Logistic Regression

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Machine Learning

Outline

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Motivation

Objectives

1. Determine the existence/absence of relationship between independent variables and a dependent variable
2. Use the identified variables to predict the probability of the response taking each value, as a function of the predictor values
3. Use these probabilities to classify future observations

Approach

What

- Since '67, standard for regression with dichotomic data (Health Sciences)
- We have: $\boxed{Y = C = 0, 1}$ $\boxed{X_1, ..., X_n}$
- N observations like
  $\mathcal{D} = \{(c^j, x_1^j, ..., x_n^j) = (c^j, \mathbf{x}^j), j = 1, ..., N\}$ with
  $c^j = 1$: observation j has the characteristic;
  $c^j = 0$: it hasn't
- Dependent variable is
  $\pi^j = p(C = 1|\mathbf{x}^j) = p(C = 1|X_1 = x_1^j, \ldots, X_n = x_n^j)$
  and since C is Bernoulli, its mean is $E(C|\mathbf{x}^j) = \pi^j$

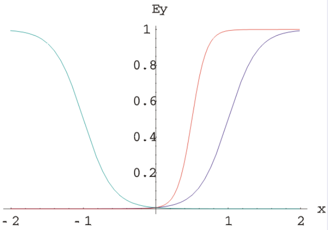
$\Rightarrow$ We look for a relationship between the response mean and the predictors

$\Rightarrow$ Scatterplots are not useful: no relation between y-axis and data

Intuitions

If $n = 1$, $C = 1$ =heart attack, X =cholesterol level, what relationship we expect between π and x?

- $\pi \approx 1$ for large x values; $\pi \approx 0$ for small x values
- Non-linear for many values of X: for medium x's, almost linear; asymptotic in extremes



$\beta_1 = 5$
$\beta_1 = 10$
$\beta_1 = -5$

$$\pi = \frac{e^{\beta_0+\beta_1 x}}{1 + e^{\beta_0+\beta_1 x}}$$

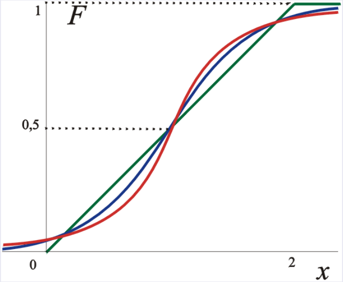
$\Rightarrow$ satisfies $\pi \in [0, 1]$

Intuitions

In general

- In general, to guarantee $\pi \in [0, 1]$, we apply a nonlinear transformation: $\pi = F(\boldsymbol{\beta}^t \mathbf{x})$

  - F any distribution function
  - $\boldsymbol{\beta} = (\beta_1, ..., \beta_n)$ vector of coefficients
  - $\mathbf{x}^j = (x_1^j, ..., x_n^j)$ data



Expressions: π and $1-\pi$

Logistic model

$\forall j = 1, ..., N$:

$$\boxed{\pi^j = p(C=1|\mathbf{x}^j) = \frac{e^{\beta^t \mathbf{x}^j}}{1+e^{\beta^t \mathbf{x}^j}} = \frac{1}{1+e^{-(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}}}$$

$$\Rightarrow \; 1-\pi^j = p(C=0|\mathbf{x}^j) = \frac{1}{1+e^{(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}}$$

- $\beta_0, \beta_1, \ldots, \beta_n$ are the parameters, to be estimated from data
- Decision boundary is linear:
  $p(C=1|\mathbf{x}^j) = p(C=0|\mathbf{x}^j) \iff p(C=1|\mathbf{x}^j) = 0.5$
  $\iff \beta_0 + \beta_1 x_1^j + \cdots + \beta_n x_n^j = 0$

Expressions: Risk Ratio $RR(\mathbf{x}, \mathbf{x}')$

Example

- Variables: C `Coronary Disease` (1 yes, 0 no); X_1 `Cholesterol` (1 high, 0 low), X_2 `Age`, and X_3 `Electrocardiogram res.` (1 abnormal, 0 normal)
- Parameters ($N = 609$ obs): $\widehat{\beta_0} = -3.911$ $\widehat{\beta_1} = 0.652$ $\widehat{\beta_2} = 0.029$ $\widehat{\beta_3} = 0.342$
- Compare the risk for two patterns: $\mathbf{x} = (1, 40, 0)$ and $\mathbf{x}' = (0, 40, 0)$:
  - $p(C = 1|\mathbf{x}) = p(C = 1|X_1 = 1, X_2 = 40, X_3 = 0) =$ $= \frac{1}{1+e^{-(-3.911+0.652(1)+0.029(40)+0.342(0))}} = 0.109$
  - $p(C = 1|\mathbf{x}') = p(C = 1|X_1 = 0, X_2 = 40, X_3 = 0) =$ $= \frac{1}{1+e^{-(-3.911+0.652(0)+0.029(40)+0.342(0))}} = 0.060$
- $RR(\mathbf{x}, \mathbf{x}') = \frac{p(C=1|\mathbf{x})}{p(C=1|\mathbf{x}')} = \frac{p(C=1|X_1=1,X_2=40,X_3=0)}{p(C=1|X_1=0,X_2=40,X_3=0)} = \frac{0.109}{0.060} = 1.82$
- For a person who is 40 years old and with normal electrocardiogram, the risk is multiplied by almost 2 when going from low `Cholesterol` level (0) to high (1)

Expressions: Odds and logit

Logistic model in *logit* form

- $$\boxed{\mathrm{Odds}(\mathbf{x}) = \frac{p(C=1|\mathbf{x})}{1-p(C=1|\mathbf{x})} = e^{(\beta_0+\beta_1 x_1+\cdots+\beta_n x_n)}}$$

  Increasig 1 unit x_1, $\frac{p(C=1|\mathbf{x})}{1-p(C=1|\mathbf{x})}$ multiplies by the factor e^{β_1}.
  Not very interpretable

- *logit* form:

$$\boxed{\mathrm{logit}(p(C=1|\mathbf{x})) = \ln \mathrm{Odds}(\mathbf{x}) = \ln\left[\frac{p(C=1|\mathbf{x})}{1-p(C=1|\mathbf{x})}\right] = \beta_0+\beta_1 x_1+\cdots+\beta_n x_n}$$

  A linear model with this transformation, that represents in a logarithmic scale the difference between the probabilities of belonging to both classes. Interpretable in this scale

- Example: $\mathrm{logit}(p(C=1|\mathbf{0})) = \ln \mathrm{Odds}(\mathbf{0}) = \beta_0$

Interpreting parameters β_i

Proposition: *In a logistic regression model, coefficient β_i represents the logit change when the i-th variable X_i $(i = 1, \ldots, n)$ increases 1 unit*

Proof: Let $\mathbf{x}$ and $\mathbf{x}'$ be vectors such that $x_l = x'_l$ for all $l \neq i$ and $x'_i = x_i + 1$, then

$$\mathrm{logit}(p(C = 1|\mathbf{x}')) - \mathrm{logit}(p(C = 1|\mathbf{x})) =$$

$$\beta_0 + \sum_{l=1}^{n} \beta_l x'_l - \left(\beta_0 + \sum_{l=1}^{n} \beta_l x_l\right) = \beta_i x'_i - \beta_i x_i = \beta_i (x_i + 1 - x_i) = \beta_i$$

- In the example: $\mathbf{x} = (1, 40, 0), \mathbf{x}' = (0, 40, 0)$
  $\mathrm{logit}(p(C = 1|\mathbf{x})) = \beta_0 + 1 \cdot \beta_1 + 40 \cdot \beta_2 + 0 \cdot \beta_3$
  $\mathrm{logit}(p(C = 1|\mathbf{x}')) = \beta_0 + 0 \cdot \beta_1 + 40 \cdot \beta_2 + 0 \cdot \beta_3$
  $\Rightarrow \mathrm{logit}(p(C = 1|\mathbf{x})) - \mathrm{logit}(p(C = 1|\mathbf{x}')) = \beta_1$

Multi-class logistic regression: $\Omega_C = \{1, ..., R\}, R > 2$

- $C|\mathbf{x} \sim$ categorical distribution (rather than Bernoulli)
- Equation of the logit is now a set of $R-1$ logit transformations:

$$\begin{aligned}
\ln \frac{p(C=1|\mathbf{x})}{p(C=R|\mathbf{x})} &= \beta_{10} + \beta_{11}x_1 + \cdots + \beta_{1n}x_n \\
&\vdots \\
\ln \frac{p(C=R-1|\mathbf{x})}{p(C=R|\mathbf{x})} &= \beta_{(R-1)0} + \beta_{(R-1)1}x_1 + \cdots + \beta_{(R-1)n}x_n
\end{aligned}$$

- Convention: using the last category R as the denominator (estimates do not vary under other choice). We get:

$$\begin{aligned}
p(C=r|\mathbf{x}) &= \frac{e^{\beta_{r0}+\beta_{r1}x_1+\cdots+\beta_{rn}x_n}}{1+\sum_{l=1}^{R-1} e^{\beta_{l0}+\beta_{l1}x_1+\cdots+\beta_{ln}x_n}}, \; r = 1, ..., R-1 \\
p(C=R|\mathbf{x}) &= \frac{1}{1+\sum_{l=1}^{R-1} e^{\beta_{l0}+\beta_{l1}x_1+\cdots+\beta_{ln}x_n}}
\end{aligned}$$

which add up to 1. There are $(n+1)(R-1)$ parameters: $\{\beta_{10}, ..., \beta_{(R-1)n}\}$

Feature subset selection

Multicollinearity among predictors

- Important to remove it, as done in linear regression
  $\Rightarrow$ Unstable $\hat{\beta}_i$ (correlated, high std error)
- Detect it as usually
- Remove correlated predictors

Outline

Maximum likelihood estimates

(Conditional) likelihood function $\mathcal{L}$

- Probability function: $p(C = c^j|\mathbf{x}^j) = (\pi^j)^{c^j}(1-\pi^j)^{1-c^j}, \quad c^j = 0,1$
(each obs is a Bernoulli trial)

- $\mathcal{L}(\beta|\mathcal{D}) = \prod_{j=1}^{N} p(C = c^j|\mathbf{x}^j) = \prod_{j=1}^{N} (\pi^j)^{c^j}(1-\pi^j)^{1-c^j}$

- Conditional log-likelihood: $\ln\mathcal{L}(\beta|\mathcal{D}) = \sum_{j=1}^{N} \ln p(C = c^j|\mathbf{x}^j)$

$$= \sum_{j=1}^{N} \left[c^j \ln \pi^j + (1-c^j)\ln(1-\pi^j)\right]$$

$$= \sum_{j=1}^{N} c^j \ln \frac{\pi^j}{1-\pi^j} + \sum_{j=1}^{N} \ln(1-\pi^j)$$

$$= \sum_{j=1}^{N} c^j \left(\beta_0 + \beta_1 x_1^j + \cdots + \beta_n x_n^j\right) - \sum_{j=1}^{N} \ln\left(1 + e^{(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}\right)$$

Maximum likelihood estimates

MLE $\hat{\beta}_i$ for β_i

- If the derivative is equal to zero: –*likelihood equations*–

$$
\begin{aligned}
\frac{\partial \ln \mathcal{L}(\boldsymbol{\beta})}{\partial \beta_0} &= \sum_{j=1}^{N} c^j - \sum_{j=1}^{N} \frac{e^{(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}}{1+e^{(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}} = 0 \\
\frac{\partial \ln \mathcal{L}(\boldsymbol{\beta})}{\partial \beta_1} &= \sum_{j=1}^{N} c^j x_1^j - \sum_{j=1}^{N} x_1^j \frac{e^{(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}}{1+e^{(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}} = 0 \\
&\vdots \\
\frac{\partial \ln \mathcal{L}(\boldsymbol{\beta})}{\partial \beta_n} &= \sum_{j=1}^{N} c^j x_n^j - \sum_{j=1}^{N} x_n^j \frac{e^{(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}}{1+e^{(\beta_0+\beta_1 x_1^j+\cdots+\beta_n x_n^j)}} = 0
\end{aligned}
$$

Non-linear in $\boldsymbol{\beta}$

Maximum likelihood estimates

MLE $\hat{\beta}_i$ for β_i

- It is impossible to have a closed formula (analytic solution) for MLE
- Newton-Raphson's numeric algorithm is traditionally used, with an updating formula given by

$$\widehat{\boldsymbol{\beta}}^{\mathbf{new}} = \widehat{\boldsymbol{\beta}}^{\mathbf{old}} + (\mathbf{Z}^{\mathbf{t}}\mathbf{W}^{\mathbf{old}}\mathbf{Z})^{-1}\mathbf{Z}^{\mathbf{t}}(\mathbf{c} - \widehat{\boldsymbol{\pi}}^{\mathbf{old}})$$

c is N-vector of response values c^j, $j = 1, \ldots, N$
X is $N \times n$-matrix with rows $\mathbf{x}^j$
Z is the matrix $[\mathbf{u}|\mathbf{X}]$, with **u** the N-vector of ones
$\widehat{\boldsymbol{\pi}}^{\text{old}}$ is N-vector of estimated values at that iteration, i.e. its jth-component is

$$(\hat{\pi}^j)^{\text{old}} = [1 + e^{-(\hat{\beta}_0^{\text{old}} + \hat{\beta}_1^{\text{old}} x_1^j + \cdots + \hat{\beta}_n^{\text{old}} x_n^j)}]^{-1}$$

$\mathbf{W}^{\mathbf{old}}$ is a diagonal matrix with elements $(\hat{\pi}^j)^{\text{old}}(1 - (\hat{\pi}^j)^{\text{old}})$
Initialize e.g. with $\widehat{\boldsymbol{\beta}} = (0, \ldots, 0)$

  - ...until convergence

Classifying

Steps

1. Fix a cutoff value $\hat{\pi}^*$ for $\hat{\pi}$
2. Assign $\hat{c}^j = 1$ if $\hat{\pi}^j \geq \hat{\pi}^*$. Otherwise, $\hat{c}^j = 0$ (predicted class)
3. Build the confusion matrix:

	$\hat{c} = 1$	$\hat{c} = 0$
$c = 1$	N_1	N_2
$c = 0$	N_3	N_4

$$N = N_1 + N_2 + N_3 + N_4$$

Assess the model utility:

% correctly classified = $100\,(N_1 + N_4)/N$

sensitivity = $100\,N_1/(N_1 + N_2)$

specificity = $100\,N_4/(N_3 + N_4)$

Outline

Software

Logistic regression with WEKA

`Classifier` $\Rightarrow$ `Functions`

Logistic

- Binary case $\rightarrow e^{\beta_i}$ is the odds ratio in Weka (> 1 for $\beta_i > 0$, and < 1 for $\beta_i < 0$). Increasing X_i in 1 unit (the remaining variables do not change), the ratio $p(C = 1|\mathbf{x})/p(C = 0|\mathbf{x})$ multiplies by e^{β_i}.
- Multi-class case $\rightarrow e^{\beta_{1i}}$: Increasing X_i in 1 unit (the remaining variables do not change), the ratio $p(C = 1|\mathbf{x})/p(C = R|\mathbf{x})$ multiplies by $e^{\beta_{1i}}$. If $e^{\beta_{1i}} > 1 (\beta_{1i} > 0)$ then $C = 1$ becomes more likely than $C = R$ for each increment in X_i

Conclusions

Statistical paradigm

- Discriminative model: maximize conditional probability
- Assign to each instance the posterior probability of belonging to each class
- Interpretation of parameters
- Estimation of parameters by maximum likelihood. Approximate them via iterative numerical methods

Bibliography

Texts

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