Chapter 4: Classification

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

e.g. eye color
cancer diagnosis
product purchase.

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-driving car you are riding in. The car must 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**).

fit a model

most importantly!

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.

↓

yes or no ⇒ categorical.

head(Default)

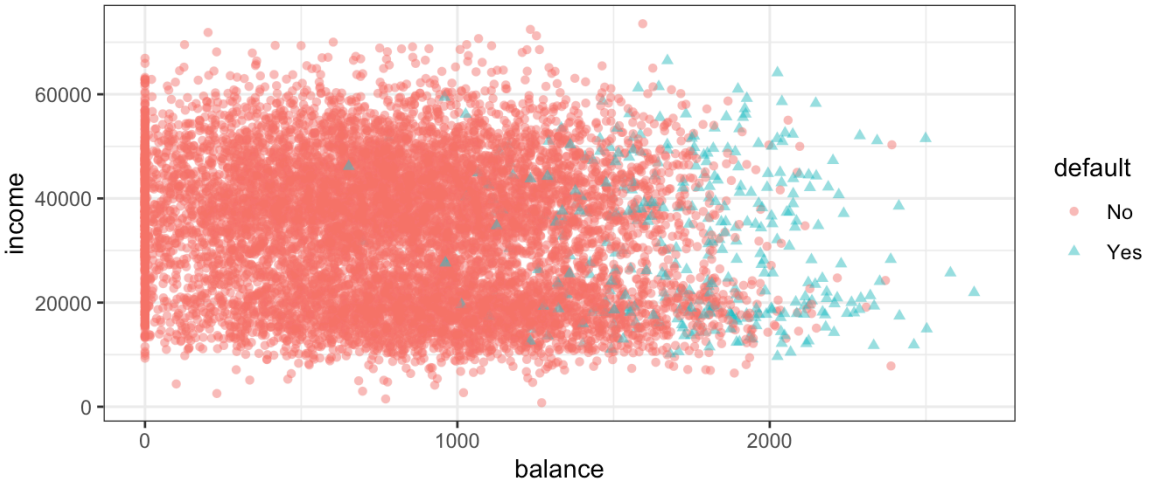
focus on these first.

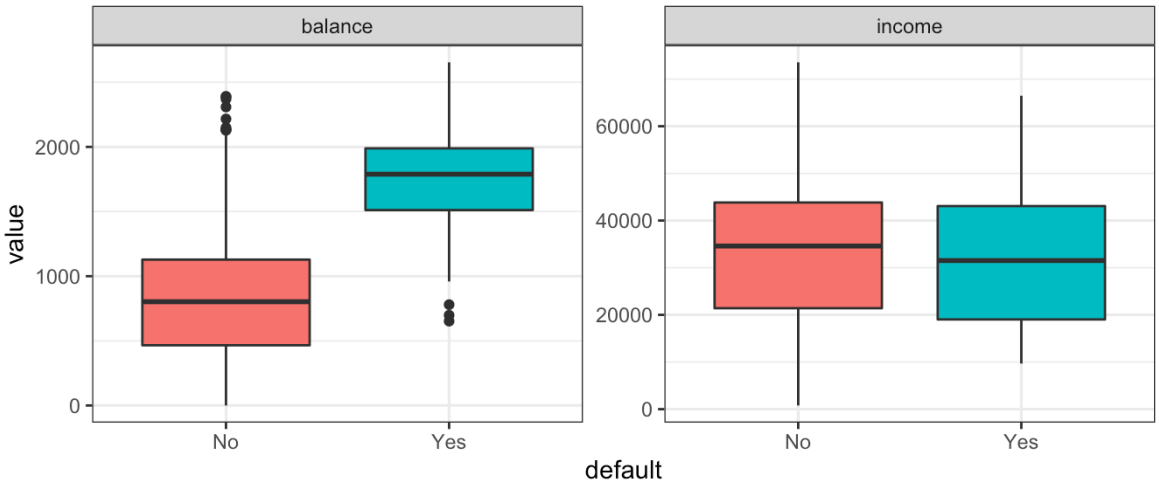
```
##   default student   balance     income
## 1      No      No  729.5265 44361.625
## 2      No     Yes  817.1804 12106.135
## 3      No      No 1073.5492 31767.139
## 4      No      No  529.2506 35704.494
## 5      No      No  785.6559 38463.496
## 6      No     Yes  919.5885  7491.559
```

↑ y

features

some separation





pronounced relationship btw/ balance and default

↳ in most problems, this relationship is not so clear.

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

$$Y = \begin{cases} 1 & \text{if } \texttt{default} \\ 0 & \text{otherwise} \end{cases}$$

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 $Y = \begin{cases} 0 & \text{default} \\ 1 & \text{don't default} \end{cases}$

$Y = \begin{cases} 0 & \text{default} \\ 100 & \text{don't} \end{cases}$

there is no natural reason to use 0/1 encoding. but it has an advantage!

Using the dummy encoding (0/1), we can get a rough estimate of $P(\texttt{default}|X)$, but it is not guaranteed to be scaled correctly.

↓

doesn't need to be between 0 and 1

but will provide an ordering.

Real problem: this cannot 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.

e.g. $P(\text{default} = \text{yes} \mid \text{balance})$

which we can abbreviate $p(\text{balance}) \in [0, 1]$.

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

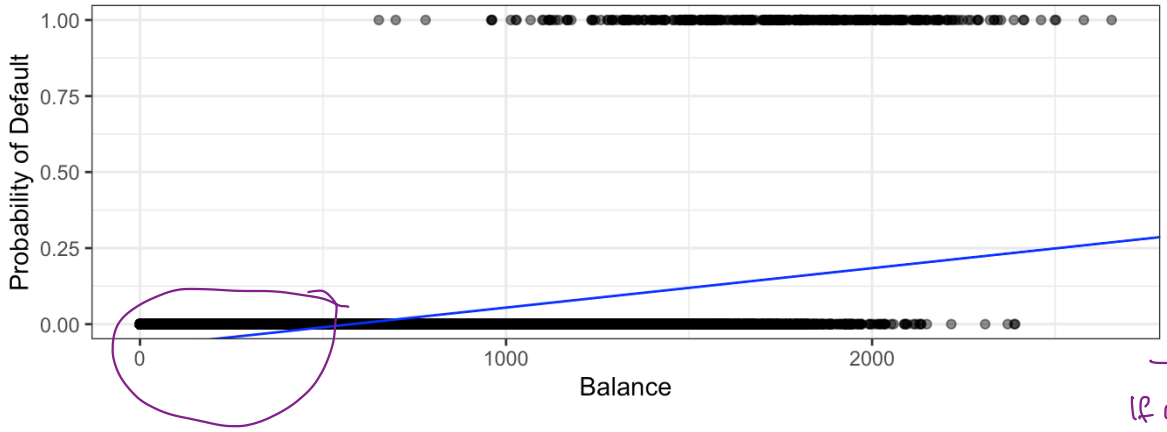
e.g. predict default = yes if $p(\text{balance}) > 0.5$

or the company could be more conservative and predict default = yes if $p(\text{balance}) > 0.1$ (threshold)

2.1 The Model

How should we model the relationship between $p(X) = P(Y = 1|X)$ (using 0/1 encoding) and X? We could use a linear regression model to represent those probabilities

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



problem: for balances close to 0 we predict negative probability

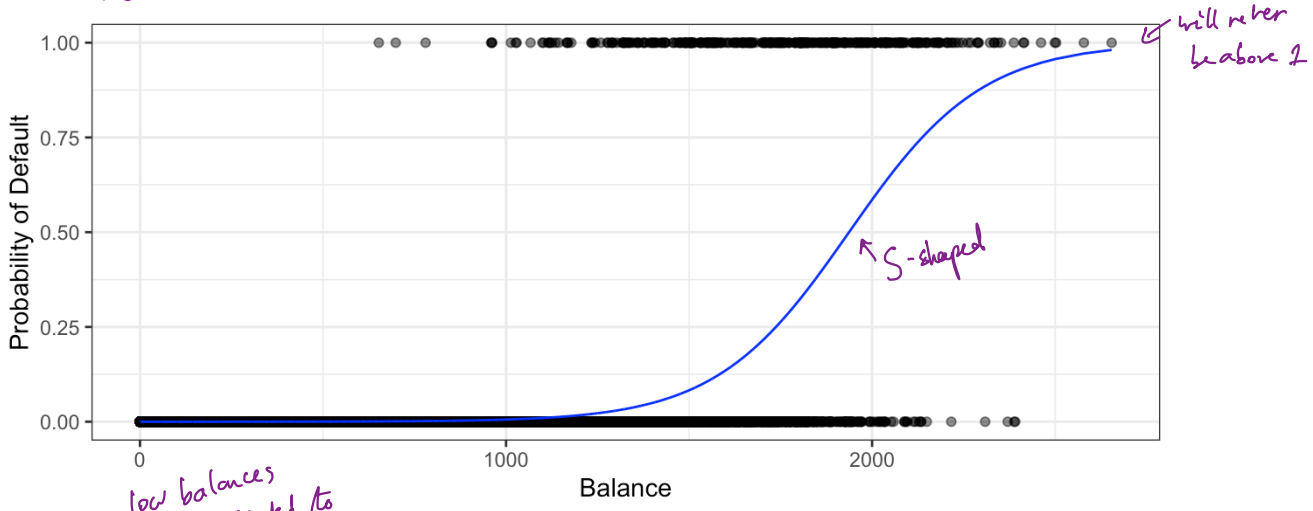
If we had balances very large would be predicting probability above 1

neither of these things make sense!

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,

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

We will use maximum likelihood estimation to estimate coefficients (β_0, β_1) – later.



After a bit of manipulation,

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

"odds" → can take any value between 0 and ∞

⇒ low prob. of default

⇒ high prob. of default.

e.g. if $p(X) = 0.2$ (1 in 5 ppl default)

$$\Rightarrow \text{odds} = \frac{0.2}{1-0.2} = \frac{1}{4}$$

By taking the logarithm of both sides we see,

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

"log-odds" / "logit"

log-odds are linear in X.

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,

increasing X by one unit changes log-odds by β_1

$\Longleftrightarrow$

increasing X by one unit multiplies the odds by e^{β_1}

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 β_1 is positive $\Rightarrow$ increasing X increases $p(X)$

If β_1 is negative $\Rightarrow$ increasing X decreases $p(X)$.

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 β_0 and β_1 such that the predicted probability $\hat{p}(x_i)$ of default for each individual corresponds as closely as possible to the individual's observed default status.

to do this, use the likelihood function $\ell(\beta_0, \beta_1) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0} (1 - p(x_i))$

$= \prod_{i:y_i=1} \frac{e^{\beta_0+\beta_1 x_i}}{1+e^{\beta_0+\beta_1 x_i}} \prod_{i:y_i=0} \frac{1}{1+e^{\beta_0+\beta_1 x_i}}$

$\hat{\beta}_0$ and $\hat{\beta}_1$ chosen to maximize $\ell(\beta_0, \beta_1)$.

in fact least squares method is equivalent to maximum likelihood

```
logistic_spec <- logistic_reg()

logistic_fit <- logistic_spec |>
  fit(default ~ balance, family = "binomial", data = Default)

logistic_fit |>
  pluck("fit") |>
  summary()
```

formula as before.

Y takes values in $\{0,1\}$.

```
##
## Call:
## stats::glm(formula = default ~ balance, family = stats::binomial,
##     data = data)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -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  -29.49   <2e-16 ***
## balance      5.499e-03  2.204e-04   24.95   <2e-16 ***
## ---
## 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: 1596.5  on 9998  degrees of freedom
## AIC: 1600.5
##
## Number of Fisher Scoring iterations: 8
```

accuracy of estimates

test statistic $\hat{\beta}_i / \widehat{se}(\hat{\beta}_i)$

hypothesis test $H_0: \beta_i = 0$ $i = 0, 1$

$H_a: \beta_i \neq 0$ for $i = 1$, H_0 implies $p(X) = \frac{e^{\beta_0}}{1+e^{\beta_0}}$ doesn't depend on X (i.e. no relationship between $p(X)$ and X)

$\hat{\beta}_0$ $\hat{\beta}_1$

there is a significant relationship between default & balance.

$\hat{\beta}_1 = 0.0055 \Rightarrow$ increase in balance of \$1 is associated w/ increase in prob of default

↳ increase in log-odds of default by .0055 units.

↳ multiplicative increase in P(default) by $e^{.0055}$

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

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

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

$$\hat{p}(X) = \frac{e^{\hat{\beta}_0+\hat{\beta}_1 X}}{1+e^{\hat{\beta}_0+\hat{\beta}_1 X}} = \frac{e^{-10.6513+0.0055\times 2000}}{1+e^{-10.6513+0.0055\times 2000}} = 0.586$$

58.6% > 50% ⇒ maybe we would predict default = yes if threshold = 0.5.

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,

$$\log\left(\frac{p(X)}{1-p(X)}\right) = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p$$

$$p(X) = \frac{e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}{1+e^{\beta_0+\beta_1 X_1+\cdots+\beta_p X_p}}$$

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

```
logistic_fit2 <- logistic_spec |>
  fit(default ~ ., family = "binomial", data = Default)
logistic_fit2 |>
  pluck("fit") |>
  summary()
```

```
##
## Call:
## stats::glm(formula = default ~ ., family = stats::binomial, data =
## data)
##
## Deviance Residuals:
##     Min       1Q   Median       3Q      Max
## -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 **
## balance      5.737e-03  2.319e-04  24.738  < 2e-16 ***
## income       3.033e-06  8.203e-06   0.370  0.71152
## ---
## 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
```

$\hat{\beta}_{student(Yes)} < 0 \Rightarrow$ if you are a student LESS likely to default holding balance and income constant.

Student confounded w/ balance – if you are a student you are more likely to have a higher balance) but if you are a non-student w/ same 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

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

$$= 0.058$$

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

$$\hat{p}(X) = \frac{e^{-10.869 + 0.00574 \times 1500 + 0.000003 \times 40000 + (-0.6468) \cdot 0}}{1 + e^{-10.869 + 0.00574 \times 1500 + 0.000003 \times 40000 + (-0.6468) \cdot 0}}$$

$$= 0.105$$

see augment or predict in R

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 X separately in each of the response classes (given Y) and the use Bayes theorem to flip these probabilities and get estimates for $P(Y=k|X=x)$

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

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

1. When classes are well separated, the parameter estimates for logistic regression are surprisingly unstable.

2. If n is small (and distributions of X approximately match what we 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.

notation

π_k — overall or "prior" probability that a randomly chosen observation comes from the k^{th} class.

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

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

$P(Y = k|X = x) = \dfrac{\pi_k f_k(x)}{\sum_{\ell=1}^{K} \pi_\ell f_\ell(x)}$ (Bayes theorem)

$\pi_k = P(Y=k)$, $f_k(x) = P(X=x \mid Y=k)$, $P(X=x) = \sum_{\ell=1}^{K} \pi_\ell f_\ell(x)$

We will use the abbreviation $p_k(x)$ as before to denote $P(Y=k \mid X=x)$ — "posterior probability" that an obs $X=x$ comes from class k

In general, estimating π_k is easy if we have a random sample of Y's from the population.

Compute fraction of training observations that come from k^{th} class.

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

If we can estimate $f_k(x)$ we can develop a classifier that is close to the "best" classifier (more later).

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

$$f_k(x) = \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left(-\frac{1}{2\sigma_k^2}(x-\mu_k)^2\right)$$

μ_k and σ_k^2 are mean and variance parameters for k^{th} class.

Let's also assume (for now) $\sigma_1^2 = \dots = \sigma_K^2 = \sigma^2$ (shared variance term).

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

$$p_k(x) = \frac{\pi_k \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu_k)^2\right)}{\sum_{l=1}^{K} \pi_l \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu_l)^2\right)}$$

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

(log + rearranging)

assign obs to class for which

$$\delta_k(x) = x\frac{\mu_k}{\sigma^2} - \frac{\mu_k^2}{2\sigma^2} + \log(\pi_k).$$

is largest.

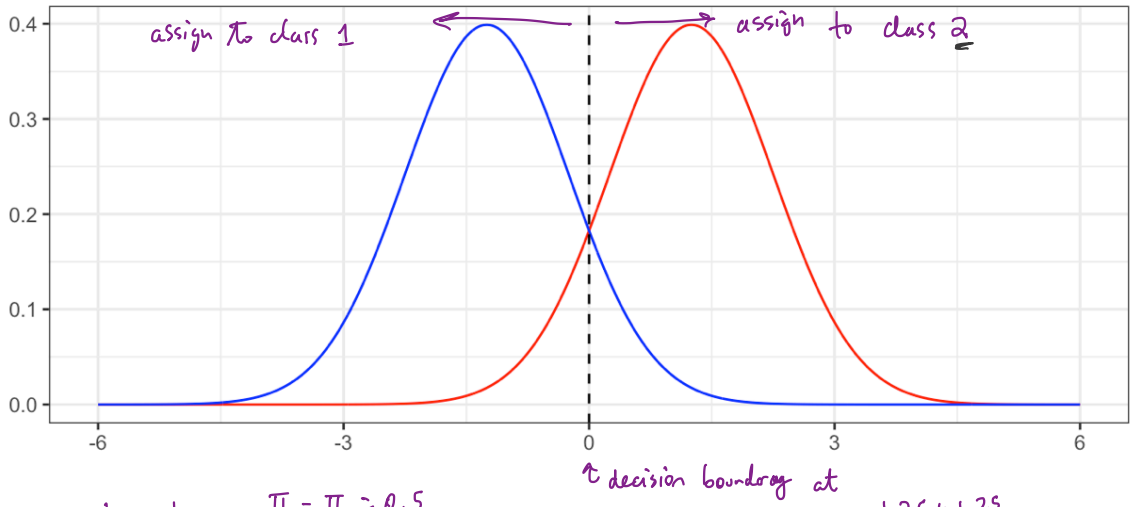
Example 3.1 Let $K = 2$ and $\pi_1 = \pi_2$. When does the Bayes classifier assign an observation to class 1?

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

$$\Leftrightarrow \quad x\frac{\mu_1}{\sigma^2} - \frac{\mu_1^2}{2\sigma^2} + \log(\pi_1) > x\frac{\mu_2}{\sigma^2} - \frac{\mu_2^2}{2\sigma^2} + \log(\pi_2)$$

$$\Leftrightarrow \quad 2x(\mu_1 - \mu_2) > \mu_1^2 - \mu_2^2$$

$$\Leftrightarrow \quad x > \frac{\mu_1 + \mu_2}{2}$$



example where $\pi_1 = \pi_2 = 0.5$

$\mu_1 = -1.25$, $\mu_2 = 1.25$, $\sigma = 1$

$\frac{-1.25 + 1.25}{2} = 0$

In this case, we know $f_k(x) \sim N(\mu_k, \sigma^2)$, $\pi_k \Rightarrow$ we can create the Bayes classifier!

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 Bayes classifier

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

$$\hat{\mu}_k = \frac{1}{n_k} \sum_{i: y_i = k} x_i$$ ← average of training observations in class k

$$\hat{\sigma}^2 = \frac{1}{n-K} \sum_{k=1}^{K} \sum_{i: y_i = k} (x_i - \hat{\mu}_k)^2$$ ← weighted average of class variances.

n = total training obs.

n_k = # training obs in class k.

Sometimes we have knowledge of class membership probabilities $\pi_1, \ldots, \pi_K$ 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. ↑ from "science" or directly from problem.

$$\hat{\pi}_k = \frac{n_k}{n}$$

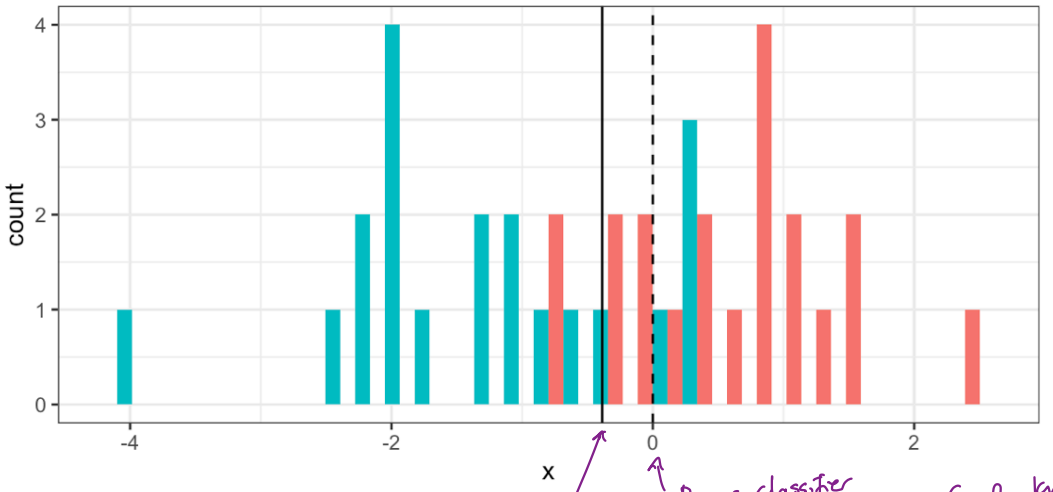
The LDA classifier assigns an observation $X = x$ to the class with the highest value of

$$\hat{\delta}_k(x) = x \frac{\hat{\mu}_k}{\hat{\sigma}^2} - \frac{\hat{\mu}_k^2}{2\hat{\sigma}^2} + \log(\hat{\pi}_k)$$

↑ linear in x ⇒ "linear discriminant analysis"

Histogram of randomly sampled points from class 1 & 2 (prev. plot).

$n_1 = n_2 = 20$



LDA boundary (based on training data)

Bayes classifier decision boundary (only know b/c I simulated the data)

$\frac{\hat{\mu}_1 + \hat{\mu}_2}{2}$

```
##      pred
## y       1     2
## 1   18966  1034
## 2    3855 16145
```

predicted; got wrong; got right; true value

"confusion matrix" on simulated many test points (20k from each class)

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 best we could possibly do in this 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.

we will relax this assumption later

3.3 p > 1

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

$X = (X_1, \ldots, X_p)$ drawn from Multivariate Normal dsn w/ class specific mean vector & common covariance

↳ each individual component follows Normal dsn and some covariance between components.

$p \times 1$ vector, $p \times p$ matrix

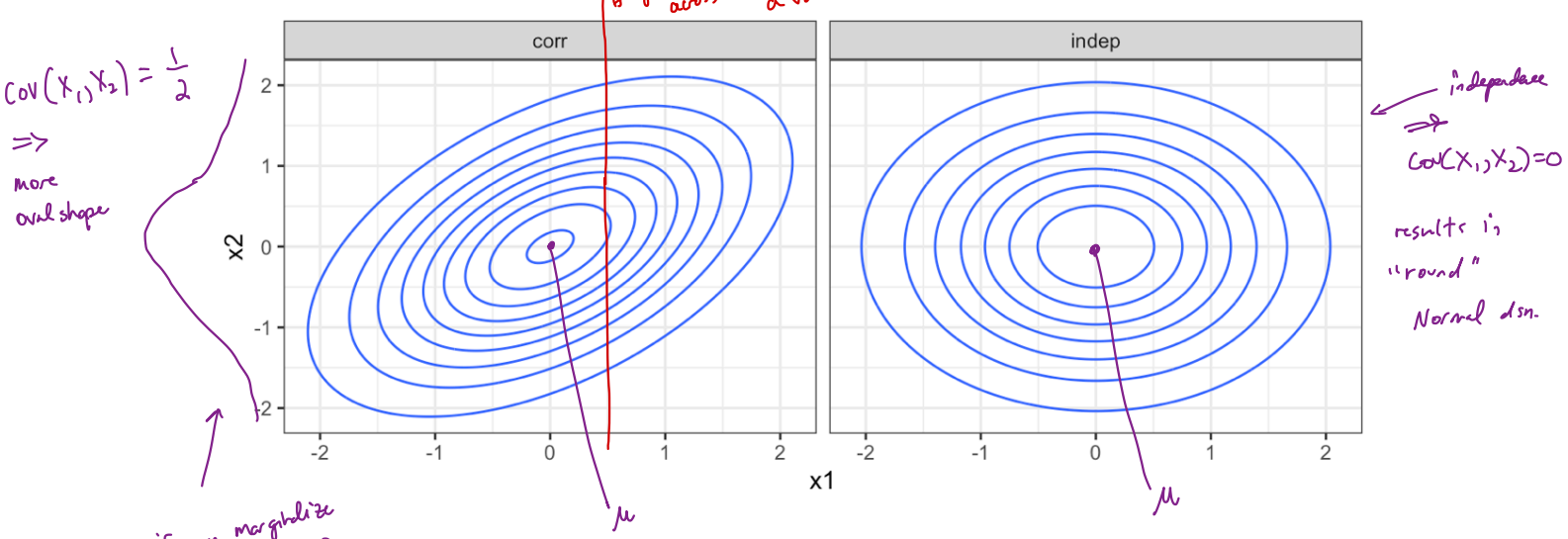
$$X \sim N_p(\mu, \Sigma) \Rightarrow \begin{aligned} EX &= \mu \\ \text{Cov}(X) &= \Sigma \end{aligned}$$

Formally the multivariate Gaussian (≈ Normal) density is defined as

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

"transpose" ↑ matrix inverse.

↑ "trace" ↳ sum of diagonal elements



$\text{Cov}(X_1, X_2) = \frac{1}{2}$ ⇒ more oval shape

independence ⇒ $\text{Cov}(X_1, X_2) = 0$

results in "round" Normal dsn.

if you marginalize out X_1 (or X_2) ⇒ Normal dsn

$p = 2$ Gaussian density w/ $\mu = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$ and 2 Σs.

In the case of $p > 1$ predictors, the LDA classifier assumes the observations in the kth class are drawn from a multivariate Gaussian distribution $N(\boldsymbol{\mu}_k, \boldsymbol{\Sigma})$. common covariance.

↑class specific mean

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

assign an observation $X = \underline{x}$ to class which maximizes

$$\delta_k(x) = \underline{x}^T \boldsymbol{\Sigma}^{-1} \underline{\mu}_k - \frac{1}{2} \underline{\mu}_k^T \boldsymbol{\Sigma}^{-1} \underline{\mu}_k + \log \pi_k$$

This decision rule is still linear in $\underline{x}$

Once again, we need to estimate the unknown parameters $\boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_K, \pi_1, \ldots, \pi_K, \boldsymbol{\Sigma}$.

use similar formulas as for $p=1$ case.

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 $\hat{\delta}_k(x)$, choose k which maximizes (i.e. estimating Bayes classifier)

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")
```

"LDA" — package actually performing LDA.

```
lda_fit <- lda_spec |>
  fit(default ~ student + balance, data = Default)

lda_fit |>
  pluck("fit")
```

formula just like linear & logistic regression: y ~ x

```
## Call:
## lda(default ~ student + balance, data = data)
##
## Prior probabilities of groups:
##     No    Yes
## 0.9667 0.0333
##
## Group means:
##     studentYes   balance
## No   0.2914037  803.9438
## Yes  0.3813814 1747.8217
##
## Coefficients of linear discriminants:
##                      LD1
## studentYes -0.249059498
## balance     0.002244397
```

$\hat{\pi}_k$ based on training data

$\hat{\underline{\mu}}_1$

$\hat{\underline{\mu}}_2$

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

```
# training data confusion matrix
lda_fit |>
  augment(new_data = Default) |>
  conf_mat(truth = default, estimate = .pred_class)
```

predict on new_data; training data; confusion matrix; columnames; column names

overall training error rate = 2.75%

```
##             Truth
## Prediction    No  Yes
##        No   9644  252
##        Yes    23   81
```

got wrong; got right

For Default = Yes only got $\frac{81}{252+81}$ = 24% right!

Why does the LDA classifier do such a poor job of classifying the customers who default?

Only 3.33% of individuals in training data defaulted!
⇒ A simple (but useless) classifier that predicts default = NO get only 3.33% wrong

LDA is trying to approximate Bayes classifier ⇒ yield smallest possible overall error rate

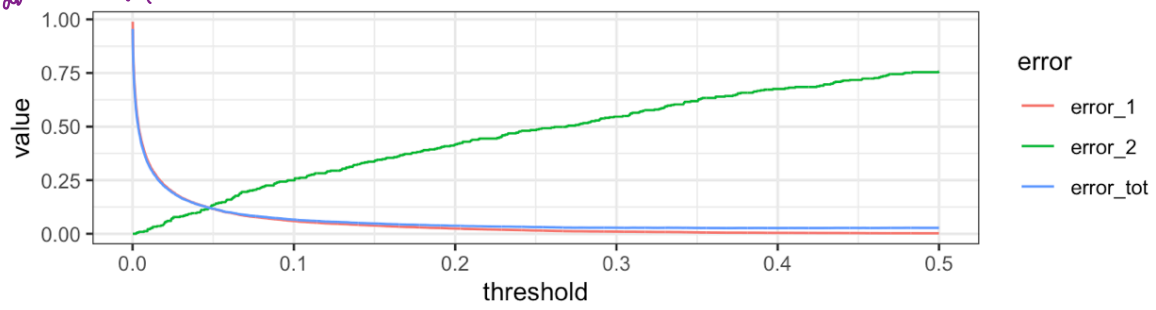
A CC company may want to avoid miss classifying default = YES people so can adjust how to select classes.

```
lda_fit |>
  augment(new_data = Default) |>
  mutate(pred_lower_cutoff = factor(ifelse(.pred_Yes > 0.2, "Yes",
         "No"))) |>
  conf_mat(truth = default, estimate = pred_lower_cutoff)
```

can adjust threshold ⇒ no longer approximating Bayes classifier.

```
##             Truth
## Prediction    No  Yes
##        No   9432  138
##        Yes   235  195
```

do worse at default = No.; better at default = Yes



as threshold ↑, error (default = NO) ↓
error (default = YES) ↑

How to choose? Domain knowledge.
(or pick 0.5 because has some theoretical 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.

an observation from class k ; covariance matrix for k^{th} class.

$$X \sim N_p(\mu_k, \Sigma_k)$$

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

$$\delta_k(x) = -\frac{1}{2}(\underline{x}-\underline{\mu}_k)^T \Sigma_k^{-1}(\underline{x}-\underline{\mu}_k) - \frac{1}{2}\log|\Sigma_k| + \log \pi_k$$

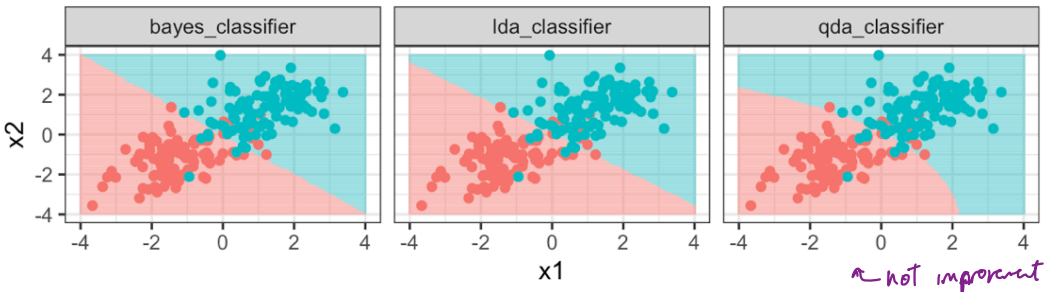
$$= -\frac{1}{2}\underline{x}^T\Sigma_k^{-1}\underline{x} + \underline{x}^T\Sigma_k^{-1}\underline{\mu}_k - \frac{1}{2}\underline{\mu}_k^T\Sigma_k^{-1}\underline{\mu}_k - \frac{1}{2}\log|\Sigma_k| + \log\pi_k$$

quadratic in $\underline{x}$ $\Rightarrow$ "quadratic discriminant analysis"

When would we prefer QDA over LDA?

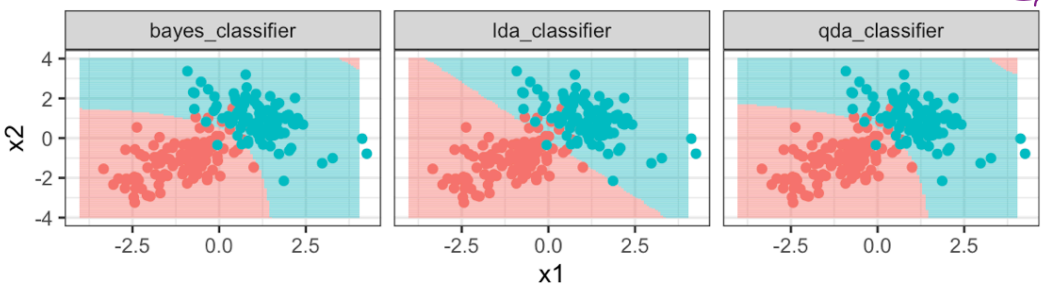
= plug in estimates for Σ_k, μ_k, π_k and take $\underset{k}{\text{argmax}}\ \hat{\delta}_k(x)$.

common covariance of 0.5 $\Rightarrow$ LDA similar to Bayes classifier



not improvement over LDA more flexible $\Rightarrow$ overfitting (capturing noise in data).

different Σ_k matrices $\Rightarrow$ QDA similar to Bayes classifier



not flexible enough!

When we have p predictors, estimating Σ_k requires estimating $\frac{p(p+1)}{2}$ parameters. $\Rightarrow$ $K\frac{p(p+1)}{2}$ parameters.

LDA is linear in k $\Rightarrow$ only have $k \cdot p$ parameters to estimate

$\Rightarrow$ LDA is much less flexible than QDA

- if don't have many training obs LDA > QDA.
- if we do have enough and assumption of global variance is bad, then LDA predictions can be wildly off!

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 $\mathcal{N}(x)$.

neighborhood

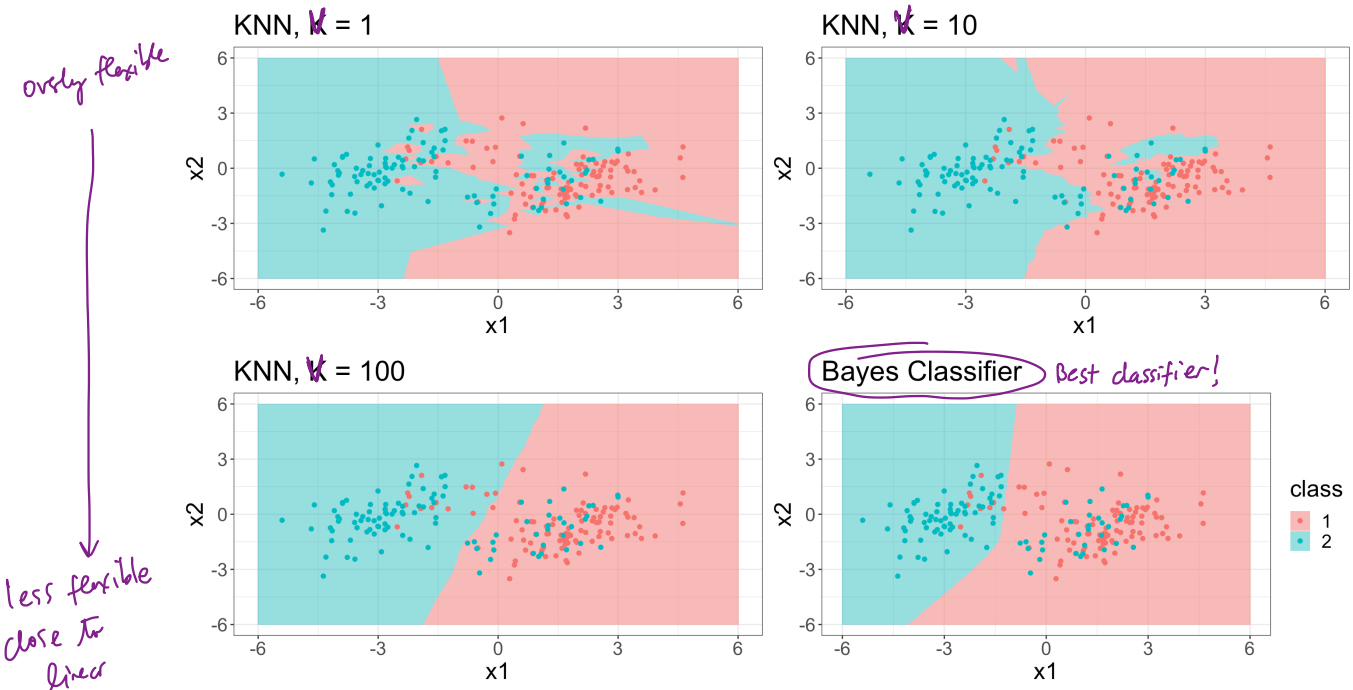
Then we can estimate $P(Y = k \mid X = x)$ as.

$$\frac{1}{K} \sum_{i \in \mathcal{N}(x)} \mathbb{I}(y_i = k)$$

class k.

points in neighborhood

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



- choosing correct level of flexibility is crucial to our success! (KNN; LDA vs QDA, logistic regression).

- How to choose (ch. 5)
  Next!

5 Comparison

LDA vs. Logistic Regression

prob of observing obs. in class 1.

LDA & logistic regression are closely related. Consider $K=2$, $p=1$ and $p_1(x)$, $p_2(x) = 1-p_1(x)$

LDA: $\log\left(\frac{p_1(x)}{1-p_1(x)}\right) = \log\left(\frac{p_1(x)}{p_2(x)}\right) = \log\left[\frac{\pi_1}{\pi_2}\exp\left[-\frac{1}{2\sigma^2}\left[(x-\mu_1)^2-(x-\mu_2)^2\right]\right]\right]$

$= \log\pi_1 - \log\pi_2 - \frac{1}{2\sigma^2}\left[x^2 - 2x\mu_1 + \mu_1^2 - x^2 + 2x\mu_2 - \mu_2^2\right]$

$= c_0 + c_1 x$

logistic regression: $\log\left(\frac{p_1(x)}{1-p_1(x)}\right) = \beta_0 + \beta_1 x$

Should give similar results!

BUT LDA assumes Gaussian dsn w/ common variance and logistic regression does not

$\Rightarrow$ which assumptions hold should give better results.

(LDA & Logistic Regression) vs. KNN

KNN $\rightarrow$ non parametric $\Rightarrow$ no assumption made about shape of decision boundary.

$\Rightarrow$ should outperform LDA & logistic regression when decision boundary is highly non linear

KNN doesn't tell us which variables are important (relationship btw/ response & predictors).

QDA

Compromise btw/ KNN & LDA, logistic regression.

Quadratic decision boundary $\Rightarrow$ more flexibility.

Not as flexible as KNN $\Rightarrow$ problems w/ slightly less training data can have improvements on test data vs. KNN.