Week 5: Logistic Regression

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Logistic Regression Overview

- Logistic regression is used for binary classification
- Logistic regression outputs probability $\in (0, 1)$
- Example: cancer prediction (Yes/No) based on tumor size

Intuition

- Linear regression cannot bound output between 0 and 1, i.e. unbounded: $(-\infty, +\infty)$
- Apply sigmoid function $\sigma(z)$ to squash the linear regression output into $(0, 1)$

  Given, $z = \theta^T x$

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

- S-shaped curve centered at $z = 0$

Linear VS Logistic Regression

- Linear regression: $h_\theta(x) = \theta^T x$
- Logistic regression: $h_\theta(x) = \sigma(\theta^T x)$

Decision Boundary

Suppose we predict:

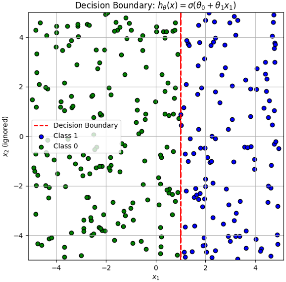
- $y = 1$ if $h_\theta(x) \geq 0.5$
- $y = 0$ if $h_\theta(x) < 0.5$

$$h_\theta(x) = \sigma(\theta_0 + \theta_1 x_1)$$

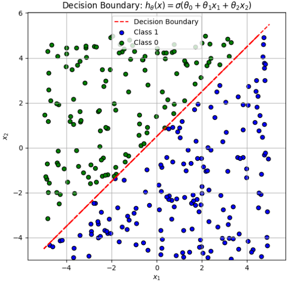
$$h_\theta(x) = \sigma(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$$

$$h_\theta(x) = \sigma(-1 + x_1^2 + x_2^2)$$

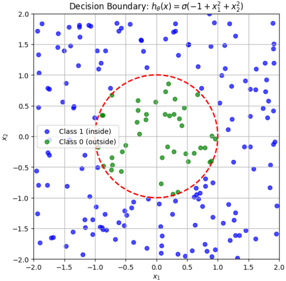
Three Decision Boundaries



$h_\theta(x) = \sigma(\theta_0 + \theta_1 x_1)$



$h_\theta(x) = \sigma(\theta_0 + \theta_1 x_1 + \theta_2 x_2)$



$h_\theta(x) = \sigma(-1 + x_1^2 + x_2^2)$

Ref: figures source

Cost function for Logistic Regression?

- MSE (Mean Squared Error) is used in linear regression:

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N}(h_\theta(x_i) - y_i)^2$$

- Not ideal for logistic regression because
  - Non-convex cost surface
  - Poor convergence properties

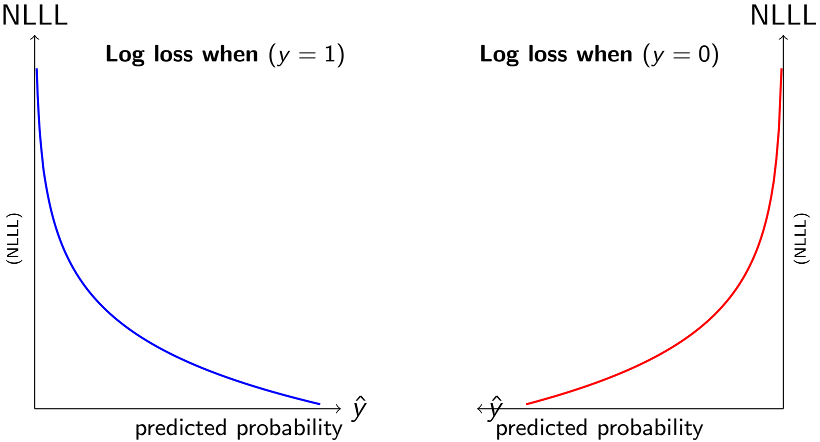
Cross-Entropy Loss

- Measures performance of classification model (output is probability)
- NLLLoss increases when prediction is wrong
- Example:

$$y = 1, \quad \hat{y} = 0.012 \Rightarrow \text{Loss} = -\log(0.012) \approx 4.42$$

- Visualization shows steep increase in loss when $\hat{y} \to 0$ (for $y = 1$)

Cross-Entropy Loss



Negative Log Likelihood Loss

- General form:

$$J(\theta) = \frac{1}{N}\sum_{i=1}^{N} \text{Cost}(h_\theta(x_i), y_i)$$

- Case-based definition:

$$\text{Cost}(h_\theta(x), y) = \begin{cases} -\ln(h_\theta(x)) & \text{if } y = 1 \\ -\ln(1 - h_\theta(x)) & \text{if } y = 0 \end{cases}$$

- Combined:

$$J(\theta) = -\frac{1}{N}\sum_{i=1}^{N} [y_i \ln h_\theta(x_i) + (1 - y_i)\ln(1 - h_\theta(x_i))]$$

- Based on Bernoulli distribution likelihood

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

$$\log\left(P(y_i \mid x_i; \theta)\right) = y_i \ln\left(h_\theta(x_i)\right) + (1 - y_i)\ln\left(1 - h_\theta(x_i)\right)$$

Derivation of Gradient (1)

$$J(\theta) = -\frac{1}{N}\sum_{i=1}^{N}\left(y_i \log(h_\theta(x_i)) + (1-y_i)\log(1-h_\theta(x_i))\right)$$

$$\Rightarrow \frac{\partial J(\theta)}{\partial \theta_j} = -\frac{1}{N}\sum_{i=1}^{N}\left(y_i \cdot \frac{1}{h_\theta(x_i)} \cdot \frac{\partial h_\theta(x_i)}{\partial \theta_j} + (1-y_i) \cdot \frac{1}{1-h_\theta(x_i)} \cdot \frac{\partial(1-h_\theta(x_i))}{\partial \theta_j}\right)$$

Note: $\frac{\partial \sigma(x)}{\partial x} = \sigma(x)(1-\sigma(x))$

Derivation of Gradient (2)

$$\frac{\partial J(\theta)}{\partial \theta_j} = -\frac{1}{N}\sum_{i=1}^{N}\left(y_i \cdot \frac{1}{h_\theta(x_i)} \cdot \frac{\partial \sigma(\theta^T x)}{\partial \theta_j} + (1-y_i) \cdot \frac{1}{1-h_\theta(x_i)} \cdot (-1) \cdot \frac{\partial \sigma(\theta^T x)}{\partial \theta_j}\right)$$

$$= -\frac{1}{N}\sum_{i=1}^{N}\left(y_i \cdot \frac{1}{h_\theta(x_i)} \cdot \sigma(\theta^T x)(1-\sigma(\theta^T x))x_{ij} + (1-y_i) \cdot \frac{-1}{1-h_\theta(x_i)} \cdot \sigma(\theta^T x)(1-\sigma(\theta^T x))x_{ij}\right)$$

Chain Rule on Sigmoid

$$\frac{\partial \sigma(\theta^T x)}{\partial \theta_j} = \frac{\partial \sigma(\theta^T x)}{\partial (\theta^T x)} \cdot \frac{\partial (\theta^T x)}{\partial \theta_j}$$

$$= \sigma(\theta^T x)(1 - \sigma(\theta^T x)) \cdot x_j = h_\theta(x_i)(1 - h_\theta(x_i))x_{ij}$$

Simplified Gradient Expression

$$= -\frac{1}{N}\sum_{i=1}^{N}(y_i(1-h_\theta(x_i))x_{ij} + (1-y_i)(-1)h_\theta(x_i)x_{ij})$$

$$= -\frac{1}{N}\sum_{i=1}^{N}(y_i x_{ij} - y_i h_\theta(x_i)x_{ij} - h_\theta(x_i)x_{ij} + y_i h_\theta(x_i)x_{ij})$$

$$= -\frac{1}{N}\sum_{i=1}^{N}(y_i x_{ij} - h_\theta(x_i)x_{ij}) = -\frac{1}{N}\sum_{i=1}^{N}(y_i - h_\theta(x_i))x_{ij}$$

$$\Rightarrow \frac{\partial J(\theta)}{\partial \theta_j} = \frac{1}{N}\sum_{i=1}^{N}(h_\theta(x_i) - y_i)x_{ij} \quad \text{for } j = 0, \ldots, d$$

*** Same form as BGD with MSE**

Linear vs Logistic Regression

Linear Regression	Logistic Regression
$h_\theta(x) = \theta^T x$	$h_\theta(x) = \sigma(\theta^T x)$
$J(\theta) = \frac{1}{N}\sum(h_\theta(x_i) - y_i)^2$	$J(\theta) = -\frac{1}{N}\sum\left(y_i \log(h_\theta(x_i)) + (1 - y_i)\log(1 - h_\theta(x_i))\right)$
MSE	NLLoss
MSE, R^2, MAE	Accuracy, Precision, Recall, F1, AUC
$\theta_j^{(t+1)} = \theta_j^{(t)} - \eta \cdot \frac{1}{N}\sum(h_\theta(x_i) - y_i)x_{ij}$	$\theta_j^{(t+1)} = \theta_j^{(t)} - \eta \cdot \frac{1}{N}\sum(h_\theta(x_i) - y_i)x_{ij}$

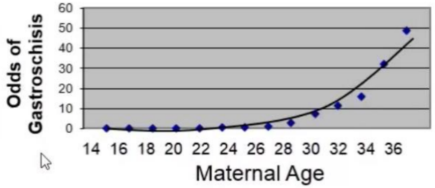
Appendix: Odds

- Odds refer to the probability of an event happening divided by the probability of it not happening.

$$\text{Odds} = \frac{P(\text{event=success})}{1 - P(\text{event=success})}$$

- Examples:

$$\frac{0.8}{0.2} = 4, \quad \frac{0.9}{0.1} = 9, \quad \frac{0.5}{0.5} = 1, \quad \frac{0.2}{0.8} = 0.25$$



Maternal age VS Odds of Gastroschisis

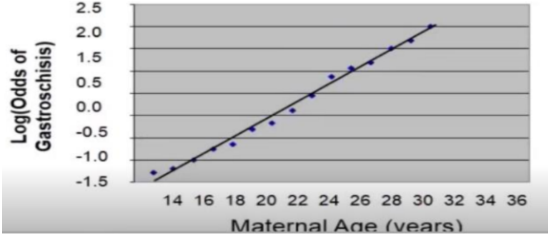
Gastroschisis

Appendix: Logit Function

Take log(.) to the chart above, we the obain the linear relationship.

$$\text{Log(Odds of Gastroschisis)} = \theta_0 + \theta_1 \cdot \text{Age}$$

This is called a logit function.



Appendix: Logistic Regression

$$logit(p) = log(\frac{p}{1-p}) = \beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k.$$

Exponentiate and take the multiplicative inverse of both sides,

$$\frac{1-p}{p} = \frac{1}{exp(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k)}.$$

Partial out the fraction on the left-hand side of the equation and add one to both sides,

$$\frac{1}{p} = 1 + \frac{1}{exp(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k)}.$$

Change 1 to a common denominator,

$$\frac{1}{p} = \frac{exp(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k) + 1}{exp(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k)}.$$

Finally, take the multiplicative inverse again to obtain the formula for the probability $P(Y = 1)$,

$$p = \frac{exp(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k)}{1 + exp(\beta_0 + \beta_1 x_1 + \cdots + \beta_k x_k)}.$$

ref: link

Reference

- Sperandei,S.(2014).Understandinglogisticregression analysis.Biochemiamedica,24(1),12-18.