STA 314: Statistical Methods for Machine Learning I

Lecture - Logistic Regression in Binary Classification

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Review

- In classification, $X \in \mathcal{X}$ and $Y \in C = \{0, 1, \ldots, K-1\}$.

- The Bayes rule

$$f^*(\mathbf{x}) = \arg\max_{k \in C} \mathbb{P}\{Y = k \mid X = \mathbf{x}\}, \qquad \forall \mathbf{x} \in \mathcal{X}$$

  has the smallest expected error rate.

- For binary classification, our goal is to estimate

$$p(\mathbf{x}) := \mathbb{P}(Y = 1 \mid X = \mathbf{x}), \qquad \forall \mathbf{x} \in \mathcal{X}$$

Logistic Regression

Logistic Regression is a parametric approach that postulates parametric structure on the function $p : \mathcal{X} \mapsto [0, 1]$.

- It is assumed that

$$p(\mathbf{x}) := p(\mathbf{x}; \boldsymbol{\beta}) = \frac{e^{\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p}}{1 + e^{\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p}}, \qquad \forall \mathbf{x} \in \mathcal{X}.$$

  The function $f(t) = e^t/(1 + e^t)$ is called the logistic function. $\beta_0, \ldots, \beta_p$ are the parameters.

- We always have $0 \leq p(\mathbf{x}) \leq 1$.

- Note that $p(\mathbf{x}; \boldsymbol{\beta})$ is **NOT** a linear function either in $\mathbf{x}$ or in $\boldsymbol{\beta}$.

Logistic Regression

- A bit of rearrangement gives

$$\underbrace{\frac{p(\mathbf{x})}{1-p(\mathbf{x})}}_{\text{odds}} = e^{\beta_0+\beta_1 x_1+\cdots+\beta_p x_p},$$

$$\underbrace{\log\left[\frac{p(\mathbf{x})}{1-p(\mathbf{x})}\right]}_{\text{log-odds (a.k.a. logit)}} = \beta_0+\beta_1 x_1+\cdots+\beta_p x_p.$$

odds $\in [0,\infty)$ and log-odds $\in (-\infty,\infty)$.

- Similar interpretation as linear models[1]

[1] Each β_j represents the change of log-odds for one unit increase in X_j (with other features held fixed).

Logistic regression

Our interests:

- **Prediction**: for any $\mathbf{x}_0 \in \mathcal{X}$, classify its corresponding label y_0.
- **Estimation**: how to estimate the vector of β by using our training data?

Prediction at **different levels** under logistic regression

Let $\hat{\boldsymbol{\beta}} = (\hat{\beta}_0, \ldots, \hat{\beta}_p)$ be any estimates of $\boldsymbol{\beta}$.

- Prediction of **the logit** at $\mathbf{x} \in \mathcal{X}$:

$$\widehat{\text{logit}}(\mathbf{x}) = \hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p.$$

- Prediction of **the conditional probability** $p(\mathbf{x}) = \mathbb{P}(Y = 1 | X = \mathbf{x})$:

$$\hat{p}(\mathbf{x}) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 x_1 + \cdots + \hat{\beta}_p x_p}}$$

- Classify **the label** Y at $X = \mathbf{x}$:

$$\hat{y} = \begin{cases} 1, & \text{if } \hat{p}(\mathbf{x}) \geq 0.5; \\ 0, & \text{otherwise.} \end{cases}$$

Maximum Likelihood Estimator (MLE)

Given $\mathcal{D}^{train} = \{(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\}$ with $y_i \in \{0, 1\}$, we estimate the parameters by **maximizing the likelihood** of $\mathcal{D}^{train}$.

The maximum likelihood principle

We seek the estimates of parameters such that the fitted probability are the closest to the individual's observed outcome.

Computation of the MLE under Logistic Regression

General steps of computing the MLE:

- Write down the likelihood, as always!
- Solve the optimization problem.

Likelihood under Logistic Regression

For simplicity, let us set $\beta_0 = 0$ such that

$$p(\mathbf{x}; \boldsymbol{\beta}) = \frac{e^{\mathbf{x}^\top \boldsymbol{\beta}}}{1 + e^{\mathbf{x}^\top \boldsymbol{\beta}}}, \qquad 1 - p(\mathbf{x}; \boldsymbol{\beta}) = \frac{1}{1 + e^{\mathbf{x}^\top \boldsymbol{\beta}}}.$$

The data consists of $(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)$ with

$$y_i \sim \text{Bernoulli}(p(\mathbf{x}_i; \boldsymbol{\beta})), \qquad 1 \le i \le n.$$

- What is the likelihood of $(\mathbf{x}_i, y_i)$?

Likelihood under Logistic Regression

The likelihood of each data point $(\mathbf{x}_i, y_i)$ at any $\boldsymbol{\beta}$ is

$$L(\boldsymbol{\beta}; \mathbf{x}_i, y_i) \propto \left[p(\mathbf{x}_i; \boldsymbol{\beta})\right]^{y_i} \left[1 - p(\mathbf{x}_i; \boldsymbol{\beta})\right]^{1-y_i}$$

with

$$p(\mathbf{x}_i; \boldsymbol{\beta}) = \frac{e^{\mathbf{x}_i^\top \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i^\top \boldsymbol{\beta}}}.$$

The sign $\propto$ means "proportional to, up to some multiplicative term that does not involve the parameter $\boldsymbol{\beta}$.

The joint likelihood of all data points is

$$L(\boldsymbol{\beta}) = \prod_{i=1}^{n} \left[p(\mathbf{x}_i; \boldsymbol{\beta})\right]^{y_i} \left[1 - p(\mathbf{x}_i; \boldsymbol{\beta})\right]^{1-y_i}.$$

Log-likelihood under Logistic Regression

The log-likelihood at any $\boldsymbol{\beta}$ is

$$
\begin{aligned}
\ell(\boldsymbol{\beta}) &= \log\left\{\prod_{i=1}^{n}\left[p(\mathbf{x}_i;\boldsymbol{\beta})\right]^{y_i}\left[1-p(\mathbf{x}_i;\boldsymbol{\beta})\right]^{1-y_i}\right\} \\
&= \sum_{i=1}^{n}\left[y_i \log(p(\mathbf{x}_i;\boldsymbol{\beta})) + (1-y_i)\log(1-p(\mathbf{x}_i;\boldsymbol{\beta}))\right] \\
&= \sum_{i=1}^{n}\left[y_i \log\left(\frac{p(\mathbf{x}_i;\boldsymbol{\beta})}{1-p(\mathbf{x}_i;\boldsymbol{\beta})}\right) + \log(1-p(\mathbf{x}_i;\boldsymbol{\beta}))\right] \\
&= \sum_{i=1}^{n}\left[y_i \mathbf{x}_i^\top \boldsymbol{\beta} - \log\left(1+e^{\mathbf{x}_i^\top \boldsymbol{\beta}}\right)\right].
\end{aligned}
$$

How to compute the MLE?

How do we maximize the log-likelihood

$$\ell(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left[y_i \mathbf{x}_i^\top \boldsymbol{\beta} - \log\left(1 + e^{\mathbf{x}_i^\top \boldsymbol{\beta}}\right) \right]$$

for logistic regression?

- It is equivalent to minimize $-\ell(\boldsymbol{\beta})$ over $\boldsymbol{\beta}$.
- No direct solution: taking derivatives of $\ell(\boldsymbol{\beta})$ w.r.t. $\boldsymbol{\beta}$ and setting them to 0 doesn't have an explicit solution.
- Need to use iterative procedure.

Gradient descent for solving the MLE under logistic regression

Recall we would like to solve

$$\min_{\boldsymbol{\beta} \in \mathbb{R}^p} -\ell(\boldsymbol{\beta})$$

where

$$-\ell(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left[-y_i \mathbf{x}_i^\top \boldsymbol{\beta} + \log\left(1 + e^{\mathbf{x}_i^\top \boldsymbol{\beta}}\right) \right].$$

The gradient at any $\boldsymbol{\beta}$ is that, for any $j \in \{1, \ldots, p\}$,

$$-\frac{\partial \ell(\boldsymbol{\beta})}{\partial \beta_j} = \sum_{i=1}^{n} \left[-y_i + \frac{e^{\mathbf{x}_i^\top \boldsymbol{\beta}}}{1 + e^{\mathbf{x}_i^\top \boldsymbol{\beta}}} \right] x_{ij} \qquad \text{(verify this!)}$$

Updates and stopping criteria

Therefore, at the $(k+1)$th iteration, with the learning rate α,

$$\hat{\boldsymbol{\beta}}^{(k+1)} = \hat{\boldsymbol{\beta}}^{(k)} - \alpha \sum_{i=1}^{n} \left[-y_i + \frac{e^{\mathbf{x}_i^\top \hat{\boldsymbol{\beta}}^{(k)}}}{1 + e^{\mathbf{x}_i^\top \hat{\boldsymbol{\beta}}^{(k)}}} \right] \mathbf{x}_i.$$

Initialization $\boldsymbol{\beta}^{(0)} = 0$.

- The objective value stops changing: $|\ell(\hat{\boldsymbol{\beta}}^{(k+1)}) - \ell(\hat{\boldsymbol{\beta}}^{(k)})|$ is small, say, $\leq 10^{-6}$.
- The parameter stops changing: $||\hat{\boldsymbol{\beta}}^{(k+1)} - \hat{\boldsymbol{\beta}}^{(k)}||_2$ is small or $||\hat{\boldsymbol{\beta}}^{(k+1)} - \hat{\boldsymbol{\beta}}^{(k)}||_2 / ||\hat{\boldsymbol{\beta}}^{(k)}||_2$ is small.
- Stop after M iterations for some specified M, e.g. $M = 1000$.

Gradient descent for solving the MLE under logistic regression

- The negative log-likelihood

$$-\ell(\boldsymbol{\beta}) = \sum_{i=1}^{n} \left[-y_i \mathbf{x}_i^\top \boldsymbol{\beta} + \log\left(1 + e^{\mathbf{x}_i^\top \boldsymbol{\beta}}\right) \right]$$

  is convex in $\boldsymbol{\beta}$ (check this).

- So we can use gradient descent to find the MLE.

Why MLE?

The MLE, whenever can be computed, has many nice properties!

- Asymp. consistent

$$\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta} \to 0, \quad \text{in probability as } n \to \infty.$$

- Asymp. normal

$$\sqrt{n}\left(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta}\right) \to N(0, \Sigma) \quad \text{in distribution as } n \to \infty.$$

- Asymp. efficient:

Σ is the "smallest" among all asymptotic unbiased estimators.

Any downsides? computation, model misspecification ...

Inference under logistic regression

Let $\hat{\boldsymbol{\beta}}$ be the MLE of $\boldsymbol{\beta}$.

- Z-statistic is similar to t-statistic in regression, and is defined as

$$\frac{\hat{\beta}_j}{SE(\hat{\beta}_j)}, \qquad \forall j \in \{0, 1, \ldots, p\}$$

  where $SE(\hat{\beta}_j)$ is the asymp. variance of $\hat{\beta}_j$ (equal to $\hat{\Sigma}_{jj}/n$ in the previous slide).

- It produces p-value for testing the null hypothesis

$$H_0 : \beta_j = 0 \quad \text{v.s.} \quad H_1 : \beta_j \neq 0.$$

  A large (absolute) value of the z-statistic or small p-value indicates evidence against H_0.

Example: Default data

Suppose that we are interested in predicting

the probability of default for a given customer

by using **student status** as the only feature.

By encoding $x_i = 1\{\text{the } i\text{th customer is student}\}$ and, $y_i = 1$ if default happens and 0 otherwise. Fit the logistic regression model

$$y_i \sim \text{Bernoulli}(p(x_i)), \qquad p(x_i) = \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}}.$$

Prediction of $p(x)$

The fitted maximum likelihood estimates of β_0 and β_1 satisfy:

	Coefficient	Std.Error	Z-statistic	P-value
Intercept	-3.5	0.071	-49.55	<0.0001
student[Yes]	0.405	0.115	3.52	0.0004

$$\hat{p}(x = 1) = \hat{\mathbb{P}}(\text{default} \mid \text{student}) = \frac{e^{-3.5+0.405\times1}}{1 + e^{-3.5+0.405\times1}} \approx 0.043$$

$$\hat{p}(x = 0) = \hat{\mathbb{P}}(\text{default} \mid \text{non-student}) = \frac{e^{-3.5+0.405\times0}}{1 + e^{-3.5+0.405\times0}} \approx 0.029$$

Example: Default data

Consider using more predictors: **balance**(X_1), **income**(X_2), and **student status**(X_3).

$$\log\left(\frac{p(\mathbf{x}_i)}{1-p(\mathbf{x}_i)}\right) = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3}$$

The maximum likelihood estimates yield:

	Coefficient	Std.Error	Z-statistic	P-value
Intercept	-10.87	0.492	-22.08	<0.0001
balance	0.006	0.0002	24.74	<0.0001
income	0.003	0.0082	0.37	0.712
student[Yes]	-0.647	0.2362	-2.74	0.0062

Question: how does the coefficient of student status changes?

Metrics used for evaluating classifiers

In classification, we have several metrics that can be used to evaluate a given classifier.

- The most commonly used metric is the overall classification accuracy.
- For **binary** classification, there are a few more out there.....

Cont'd example: the Default Data

- Classify whether or not an individual will default on the basis of credit card balance and student status.

- **The confusion matrix** of fitted logistic regression

		True default status		
		No	Yes	Total
Predicted default status	No	9,644	252	9,896
	Yes	23	81	104
	Total	9,667	333	10,000

- The training error rate is $(23 + 252)/10000 = 2.75\%$.

Type of Errors for binary classification

		True default status		
		No	Yes	Total
Predicted	No	9,644	252	9,896
default status	Yes	23	81	104
	Total	9,667	333	10,000

1. **False positive rate (FPR)**: The fraction of negative examples that are classified as positive: 23/9667 = 0.2% in default data.
2. **False negative rate (FNR)**: The fraction of positive examples that are classified as negative: 252/333 = 75.7% in default data.[2]

[2] For a credit card company that is trying to identify high-risk individuals, the error rate 75.7% among individuals who default is unacceptable.

Control the false negative rate

Q: How to modify the logistic classifier to lower the false negative rate?

the fraction of **positive** examples as **negative**

the fraction of **default** examples classified as **non-default**

- The current classifier is based on the rule

$$\begin{aligned} \hat{y}_i &= 1 \quad \text{(default)}, && \text{if} \quad \hat{\mathbb{P}}(\text{default} = \textit{yes} \mid X = \mathbf{x}_i) \geq 0.5 \\ \hat{y}_i &= 0 \quad \text{(non-default)}, && \text{otherwise.} \end{aligned}$$

Control the false negative rate

- To lower FNR, we reduce the number of negative predictions. Classify $X = \mathbf{x}$ to *yes* if

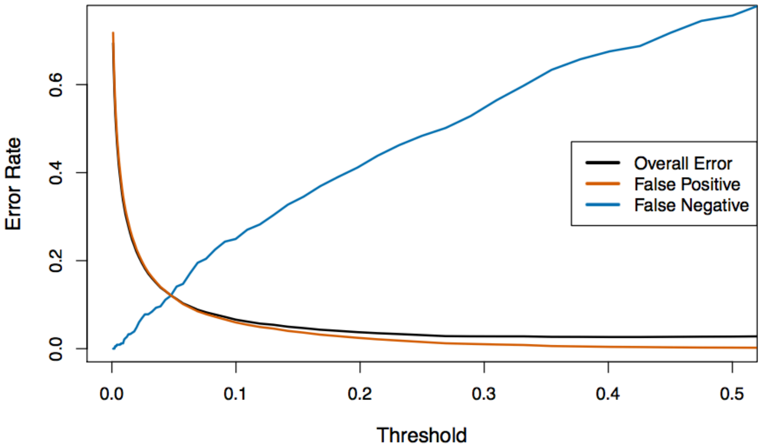
$$\hat{\mathbb{P}}(Y = yes \mid X = \mathbf{x}) \geq t.$$

for some $0 \leq t < 0.5$.

  - Why starts with $t = 0.5$?
  - What happens for $t = 0$?
  - What happens for $t = 1$?

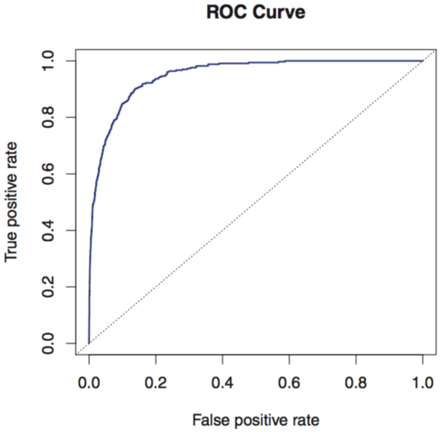
Trade-off between FPR and FNR

We can achieve better balance between FPR and FNR by varying the threshold t:



ROC Curve

The **ROC curve** is a popular graphic for simultaneously displaying FPR and TPR = 1 - FNR for all possible thresholds.



The overall performance of a classifier, summarized over all thresholds, is given by the area under the curve (**AUC**). High AUC is good.

More metrics in the binary classification

		Predicted class		
		− or Null	+ or Non-null	Total
True class	− or Null	True Neg. (TN)	False Pos. (FP)	N
	+ or Non-null	False Neg. (FN)	True Pos. (TP)	P
	Total	N^*	P^*	

Name	Definition	Synonyms
False Pos. rate	FP/N	Type I error, 1−Specificity
True Pos. rate	TP/P	1−Type II error, power, sensitivity, recall
Pos. Pred. value	TP/P^*	Precision, 1−false discovery proportion
Neg. Pred. value	TN/N^*	

The above also defines **sensitivity** and **specificity**.