Predictive Modelling

Classification - Logistic Regression

Jonathan Mwaura

Khoury College of Computer Sciences

July 23, 2024

The Roux Institute
at Northeastern University

Introduction

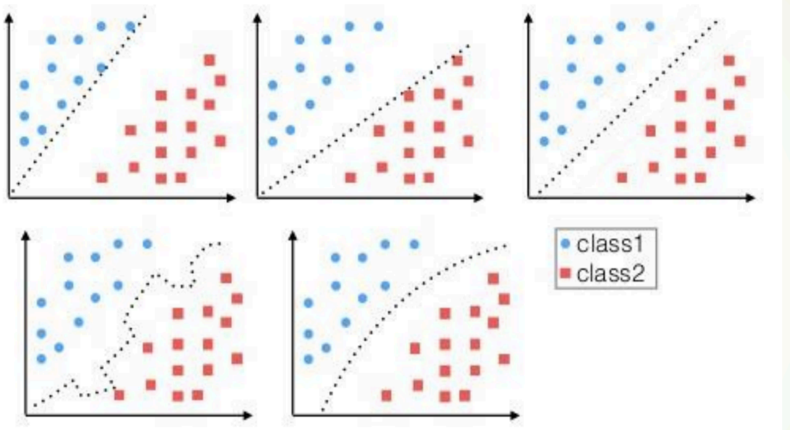
Textbook

Reading: Chapter 4 of: Gareth James et al (2021) . An Introduction to Statistical Learning (2nd Edition) .
`https://www.statlearning.com/`

Acknowledgements

These slides have been adapted from the following Professors:
1) Andrew Ng - Stanford
2) Eric Eaton - UPenn
3) David Sontag - MIT
4) Alina Oprea - Northeastern

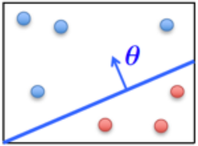
Linear vs Non-Linear Classifiers



Linear Classifiers

- **Linear classifiers:** represent decision boundary by hyperplane

$$\boldsymbol{\theta} = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_d \end{bmatrix} \quad \boldsymbol{x}^\intercal = \begin{bmatrix} 1 & x_1 & \ldots & x_d \end{bmatrix}$$



$h_\theta(x) = f(\theta^T x)$ linear function

- If $\theta^T x > 0$ classify 1
- If $\theta^T x < 0$ classify 0

All the points x on the hyperplane satisfy: $\theta^T x = 0$

Linear Classifiers

$$h_\theta(x) = f(\theta^T x)$$

- Examples: perceptron, LDA
- Pros

  - Very compact model (size *d*)
- Cons of linear models studied so far
  - Perceptron depend on the order of training data and it could take many steps for convergence

  - LDA assumes normal distribution of features

Classification Based on Probability

- Instead of just predicting the class, give the *probability of the instance being in that class*
  - Learn $P(Y|X)$
- Consider binary classifier with classes 0 and 1
  - $P(Y = 1|X) + P(Y = 0|X) = 1$
  - Sufficient to learn $P(Y = 1|X)$
- Advantages: interpretability and confidence of output

Logistic Regression

- Setup
  - Training data: $\{x_i, y_i\}$, for $i = 1, \ldots, N$
  - Labels: $y_i \in \{0,1\}$
- Goals
  - Learn $P(Y = 1|X = x)$
- Highlights
  - Probabilistic output
  - At the basis of more complex models (e.g., neural networks)
  - Supports regularization (Ridge, Lasso)
  - Can be trained with Gradient Descent

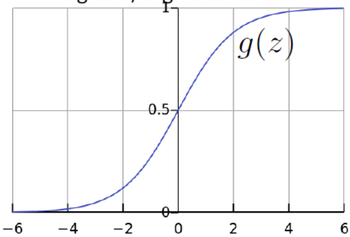
Logistic Regression

- Takes a probabilistic approach to learning discriminative functions (i.e., a classifier)
- $h_{\boldsymbol{\theta}}(\boldsymbol{x})$ should give $P(Y = 1|X; \theta)$
  - Want $0 \leq h_{\boldsymbol{\theta}}(\boldsymbol{x}) \leq 1$
- Logistic regression model:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^{\mathsf{T}}\boldsymbol{x}\right)$$

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

Logistic / Sigmoid Function



Interpretation of Model Output

$h_{\boldsymbol{\theta}}(\boldsymbol{x})$ = estimated $P(Y = 1|X;\theta)$

Example: Cancer diagnosis from tumor size

$$\boldsymbol{x} = \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 1 \\ \text{tumorSize} \end{bmatrix}$$

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = 0.7$$

→ Tell patient that 70% chance of tumor being malignant

Note that: $P(Y = 0|X;\theta) + P(Y = 1|X;\theta) = 1$

Therefore, $P(Y = 0|X;\theta) = 1 - P(Y = 1|X;\theta)$

LR is a Linear Classifier!

- Predict $Y = 1$ if:
  - $\mathrm{P}[Y = 1|X = x; \theta] > \mathrm{P}[Y = 0|X = x; \theta]$
  - $\mathrm{P}[Y = 1|X = x; \theta] > \frac{1}{2}$

$$\frac{1}{1 + e^{-\theta^T x}} > \frac{1}{2}$$

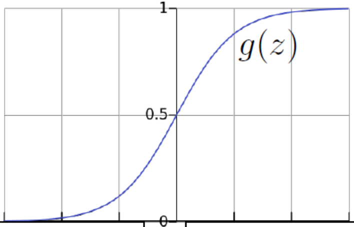
- Equivalent to:
  - $e^{\theta_0 + \sum_{j=1}^{d} \theta_j x_j} > 1$
  - $\theta_0 + \sum_{j=1}^{d} \theta_j x_j > 0$

Logistic Regression is a linear classifier!

Logistic Regression

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = g\left(\boldsymbol{\theta}^\intercal \boldsymbol{x}\right)$$

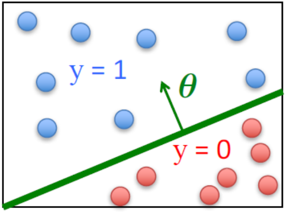
$$g(z) = \frac{1}{1 + e^{-z}}$$



$\boldsymbol{\theta}^\intercal \boldsymbol{x}$ should be large negative values for negative instances

$\boldsymbol{\theta}^\intercal \boldsymbol{x}$ should be large positive values for positive instances

- Assume a threshold and...
  - Predict $Y = 1$ if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \geq 0.5$
  - Predict $Y = 0$ if $h_{\boldsymbol{\theta}}(\boldsymbol{x}) < 0.5$



Logistic Regression is a linear classifier!

Logistic Regression Objective

- Can't just use squared loss as in linear regression:

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

  - Using the logistic regression model

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\top \boldsymbol{x}}}$$

    results in a non-convex optimization

Maximum Likelihood Estimation (MLE)

Given training data $X = \{x_1, \dots, x_N\}$ with labels $\mathrm{Y} = \{y_1, \dots, y_N\}$

What is the likelihood of training data for parameter θ?

Define likelihood function

$$Max_\theta\, L(\theta) = P[Y|X;\theta]$$

Assumption: training points are independent

$$L(\theta) = \prod_{i=1}^{n} P[Y = y_i | X = x_i; \theta]$$

General probabilistic method for classifier training

Log Likelihood

- Max likelihood is equivalent to maximizing log of likelihood

$$L(\theta) = \prod_{i=1}^{N} P[Y = y_i | X = x_i; \theta]$$

$$\log L(\theta) = \sum_{i=1}^{N} \log P[Y = y_i | X = x_i; \theta]$$

- They both have the same maximum θ_{MLE}

MLE for Logistic Regression

$$\mathrm{P}(Y = y_i | X = x_i; \theta) = h_\theta(x_i)^{y_i} \left(1 - h_\theta(x_i)\right)^{1-y_i}$$

$$\theta_{MLE} = \mathrm{argmax}_\theta \sum_{i=1}^{N} \log P[Y = y_i | X = x_i; \theta]$$

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

Logistic regression objective

$$\min_\theta J(\theta)$$

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

Cross-Entropy Objective

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

- Cost of a single instance:

$$\operatorname{cost}(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = \begin{cases} -\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 1 \\ -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 0 \end{cases}$$

- Can re-write objective function as

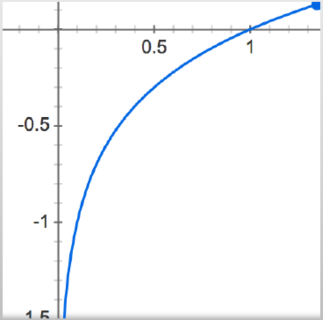
$$J(\boldsymbol{\theta}) = \sum_{i=1}^{n} \underbrace{\operatorname{cost}\left(h_\theta(x_i), y_i \right)}_{\text{Cross-entropy loss}}$$

The Roux Institute
at Northeastern University

Intuition

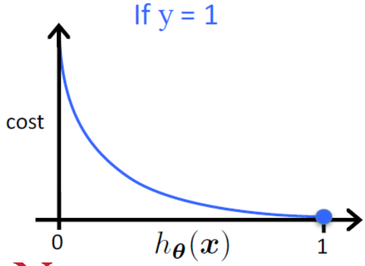
$$\text{cost}\left(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y\right) = \begin{cases} -\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 1 \\ -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) & \text{if } y = 0 \end{cases}$$

Aside: Recall the plot of log(z)



Intuition

$$\text{cost}\left(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y\right) = \begin{cases} \boxed{-\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) \quad \text{if } y = 1} \\ -\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) \quad \text{if } y = 0 \end{cases}$$

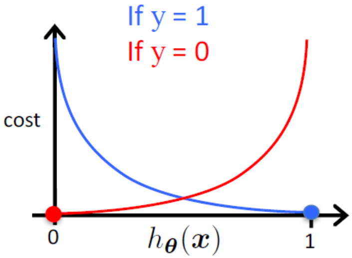


If y = 1

- Cost = 0 if prediction is correct
- As $h_{\boldsymbol{\theta}}(\boldsymbol{x}) \rightarrow 0$, cost $\rightarrow \infty$
- Captures intuition that larger mistakes should get larger penalties
  - e.g., predict $h_{\boldsymbol{\theta}}(\boldsymbol{x}) = 0$, but y = 1

Intuition

$$\text{cost}\,(h_{\boldsymbol{\theta}}(\boldsymbol{x}), y) = \begin{cases} \boxed{-\log(h_{\boldsymbol{\theta}}(\boldsymbol{x})) \quad \text{if } y = 1} \\ \boxed{-\log(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) \quad \text{if } y = 0} \end{cases}$$



If y = 0

- Cost = 0 if prediction is correct
- As $(1 - h_{\boldsymbol{\theta}}(\boldsymbol{x})) \rightarrow 0, \text{cost} \rightarrow \infty$
- Captures intuition that larger mistakes should get larger penalties

Gradient Descent for Logistic Regression

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

$$J(\theta) = -\sum_{i=1}^{n} C_i$$

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update for j = 0 ... d

Computing Gradients

- Derivative of sigmoid
  - $g(z) = \frac{1}{1+e^{-z}}$; $g'(z) = \frac{e^{-z}}{(1+e^{-z})^2} = g(z)(1 - g(z))$
- Derivative of hypothesis
  - $h_\theta(x) = g(\theta^T x) = g(\theta_j x_j + \sum_{k \neq j} \theta_k x_k)$
  - $\frac{\partial h_\theta(x)}{\partial \theta_j} = \frac{\partial g(\theta^T x)}{\partial \theta_j} x_j = g(\theta^T x)\big(1 - g(\theta^T x)\big)x_j$
- Derivation of C_i
  - $\frac{\partial C_i}{\partial \theta_j} = y_i \frac{1}{h_\theta(x_i)} \mathrm{g}(\theta^T x_i)\big(1 - \mathrm{g}(\theta^T x_i)\big)x_{ij}$ -

$$(1 - y_i)\frac{1}{1-h_\theta(x_i)} \mathrm{g}(\theta^T x_i)\big(1 - \mathrm{g}(\theta^T x_i)\big)x_{ij}$$

$$= \big(y_i - h_\theta(x_i)\big)x_{ij}$$

Gradient Descent for Logistic Regression

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

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence (simultaneous update for j = 0 ... d)

$$\theta_0 \leftarrow \theta_0 - \alpha \textstyle\sum_{i=1}^{N}(h_\theta(x_i) - y_i)$$

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

Gradient Descent for Logistic Regression

Want $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence (simultaneous update for j = 0 ... d)

$$\theta_0 \leftarrow \theta_0 - \alpha \sum_{i=1}^{N} (h_\theta(x_i) - y_i)$$

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

This looks IDENTICAL to Linear Regression!

- However, the form of the model is very different:

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \frac{1}{1 + e^{-\boldsymbol{\theta}^\mathsf{T} \boldsymbol{x}}}$$

Regularized Logistic Regression

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

- We can regularize logistic regression exactly as before:

$$\begin{aligned} J_{\text{regularized}}(\boldsymbol{\theta}) &= J(\boldsymbol{\theta}) + \lambda\sum_{j=1}^{d}\theta_j^2 \\ &= J(\boldsymbol{\theta}) + \lambda\|\boldsymbol{\theta}_{[1:d]}\|_2^2 \end{aligned}$$

L2 regularization