Lecture 5: LDA and Logistic Regression

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Outline

- Two Popular Linear Models for Classification
  - Linear Discriminant Analysis (LDA)
  - Logistic Regression Models
- Take-home message:
  - Both LDA and Logistic regression models rely on the linear-odd assumption, indirectly or directly. However, they estimate the coefficients in a different manner.

Linear Classifier

Linear methods: The decision boundary is linear.
Common linear classification methods:

- Linear regression methods (covered in Lecture 3)
- Linear log-odds (logit) models
  - Linear logistic models
  - Linear discriminant analysis (LDA)
- separating hyperplanes (introduced later)
  - perceptron model (Rosenblatt 1958)
  - Optimal separating hyperplane (Vapnik 1996) – SVMs

From now on, we assume equal costs (by default).

Odds, Logit, and Linear Odds Models Linear

Some terminologies

- Call the term $\frac{\Pr(Y=1|\mathbf{X}=\mathbf{x})}{\Pr(Y=0|\mathbf{X}=\mathbf{x})}$ is called odds
- Call $\log \frac{\Pr(Y=1|\mathbf{X}=\mathbf{x})}{\Pr(Y=0|\mathbf{X}=\mathbf{x})}$ log of the odds, or logit function

Linear odds models assume: the logit is linear in $\mathbf{x}$, i.e.,

$$\log \frac{\Pr(Y=1|\mathbf{X}=\mathbf{x})}{\Pr(Y=0|\mathbf{X}=\mathbf{x})} = \beta_0 + \beta_1^T \mathbf{x}.$$

Examples: LDA, Logistic regression

Classifier Based on Linear Odd Models

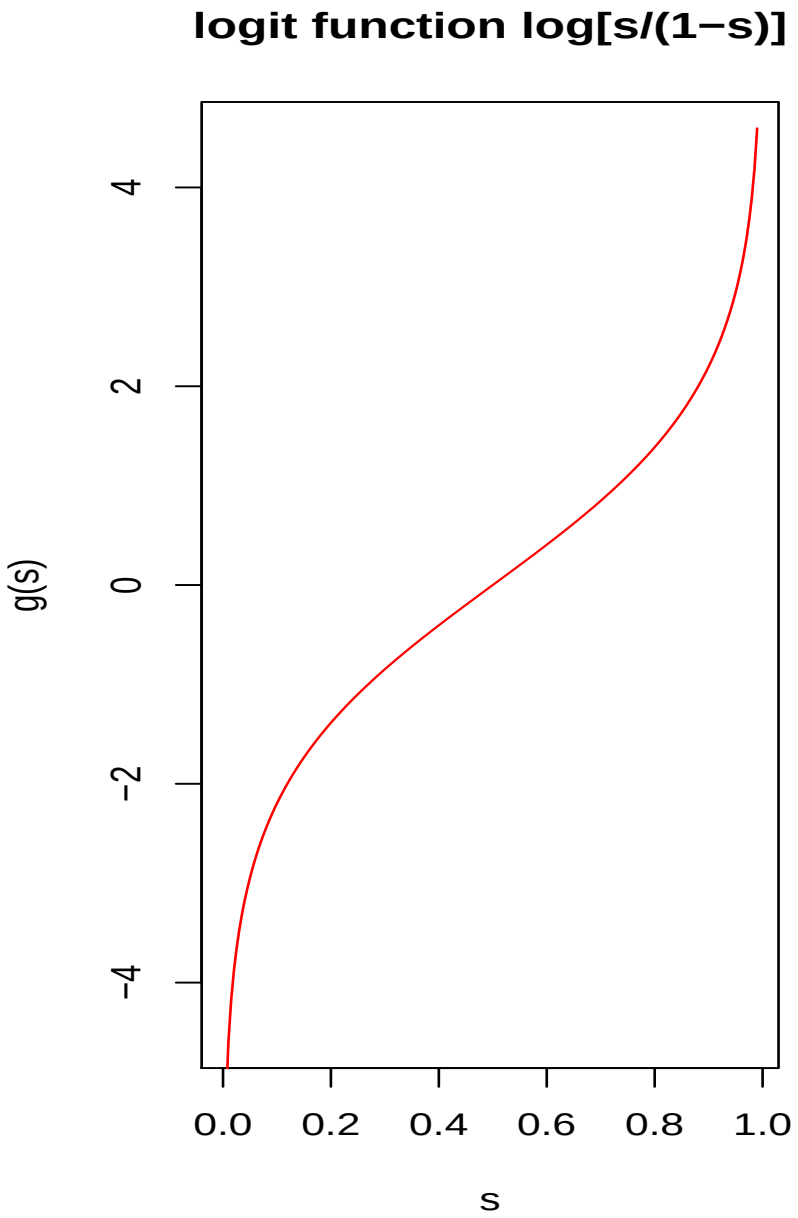
From the linear odds, we can obtain posterior class probabilities

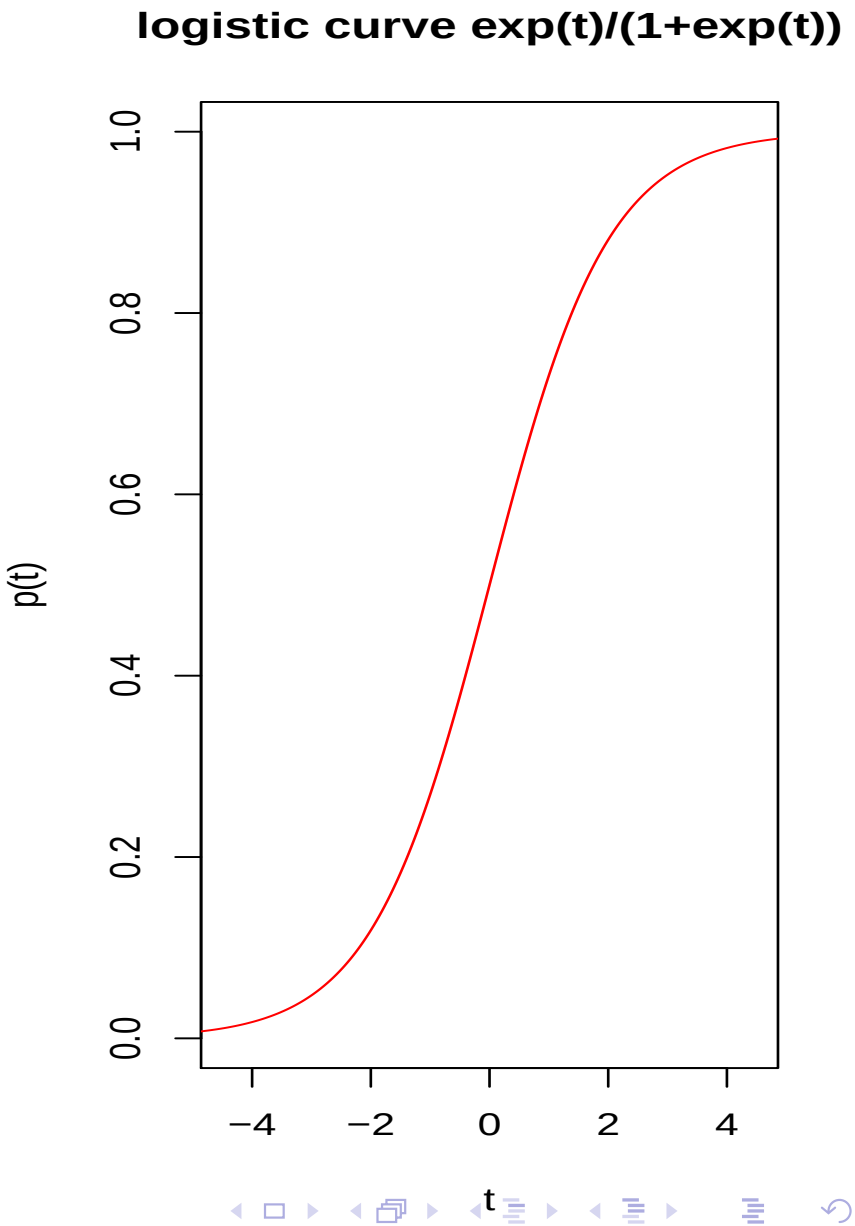
$$\begin{aligned} \Pr(Y=1|\mathbf{x}) &= \frac{\exp\left(\beta_0+\beta_1^T\mathbf{x}\right)}{1+\exp\left(\beta_0+\beta_1^T\mathbf{x}\right)} \\ \Pr(Y=0|\mathbf{x}) &= \frac{1}{1+\exp\left(\beta_0+\beta_1^T\mathbf{x}\right)} \end{aligned}$$

Assuming equal costs, the decision boundary is given by

$$\{\mathbf{x}|P(Y=1|\mathbf{x})=0.5\}=\{\mathbf{x}|\beta_0+\beta_1^T\mathbf{x}=0\},$$

which can be interpreted as "zero log-odds"


logit function log[s/(1−s)]
g(s)
4
2
0
−2
−4
0.0
0.2
0.4
0.6
0.8
1.0
s


logistic curve exp(t)/(1+exp(t))
p(t)
1.0
0.8
0.6
0.4
0.2
0.0
−4
−2
0
2
4
t

Linear Discriminant Analysis (LDA)

LDA assumes

- Assume each class density is multivariate Gaussian, i.e.,

$$X|Y_j \sim N(\mu_j, \Sigma_j), \quad j = 0, 1.$$

- Equal covariance assumption

$$\Sigma_j = \Sigma, \quad j = 0, 1.$$

In other words,

- both classes are from Gaussian and they have the same covariance matrix.

Linear Discriminant Function

Under the mixture Gaussian assumption, the log-odd is

$$\begin{aligned} & \log \frac{\Pr(Y=1|\mathbf{X}=\mathbf{x})}{\Pr(Y=0|\mathbf{X}=\mathbf{x})} \\ = \quad & \log \frac{\pi_1}{\pi_0} - \frac{1}{2}(\mu_1+\mu_0)^T\Sigma^{-1}(\mu_1-\mu_0) + \mathbf{x}^T\Sigma^{-1}(\mu_1-\mu_0) \end{aligned}$$

Under equal costs, the LDA classifies to "1" if and only if

$$\left[\log \frac{\pi_1}{\pi_0} - \frac{1}{2}(\mu_1+\mu_0)^T\Sigma^{-1}(\mu_1-\mu_0)\right] + \mathbf{x}^T\Sigma^{-1}(\mu_1-\mu_0) > 0.$$

It has a linear boundary $\{\mathbf{x} : \beta_0 + \mathbf{x}^T\boldsymbol{\beta}_1 = 0\}$, with

$$\begin{aligned} \beta_0 &= \log \frac{\pi_1}{\pi_0} - \frac{1}{2}(\mu_1+\mu_0)^T\Sigma^{-1}(\mu_1-\mu_0), \\ \boldsymbol{\beta}_1 &= \Sigma^{-1}(\mu_1-\mu_0). \end{aligned}$$

Parameter Estimation in LDA

In practice, $\pi_1, \pi_0, \mu_0, \mu_1, \Sigma$ are unknown

- We estimate the parameters from the training data, using MLE or the moment estimator
  - $\hat{\pi}_j = n_j/n$, where n_k is the size size of class j.
  - $\hat{\mu}_j = \sum_{Y_i=j} \mathbf{x}_i/n_j$ for $j = 0, 1$.
  - The sample covariance matrix is

$$S_j = \frac{1}{n_j - 1} \sum_{Y_i=j} (\mathbf{x}_i - \hat{\mu}_j)(\mathbf{x}_i - \hat{\mu}_j)^T$$

  - (Unbiased) pooled sample covariance is a weighted average

$$\begin{aligned} \hat{\Sigma} &= \frac{n_0 - 1}{(n_0 - 1) + (n_1 - 1)} S_0 + \frac{n_1 - 1}{(n_0 - 1) + (n_1 - 1)} S_1 \\ &= \sum_{j=0}^{1} \sum_{Y_i=j} (\mathbf{x}_i - \hat{\mu}_j)(\mathbf{x}_i - \hat{\mu}_j)^T/(n-2) \end{aligned}$$

R code for LDA Fitting (I)

There are two ways to call the function "lda". The first way is to use a formula and an optional data frame.

```
library(MASS)
lda(formula, data,subset)
```

Arguments:

- *formula*: the form "groups $\sim x_1 + x_2 + \ldots$", where the response is the grouping factor and the right hand side specifies the (non-factor) discriminators.
- *data*: data frame from which variables specified
- *subset*: An index vector specifying the cases to be used in the training sample.

Output:

- an object of class "lda" with multiple components

R code for LDA Fitting (II)

The second way is to use a matrix and group factor as the first two arguments.

```
library(MASS)
lda(x, grouping, prior = proportions, CV = FALSE)
```

Arguments:

- *x*: a matrix or data frame or Matrix containing predictors.
- *grouping*: a factor specifying the class for each observation.
- *prior*: the prior probabilities of class membership. If unspecified, the class proportions for the training set are used.

Output:

- If CV = TRUE, the return value is a list with components "class" (the MAP classification, a factor) and "posterior" (posterior probabilities for the classes).

R code for LDA Prediction

We use the "predict" or "predict.lda" function to classify multivariate observations with lda

```
predict(object, newdata, ...)
```

Arguments:

- *object*: object of class "lda"
- *newdata*: data frame of cases to be classified or, if "object" has a formula, a data frame with columns of the same names as the variables used.

Output:

- a list with the components "class" (the MAP classification, a factor) and "posterior" (posterior probabilities for the classes)

Fisher's Iris Data (Three-Classification Problems)

Fisher (1936) "The use of multiple measurements in taxonomic problems".

- Three species: Iris setosa, Iris versicolor, Iris verginica
- Four features: the length and the width of the sepals and petals, in centimeters.
- 50 samples from each species

In the following analysis, we randomly select 50% of the data points as the training set, and the rest as the test set.

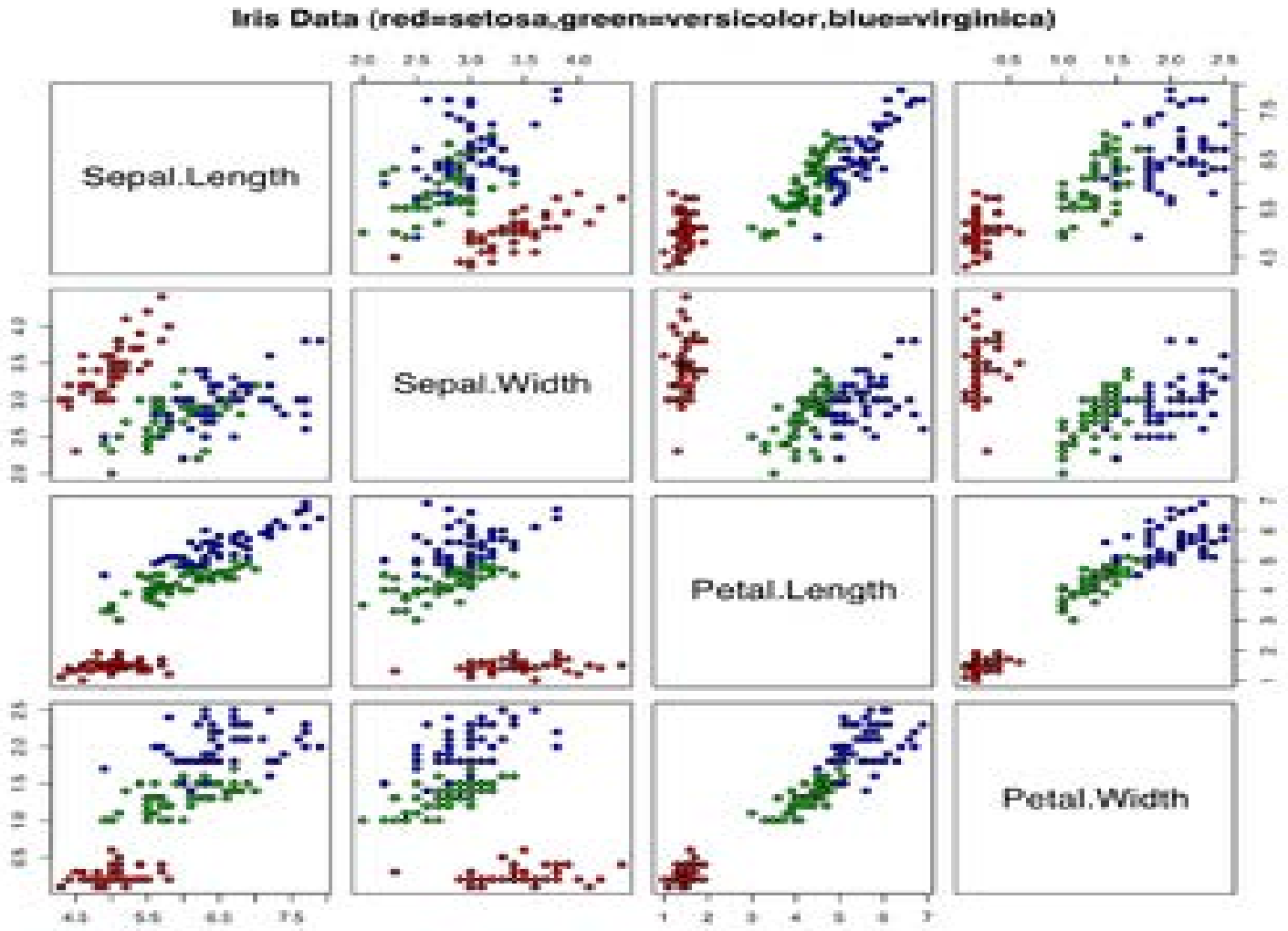

Iris Data (red=setosa,green=versicolor,blue=virginica)
Sepal.Length
Sepal.Width
Petal.Length
Petal.Width

Illustration 1

```
Iris <- data.frame(rbind(iris3[,,1], iris3[,,2],
   iris3[,,3]), Sp = rep(c("s","c","v"), rep(50,3)))
train <- sample(1:150, 75)
table(Iris$Sp[train])
z <- lda(Sp ~ ., Iris, prior = c(1,1,1)/3, subset = train)
```

Training Error and Test Error

```
#training error rate
ytrain <- predict(z, Iris[train, ])$class
table(ytrain, Iris$Sp[train])
train_err <- mean(ytrain!=Iris$Sp[train])
#test error rate
ytest <- predict(z, Iris[-train, ])$class
table(ytest, Iris$Sp[-train])
test_err <- mean(ytest!=Iris$Sp[-train])
```

Illustration 2

```
tr <- sample(1:50, 25)
train <- rbind(iris3[tr,,1], iris3[tr,,2], iris3[tr,,3])
test <- rbind(iris3[-tr,,1], iris3[-tr,,2], iris3[-tr,,3])
cl <- factor(c(rep("s",25), rep("c",25), rep("v",25)))
z <- lda(train, cl)
ytest <- predict(z, test)$class
```

Logistic Regression

Model assumption: the log-odd is linear in $\mathbf{x}$.

$$\log \frac{\Pr(Y=1|\mathbf{X}=\mathbf{x})}{\Pr(Y=0|\mathbf{X}=\mathbf{x})} = \beta_0 + \boldsymbol{\beta}_1^T \mathbf{x}.$$

Define

$$p(\mathbf{x};\boldsymbol{\beta}) \equiv= \frac{\exp(\beta_0 + \boldsymbol{\beta}_1^T \mathbf{x})}{1+\exp(\beta_0 + \boldsymbol{\beta}_l^T \mathbf{x})}$$

Write $\boldsymbol{\beta} = (\beta_0, \boldsymbol{\beta}_1)$. The posterior class probabilities can be calculated as

$$\begin{aligned} p_1(\mathbf{x}) &= \Pr(Y=1|\mathbf{x}) = p(\mathbf{x};\boldsymbol{\beta}), \\ p_0(\mathbf{x}) &= \Pr(Y=0|\mathbf{x}) = 1 - p(\mathbf{x};\boldsymbol{\beta}). \end{aligned}$$

The classification boundary is given by: $\{\mathbf{x} : \beta_0 + \boldsymbol{\beta}_1^T \mathbf{x} = 0\}$.

Model Interpretation

- Denote $\mu = E(Y|\mathbf{X}) = P(Y = 1|\mathbf{X})$
- By assuming

$$g(\mu) = \log[\mu/(1-\mu)] = \beta_0 + \beta_1^T \mathbf{X},$$

  the logit g connects μ with the linear predictor $\beta_0 + \beta_1^T \mathbf{X}$.
- We call g the link function
- $Var(Y|\mathbf{X}) = \mu(1-\mu)$.

Interpretation of β_j

In logistic regression,

$$\text{odds}_{X_j} = \frac{\text{odds}(\ldots, X_j = x+1, \ldots)}{\text{odds}(\ldots, X_j = x, \ldots)} = e^{\beta_j}.$$

- If $X_j = 0$ or 1, then odds for group with $X_j = 1$ are e^{β_j} higher than for group with $X_j = 0$, with other parameters fixed.

For rare diseases,

- when incidence is rare, $Pr(Y = 0) \approx 1$, then odds $\approx Pr(Y = 1)$

$$e^{\beta_j} = \text{odds}_{X_j} \approx \frac{\text{Pr}(\ldots, X_j = x+1, \ldots)}{\text{Pr}(\ldots, X_j = x, \ldots)}.$$

- in a cancer study, an log-OR of 5 means that smokers are $e^5 \approx 150$ times more likely to develop the cancer

Maximum Likelihood Estimate (MLE) for Logistic Models

The joint conditional likelihood of y_i given $\mathbf{x}_i$ is

$$l(\beta) = \sum_{i=1}^{n} \log p_{y_i}(\mathbf{x}; \beta),$$

where

$$p_y(\beta; \mathbf{x}) = p(\mathbf{x}; \beta)^y [1 - p(\mathbf{x}; \beta)]^{1-y}.$$

In details,

$$\begin{aligned} l(\beta) &= \sum_{i=1}^{n} \{y_i \log p(\mathbf{x}_i; \beta) + (1 - y_i) \log[1 - p(\mathbf{x}_i, \beta)]\} \\ &= \sum_{i=1}^{n} \{y_i(\beta_{10} + \beta_1^T \mathbf{x}_i) - \log[1 + \exp(\beta_{10} + \beta_1^T \mathbf{x}_i)]. \end{aligned}$$

.

Score Equations

For simplicity, now assume $\mathbf{x}_i$ has 1 in its first component.

$$\frac{\partial l(\beta)}{\partial \beta} = \sum_{i=1}^{n} \mathbf{x}_i [y_i - p(\mathbf{x}_i; \beta)] = 0,$$

Totally (d+1) nonlinear equations. The first equation

$$\sum_{i=1}^{n} y_i = \sum_{i=1}^{n} p(\mathbf{x}_i; \beta),$$

expected number of 1's = *observed* number in sample.

$$\begin{aligned} \mathbf{y} &= [y_1, \cdots, y_n]^T \\ \mathbf{p} &= [p(\mathbf{x}_1; \beta^{\text{old}}), \cdots, p(\mathbf{x}_n; \beta^{\text{old}})]^T. \\ W &= \text{diag}\left\{ p(\mathbf{x}_i; \beta^{\text{old}})(1 - p(\mathbf{x}_i; \beta^{\text{old}})) \right\}. \end{aligned}$$

Newton-Raphson Algorithm

The second-derivative (Hessian) matrix

$$\frac{\partial^2 l(\beta)}{\partial \beta \partial \beta^T} = -\sum_{i=1}^{n} \mathbf{x}_i \mathbf{x}_i^T p(\mathbf{x}_i; \beta)[1 - p(\mathbf{x}_i; \beta)].$$

1. Choose an initial value β^0
2. Update β by

$$\beta^{\text{new}} = \beta^{\text{old}} - \left[\frac{\partial^2 l(\beta)}{\partial \beta \partial \beta^T}\right]^{-1}_{\beta^{\text{old}}} \frac{\partial l(\beta)}{\partial \beta}_{\beta^{\text{old}}}$$

Using matrix notations, we have

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

Iteratively Re-weighted Least Squares (IRLS)

Newton-Raphson step

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

where we defined the *adjusted response*

$$\mathbf{z} = X\beta^{\text{old}} + W^{-1}(\mathbf{y} - \mathbf{p})$$

- Repeatedly solve weighted least squares till convergence.

$$\beta^{\text{new}} = \arg\min_{\beta} (\mathbf{z} - X\beta)^T W (\mathbf{z} - X\beta),$$

  Weight W, response $\mathbf{z}$, and $\mathbf{p}$ change in each iteration.
- The algorithm can be generalized to $K \geq 3$ case.

Quadratic Approximations

$\widehat{\beta}$ satisfies a self-consistency relationship: it solves a weighted least square fit with response

$$z_i = \mathbf{x}_i^T \widehat{\beta} + \frac{(y_i - \hat{p}_i)}{\hat{p}_i(1 - \hat{p}_i)}$$

and the weight $w_i = \hat{p}_i(1 - \hat{p}_i)$.

- $\beta = 0$ seems to be a good starting value
- Typically the algorithm converges, but it is never guaranteed.
- The weighted residual sum-of-squared is **Pearson chi-square** statistic

$$\sum_{i=1}^{n} \frac{(y_i - \hat{p}_i)^2}{\hat{p}_i(1 - \hat{p}_i)},$$

a quadratic approximation to the deviance.

Statistical Inferences

Using the weighted least squares formulation, we have

- Asymptotic likelihood theory says: if the model is correct, $\widehat{\beta}$ is consistent
- Using central limit theorem, the distribution of $\widehat{\beta}$ converges to $N(\beta, (X^T W X)^{-1})$
- Model building is costly due to iterations, popular shortcuts:
  - For inclusion of a term, use *Rao score test*.
  - For exclusion of a term, use *Wald test*.

  Neither of these two algorithms require iterative fitting, and are based on the maximum likelihood fit of the current model.

R Code for Logistic Regression

```
logist <- glm(formula, family, data, subset, ...)
predict(logist)
```

Arguments:

- *formula*: an object of class "formula"
- *family*: a description of the error distribution and link function to be used in the model.
- *data*: an optional data frame, list or environment containing the variables in the model.
- *subset*: an optional vector specifying a subset of observations to be used in the fitting process.

Output:

- returns an object of class inheriting from "glm" and "lm"

R Code for Logistic Prediction

```
logist <- glm(y~x, data, family=binomial(link="logit"))
predict(logist, newdata)
summary(logist)
anova(logist)
```

- The function "predict" gives the predicted values, newdata is a data frame
- The function "summary" is used to obtain or print a summary of the results
- The function "anova" produces an analysis of variance table.

Relationship between LDA and Least Squares (LS)

For two-class problems, both LDA and least squares fit a linear boundary $\beta_0 + \boldsymbol{\beta}^T \mathbf{x}$. Their solutions have the following relationship:

- The least square regression coefficient $\hat{\boldsymbol{\beta}}$ is proportional to the LDA direction, i.e.,

$$\hat{\boldsymbol{\beta}} \propto \hat{\Sigma}^{-1}(\hat{\boldsymbol{\mu}}_1 - \hat{\boldsymbol{\mu}}_0),$$

  where $\hat{\Sigma}$ is the pooled sample covariance matrix, and $\hat{\boldsymbol{\mu}}_k$ is the sample mean of points from class $k, k = 0, 1$. In other words, their slope coefficients are identical, up to a scalar multiple. (Exercise 4.2 in textbook)
- The LS intercept $\hat{\beta}_0$ is generally different from that of LDA, unless $n_1 = n_0$.

In general, they have different decision rules (unless $n_1 = n_2$).

Common Feature of LDA and Logistic Regression Models

For both LDA and logistic regression, the logit has a linear form

$$\log \frac{\Pr(Y=1|\mathbf{x})}{\Pr(Y=0|\mathbf{x})} = \beta_0 + \boldsymbol{\beta}_1^T \mathbf{x}.$$

Or equivalently, for both estimators, their posterior class probability can be expressed in the form of

$$\Pr(Y=1|\mathbf{x}) = \frac{\exp\left(\beta_0 + \boldsymbol{\beta}_1^T \mathbf{x}\right)}{1 + \exp\left(\beta_0 + \boldsymbol{\beta}_1^T \mathbf{x}\right)}.$$

They have exactly same forms. Are they same estimators?

Major Differences of LDA and Logistsics Regresion

Main differences of two estimators include

- Where is the linear-logit from?
- What assumptions are made on the data distribution? (Difference on data distribution)
- How to estimate the linear coefficients? (Difference in parameter estimation)
- Any assumption on the marginal density of $\mathbf{X}$? (flexibility of model)

Where is Linear-logit from?

For LDA, the linear logit is due to the equal-covariance Gaussian assumption on data

$$\begin{aligned} \log \frac{\Pr(Y=1|\mathbf{x})}{\Pr(Y=0|\mathbf{x})} &= \log \frac{\pi_1}{\pi_0} - \frac{1}{2}(\boldsymbol{\mu}_1+\boldsymbol{\mu}_0)^T\Sigma^{-1}(\boldsymbol{\mu}_1+\boldsymbol{\mu}_0) \\ &\quad +\mathbf{x}^T\Sigma^{-1}(\boldsymbol{\mu}_1-\boldsymbol{\mu}_0) \\ &= \beta_0+\boldsymbol{\beta}_1^T\mathbf{x} \end{aligned}$$

For Logistic model, the linear logit is due to construction

$$\log \frac{\Pr(Y=1|\mathbf{x})}{\Pr(Y=0|\mathbf{x})} = \beta_0+\boldsymbol{\beta}_1^T\mathbf{x}$$

Difference in Marginal Density Assumption

The assumptions on Pr($\mathbf{X}$):

- The logistic model leaves the marginal density of $\mathbf{X}$ arbitrary and unspecified.
- The LDA model assumes a Gaussian density

$$\Pr(\mathbf{X}) = \sum_{j=0}^{1} \pi_j \phi(\mathbf{X}; \boldsymbol{\mu}_j, \Sigma)$$

Conclusion: The logistic model makes less assumptions about the data, and hence is more general.

Difference in Parameter Estimation

Logistic regression

- Maximizing the conditional likelihood, the multinomial likelihood with probabilities $\Pr(Y = k|\mathbf{X})$
- The marginal density Pr(X) is totally ignored (fully nonparametric using the empirical distribution function which places $1/n$ at each observation)

LDA

- Maximizing the full log-likelihood based on the joint density

$$\Pr(\mathbf{X}, Y = j) = \phi(\mathbf{X}; \mu_j, \Sigma)\pi_j,$$

  Standard MLE theory leads to estimators $\hat{\boldsymbol{\mu}}_j, \hat{\Sigma}, \hat{\pi}_j$
- Marginal density does play a role

More Comments

- LDA is easier to compute than logistic regression.
- If the true $f_k(\boldsymbol{x})$'s are Gaussian, LDA is better.
  - Logistic regression may lose efficiency around 30% asymptotically in error rate (by Efron 1975)
- Robustness?
  - LDA uses all the points to estimate the covariance matrix; more information but not robust against outliers
  - Logistic regression down-weights points far from decision boundary (recall the weight is $p_i(1-p_i)$; more robust and safer
- In practice, these two methods often give similar results (for approximately normal distributed data)

Two-dimensional Linear Example

Consider the following scenarios for a two-class problem:

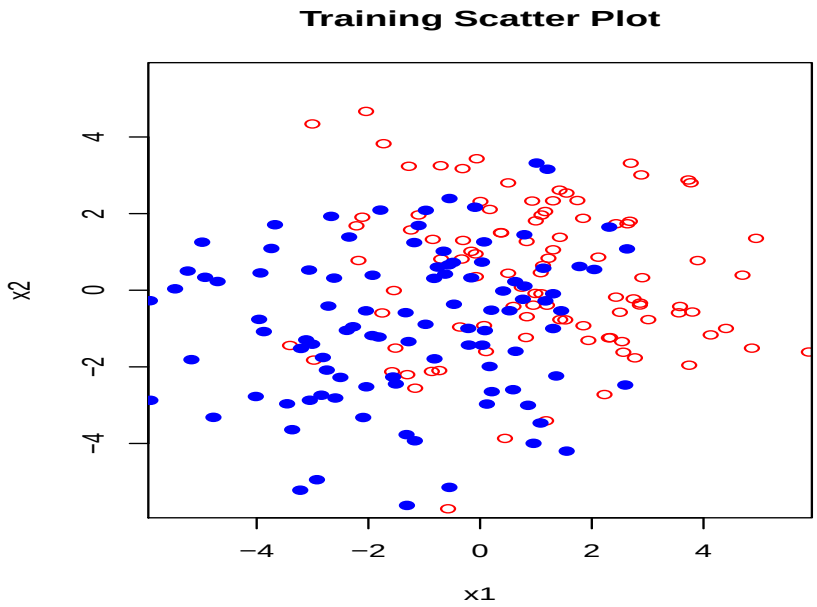
- $\pi_1 = \pi_0 = 0.5$.
- Class 1: $\mathbf{X} \sim N_2((1,1)^T, 4\mathbf{I})$
- Class 2: $\mathbf{X} \sim N_2((-1,-1)^T, 4\mathbf{I})$

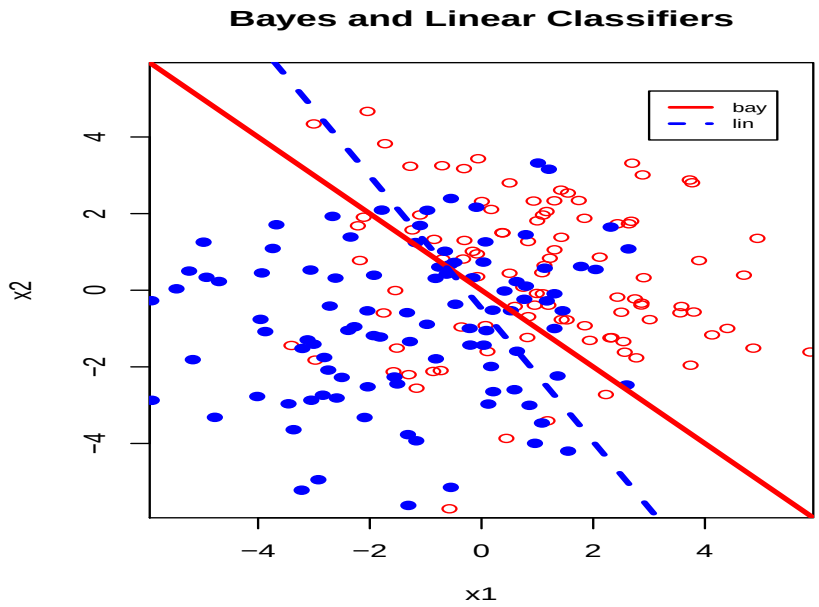
The Bayes boundary is

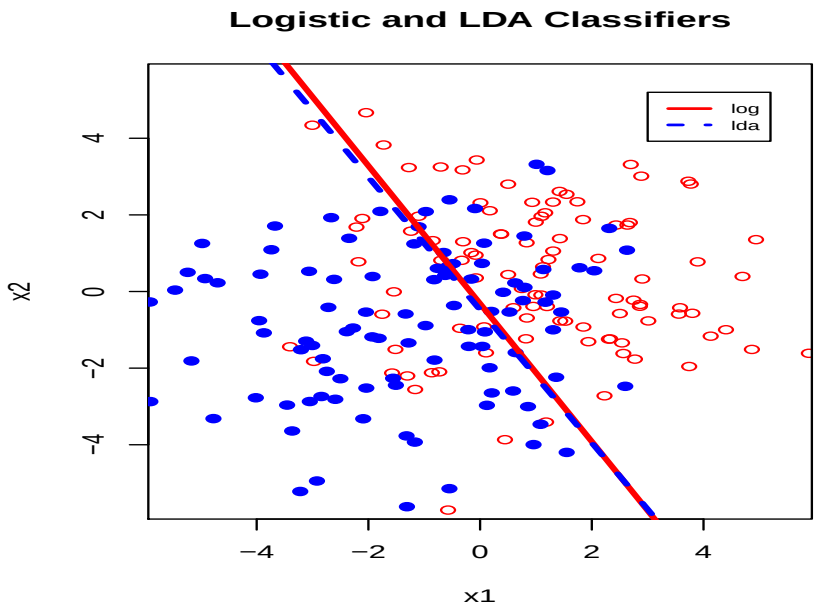
$$\{\mathbf{x} : x_1 - x_2 = 0\}.$$

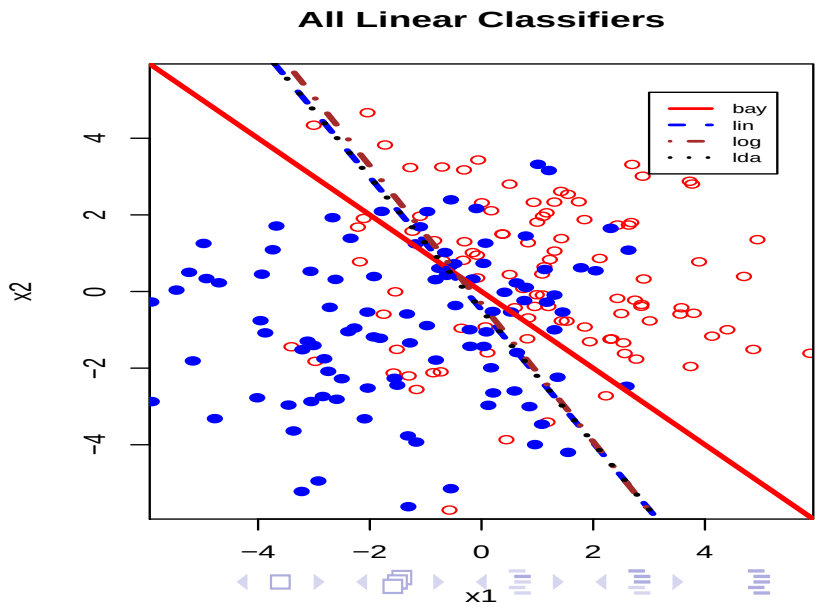
We generate

- the "training set" of $n = 200, 400$ to fit the classifier
- the "testing set" of $n' = 2000$ " to evaluate its prediction performance.


Training Scatter Plot
x2
x1
−4
−2
0
2
4


Bayes and Linear Classifiers
bay
lin
x2
x1
−4
−2
0
2
4


Logistic and LDA Classifiers
log
lda
x2
x1
−4
−2
0
2
4


All Linear Classifiers
bay
lin
log
lda
x2
x1
−4
−2
0
2
4

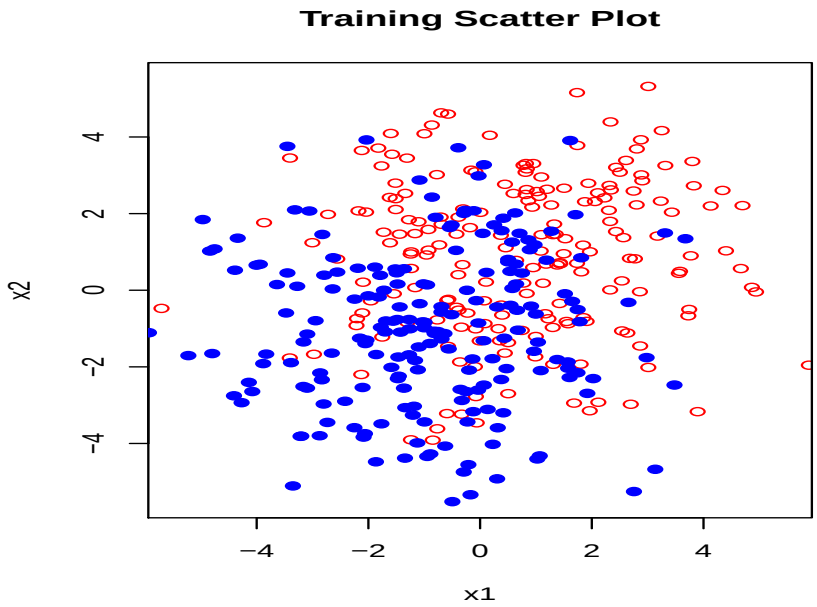
Performance of Various Classifiers (n=200)

	Bayes	Linear	Logistic	LDA
Train Error	0.250	0.255	0.255	0.255
Test Error	0.240	0.247	0.242	0.247

Fitted classification boundaries:

Linear & LDA: $x_2 = -0.48 - 1.73x_1$

Logistic: $x_2 = -0.32 - 1.80x_1$.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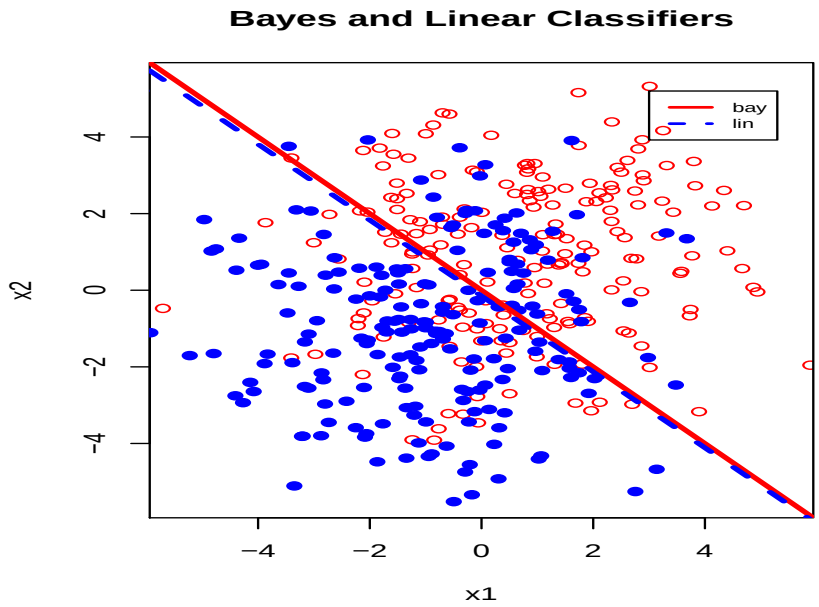
4


Bayes and Linear Classifiers
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x1
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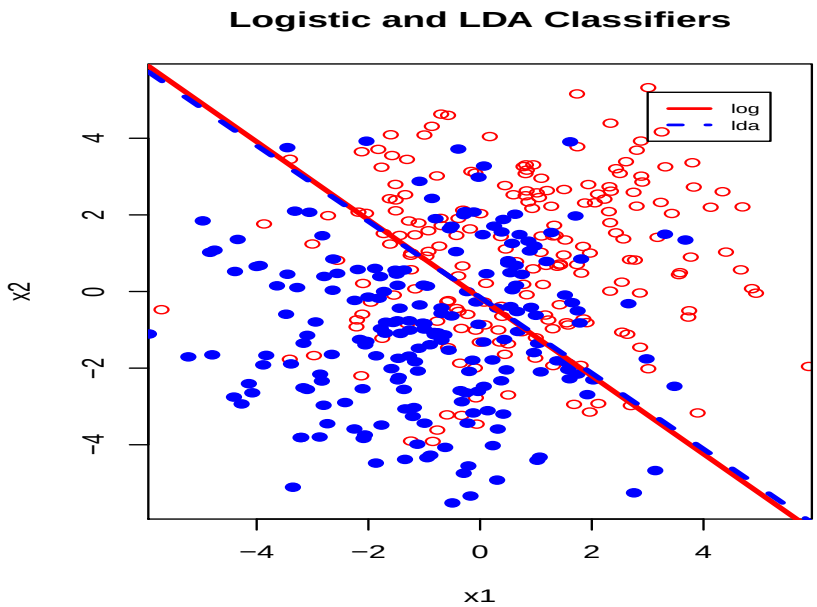
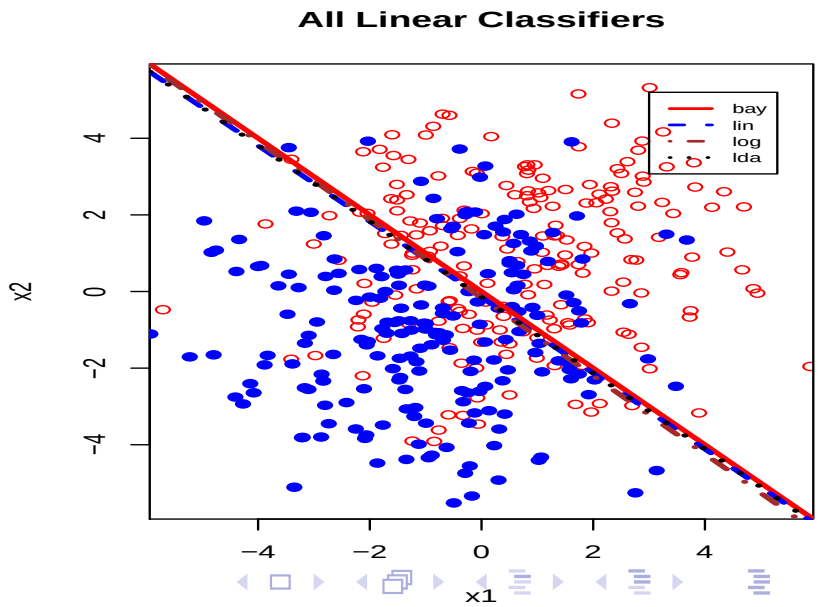
−2
0
2
4


Logistic and LDA Classifiers
log
lda
x2
x1
−4
−2
0
2
4


All Linear Classifiers
bay
lin
log
lda
x2
x1
−4
−2
0
2
4