Chapter 4: Classification

The linear model in Ch. 3 assumes the response variable Y is quantitative. But in many situations, the response is categorical.

e.g. eye color cancer diagnosi's which product a customer would purchase.

In this chapter we will look at approaches for predicting <u>categorical responses</u>, a process known as *classification*.

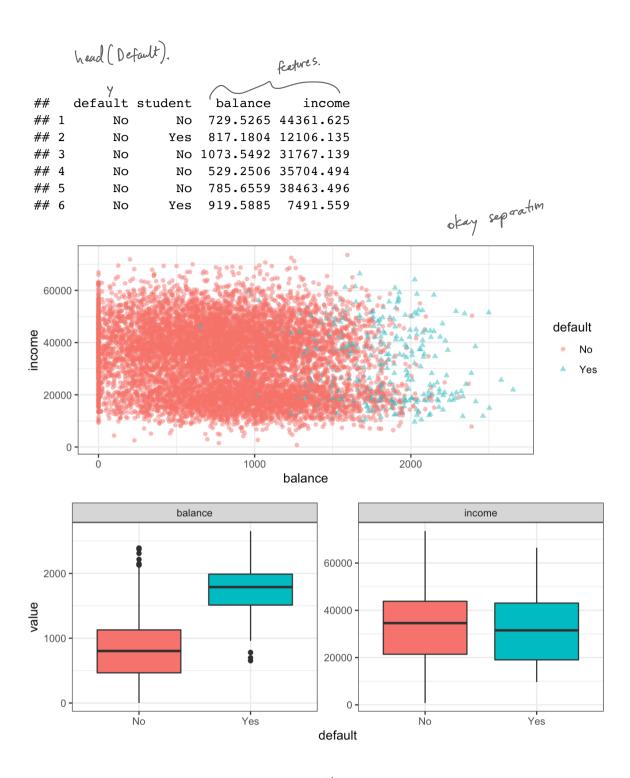
Classification problems occur often, perhaps even more so than regression problems. Some examples include

- 1. A person arrives in the emerging room of set of symptoms that could be attributed to 3 root cances. predict which undition the person bas.
- 2. An online banking service must be able the determine it a transaction is fraudulent or not on The basis of 16 address, past transaction history, etc.
- 3. Something is in the street in front of a salf-driving car you are riding in. The car must determine if if B a human or another car.

As with regression, in the classification setting we have a set of training observations $(x_1, y_1), \ldots, (x_n, y_n)$ that we can use to build a classifier. We want our classifier to perform well on the training data and also on data not used to fit the model (**test data**).

We will use the Default data set in the ISLR package for illustrative purposes. We are interested in predicting whether a person will default on their credit card payment on the basis of annual income and credit card balance.

fit a model



relationship between balance and default

(in most real world problems the relationship is not so cleer).

1 Why not Linear Regression?

I have said that linear regression is not appropriate in the case of a categorical response. Why not?

Let's try it anyways. We could consider encoding the values of default in a quantitative repsonse variable Y

$$Y = egin{cases} 1 & ext{if default} \ 0 & ext{otherwise} \end{cases}$$

Using this coding, we could then fit a linear regression model to predict Y on the basis of **income** and **balance**. This implies an ordering on the outcome, not defaulting comes first before defaulting and insists the difference between these two outcomes is 1 unit. In practice, there is no reason for this to be true.

We could let
$$Y = \begin{cases} 0 & \text{if default} \\ 1 & \text{otherwise} \end{cases}$$
 there is no natural reason the choose $f(1)$,
 $y = \begin{cases} 1 & \text{if default} \\ 0 & \text{otherwise} \end{cases}$ but it has an advartage:

Using the dummy encoding, we can get a rough estimate of P(default|X), but it is not guaranteed to be scaled correctly.

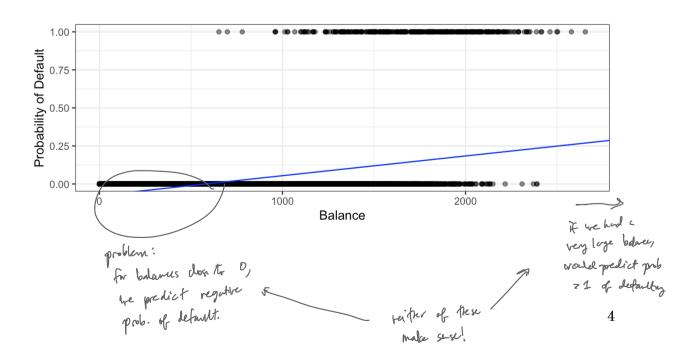
2 Logistic Regression

Let's consider again the default variable which takes values Yes or No. Rather than modeling the response directly, logistic regression models the *probability* that Y belongs to a particular category.

For any given value of balance, a prediction can be made for default.

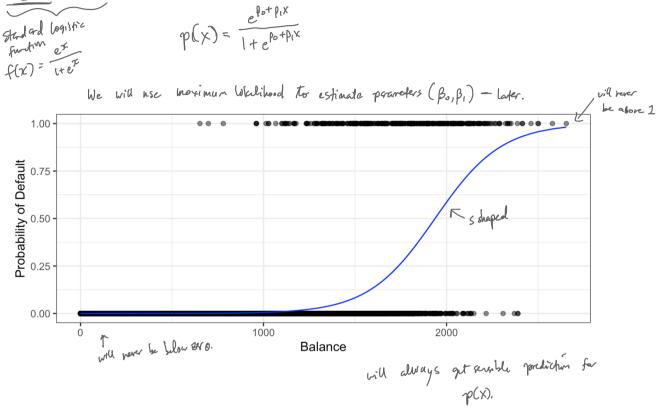
2.1

How should we model the relationship between p(X) = P(Y = 1 | X) and X? We could use a linear regression model to represent those probabilities



$$p(\mathbf{X}) = \beta_0 + \beta_1 \mathbf{X}$$

To avoid this, we must model p(X) using a function that gives outputs between 0 and 1 for all values of X. Many functions meet this description, but in *logistic* regression, we use the *logistic* function,



After a bit of manipulation,

$$\frac{p(sc)}{1-p(x)} = e^{f_0 + f_1 \cdot x}$$

$$\int_{1}^{1} e^{pob \, dt} \frac{p + p \cdot b}{p \cdot b} dt \frac{p \cdot b}{p \cdot b} dt \frac{$$

$$e_x$$
; $p(x) = 0.2$ ([in 5 people default) => odds = $\frac{0.2}{1-0.2} = \frac{1}{4}$

By taking the logarithm of both sides we see,

$$\log\left(\frac{p(x)}{1-p(x)}\right) = \beta_0 + \beta_1 x$$

"(og-odds" log-odds is linear in X.
"logif" log-odds"

Recall from Ch. 3 that β_1 gives the "average change in Y associated with a one unit increase in X." In contrast, in a logistic model,

However, because the relationship between p(X) and X is not linear, β_1 does **not** correspond to the change in p(X) associated with a one unit increase in X. The amount that p(X) changes due to a 1 unit increase in X depends on the current value of X.

Regardless of the value of X,
if
$$\beta_1$$
 is positive => increasing X increases $p(X)$.
if β_1 is hegative => increasing X reduces $p(K)$.

2.2 Estimating the Coefficients

The coefficients β_0 and β_1 are unknown and must be estimated based on the available training data. To find estimates, we will use the method of *maximum likelihood*.

```
The basic intuition is that we seek estimates for \beta_0 and \beta_1 such that the predicted
 probability \hat{p}(x_i) of default for each individual corresponds as closely as possible to the
probability p(x_i) of default status. Endingeneral given the interval of particular of particular of particular of the data

to do twis, use the dividing L(\beta_0,\beta_1|\{2Y_{i_1} \ge i_{i_{i=1}}^n) = \prod_{i:y_i=1}^{TT} p(x_i) \prod_{i:y_i=0}^{TT} (1-p(x_i)).

\hat{\beta}_0 and \hat{\beta}_1 chosen to maximize L(\beta_0,\beta_1). Cuse calculus: derivatives met \beta_0,\beta_1, set =0, solve).

Use numeric optimization

\hat{\beta}_0 and \hat{\beta}_1 chosen to maximize L(\beta_0,\beta_1). Cuse calculus: derivatives met \beta_0,\beta_1, set =0, solve).

\hat{\beta}_0 and \hat{\beta}_1 chosen to maximize L(\beta_0,\beta_1). Cuse calculus: derivatives met \beta_0,\beta_1, set =0, solve).

\hat{\beta}_0 and \hat{\beta}_1 chosen to maximize \hat{\beta}_0 and \hat{\beta}_1 and \hat{\beta}_1 chosen to maximize \hat{\beta}_0 and \hat{\beta}_1 chosen to maximize \hat{\beta}_1 and \hat{\beta}_2 and \hat{\beta}_2 and \hat{\beta}_1 chosen to maximize \hat{\beta}_2 and \hat{\beta}_3 and \hat{\beta}_4 chosen to maximize \hat{\beta}_1 and \hat{\beta}_2 and \hat{\beta}_3 and \hat{\beta}_4 and \hat{\beta}_1 chosen to maximize \hat{\beta}_1 and \hat{\beta}_2 and \hat{\beta}_3 and \hat{\beta}_4 and \hat{\beta}_4 and \hat{\beta}_4 and \hat{\beta}_4 and \hat{\beta}_4 and \hat{\beta}_5 and \hat{\beta}_5 and \hat{\beta}_4 and \hat{\beta}_5 and 
     logistic spec <- logistic reg()</pre>
     logistic fit <- logistic spec |>
            fit(default ~ balance, family = "binomial", data = Default)
                                                             YNX
                                                                                                           Y takes values in 50,13
     logistic fit |>
            pluck("fit") |>
            summary()
     ##
     ## Call:
     ## stats::glm(formula = default ~ balance, family = stats::binomial,
     ##
                            data = data)
     ##
     ## Deviance Residuals:
                                                                            Median
     ##
                           Min
                                                            1Q
                                                                                                                       3Q
                                                                                                                                                 Max
              -2.2697 -0.1465 -0.0589
                                                                                                   -0.0221
     ##
                                                                                                                                        3.7589
                                                                                                                                                                      Hypothesis test Hos Bi=0
Ha: Bi =0
                                                                                             accuracy
of estimates
     ##
              Coefficients: b, b
     ##
                                                            Estimate Std. Error z value Pr(>|z|)
     ##
     ## (Intercept) -1.065e+01
                                                                                             3.612e-01
                                                                                                                                -29.49
                                                                                                                                                              <2e-16 ***
                                                                                                                                                                                                               - if H_0: \beta_1=0 bree, implies

P(X) = \frac{e^{\beta_0}}{1+e^{\beta_0}}
                                                                                                                                                              <2e-16 ***
     ## balance
                                                          5.499e-03
                                                                                          2.204e-04
                                                                                                                                    24.95
                                                                                                                                                                                                                             p(x) = \frac{e^{R_0}}{1+e^{R_0}}
     ##
              ____
     ## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
                                                                                                                                                                                                                              (doesn't depend on X =>
     ##
     ##
               (Dispersion parameter for binomial family taken to be 1)
     ##
     ##
                            Null deviance: 2920.6
                                                                                                      on 9999
                                                                                                                                    degrees of freedom
     ## Residual deviance: 1596.5 on 9998
                                                                                                                                    degrees of freedom
     ## AIC: 1600.5
     ##
     ## Number of Fisher Scoring iterations: 8
            B: = 0.0055 => ingrase in blance associated w/ increase in prob. of default.
                                                 => one unit increases in balance associated w/ overage intease of log-odds by .0055 mits.
```

2.3 Predictions

Once the coefficients have been estimated, it is a simple matter to compute the probability of default for any given credit card balance. For example, we predict that the default probability for an individual with balance of \$1,000 is

$$\hat{p}(x) = \frac{e^{\hat{h}_0 + \hat{h}_1 x}}{1 + e^{\hat{h}_0 + \hat{h}_1 x}}$$

$$\hat{p}(1000) = \frac{e^{-10.6513 + 0.0055 \times 1000}}{(1 + e^{10.6513 + 0.0055 \times 1000} = 0.00576)}$$

In contrast, the predicted probability of default for an individual with a balance of 2,000 is

$$\hat{p}(2000) = \frac{e^{-(0.6513 + 0.0055 \times 2000}}{|+e^{-(0.6513 + 0.0055 \times 2000}} = 0.586 = 0.5$$

$$maybe \ ve \ would \ predict \ default = yes \ bard \ on \ a \ threshold \ f \ 0.5.$$

(tidy models: augment predict)

2.4 Multiple Logistic Regression

We now consider the problem of predicting a binary response using multiple predictors. By analogy with the extension from simple to multiple linear regression,

$$p(x) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$

$$p(x) = \frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}}{(1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p})}$$

Just as before, we can use maximum likelihood to estimate $\beta_0, \beta_1, \ldots, \beta_p$.

```
logistic_fit2 <- logistic_spec |> specification.
  fit(default ~ ., family = "binomial", data = Default)
                   × Y N every other
> Variable industa
                                         Y is in Soli3.
logistic fit2 |>
  pluck("fit") |>
  summary()
```

```
##
## Call:
## stats::glm(formula = default ~ ., family = stats::binomial, data =
data)
##
## Deviance Residuals:
##
       Min
             10 Median
                                     3Q
                                              Max
## -2.4691 -0.1418 -0.0557 -0.0203
                                           3.7383
##
                                               Ho: B: =0
## Coefficients: \hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_3
                               SE(Bi)
                                                Ha: Bito
                  Estimate Std. Error z value Pr(>|z|)
##
## studentYes -6.468e-01 2.363e-01 -2.738 0.00619 **
## balance
                5.737e-03 2.319e-04
                                         24.738 < 2e-16 ***
## income
                 3.033e-06 8.203e-06
                                          0.370
                                                 0.71152 cm no significant
                                                             relationship
## ___
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05/'.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
##
       Null deviance: 2920.6 on 9999
                                          degrees of freedom
## Residual deviance: 1571.5 on 9996
                                          degrees of freedom
## AIC: 1579.5
##
## Number of Fisher Scoring iterations: 8
Brudet (405) <0 => if you are a student LESS likely to default holding balance & income constant.
Student confounded of income. (see "restricted regression" for more).
```

By substituting estimates for the regression coefficients from the model summary, we can make predictions. For example, a student with a credit card balance of \$1,500 and an income of \$40,000 has an estimated probability of default of

$$\hat{p}\left(\Xi = \{4es, 1500, 40000\}\right) = e_{xp}\left(-10.689 + (-0.6468) \times 1 + 0.00574 \times 1500 + 0.000003 \times 40000\right)$$

$$= 0, 058$$

A non-student with the same balance and income has an estimated probability of default of

p(z = {No, 1500, 40003) = 0, 05

2.5 Logistic Regression for > 2 Classes

We sometimes which to classify a response variable that has more than two classes. There are multi-class extensions to logistic regression ("multinomial regression"), but there are far more popular methods of performing this.

3 LDA "linear discriminant analysis"

Logistic regression involves direction modeling P(Y = k | X = x) using the logistic function for the case of two response classes. We now consider a less direct approach.

Idea:

Model the distribution of the predictors X separately in each of the response classes (given Y).
and then use Bayes theorem to flip tase and got
$$P(Y=k|X=x)$$
.
$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

Why do we need another method when we have logistic regression?

 Classes well separated, parameter estimates of predictors are surprisingly unstable
 n is small (¹/₂ × ^{apx} Normal) → LDA more stable

3. if we have 72 vesponse classes

3.1 Bayes' Theorem for Classification

Suppose we wish to classify an observation into one of K classes, where $K \ge 2$.

$$\begin{array}{l} Y - response \quad (k \quad distinct) \\ \pi_{k} \\ \Rightarrow prior \Rightarrow overall probability that an observation is \\ in class k \\ \end{array}$$

$$\begin{array}{l} F_{k(x)} = \left\{ P(X = x \mid Y = k) \right\} \Rightarrow discrete \\ (kensity of \quad (P(X in some gnall interval (Y = k)) \rightarrow continuens) \\ x in class k \\ \end{array}$$

$$\begin{array}{l} \frac{P(Y = k \mid X = x)}{P_{k}(x)} = \frac{P(X = x \mid Y = k) P(Y = k)}{P(X = x)} = \frac{f_{k}(x) \cdot \pi_{k}}{f_{k}(x)} \\ \frac{P(Y = k \mid X = x)}{P_{k}(x)} = \frac{P(X = x \mid Y = k) P(Y = k)}{f_{k}(x)} = \frac{f_{k}(x) \cdot \pi_{k}}{f_{k}(x)} \\ \frac{P(Y = k \mid X = x)}{P_{k}(x)} = \frac{P(X = x \mid Y = k) P(Y = k)}{f_{k}(x)} \\ \end{array}$$

$$\begin{array}{l} P(Y = k \mid X = x) = \frac{P(X = x \mid Y = k) P(Y = k)}{f_{k}(x)} \\ \frac{P(X = x \mid Y = k) P(Y = k)}{f_{k}(x)} \\ \end{array}$$

prior
$$\mathcal{T}_{k} = \frac{\text{# of obs. In Class k}}{\text{Total # of observations}}$$

Estimating $f_k(x)$ is more difficult unless we assume some particular forms.

If we can estimate $f_{k}(x) \rightarrow we can develop$ a classifier close to the "BEST" classifier.

3.2 p = 1

Let's (for now) assume we only have 1 predictor. We would like to obtain an estimate for $f_k(x)$ that we can plug into our formula to estimate $p_k(x)$. We will then classify an observation to the class for which $\hat{p}_k(x)$ is greatest.

Suppose we assume that $f_k(x)$ is normal. In the one-dimensional setting, the normal density takes the form

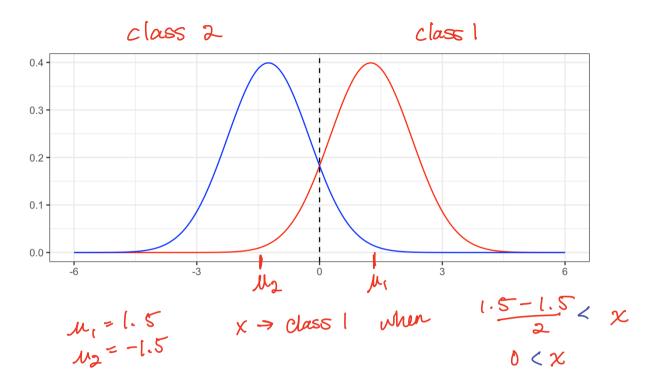
$$\begin{aligned} & \mathcal{R} \sim \mathcal{N}(\mathcal{M}_{\mathcal{K}}, \sigma_{\mu}^{\mathcal{A}}) \\ & f_{\mu}(x) = \int_{\overline{2\pi\sigma_{\mu}^{2}}}^{1} exp\left\{ -\frac{1}{2\sigma_{\mu}^{2}} \left(x - \mathcal{M}_{\mu} \right)^{2} \right\} \\ & \text{Assume for now} \quad \sigma_{\mu}^{2} = \sigma^{2} \quad \text{for all } \mathcal{K} \\ & \text{Plugging this into our formula to estimate } p_{k}(x), \\ & \mathcal{P}(x) = \mathcal{P}(1 - \mathcal{K}[x = x)) = \begin{array}{c} \mathcal{P}^{\text{rior}} & \frac{1}{\pi_{\mathcal{K}}} \left(\frac{1}{2\sigma_{\mu}^{2}\sigma^{2}} exp\left\{ -\frac{1}{2\sigma^{2}} \left(x - \mathcal{M}_{\mu} \right)^{2} \right\} \right) \\ & \mathcal{P}_{\mu}(x) = \mathcal{P}(1 - \mathcal{K}[x = x)) = \begin{array}{c} \mathcal{P}^{\text{rior}} & \frac{1}{\pi_{\mathcal{K}}} \left(\frac{1}{2\sigma_{\mu}^{2}\sigma^{2}} exp\left\{ -\frac{1}{2\sigma^{2}} \left(x - \mathcal{M}_{\mu} \right)^{2} \right\} \\ & \mathcal{P}(x - \pi_{\mathcal{K}}) = \frac{1}{2\sigma_{\mu}^{2}\sigma^{2}} exp\left\{ -\frac{1}{2\sigma^{2}} \left(x - \mathcal{M}_{\mu} \right)^{2} \right\} \\ & \mathcal{P}(x - \pi_{\mathcal{K}}) = \sum_{\mu} \mathcal{P}(x - \pi_{\mathcal{K}}) \mathcal{P}(x - \pi_{\mu}) = \sum_{\mu} \mathcal{P}(x - \pi_{\mathcal{K}}) \mathcal{P}(x - \pi_{\mu}) \\ & \mathcal{P}(x - \pi_{\mu}) = \sum_{\mu} \mathcal{P}(x - \pi_{\mu}) \mathcal{P}(x - \pi_{\mu}) \mathcal{P}(x - \pi_{\mu}) \mathcal{P}(x - \pi_{\mu}) \\ & \mathcal{P}(x - \pi_{\mu}) = \sum_{\mu} \mathcal{P}(x - \pi_{\mu}) \\ & \mathcal{P}(x - \pi_{\mu}) = \sum_{\mu} \mathcal{P}(x - \pi_{\mu}) \mathcal{P}(x$$

maximizing
$$\delta_{k}(x) = \chi \frac{\mu_{k}}{\sigma^{2}} - \frac{\mu_{k}^{2}}{2\sigma^{2}} + \log(\pi_{k}) \leftarrow \frac{\lambda_{k}}{\sigma^{2}}$$

Example 3.1 Let K = 2 and $\pi_1 = \pi_2$. When does the Bayes classifier assign an observation to class 1?

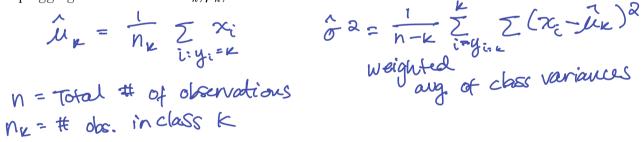
$$\begin{split} & \delta_{1}(x) > \delta_{2}(x) \\ & \delta_{1}(x) = \chi \frac{\mu_{1}}{\sigma^{2}} - \frac{\mu_{2}}{2\sigma^{2}} + \log(\pi_{1}) > \chi \frac{\mu_{2}}{\sigma^{2}} - \frac{\mu_{2}}{2\sigma^{2}} + \log(\pi_{2}) \\ & = 2\chi(\mu_{1} - \mu_{2}) > \mu_{1}^{2} - \mu_{2}^{2} \\ & \mu_{1} < \mu_{2} \\ & \chi < (\mu_{1} - \mu_{2}) > (\mu_{1} - \mu_{2})(\mu_{1} + \mu_{2}) \\ & \chi < \mu_{1} + \mu_{2} \\ & \chi > \frac{\mu_{1} + \mu_{2}}{2} \\ \end{split}$$

 $\mu_1 > \mu_2$



In practice, even if we are certain of our assumption that X is drawn from a Gaussian distribution within each class, we still have to estimate the parameters $\mu_1, \ldots, \mu_K, \pi_1, \ldots, \pi_K, \sigma^2$.

The *linear discriminant analysis* (LDA) method approximated the Bayes classifier by plugging estimates in for π_k, μ_k, σ^2 .



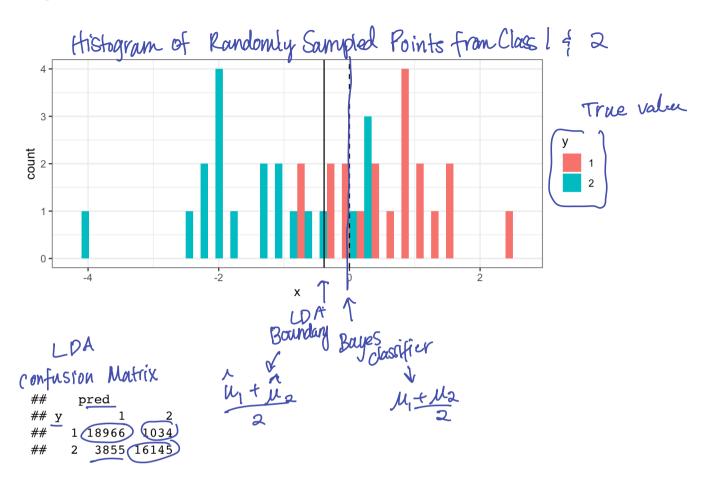
Sometimes we have knowledge of class membership probabilities π_1, \ldots, π_K that can be used directly. If we do not, LDA estimates π_k using the proportion of training observations that belong to the *k*th class.

$$\hat{\mathcal{T}}_{\mathbf{k}} = \frac{\mathbf{n}_{\mathbf{k}}}{\mathbf{n}}$$

The LDA classifier assignes an observation X = x to the class with the highest value of

$$S_{k}(x) = x \frac{\mu_{k}}{\partial 2} - \frac{\mu_{k}}{2\partial 2} + \log(\hat{\pi}_{k})$$

$$f$$
linear



The LDA test error rate is approximately 12.22% while the Bayes classifier error rate is approximately 10.52%.

$$\frac{1034+3855}{8966+1034+3855+16145} = error$$

(

The LDA classifier results from assuming that the observations within each class come from a normal distribution with a class-specific mean vector and a common variance σ^2 and plugging estimates for these parameters into the Bayes classifier.

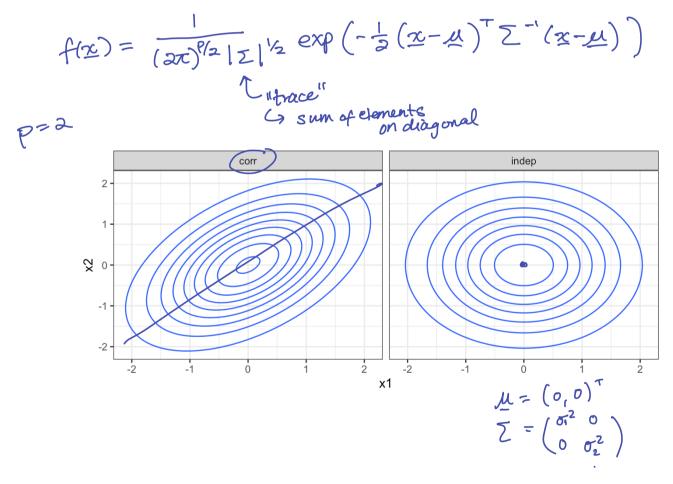
1

we will relax this.

3.3 p > 1

We now extend the LDA classifier to the case of multiple predictors. We will assume $\chi = (\chi_1, \ldots, \chi_p) \sim MNN(\mathcal{M}, \mathcal{Z})$

Formally the multivariate Gaussian density is defined as



In the case of p > 1 predictors, the LDA classifier assumes the observations in the *k*th class are drawn from a multivariate Gaussian distribution $N(\mu_k, \Sigma)$.

Plugging in the density function for the *k*th class, results in a Bayes classifier

Once again, we need to estimate the unknown parameters $\mu_1, \ldots, \mu_K, \pi_1, \ldots, \pi_K, \Sigma$.

$$\delta_{k}(x) = x^{T} \hat{\Sigma}^{T} \hat{\mu}_{k} - \frac{1}{2} \mu_{k}^{T} \hat{\Sigma}^{T} \hat{\mu}_{k} + \log \hat{\pi}_{k}$$

To classify a new value X = x, LDA plugs in estimates into $\delta_k(x)$ and chooses the class which maximized this value.

Let's perform LDA on the Default data set to predict if an individual will default on their CC payment based on balance and student status.

```
lda spec <- discrim linear(engine = "MASS")</pre>
    lda_fit <- lda_spec |>
                                 YNX
      fit(default ~ student + balance, data = Default)
                          specify formula just like lines repression or logistic regression
    lda_fit |>
      pluck("fit")
    ## Call:
    ## lda(default ~ student + balance, data = data)
                                                                      1
    ##
    ## Prior probabilities of groups:
    ##
           No
                  Yes
                             - estimates of TIK based on class membrship in training data.
    ## 0.9667 0.0333
    ##
    ## Group means:
                                              average of each predictor
-ithin each class, use to estimate me
                          balance
           studentYes
    ##
    ## No (0.2914037, 803.9438)
   ## Yes (0.3813814 1747.8217)
    ##
    ## Coefficients of linear discriminants:
    ##
                             T<sub>D</sub>1
★ ## studentYes -0.249059498
                                             F linear combinations of student and bulance
    ## balance
                    0.002244397
                                                   und now LDA decision rule.
```

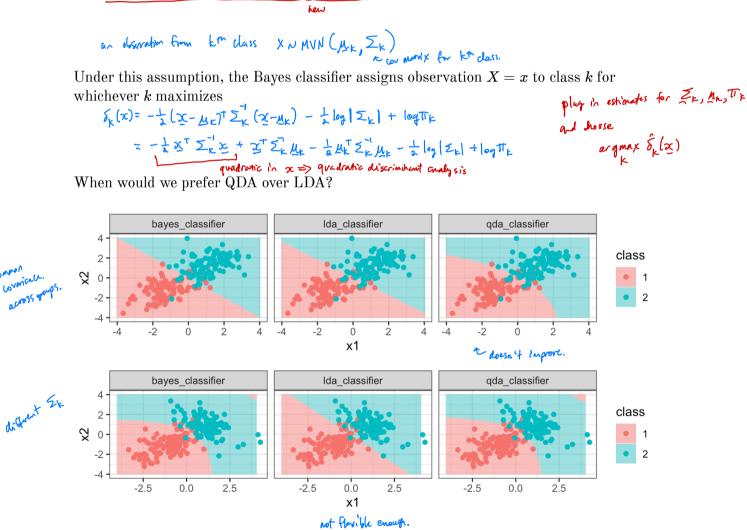
$$|da_{i}fit|^{2} \qquad \text{while a confision matrix} \\ |da_{i}fit|^{2} \qquad \text{while a confision matrix} \\ |augment(new_{i}data = Default)|^{2} \\ conf_mat(truth = default, estimate = .pred_elass) \\ \# \\ restrict \\ \# \\ restrict$$

How to choose? Domain knowledge (CV restricts), or pick 0.5 because has proverial justification,

3.4 QDA

LDA assumes that the observations within each class are drawn from a multivariate Gaussian distribution with a class-specific mean vector and a common covariance matrix across all K classes.

Quadratic Discriminant Analysis (QDA) also assumes the observations within each class are drawn from a multivariate Gaussian distribution with a class-specific mean vector but now each class has its own covariance matrix.



When here are p predictors, estimating Z_k requires estimating $\frac{p(p+1)}{2}$ granders $\implies K \frac{p(p+1)}{2}$ prometers. LDA is linear in $X \implies$ only $K \cdot p$ parameters the estimate.

> LOA is much less fluxible than QDA, but if global variance assumption is bad, LDA night be wildly off >> QDA?

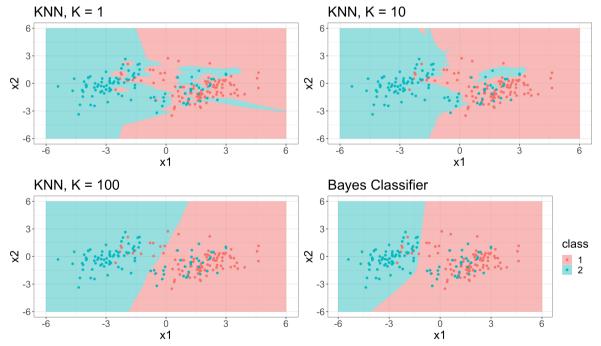
> LDA > QDA if not many praining ofs.

4 KNN

Another method we can use to estimate P(Y = k | X = x) (and thus estimate the Bayes classifier) is through the use of K-nearest neighbors.

The KNN classifier first identifies the K points in the training data that are closest to the test data point X = x, called $\mathcal{N}(x)$.

Just as with regression tasks, the choice of K (neighborhood size) has a drastic effect on the KNN classifier obtained.



5 Comparison

LDA vs. Logistic Regression

(LDA & Logistic Regression) vs. KNN $\,$

QDA