

Lecture 8: 1 February, 2024

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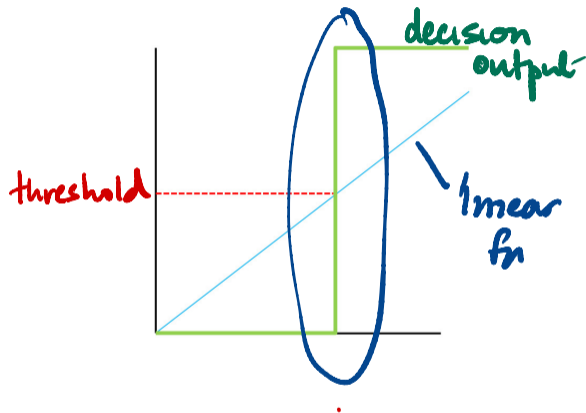
Data Mining and Machine Learning
January–April 2024

Regression for classification

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

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- Classifier output is a step function

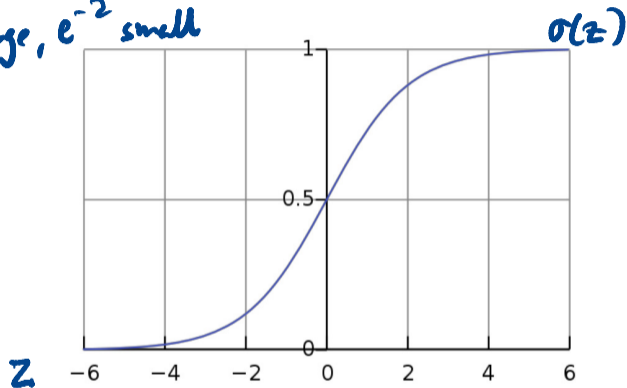


Smoothen the step

- Sigmoid function

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

z large, e^{-z} small



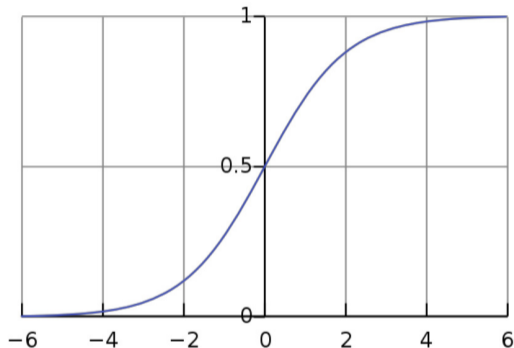
Smoothen the step

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- Input z is output of our regression

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



Smoothen the step

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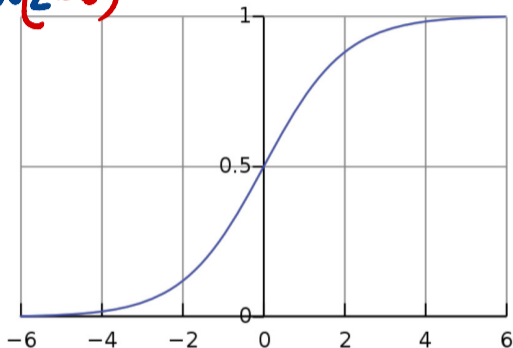
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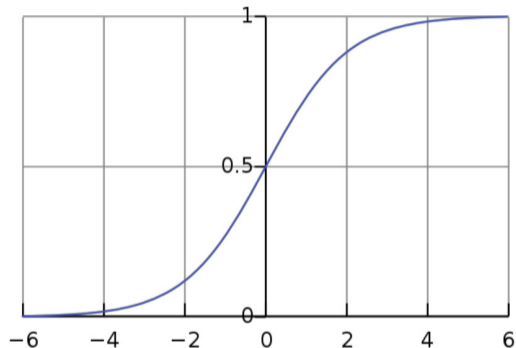
- Adjust parameters to fix horizontal position and steepness of step

$$\frac{1}{1 + e^{-100(z-b)}}$$



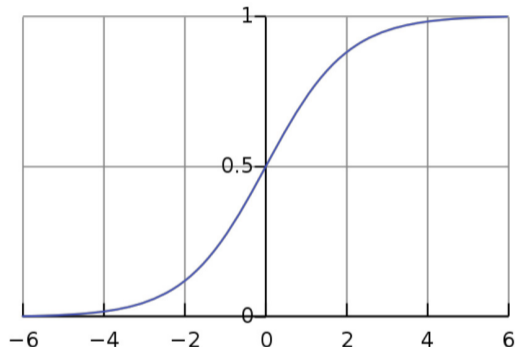
Logistic regression

- Compute the coefficients?
- Solve by gradient descent



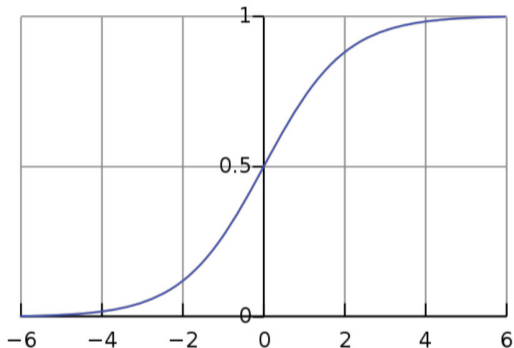
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- Need derivatives to exist
 - Hence smooth sigmoid, not step function
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Logistic regression

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 - Hence smooth sigmoid, not step function
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- Need a cost function to minimize



Loss function for logistic regression

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Loss function for logistic regression

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

$$y_i = 0 \rightarrow 1 - h_{\theta}(x_i)$$

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

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

$$-\sum p_i \log p_i$$

MSE for logistic regression and gradient descent

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

$$C = \frac{1}{n} \sum_{i=1}^n (y_i - \sigma(z_i))^2, \text{ where } z_i = \theta_0 + \theta_1 x_{i1} + \theta_2 x_{i2}$$

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- For $j = 1, 2$,

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

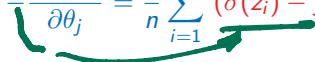
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- For $j = 1, 2$,

$$\begin{aligned} \frac{\partial C}{\partial \theta_j} &= \frac{2}{n} \sum_{i=1}^n (y_i - \sigma(z_i)) \cdot -\frac{\partial \sigma(z_i)}{\partial \theta_j} = \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \frac{\partial \sigma(z_i)}{\partial z_i} \frac{\partial z_i}{\partial \theta_j} \\ &= \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \sigma'(z_i) x_{ij} \end{aligned}$$

chain rule

MSE for logistic regression and gradient descent

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

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

MSE for logistic regression and gradient descent . . .

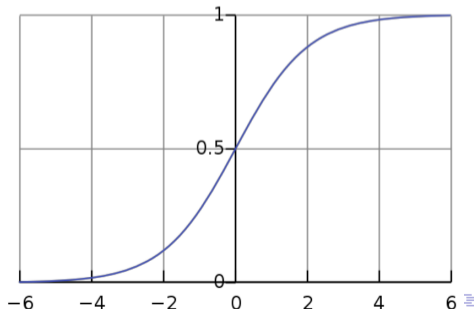
- For $j = 1, 2$, $\frac{\partial C}{\partial \theta_j} = \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \sigma'(z_i) x_j^i$, and $\frac{\partial C}{\partial \theta_0} = \frac{2}{n} \sum_{i=1}^n (\sigma(z_i) - y_i) \sigma'(z_i)$
- Each term in $\frac{\partial C}{\partial \theta_1}$, $\frac{\partial C}{\partial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

MSE for logistic regression and gradient descent . . .

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

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



Cross entropy and gradient descent

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

Cross entropy and gradient descent

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- $\frac{\partial C}{\partial \theta_j} = \frac{\partial C}{\partial \sigma} \frac{\partial \sigma}{\partial \theta_j}$

Cross entropy and gradient descent

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

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

Cross entropy and gradient descent

- $C = -[y \ln(\sigma(z)) + (1 - y) \ln(1 - \sigma(z))]$
- $$\begin{aligned} \frac{\partial C}{\partial \theta_j} &= \frac{\partial C}{\partial \sigma} \frac{\partial \sigma}{\partial \theta_j} = - \left[\frac{y}{\sigma(z)} - \frac{1 - y}{1 - \sigma(z)} \right] \frac{\partial \sigma}{\partial \theta_j} \\ &= - \left[\frac{y}{\sigma(z)} - \frac{1 - y}{1 - \sigma(z)} \right] \frac{\partial \sigma}{\partial z} \frac{\partial z}{\partial \theta_j} \end{aligned}$$

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Cross entropy and gradient descent

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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 $\sigma'(z) = \sigma(z)(1 - \sigma(z))$

Cross entropy and gradient descent ...

- $\frac{\partial C}{\partial \theta_j} = - \left[\frac{y(1 - \sigma(z)) - (1 - y)\sigma(z)}{\sigma(z)(1 - \sigma(z))} \right] \cancel{\sigma'(z)} x_j$
- Recall that $\sigma'(z) = \sigma(z)(1 - \sigma(z))$
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- Recall that $\sigma'(z) = \sigma(z)(1 - \sigma(z))$
- Therefore, $\frac{\partial C}{\partial \theta_j} = -[y(1 - \sigma(z)) - (1 - y)\sigma(z)]x_j$
 $= -[y - y\cancel{\sigma(z)} - \sigma(z) + y\cancel{\sigma(z)}]x_j$

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 $\sigma'(z) = \sigma(z)(1 - \sigma(z))$
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Cross entropy and gradient descent ...

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- Similarly, $\frac{\partial C}{\partial \theta_0} = (\sigma(z) - y)$

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

Logistic
regression

Cross entropy and gradient descent . . .

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