{y_i} \cdot (1 - h_{\theta}(x_i))^{1-y_i}$ 

• Likelihood: 
$$\mathcal{L}(\theta) = \prod_{i=1}^n h_{\theta}(x_i)^{y_i} \cdot (1 - h_{\theta}(x_i))^{1-y_i}$$

....

• Log-likelihood: 
$$\ell(\theta) = \sum_{i=1}^{n} y_i \log h_{\theta}(x_i) + (1 - y_i) \log(1 - h_{\theta}(x_i))$$

• Minimize cross entropy: 
$$-\sum_{i=1}^{n} y_i \log h_{\theta}(x_i) + (1 - y_i) \log(1 - h_{\theta}(x_i))$$

Madhavan Mukund

## MSE for logistic regression and gradient descent

- Suppose we take mean sum-squared error as the loss function.
- Consider two inputs  $x = (x_1, x_2)$

$$C = \frac{1}{n} \sum_{i=1}^{n} (y_i - \sigma(z_i))^2$$
, where  $z_i = \theta_0 + \theta_1 x_{i_1} + \theta_2 x_{i_2}$ 

• For gradient descent, we compute  $\frac{\partial C}{\partial \theta_1}$ ,  $\frac{\partial C}{\partial \theta_2}$ ,  $\frac{\partial C}{\partial \theta_0}$ 

• For 
$$j = 1, 2$$
,  

$$\frac{\partial C}{\partial \theta_j} = \frac{2}{n} \sum_{i=1}^n (y_i - \sigma(z_i)) \cdot -\frac{\partial \sigma(z_i)}{\partial \theta_j} = \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \frac{\partial \sigma(z_i)}{\partial z_i} \frac{\partial z_i}{\partial \theta_j}$$

$$= \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \sigma'(z_i) x_{i_j}$$
•  $\frac{\partial C}{\partial \theta_0} = \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \frac{\partial \sigma(z_i)}{\partial z_i} \frac{\partial z_i}{\partial \theta_0} = \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \sigma'(z_i)$ 

## MSE for logistic regression and gradient descent ...

• For 
$$j = 1, 2$$
,  $\frac{\partial C}{\partial \theta_j} = \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \sigma'(z_i) x_j^i$ , and  $\frac{\partial C}{\partial \theta_0} = \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \sigma'(z_i)$   
• Each term in  $\frac{\partial C}{\partial \theta_1}$ ,  $\frac{\partial C}{\partial \theta_2}$ ,  $\frac{\partial C}{\partial \theta_0}$  is proportional to  $\sigma'(z_i)$ 

Ideally, gradient descent should take large steps when  $\sigma(z) - y$  is large

- $\sigma(z)$  is flat at both extremes
- If  $\sigma(z)$  is completely wrong,  $\sigma(z) \approx (1-y)$ , we still have  $\sigma'(z) \approx 0$
- Learning is slow even when current model is far from optimal



7/9

#### Cross entropy and gradient descent

• 
$$C = -[y \ln(\sigma(z)) + (1 - y) \ln(1 - \sigma(z))]$$

• 
$$\frac{\partial C}{\partial \theta_j} = \frac{\partial C}{\partial \sigma} \frac{\partial \sigma}{\partial \theta_j} = -\left[\frac{y}{\sigma(z)} - \frac{1-y}{1-\sigma(z)}\right] \frac{\partial \sigma}{\partial \theta_j}$$
  
 $= -\left[\frac{y}{\sigma(z)} - \frac{1-y}{1-\sigma(z)}\right] \frac{\partial \sigma}{\partial z} \frac{\partial z}{\partial \theta_j}$   
 $= -\left[\frac{y}{\sigma(z)} - \frac{1-y}{1-\sigma(z)}\right] \sigma'(z)x_j$   
 $= -\left[\frac{y(1-\sigma(z)) - (1-y)\sigma(z)}{\sigma(z)(1-\sigma(z))}\right] \sigma'(z)x_j$ 

## Cross entropy and gradient descent ...

• 
$$\frac{\partial C}{\partial \theta_j} = -\left[\frac{y(1-\sigma(z))-(1-y)\sigma(z)}{\sigma(z)(1-\sigma(z))}\right]\sigma'(z)x_j$$

• Recall that 
$$\sigma'(z) = \sigma(z)(1 - \sigma(z))$$

• Therefore, 
$$\frac{\partial C}{\partial \theta_j} = -[y(1 - \sigma(z)) - (1 - y)\sigma(z)]x_j$$
  
=  $-[y - y\sigma(z) - \sigma(z) + y\sigma(z)]x_j$   
=  $(\sigma(z) - y)x_j$ 

- Similarly,  $\frac{\partial C}{\partial \theta_0} = (\sigma(z) y)$
- Thus, as we wanted, the gradient is proportional to  $\sigma(z) y$
- The greater the error, the faster the learning rate

Madhavan Mukund