Chapter 4: Classification

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

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

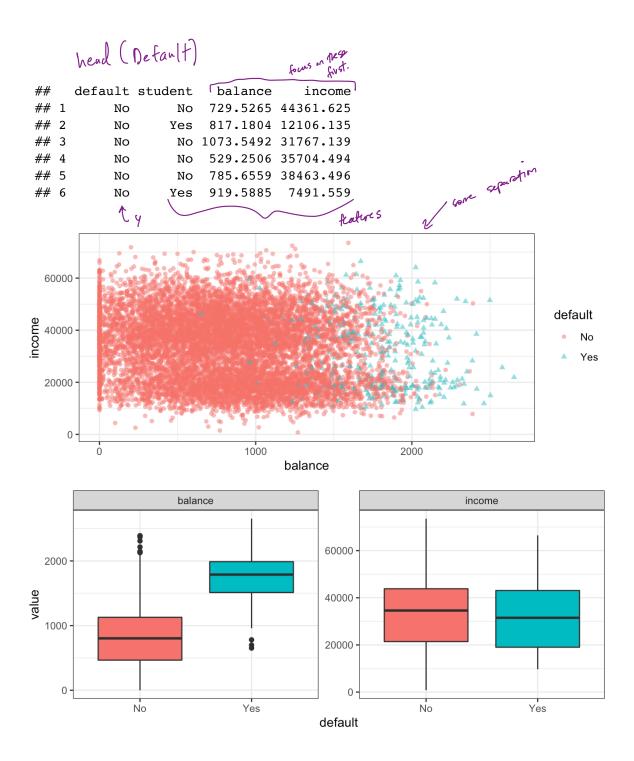
Classification problems occur often, perhaps even more so than regression problems. Some examples include

- 1. A person arrives in the ER W/ Set of symptoms that could possibly be attributed to one of 3 conditions. Which one of these conditions does the person have?
- 2. An online banking service must be able to determine if a transaction is fraudulent on basis of user's IP address, past transaction history, etc.
- 3. Something is in the street in front of the self-drinky car you are riding in.
 The cormust determine if it is 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.

sit and sul



pronounced relationship stul balance and default by in most problems, this relationship is not so dear.

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 $\mathtt{default}$ 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
$$Y = \frac{20}{21}$$
 den't default
$$Y = \frac{8}{2} \frac{0}{(00)} \frac{\text{den't}}{\text{den't}}$$

there is no notional reservation to use of emodify. but is has an advantage:

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

head problem: this connot easily be extended to more than 2 classes

We will instead use methods specifically formulated for categorical response.

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.

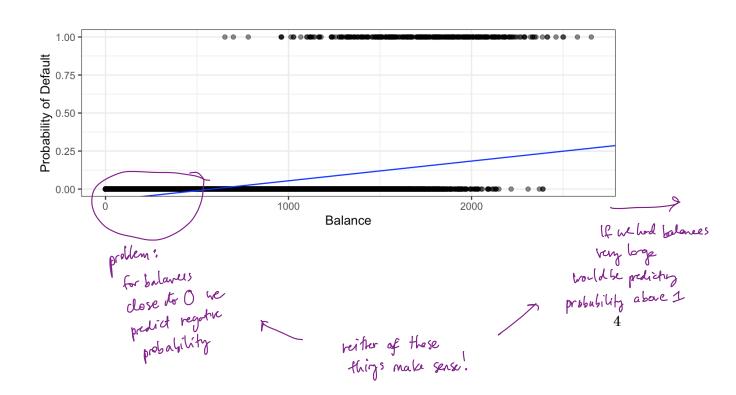
using o/1 erando

Ahreshold.

2.1 The Model

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

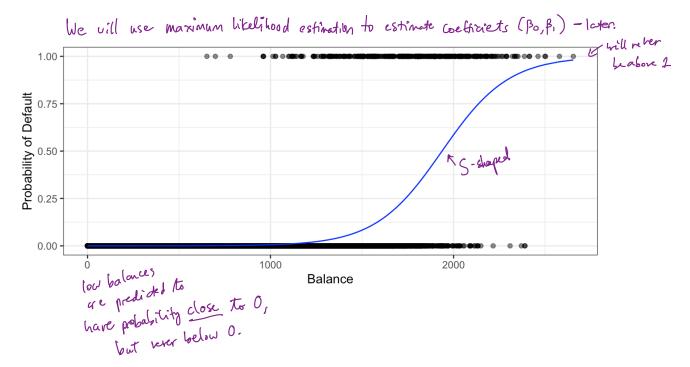
$$p(x) = \beta_0 + \beta_1 x + \varepsilon$$



2.1 The Model 5

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,

$$p(x) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}}$$



After a bit of manipulation,

$$\frac{p(x)}{1-p(x)} = e^{\beta_0 + \beta_1 x}$$

$$|-p(x)| = e^{\beta_0 + \beta$$

By taking the logarithm of both sides we see,

$$\log\left(\frac{\rho(x)}{1-\rho(x)}\right) = \beta_0 + \beta_1 \times \log_{10} - \rho(x) = \beta_0 + \rho(x) = \beta$$

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 \Rightarrow increasing X thereases $\rho(x)$

If β_1 is regardle $=$ 7 the reasing X decreases $\rho(x)$.

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
                                                                                                                                                                                                                                                 in fuct
individual's observed default status.
                                                                                                                         L(\beta_{0},\beta_{1}) = \frac{11}{1!} p(x_{i}) \prod_{\substack{i:y_{i}=0\\1:y_{i}=1}} (1-p(x_{i}))
= \prod_{\substack{i:y_{i}=0\\1:y_{i}=0}} \frac{e^{\beta_{0}+\beta_{i}x_{i}}}{1+e^{\beta_{0}+\beta_{i}x_{i}}} \prod_{\substack{i:y_{i}=0\\i:y_{i}=0}} \frac{1}{1+e^{\beta_{0}+\beta_{i}x_{i}}}
     to do this, use the likelihood function
    Fo and B, chosen to maximize l(fo, fi).
    logistic spec <- logistic reg()</pre>
                                                                                                                                                                                                                                                  Likelihood
    logistic_fit <- logistic_spec |>
           fit(default ~ balance, family = "binomial", data = Default)
                                                                                                                            Y takes Values in Eo,13
    logistic fit |>
           pluck("fit") |>
           summary()
    ##
    ## Call:
    ## stats::glm(formula = default ~ balance, family = stats::binomial,
                           data = data)
    ##
    ## Deviance Residuals:
                                                                            Median
                                                            10
             -2.2697
                                           -0.1465
                                                                         -0.0589
                                                                                                      -0.0221
                                                                                                                                        3.7589
    ## Coefficients:
                                                           Estimate Std. Error z value Pr(> z |)
    ## (Intercept)
                                                     -1.065e+01
                                                                                            3.612e-01
                                                                                                                                                               <2e-16
                                                         5.499e-03
                                                                                             2.204e-04
                                                                                                                                     24.95
                                                                                                                                                              <2e-16
                                                                                                                                                                                           0.1 ' ' 1
                                                                  0 '***' 0.001 '**' 0.01 '*'
                                                                                                                                                            0.05
             Signif. codes:
    ##
             (Dispersion parameter for binomial family taken to be 1) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( \) \( 
    ##
    ##
                           Null deviance: 2920.6
                                                                                                                                    degrees of freedom
                                                                                                      on 9999
    ## Residual deviance: 1596.5
                                                                                                  on 9998
                                                                                                                                   degrees of freedom
    ## AIC: 1600.5
    ##
    ## Number of Fisher Scoring iterations: 8
```

f: =0.0055 => increase in bulance of \$1 is associated w/imase in prob of default

Ly increase in log-odds of default by .0055

Ly multiplicative increase in PC default) by e.0055

units.

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

$$\hat{p}(x) = \frac{e^{\hat{\beta}_0 + \hat{\beta}_1 x}}{1 + e^{\hat{\beta}_0 + \hat{\beta}_1 x}} = \frac{-10.6513 + 0.0055 \times 1000}{1 + e^{10.6513 + 0.0055 \times 1000}} = 0.00575$$

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

$$\hat{p}(x) = \frac{e^{\hat{p}_0 + \hat{p}_1 x}}{1 + e^{\hat{p}_0 + \hat{p}_1 x}} = \frac{e^{(0.6513 + 0.0055 \times 2000})}{1 + e^{(0.6513 + 0.0055 \times 2000)}} = 0.586$$

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,

$$\log\left(\frac{\rho(x)}{1-\rho(x)}\right) = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p$$

$$p(x) = \frac{e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}}{1 + e^{\beta_0 + \beta_1 x_1 + \dots + \beta_p x_p}}$$
Just as before, we can use maximum likelihood to estimate $\beta_0, \beta_1, \dots, \beta_p$.

```
logistic_fit2 <- logistic_spec |> 6/1 reporte.
   fit(default ~ (), family = "binomial", data = Default)
               Y ~ every other column in data
 logistic fit2 >
   pluck("fit") |>
   summary()
 ##
 ## Call:
 ## stats::glm(formula = default ~ ., family = stats::binomial, data =
 data)
 ##
 ## Deviance Residuals:
        Min
                   1Q Median
 ## -2.4691 -0.1418 -0.0557 -0.0203
                                          3.7383
 ##
 ## Coefficients:
                   Estimate Std. Error z value Pr(>|z|)
 ## (Intercept) -1.087e+01 4.923e-01 -22.080 < 2e-16 ***
→ ## studentYes -6.468e-01 2.363e-01 -2.738 0.00619 **
                5.737e-03 2.319e-04 24.738 < 2e-16 ***
 ## balance
                                        0.370 0.71152 eno significant relationship w/ insome.
 ## income
                  3.033e-06 8.203e-06
 ## 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
```

fundet (yes) < 0 => if you are a student LESS likely to default holding balance and incorpo constant.

Student confounded w/ balance - if you are a student you are more likely to have a higher belance) but if you're a non-studet w/ save balance/income more to default.

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

$$\hat{P}(X) = \frac{-10.869 + 0.00574 \times 1500 + 0.000003 \times 40000 + (-0.6468) \cdot 1}{| + e|}$$

$$= 0.058$$

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

$$\hat{P}(X) = \frac{-10.869 + 0.00574 \times 1500 + 0.000003 \times 40000 + (-0.6468) \cdot 0}{| + e|}$$

$$= 0.105$$

pict in th

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 predictors
$$\times$$
 separately in each of the response classes (girm Y) and the use Bayes Heorem to thip these probabilities and get estimates for $P(Y=k \mid X=x)$

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

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

- 1. When classes are well separated, the parameter estimates for logistic regression are supplisingly unstable.
- 2. If n is small (and distributions of X approximately match what re assume in LDA -- Normal) LDA is more stable than logistic regression.
- 3. We might have more than 2 response classes.

3.1 Bayes' Theorem for Classification

Suppose we wish to classify an observation into one of K classes, where $K \geq 2$. Categorical Y can take on K possible distinct and unordered values.

 π_k - overall or "prior" probability that a randomly chosen observation comes from the km class.

$$f_k(x) = \begin{cases} P(X = x \mid Y = k) \\ P(x) \end{cases}$$
 discrete X prob that X falls in a small region around X given $Y = k$ (continuous X).

"density function" of
$$X$$
 for an observation that comes from class K

$$P(Y=k|X=x) = \frac{\prod_{k=1}^{K} f_k(x)}{\prod_{k=1}^{K} f_k(x)} \qquad \text{(Bayes phorem)}$$

$$\sum_{k=1}^{K} \prod_{k=1}^{K} f_k(x) \qquad \text{(Bayes phorem)}$$
We will use the approximation $f_k(x)$ as before to denote $f_k(x) = x$ from class $f_k(x) = x$.
In general, estimating $f_k(x) = x$ is easy if we have a random sample of $f_k(x) = x$ from the population.

Compute fraction of training observations but come from $f_k(x) = x$.

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

If we can estimate fk(x) we can develop a classifier that is close to he "best" classifier (more later).

3.2 p = 113

3.2 p = 1

he "Bayes

classifier is known to be "optimal"

i.e. wc con do

no better!

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. estimating the Bayes classifier!

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

$$f_k(x) = \frac{1}{\sqrt{2176_k^2}} \exp\left(-\frac{1}{26_k^2}(x-\mu_k)^2\right)$$

Mx and 62 are men and variance parameters for kth class.

Let's also assume (for now)
$$6_1^2 = \dots = 6_k^2 = 6^2$$
 (shared variance torm).

Plugging this into our formula to estimate $p_k(x)$,

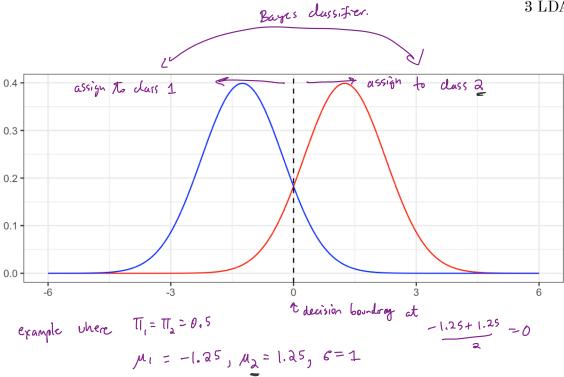
$$P_{K}(x) = \frac{\prod_{k} \frac{1}{\sqrt{2\pi}6^{2}} e_{xp} \left(-\frac{1}{26^{2}} (x - \mu_{k})^{2}\right)}{\sum_{\ell=1}^{K} \frac{1}{\sqrt{2\pi}6^{2}} e_{xp} \left(-\frac{1}{26^{2}} (x - \mu_{\ell})^{2}\right)}$$

We then assign an observation X=x to the class which makes $p_k(x)$ tthe largest. This is equivalent to

(log + tearranging) assign obs to class for which $\delta_{k}(x) = \chi \frac{\mu k}{6^{2}} - \frac{\mu k^{2}}{2r^{2}} + \log(\pi_{k}).$ is largest.

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

When
$$\delta_1(x) > \delta_2(x)$$



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

$$> \mu_1, \ldots, \mu_K, \pi_1, \ldots, \pi_K, \sigma^2$$
. to estimate the pages classifier

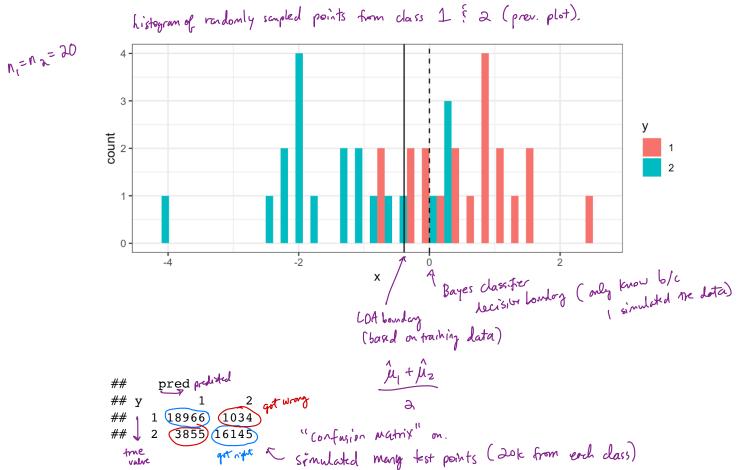
The linear discriminant analysis (LDA) method approximated the Bayes classifier by plugging estimates in for π_k, μ_k, σ^2 .

$$\frac{1}{n_{k}} = \frac{1}{n_{k}} \sum_{i:g_{i}=k}^{\infty} \sum_{k}^{\infty} \sum_{i:g_{i}=k}^{\infty} \sum_{k}^{\infty} \sum_{i:g_{i}=k}^{\infty} \sum_{k}^{\infty} \sum_{i:g_{i}=k}^{\infty} \sum_{k}^{\infty} \sum_{i:g_{i}=k}^{\infty} \sum_{i:g_{i}=k}^{$$

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 kth class.

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

$$\hat{J}_{k}(x) = \frac{\hat{\mu}_{k}}{\hat{g}^{2}} - \frac{\hat{\mu}_{k}^{2}}{2\hat{G}^{2}} + \log(\hat{T}_{k})$$
linear în $x \Rightarrow$ "linear discriminant analysis"



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

The Bayes error rate is the last he could possibly do inthis problem! (we can only estimate it because this is a simulated example)

The LDA approach did almost as well!

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.

me will relax this assumption later 16 3 LDA

3.3 p > 1

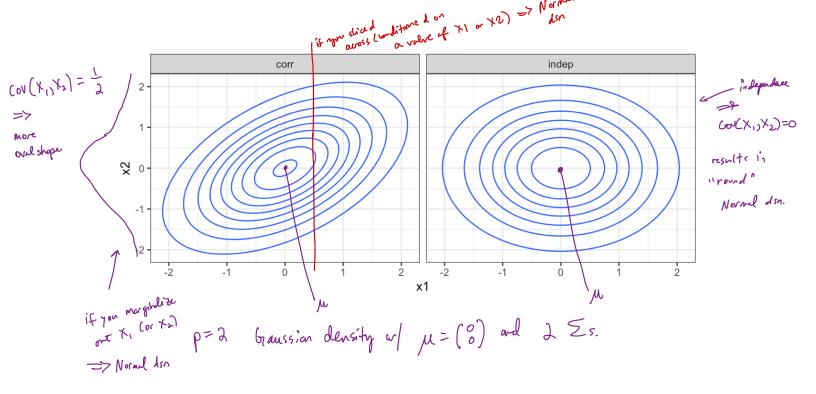
We now extend the LDA classifier to the case of multiple predictors. We will assume

X = (X1,-,,Xp) drawn from Multivariate Vormal dan W class specific mean vector & common carriance L> each individual component follows Normal dan and

$$f(x) = \frac{1}{(2\pi)^{p/2} |\Sigma|^{y_2}} \exp\left(-\frac{1}{2}(x-\mu)^T \sum_{i=1}^{p/2} (x-\mu)\right)$$

$$= \frac{1}{(2\pi)^{p/2} |\Sigma|^{y_2}} \exp\left(-\frac{1}{2}(x-\mu)^T \sum_{i=1}^{p/2} (x-\mu)^T \sum_{i=1}^{p/2} (x-\mu)\right)$$

$$= \frac{1}{(2\pi)^{p/2} |\Sigma|^{y_2}} \exp\left(-\frac{1}{2}(x-\mu)^T \sum_{i=1}^{p/2} (x-\mu)^T \sum_{i=1}$$



3.3 p > 117

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

1 dass specific mean

Plugging in the density function for the kth class, results in a Bayes classifier

assign a observation
$$X=X$$
 to class which maximizes
$$\delta_{K}(x)=X^{T}\sum_{k}\mu_{k}-\frac{1}{2}\mu_{k}^{T}\sum_{k}\mu_{k}+\log T_{k}$$
 This decision rate is still linear in X

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

To classify a new value X = x, LDA plugs in estimates into $\delta_k(x)$ and chooses the class which maximized this value. \Rightarrow get $\delta_k(x)$, choose k which maximizes (i.e. estimating Bayes 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>
                                     package actually prforming LDA.
                "LDA"
lda fit <- lda spec |>
  fit(default ~ student + balance, data = Default)
                    formula just like
lda_fit |>
  pluck("fit")
## Call:
## lda(default ~ student + balance, data = data)
##
## Prior probabilities of groups:
## 0.9667 0.0333 - Tr based on training data
## Group means:
      studentYes balance
## Coefficients of linear discriminants:
## studentYes -0.249059498
           0.002244397
## balance
```

libear combinations of student of balance use to form the LDA decision rule.

18 3 LDA

```
# training data confusion matrix
 lda_fit |>
___augment(new_data = Default) |>
    conf_mat(truth = default, estimate = .pred_class)
 ##
                 Truth
                                               For Default = Yes
 ## Prediction
                     No
             No (9644)
                                                    mly set \frac{81}{252+81} = 24\% nxtt!
 ##
Why does the LDA classifier do such a poor job of classifying the customers who default?
    only 3.33% of individuals in training lota defaulted!
     => A simple (but usuless) classifier that predicts default =NO get only 3.33% wray
    LDA is trying to approximate Bayes dassifier => yield smallest possible orall ever rate
   A CC company may want to avoid miss classifying default = YES people so can adjust
                               how to alect classes.
   how /br alect classes.

la_fit |>
augment(new_data = Default) |>
can adjust threshold => no looper
augment(pred_lower_cutoff = factor(ifelse(.pred_Yes > 0.2, "Yes", Gayes
class=F
 lda fit |>
    conf_mat(truth = default, estimate = pred_lower_cutoff)
 ##
                 Truth
 ## Prediction
                     No
                          Yes
             No 9432
                          138
             Yes 235
                            C no butter et default = Yes
   1.00
                                                                               error
  0.75
value
0.50
                                                                                  error_1
                                                                                  error_2
  0.25
                                                                                  error_tot
  0.00
```

0.3

threshold

0.4

0.5

0.1

0.0

3.4 QDA

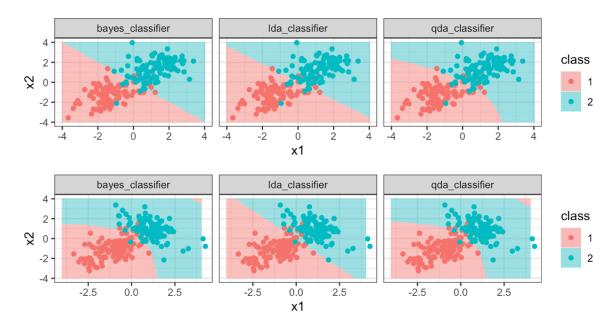
3.4 QDA

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.

Under this assumption, the Bayes classifier assigns observation X = x to class k for whichever k maximizes

When would we prefer QDA over LDA?



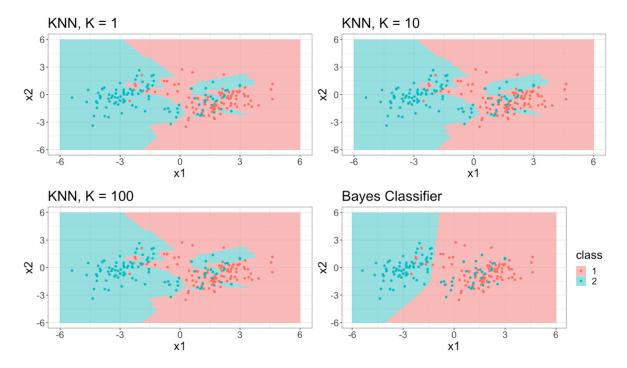
20 4 KNN

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. ${\rm KNN}$

 QDA