Logistic Regression

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Logistic Regression

Preserve linear classification boundaries.

• By the Bayes rule:

$$\hat{G}(x) = \arg\max_{k} Pr(G = k \mid X = x)$$

 Decision boundary between class k and l is determined by the equation:

$$Pr(G = k | X = x) = Pr(G = l | X = x).$$

• Divide both sides by $Pr(G=l \mid X=x)$ and take log. The above equation is equivalent to

$$\log \frac{Pr(G=k \mid X=x)}{Pr(G=l \mid X=x)} = 0.$$

Meaning of ξ_p

Since we enforce linear boundary, we can assume

$$\log \frac{Pr(G=k \mid X=x)}{Pr(G=l \mid X=x)} = a_0^{(k,l)} + \sum_{i=1}^{P} a_j^{(k,l)} x_j.$$

• For logistic regression, there are restrictive relations between $a^{(k,l)}$ for different pairs of (k,l).

Assumptions

$$\log \frac{Pr(G = 1 \mid X = x)}{Pr(G = K \mid X = x)} = \beta_{10} + \beta_1^T x$$

$$\log \frac{Pr(G = 2 \mid X = x)}{Pr(G = K \mid X = x)} = \beta_{20} + \beta_2^T x$$

$$\vdots$$

$$\log \frac{Pr(G = K - 1 \mid X = x)}{Pr(G = K \mid X = x)} = \beta_{(K-1)0} + \beta_{K-1}^T x$$

For any pair (k, l):

$$\log \frac{Pr(G = k | X = x)}{Pr(G = l | X = x)} = \beta_{k0} - \beta_{l0} + (\beta_k - \beta_l)^T x.$$

- Number of parameters: (K-1)(p+1).
- Denote the entire parameter set by

$$\theta = \{\beta_{10}, \beta_1, \beta_{20}, \beta_2, \dots, \beta_{(K-1)0}, \beta_{K-1}\}.$$

 The log ratio of posterior probabilities are called log-odds or logit transformations. Under the assumptions, the posterior probabilities are given by:

$$Pr(G = k \mid X = x) = \frac{\exp(\beta_{k0} + \beta_k^T x)}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \beta_l^T x)}$$

for k = 1, ..., K - 1

$$Pr(G = K | X = x) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \beta_l^T x)}.$$

- For Pr(G = k | X = x) given above, obviously
 - Sum up to 1: $\sum_{k=1}^{K} Pr(G = k | X = x) = 1$.
 - A simple calculation shows that the assumptions are satisfied.

Comparison with LR on Indicators

Similarities:

- Both attempt to estimate Pr(G = k | X = x).
- Both have linear classification boundaries.

Difference:

- Linear regression on indicator matrix: approximate $Pr(G=k \mid X=x)$ by a linear function of x. $Pr(G=k \mid X=x)$ is not guaranteed to fall between 0 and 1 and to sum up to 1.
- Logistic regression: Pr(G = k | X = x) is a nonlinear function of x. It is guaranteed to range from 0 to 1 and to sum up to 1.

Fitting Logistic Regression Models

- Criteria: find parameters that maximize the conditional likelihood of G given X using the training data.
- Denote $p_k(x_i; \theta) = Pr(G = k | X = x_i; \theta)$.
- Given the first input x_1 , the posterior probability of its class being g_1 is $Pr(G = g_1 | X = x_1)$.
- Since samples in the training data set are independent, the posterior probability for the N samples each having class g_i , i = 1, 2, ..., N, given their inputs $x_1, x_2, ..., x_N$ is:

$$\prod_{i=1}^{N} Pr(G = g_i \mid X = x_i).$$

 The conditional log-likelihood of the class labels in the training data set is

$$L(\theta) = \sum_{i=1}^{N} \log Pr(G = g_i | X = x_i)$$
$$= \sum_{i=1}^{N} \log p_{g_i}(x_i; \theta).$$

Binary Classification

- For binary classification, if $g_i = 1$, denote $y_i = 1$; if $g_i = 2$, denote $y_i = 0$.
- Let $p_1(x;\theta) = p(x;\theta)$, then

$$p_2(x;\theta) = 1 - p_1(x;\theta) = 1 - p(x;\theta).$$

• Since K=2, the parameters $\theta=\{\beta_{10},\beta_1\}$. We denote $\beta=(\beta_{10},\beta_1)^T$.

• If
$$y_i=1$$
, i.e., $g_i=1$,
$$\log p_{g_i}(x;\beta) = \log p_1(x;\beta)$$

$$= 1 \cdot \log p(x;\beta)$$

$$= y_i \log p(x;\beta).$$

If
$$y_i = 0$$
, i.e., $g_i = 2$,

$$\log p_{g_i}(x; \beta) = \log p_2(x; \beta) = 1 \cdot \log(1 - p(x; \beta)) = (1 - y_i) \log(1 - p(x; \beta)).$$

Since either $y_i = 0$ or $1 - y_i = 0$, we have

$$\log p_{g_i}(x;\beta) = y_i \log p(x;\beta) + (1-y_i) \log(1-p(x;\beta)).$$

The conditional likelihood

$$L(\beta) = \sum_{i=1}^{N} \log p_{g_i}(x_i; \beta)$$

$$= \sum_{i=1}^{N} [y_i \log p(x_i; \beta) + (1 - y_i) \log(1 - p(x_i; \beta))]$$

- There p+1 parameters in $\beta = (\beta_{10}, \beta_1)^T$.
- Assume a column vector form for β :

$$\beta = \begin{pmatrix} \beta_{10} \\ \beta_{11} \\ \beta_{12} \\ \vdots \\ \beta_{1n} \end{pmatrix}.$$

 Here we add the constant term 1 to x to accommodate the intercept.

$$x = \begin{pmatrix} 1 \\ x_{,1} \\ x_{,2} \\ \vdots \\ x_{,p} \end{pmatrix}$$

By the assumption of logistic regression model:

$$p(x; \beta) = Pr(G = 1 | X = x) = \frac{\exp(\beta^T x)}{1 + \exp(\beta^T x)}$$
$$1 - p(x; \beta) = Pr(G = 2 | X = x) = \frac{1}{1 + \exp(\beta^T x)}$$

• Substitute the above in $L(\beta)$:

$$L(\beta) = \sum_{i=1}^{N} \left[y_i \beta^T x_i - \log \left(1 + e^{\beta^T x_i} \right) \right]$$

• To maximize $L(\beta)$, we set the first order partial derivatives of $L(\beta)$ to zero.

$$\frac{\partial L(\beta)}{\beta_1 j} = \sum_{i=1}^{N} y_i x_{ij} - \sum_{i=1}^{N} \frac{x_{ij} e^{\beta^T x_i}}{1 + e^{\beta^T x_i}}$$

$$= \sum_{i=1}^{N} y_i x_{ij} - \sum_{i=1}^{N} p(x; \beta) x_{ij}$$

$$= \sum_{i=1}^{N} x_{ij} (y_i - p(x_i; \beta))$$

for all j = 0, 1, ..., p.

In matrix form, we write

$$\frac{\partial L(\beta)}{\partial \beta} = \sum_{i=1}^{N} x_i (y_i - p(x_i; \beta)).$$

- To solve the set of p+1 nonlinear equations $\frac{\partial L(\beta)}{\beta_1 j}$, j=0,1,...,p, use the Newton-Raphson algorithm.
- The Newton-Raphson algorithm requires the second-derivatives or Hessian matrix:

$$\frac{\partial^2 L(\beta)}{\partial \beta \partial \beta^T} = -\sum_{i=1}^N x_i x_i^T p(x_i; \beta) (1 - p(x_i; \beta)).$$

 The element on the jth row and nth column is (counting from 0):

$$\frac{\partial L(\beta)}{\partial \beta_{1j} \partial \beta_{1n}}
= -\sum_{i=1}^{N} \frac{(1 + e^{\beta^{T} x_{i}}) e^{\beta^{T} x_{i}} x_{ij} x_{in} - (e^{\beta^{T} x_{i}})^{2} x_{ij} x_{in}}{(1 + e^{\beta^{T} x_{i}})^{2}}
= -\sum_{i=1}^{N} x_{ij} x_{in} p(x_{i}; \beta) - x_{ij} x_{in} p(x_{i}; \beta)^{2}
= -\sum_{i=1}^{N} x_{ij} x_{in} p(x_{i}; \beta) (1 - p(x_{i}; \beta)).$$

• Starting with β^{old} , a single Newton-Raphson update is

$$\beta^{new} = \beta^{old} - \left(\frac{\partial^2 L(\beta)}{\partial \beta \partial \beta^T}\right)^{-1} \frac{\partial L(\beta)}{\partial \beta},$$

where the derivatives are evaluated at β^{old} .

- The iteration can be expressed compactly in matrix form.
 - Let y be the column vector of y_i.
 - Let **X** be the $N \times (p+1)$ input matrix.
 - Let **p** be the N-vector of fitted probabilities with ith element $p(x_i; \beta^{old})$.
 - Let **W** be an $N \times N$ diagonal matrix of weights with i th element $p(x_i; \beta^{old})(1-p(x_i; \beta^{old}))$.
 - Then

$$\frac{\partial L(\beta)}{\partial \beta} = \mathbf{X}^{T}(\mathbf{y} - \mathbf{p})$$
$$\frac{\partial^{2} L(\beta)}{\partial \beta \partial \beta^{T}} = -\mathbf{X}^{T}\mathbf{W}\mathbf{X}.$$

The Newton-Raphson step is

$$\begin{split} \boldsymbol{\beta}^{new} = & \boldsymbol{\beta}^{old} + (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T (\boldsymbol{y} - \boldsymbol{p}) \\ = & (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} (\mathbf{X} \boldsymbol{\beta}^{old} + \mathbf{W}^{-1} (\boldsymbol{y} - \boldsymbol{p})) \\ = & (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \boldsymbol{z}, \end{split}$$

where $z \stackrel{\triangle}{=\!\!\!=\!\!\!=} \mathbf{X} \beta^{old} + \mathbf{W}^{-1}(\boldsymbol{y} - \boldsymbol{p})$.

• If z is viewed as a response and X is the input matrix, β new is the solution to a weighted least square problem:

$$\beta^{new} \leftarrow \arg\min_{\beta} (\boldsymbol{z} - \mathbf{X}\beta)^T \mathbf{W} (\boldsymbol{z} - \mathbf{X}\beta).$$

Recall that linear regression by least square is to solve

$$\arg\min_{\beta}(\mathbf{z}-\mathbf{X}\beta)^{T}(\mathbf{z}-\mathbf{X}\beta).$$

- z is referred to as the adjusted response.
- The algorithm is referred to as iteratively reweighted least squares or IRLS.



Pseudo Code

- 1. $\mathbf{0} \rightarrow \beta$
- 2. Compute y by setting its elements to

$$y_i = \left\{ \begin{array}{ll} 1 & \text{if } g_i = 1 \\ 0 & \text{if } g_i = 2 \end{array} \right., \ i = 1, 2, ..., N.$$

3. Compute p by setting its elements to

$$p(x_i; \beta) = \frac{e^{\beta T x_i}}{1 + e^{\beta T x_i}} \quad i = 1, 2, ..., N.$$

- 4. Compute the diagonal matrix **W**. The *i*th diagonal element is $p(x_i; \beta)(1-p(x_i; \beta)), i = 1, 2, ..., N$.
- 5. $z \leftarrow X\beta + W^{-1}(y p)$.
- 6. $\beta \leftarrow (\mathbf{X}^T \mathbf{W} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{W} \mathbf{z}$.
- 7. If the stopping criteria is met, stop; otherwise go back to step 3.



Computational Efficiency

- Since W is an $N \times N$ diagonal matrix, direct matrix operations with it may be very inefficient.
- A modified pseudo code is provided next.

- 1. $0 \rightarrow \beta$
- 2. Compute y by setting its elements to

$$y_i = \left\{ \begin{array}{ll} 1 & \text{if } g_i = 1 \\ 0 & \text{if } g_i = 2 \end{array} \right., \ i = 1, 2, ..., N.$$

3. Compute p by setting its elements to

$$p(x_i; \beta) = \frac{e^{\beta T x_i}}{1 + e^{\beta T x_i}} \quad i = 1, 2, ..., N.$$

4. Compute the $N \times (p+1)$ matrix \mathbf{X} by multiplying the ith row of matrix \mathbf{X} by $p(x_i; \beta)(1-p(x_i; \beta)), i=1,2,...,\mathbf{N}$:

$$\mathbf{X} = \begin{pmatrix} x_1^T \\ x_2^T \\ \dots \\ x_N^T \end{pmatrix} \quad \tilde{\mathbf{X}} = \begin{pmatrix} p(x_1; \beta)(1 - p(x_1; \beta))x_1^T \\ p(x_2; \beta)(1 - p(x_2; \beta))x_2^T \\ \dots \\ p(x_N; \beta)(1 - p(x_N; \beta))x_N^T \end{pmatrix}$$

- 5. $\beta \leftarrow \beta + (\mathbf{X}^T \tilde{\mathbf{X}})^{-1} \mathbf{X}^T (\mathbf{y} \mathbf{p}).$
- 6. If the stopping criteria is met, stop; otherwise go back to step 3.

Example

Diabetes data set

- Input X is two dimensional. X_1 and X_2 are the two principal components of the original 8 variables.
- Class 1: without diabetes; Class 2: with diabetes.
- Applying logistic regression, we obtain

$$\beta = (0.7679, -0.6816, -0.3664)^{T}.$$

The posterior probabilities are:

$$Pr(G = 1 \mid X = x) = \frac{e^{0.7679 - 0.6816X_1 - 0.3664X_2}}{1 + e^{0.7679 - 0.6816X_1 - 0.3664X_2}}$$
$$Pr(G = 2 \mid X = x) = \frac{1}{1 + e^{0.7679 - 0.6816X_1 - 0.3664X_2}}$$

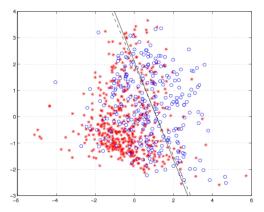
The classification rule is:

$$\hat{G}(x) = \begin{cases} 1 & 0.7679 - 0.6816X_1 - 0.3664X_2 \geqslant 0 \\ 2 & 0.7679 - 0.6816X_1 - 0.3664X_2 < 0 \end{cases}$$

Solid line: decision boundary obtained by logistic regression. Dash line: decision boundary obtained by LDA.

Within training data set classification error rate: 28.12%.

Sensitivity: 45.9%.Specificity: 85.8%.



Multiclass Case $(K \geqslant 3)$

• When $K \geqslant 3$, β is a (K-1)(p+1)-vector:

$$\beta = \begin{pmatrix} \beta_{10} \\ \beta_{1} \\ \beta_{20} \\ \beta_{2} \\ \vdots \\ \beta_{(K-1)0} \\ \beta_{K-1} \end{pmatrix} = \begin{pmatrix} \beta_{10} \\ \beta_{11} \\ \vdots \\ \beta_{1p} \\ \beta_{20} \\ \vdots \\ \beta_{2p} \\ \vdots \\ \beta_{(K-1)p} \\ \vdots \\ \beta_{(K-1)p} \end{pmatrix}$$

- Let $\bar{\beta}_I = \begin{pmatrix} \beta_{I0} \\ \beta_I \end{pmatrix}$.
- The likelihood function becomes

$$L(\beta) = \sum_{i=1}^{N} \log p_{g_i}(x_i; \beta)$$

$$= \sum_{i=1}^{N} \log \left(\frac{e^{\bar{\beta}_{g_i}^T x_i}}{1 + \sum_{I=1}^{K-1} e^{\bar{\beta}_l^T x_i}} \right)$$

$$= \sum_{i=1}^{N} \left[\bar{\beta}_{g_i}^T x_i - \log \left(1 + \sum_{I=1}^{K-1} e^{\bar{\beta}_l^T x_i} \right) \right]$$

- Note: the indicator function $I(\cdot)$ equals 1 when the argument is true and 0 otherwise.
- First order derivatives:

$$\frac{\partial L(\beta)}{\partial \beta_{kj}} = \sum_{i=1}^{N} \left[I(g_i = k) x_{ij} - \frac{e^{\bar{\beta}_{g_i}^T x_i}}{1 + \sum_{I=1}^{K-1} e^{\bar{\beta}_I^T x_i}} \right]$$
$$= \sum_{i=1}^{N} x_{ij} (I(g_i = k) - p_k(x_i; \beta))$$

Second order derivatives:

$$\frac{\partial^{2} L(\beta)}{\partial \beta_{kj} \partial \beta_{mn}} = \sum_{l=1}^{N} x_{ij} \cdot \frac{1}{(1 + \sum_{l=1}^{K-1} e^{\bar{\beta}_{l}^{T} x_{i}})^{2}} \cdot \left[-e^{\bar{\beta}_{k}^{T} x_{i}} I(k = m) x_{in} \left(1 + \sum_{l=1}^{K-1} e^{\bar{\beta}_{l}^{T} x_{i}} \right) + e^{\bar{\beta}_{k}^{T} x_{i}} e^{\bar{\beta}_{m}^{T} x_{i}} x_{in} \right] \\
= \sum_{i=1}^{N} x_{ij} x_{in} (-p_{k}(x_{i}; \beta) I(k = m) + p_{k}(x_{i}; \beta) p_{m}(x_{i}; \beta)) \\
= -\sum_{i=1}^{N} x_{ij} x_{in} p_{k}(x_{i}; \beta) [I(k = m) - p_{m}(x_{i}; \beta)].$$

- Matrix form.
 - y is the concatenated indicator vector of dimension N × (K−1).

$$egin{aligned} oldsymbol{y} = egin{pmatrix} oldsymbol{y}_1 \\ oldsymbol{y}_2 \\ dots \\ oldsymbol{y}_{K-1} \end{pmatrix} & oldsymbol{y}_k = egin{pmatrix} l(g_1 = k) \\ l(g_2 = k) \\ dots \\ l(g_N = k) \end{pmatrix} \\ 1 \le k \le K - 1 \end{aligned}$$

 p is the concatenated vector of fitted probabilities of dimension N × (K-1).

$$oldsymbol{p} = egin{pmatrix} oldsymbol{p}_1 \ oldsymbol{p}_2 \ dots \ oldsymbol{p}_{K-1} \end{pmatrix} \quad oldsymbol{p}_k = egin{pmatrix} p_k(x_1;eta) \ p_k(x_2;eta) \ dots \ p_k(x_N;eta) \end{pmatrix}$$

• $\tilde{\mathbf{X}}$ is an $N(K-1) \times (p+1)(K-1)$ matrix:

$$ilde{\mathbf{X}} = egin{pmatrix} \mathbf{X} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{X} & \cdots & \mathbf{0} \\ \cdots & \cdots & \cdots & \cdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{X} \end{pmatrix}$$

• Matrix **W** is an $N(K-1) \times N(K-1)$ square matrix:

$$\mathbf{W} = \begin{pmatrix} \mathbf{W}_{11} & \mathbf{W}_{12} & \cdots & \mathbf{W}_{1(K-1)} \\ \mathbf{W}_{21} & \mathbf{W}_{22} & \cdots & \mathbf{W}_{2(K-1)} \\ \cdots & \cdots & \cdots & \cdots \\ \mathbf{W}_{(K-1),1} & \mathbf{W}_{(K-1),2} & \cdots & \mathbf{W}_{(K-1),(K-1)} \end{pmatrix}$$

- Each submatrix \mathbf{W}_{km} , $1 \leqslant k$, $m \leqslant K-1$, is an $N \times N$ diagonal matrix.
- When k=m, the i th diagonal element in \mathbf{W}_{kk} is $p_k(x_i;\beta^{old})(1-p_k(x_i;\beta^{old}))$.
- When $k \neq m$, the i th diagonal element in \mathbf{W}_{km} is $-p_k(x_i; \beta^{old})p_m(x_i; \beta^{old})$.

Similarly as with binary classification

$$\begin{split} \frac{\partial L(\beta)}{\partial \beta} &= \tilde{\mathbf{X}}^T (\boldsymbol{y} - \boldsymbol{p}) \\ \frac{\partial^2 L(\beta)}{\partial \beta \partial \beta^T} &= -\tilde{\mathbf{X}}^T \mathbf{W} \tilde{\mathbf{X}}. \end{split}$$

• The formula for updating β^{new} in the binary classification case holds for multiclass.

$$\beta^{new} = (\tilde{\mathbf{X}}^T \mathbf{W} \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T \mathbf{W} \mathbf{z},$$

where
$$z \stackrel{\triangle}{=\!\!\!=\!\!\!=} \tilde{\mathbf{X}} \beta^{old} + \mathbf{W}^{-1}(y-p)$$
. Or simply:

$$\beta^{new} = \beta^{old} + (\tilde{\mathbf{X}}^T \mathbf{W} \tilde{\mathbf{X}})^{-1} \tilde{\mathbf{X}}^T (\boldsymbol{y} - \boldsymbol{p}).$$

Computation Issues

- Initialization: one option is to use $\beta = 0$.
- Convergence is not guaranteed, but usually is the case.
- Usually, the log-likelihood increases after each iteration, but overshooting can occur.
- In the rare cases that the log-likelihood decreases, cut step size by half.

Connection with LDA

• Under the model of LDA:

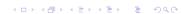
$$\log \frac{Pr(G = k | X = x)}{Pr(G = K | X = x)}$$

$$= \log \frac{\pi_k}{\pi_k} - \frac{1}{2} (\mu_k + \mu_K)^T \sum_{k=0}^{T} (\mu_k - \mu_K)$$

$$+ x^T \sum_{k=0}^{T} (\mu_k - \mu_K)$$

$$= a_{k0} + a_k^T x.$$

- The model of LDA satisfies the assumption of the linear logistic model.
- The linear logistic model only specifies the conditional distribution $Pr(G=k \mid X=x)$. No assumption is made about Pr(X).



• The LDA model specifies the joint distribution of X and G. Pr(X) is a mixture of Gaussians:

$$Pr(x) = \sum_{k=1}^{K} \pi_k \phi\left(X; \mu_k, \sum\right).$$

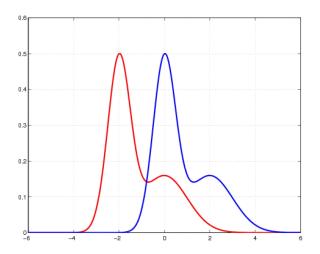
where ϕ is the Gaussian density function.

- Linear logistic regression maximizes the conditional likelihood of G given X: Pr(G = k | X = x).
- LDA maximizes the joint likelihood of G and X: Pr(X = x, G = k).

- If the additional assumption made by LDA is appropriate, LDA tends to estimate the parameters more efficiently by using more information about the data.
- Samples without class labels can be used under the model of LDA.
- LDA is not robust to gross outliers.
- As logistic regression relies on fewer assumptions, it seems to be more robust.
- In practice, logistic regression and LDA often give similar results.

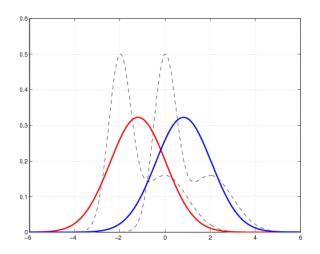
Simulation

- Assume input X is 1-D.
- Two classes have equal priors and the class-conditional densities of X are shifted versions of each other.
- Each conditional density is a mixture of two normals:
 - Class 1 (red): $0.6N(-2,\frac{1}{4}) + 0.4N(0,1)$.
 - Class 2 (blue): $0.6N(0,\frac{1}{4}) + 0.4N(2,1)$.
- The class-conditional densities are shown below.



LDA Result

- Training data set: 2000 samples for each class.
- Test data set: 1000 samples for each class.
- The estimation by LDA: $\hat{\mu}_1 = -1.1948$, $\hat{\mu}_2 = 0.8224$, $\hat{\sigma}_2 = 1.5268$. Boundary value between the two classes is $(\hat{\mu}_1 + \hat{\mu}_2)/2 = -0.1862$.
- The classification error rate on the test data is 0.2315.
- Based on the true distribution, the Bayes (optimal) boundary value between the two classes is -0.7750 and the error rate is 0.1765.



Logistic Regression Result

Linear logistic regression obtains

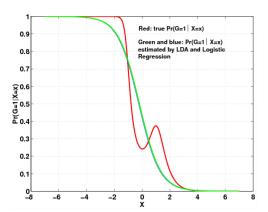
$$\beta = (-0.3288, -1.3275)^T.$$

The boundary value satisfies -0.3288-1.3275X=0, hence equals -0.2477.

- The error rate on the test data set is 0.2205.
- The estimated posterior probability is:

$$Pr(G=1 \mid X=x) = \frac{e^{-0.3288-13275x}}{1+e^{-0.3288-1.3275x}}.$$

The estimated posterior probability $Pr(G=1 \mid X=x)$ and its true value based on the true distribution are compared in the graph below.



Thank you!