Chapter 5: Assessing Model Accuracy

One of the key aims of this course is to introduce you to a wide range of statistical learning techniques. Why so many? Why not just the "best one"?

There is no best one for every situation!

exception: if you know the TRUE model that your data comes from

You won't know this.

Hence, it's important to decide for any given set of data which method produces the best results.

How to decide?

this is NOT how we will decide!

https://xkcd.com/1838/

1 Measuring Quality of Fit

With linear regression we talked about some ways to measure fit of the model

R^2, Residual standard error.

In general, we need a way to measure fit and compare *across models*.

not just linear regression.

One way could be to measure how well its predictions match the observed data. In a regression session, the most commonly used measure is the *mean-squared error (MSE)*

$$MSE = \frac{1}{n}\sum_{i=1}^{n}\underbrace{(y_i - \hat{f}(x_i))^2}_{\text{squared error}}$$

true response for ith observation

prediction for ith observation

small if predictions are close to the responses.

This is based on training data (data used to fit the model). "training MSE"

We don't really care how well our methods work on the training data.

kind of care about relationships

Instead, we are interested in the accuracy of the predictions that we obtain when we apply our method to previously unseen data. Why?

↳ test data.

We already know response values in our training data!

Suppose we fit our learning model on training data $\{(x_1, y_1), \dots, (x_n, y_n)\}$ and obtain an estimate $\hat{f}$

We can compute $\hat{f}(x_i)$. If these are close to our response y_i => small training MSE.

But we care about:

$\hat{f}(x_0) \approx y_0$ for (x_0, y_0) unseen data not used to fit the model.

Want to choose the model w/ lowest test MSE

$\text{Ave}((y_0 - \hat{f}(x_0))^2)$ over a large # of test observations (x_0, y_0).

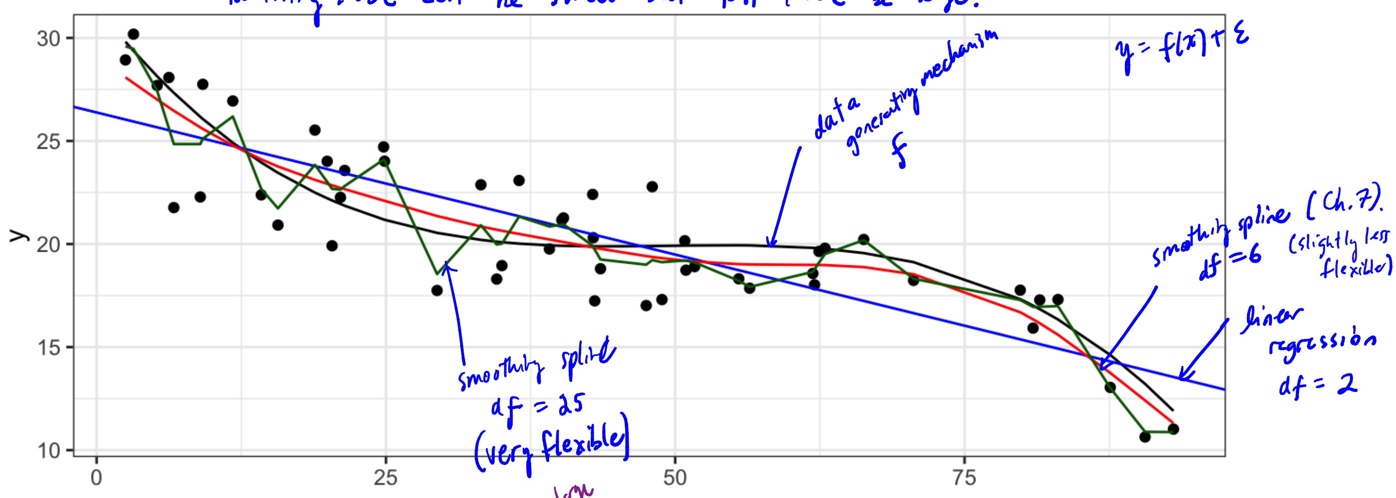
So how do we select a method that minimizes the test MSE?

Sometimes we have a test data set available to us based on scientific problem.
↳ access to set of obs. that were not used to fit model.

But what if we don't have a test set available?

Maybe we just minimize train MSE

Problem: there is no guarantee lowering training MSE lowers test MSE
because statistical learning methods are fit to lower training MSE.
⇒ training MSE can be small but test MSE be large!



estimate using a large # of draws from $f(x)+\varepsilon$ not used to fit the model.

← predict each training point $\hat{y}_i$, train MSE $= \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$

least flexible ↓ most flexible,

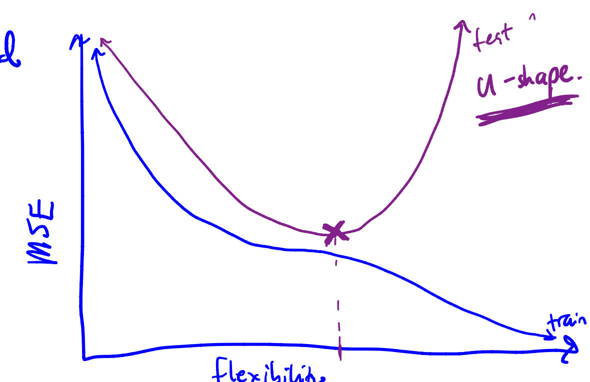
model	df	Test MSE	Train MSE
Linear Regression	2	36.0399	4.9654
Smoothing Spline	6	40.2160	3.5441
Smoothing Spline	25	38.8952	1.8645

linear regression has worst training MSE.

best training MSE fits data the best!

linear best test MSE

In general



How to choose the best model?
need to estimate test MSE!
(next).

1.1 Classification Setting

quantitative response.

So far, we have talked about assessing model accuracy in the regression setting, but we also need a way to assess the accuracy of classification models.

categorical responses.

Suppose we seek to estimate f on the basis of training observations where now the response is categorical. The most common approach for quantifying the accuracy is the training error rate.

$$\frac{1}{n}\sum_{i=1}^{n}\mathbb{I}(y_i \neq \hat{y}_i) \quad \text{where} \quad \mathbb{I}(y_i \neq \hat{y}_i) = \begin{cases} 1 & y_i \neq \hat{y}_i \\ 0 & \text{o.w. (correctly classify point } i) \end{cases}$$

true label for ith observation

predicted value for ith observation

This is called the *training error rate* because it is based on the data that was used to train the classifier.

As with the regression setting, we are more interested in error rates for data *not* in our training data; i.e. test data (x_0, y_0)

Test error rate is

$$\text{Ave}\left(\mathbb{I}(y_0 \neq \hat{y}_0)\right)$$

predicted class for test observation w/ predictor x_0 $= \hat{f}(x_0)$.

A good classifier is one for which this quantity is small.

If we want a good estimate of test error, we should use many test data points.

1.2 Bias-Variance Trade-off

or in test error

The U-shape in the test MSE curve compared with flexibility is the result of two competing properties of statistical learning methods. It is possible to show that the expected test MSE, for a given test value x_0, can be decomposed

irreducible error

$$E\left[(y_0 - \hat{f}(x_0))^2\right] = \underbrace{\mathrm{Var}(\hat{f}(x_0))}_{\geq 0} + \underbrace{\left[\mathrm{Bias}(\hat{f}(x_0))\right]^2}_{\geq 0} + \mathrm{Var}\,\varepsilon$$

average test MSE we would obtain if we repeatedly measure f at many training data sets and predict x_0.

overall expected test MSE obtained by averaging $E\left[(y_0 - \hat{f}(x_0))^2\right]$ over many test points. (x_0, y_0).

This tells us in order to minimize the expected test error, we need to select a statistical learning method that simulatenously achieves *low variance* and *low bias*.

Variance – the amount by which $\hat{f}$ would change if we estimated it using different training data.
In general, more flexible methods have higher variance because they fit data so closely
$\Rightarrow$ new data would result in bigger change in $\hat{f}$

Bias – the error that is introduced by approximating a real life problem by a much simpler model.

ex: linear regression assumes linear form. It is unlikely that any real-world problems are actually linear $\Rightarrow$ there will introduce bias.

In general: $\uparrow$ flexibility $\Rightarrow$ $\underbrace{\downarrow \text{bias} \ \& \ \uparrow \text{variance}}_{\text{how much these change}}$ determine test MSE

Similar ideas hold for classification setting and test error.

2 Cross-Validation

As we have seen, the test error can be easily calculated when there is a test data set available.

Unfortunately, this is not usually the case.

In contrast, the training error can be easily calculated.

But training error can wildly underestimate test error rate.

In the absense of a very large designated test set that can be used to estimate the test error rate, what to do?

Brainstorm:

split the training set and use part of it as the "test set"

as long as we are careful about not systematically biasing our test vs. training.

For now we will assume we are in the regression setting (quantitative response), but concepts are the same for classification.

categorical response.

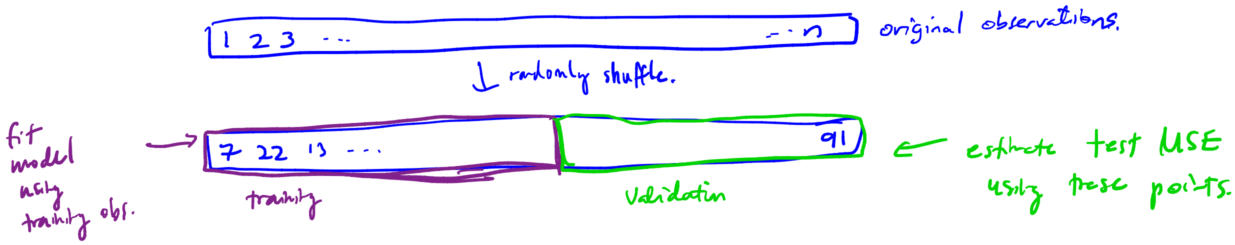
2.1 Validation Set

test MSE

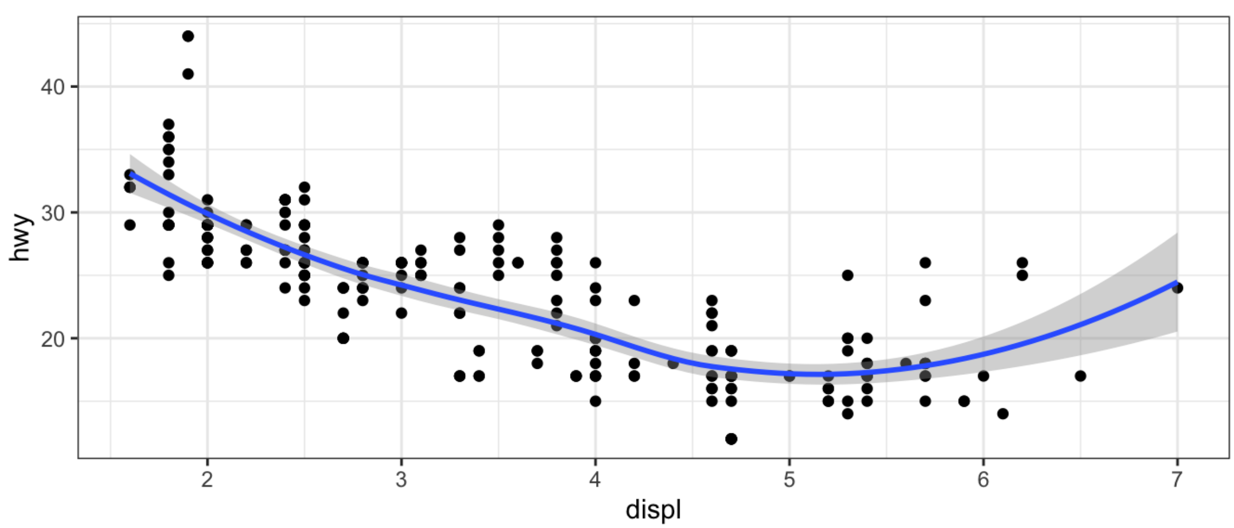
Suppose we would like to estimate the test error rate for a particular statistical learning method on a set of observations. What is the easiest thing we can think to do?

We could randomly divide the available data set into two parts: training and validation

typically 50-50



Let's do this using the `mpg` data set. Recall we found a non-linear relationship between `displ` and `hwy` mpg.



We fit the model with a squared term $\texttt{displ}^2$, but we might be wondering if we can get better predictive performance by including higher power terms!

displ^3, displ^4

often you will see 50/50.

indices of length ≈ 60% of # of observations.

"seq length"

```
## get index of training observations
# take 60% of observations as training and 40% for validation
n <- nrow(mpg)
trn <- seq_len(n) %in% sample(seq_len(n), round(0.6*n))

## fit models
m0 <- lm(hwy ~ displ, data = mpg[trn, ])
m1 <- lm(hwy ~ displ + I(displ^2), data = mpg[trn, ])
m2 <- lm(hwy ~ displ + I(displ^2) + I(displ^3), data = mpg[trn, ])
m3 <- lm(hwy ~ displ + I(displ^2) + I(displ^3) + I(displ^4), data =
  mpg[trn, ])

## predict on validation set
pred0 <- predict(m0, mpg[!trn, ])
pred1 <- predict(m1, mpg[!trn, ])
pred2 <- predict(m2, mpg[!trn, ])
pred3 <- predict(m3, mpg[!trn, ])

## estimate test MSE
true_hwy <-  mpg[!trn, ]$hwy # truth vector

data.frame(terms = 2, model = "linear", true = true_hwy, pred =
  pred0) %>%
   bind_rows(data.frame(terms = 3, model = "quadratic", true =
  true_hwy, pred = pred1)) %>%
   bind_rows(data.frame(terms = 4, model = "cubic", true = true_hwy,
  pred = pred2)) %>%
   bind_rows(data.frame(terms = 5, model = "quartic", true = true_hwy,
  pred = pred3)) %>% ## bind predictions together
   mutate(se = (true - pred)^2) %>% # squared errors
   group_by(terms, model) %>% # group by model
   summarise(test_mse = mean(se)) %>% ## get test mse
   kable() ## pretty table
```

4 models increasing in flexibility.

training set

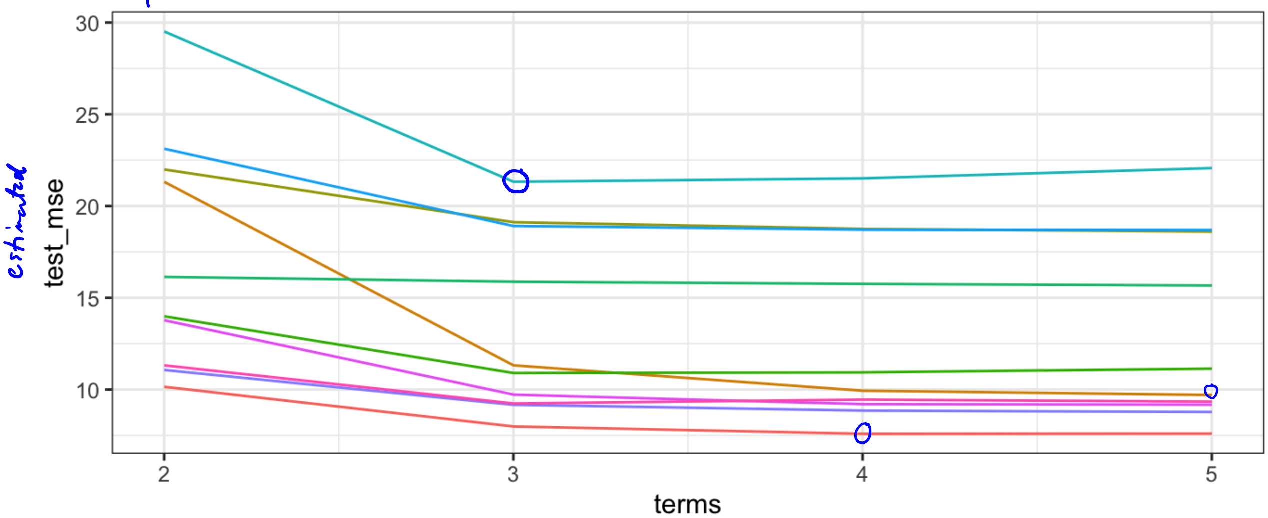
validation

terms	model	test_mse
2	linear	14.17119
3	quadratic	11.26710
4	cubic	11.08535
5	quartic	11.04907

close

best model based on this split of the data

Repeated process 10x.



a lot of variability here! sometimes squared model is the best!

- The validation estimate of the test error is highly variable! Depends on which observations we held out.

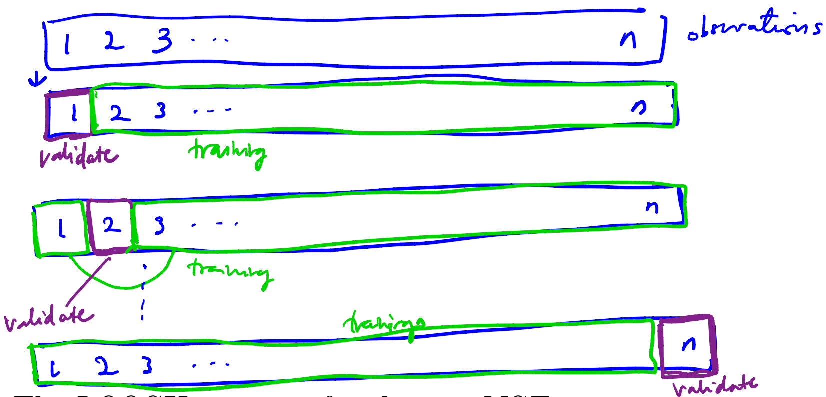
- Only a subset used to fit model. Since statistical models tend to do better with more data, the validation test error can overestimate the test error.

$\Rightarrow$ cross-validation is a method to address these weaknesses...

2.2 Leave-One-Out Cross Validation

Leave-one-out cross-validation (LOOCV) is closely related to the validation set approach, but it attempts to address the method's drawbacks.

LOOCV still splits data into 2 parts, but now a single observation is used for validation.



① fit model on $n-1$ observations

② $\hat{y}_i$: prediction for held out validation point

$$MSE_i = (y_i - \hat{y}_i)^2$$

unbiased for test error but highly variable.

The LOOCV estimate for the test MSE is

$$CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n} MSE_i = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

LOOCV has a couple major advantages and a few disadvantages. over the validation method.

Advantages
- less bias
- since we fit using $n-1$ observations (instead of $\approx \frac{n}{2}$ for validation approach)
  - $\Rightarrow$ LOOCV doesn't overestimate the test error as much as validation approach.
- No randomness in this approach $\Rightarrow$ will get the same results every time.

Disadvantage:

- Sometimes stat learning models can be expensive to fit (i.e. order of days)

  LOOCV requires us to fit the model n times.

  $\Rightarrow$ could be very very slow!

Let's fit models of increasing complexity/flexibility on mpg to learn relationship betw/ hwy + displ

```
## perform LOOCV on the mpg dataset
res <- data.frame() ## store results
for(i in seq_len(n)) { # repeat for each observation
  trn <- seq_len(n) != i # leave one out
          length n boolean vectors (only have 1 FALSE).

  ## fit models                        training data
  m0 <- lm(hwy ~ displ, data = mpg[trn, ])
  m1 <- lm(hwy ~ displ + I(displ^2), data = mpg[trn, ])
  m2 <- lm(hwy ~ displ + I(displ^2) + I(displ^3), data = mpg[trn, ])
  m3 <- lm(hwy ~ displ + I(displ^2) + I(displ^3) + I(displ^4), data =
 mpg[trn, ])
                                         left out
  ## predict on validation set          observation
  pred0 <- predict(m0, mpg[!trn, ])      i=1,...,n
  pred1 <- predict(m1, mpg[!trn, ])
  pred2 <- predict(m2, mpg[!trn, ])
  pred3 <- predict(m3, mpg[!trn, ])

  ## estimate test MSE
  true_hwy <- mpg[!trn, ]$hwy # get truth vector

  res %>% ## store results for use outside the loop
    bind_rows(data.frame(terms = 2, model = "linear", true =
 true_hwy, pred = pred0)) %>%
    bind_rows(data.frame(terms = 3, model = "quadratic", true =
 true_hwy, pred = pred1)) %>%
    bind_rows(data.frame(terms = 4, model = "cubic", true = true_hwy,
 pred = pred2)) %>%
    bind_rows(data.frame(terms = 5, model = "quartic", true =
 true_hwy, pred = pred3)) %>% ## bind predictions together
    mutate(mse = (true - pred)^2) -> res
}

res %>%
  group_by(terms, model) %>%
  summarise(LOOCV_test_MSE = mean(mse)) %>%
  kable()
```

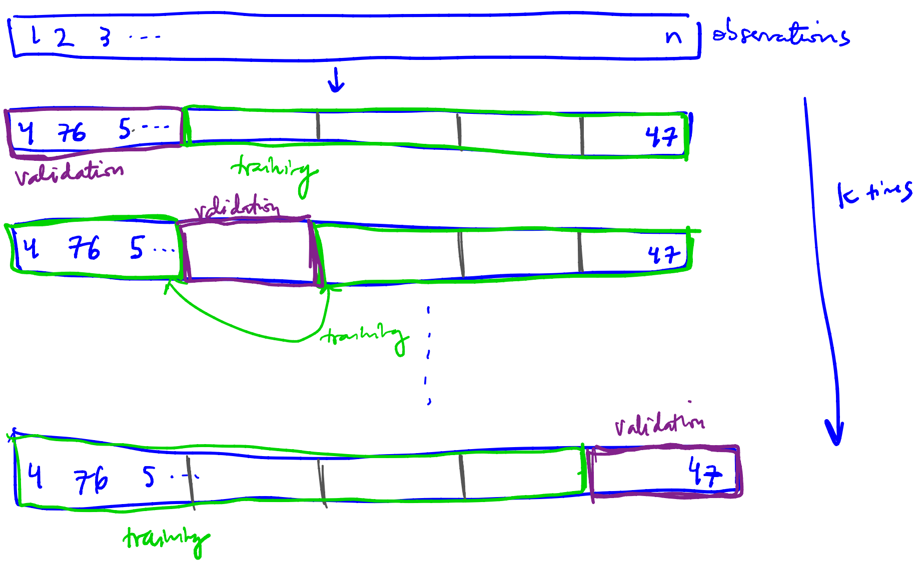
$$CV_{(n)} = \frac{1}{n}\sum_{i=1}^{n} MSE_i$$

terms	model	LOOCV_test_MSE
2	linear	14.92437
3	quadratic	11.91775
4	cubic	11.78047
5	quartic	11.93978

We would choose the level of flexibility w/ lowest $CV_{(n)}$ estimate of test error.

2.3 k-Fold Cross Validation

An alternative to LOOCV is *k*-fold CV. → randomly divide the observations into k groups or "folds"



① hold out 1 fold
fit model on remaining k-1 folds.

② predict the held out fold

get MSE_i for left out fold

Ave $(y_j - \hat{y}_j)^2$

for $j \in k^{th}$ fold.

The *k*-fold CV estimate is computed by averaging

$$CV_{(k)} = \frac{1}{k}\sum_{i=1}^{k} MSE_i = \frac{1}{k}\sum_{i=1}^{k} \underbrace{\frac{1}{|F_i|}}_{\text{fold } i} \sum_{j \in F_i} (y_j - \hat{y}_j)^2$$

Usually we use $k=5$ or $k=10$.

Why *k*-fold over LOOCV?

LOOCV is a special case of k-fold CV w/ $k=n$.

Computational advantage! Now have to fit k models not n models.

Another advantage due to bias-variance trade-off (more later).

```r
## perform k-fold on the mpg dataset
res <- data.frame() ## store results

## get the folds
k <- 10
```

10-Fold

n samples

assign each obs. to a fold.

```r
folds <- sample(seq_len(10), n, replace = TRUE) ## approximately
  equal sized
```

labels 1,...,10

vector of length n values will be 1,...,10

1,...,10

```r
for(i in seq_len(k)) { # repeat for each observation
  trn <- folds != i # leave ith fold out
```

vector of length n, booleans FALSE for ith fold positions.

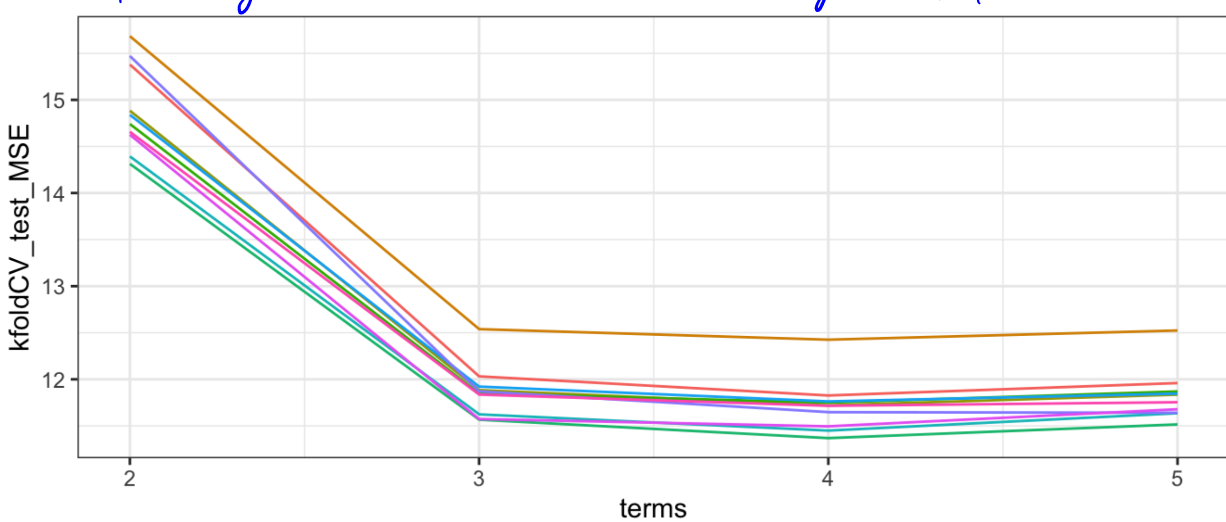
```r
  ## fit models
  m0 <- lm(hwy ~ displ, data = mpg[trn, ])
  m1 <- lm(hwy ~ displ + I(displ^2), data = mpg[trn, ])
  m2 <- lm(hwy ~ displ + I(displ^2) + I(displ^3), data = mpg[trn, ])
  m3 <- lm(hwy ~ displ + I(displ^2) + I(displ^3) + I(displ^4), data =
 mpg[trn, ])

  ## predict on validation set
  pred0 <- predict(m0, mpg[!trn, ])
  pred1 <- predict(m1, mpg[!trn, ])
  pred2 <- predict(m2, mpg[!trn, ])
  pred3 <- predict(m3, mpg[!trn, ])

  ## estimate test MSE
  true_hwy <- mpg[!trn, ]$hwy # get truth vector

  data.frame(terms = 2, model = "linear", true = true_hwy, pred =
 pred0) %>%
    bind_rows(data.frame(terms = 3, model = "quadratic", true =
 true_hwy, pred = pred1)) %>%
    bind_rows(data.frame(terms = 4, model = "cubic", true = true_hwy,
 pred = pred2)) %>%
    bind_rows(data.frame(terms = 5, model = "quartic", true =
 true_hwy, pred = pred3)) %>% ## bind predictions together
    mutate(mse = (true - pred)^2) %>%
    group_by(terms, model) %>%
    summarise(mse = mean(mse)) -> test_mse_k

  res %>% bind_rows(test_mse_k) -> res
}
```

```
res %>%
  group_by(terms, model) %>%
  summarise(kfoldCV_test_MSE = mean(mse)) %>%
  kable()
```

terms	model	kfoldCV_test_MSE
2	linear	14.77098
3	quadratic	12.14423
4	cubic	11.94037
5	quartic	11.78830

Now again there is randomness in the assignment to folds.

repeated 10 x



very similar results across different selection of folds.

When we perform CV, we are interested in estimating the test error.

More often we use it to find minimum estimated test error to help us choose a model (or a set of parameters)

called "tuning the model"

2.4 Bias-Variance Trade-off for k-Fold Cross Validation

k-Fold CV with $k < n$ has a computational advantace to LOOCV.

There is also a less obvious advantage (potentially more important)

- often the that k-fold CV give us a more accurate estimate of test error rate than LOOCV.

We know the validation approach can overestimate the test error because we use only half of the data to fit the statistical learning method.

By this logic, LOOCV gives approximately unbiased estimates of the test error rate (uses $n-1 \approx n$ points to fit).

k-fold give intermediate level of bias (use $\frac{k-1}{k}n$ obs. to fit)

LOOCV gives lowest bias!

But we know that bias is only half the story! We also need to consider the procedure's variance.

LOOCV have higher variance than k-fold CV when $k<n$.

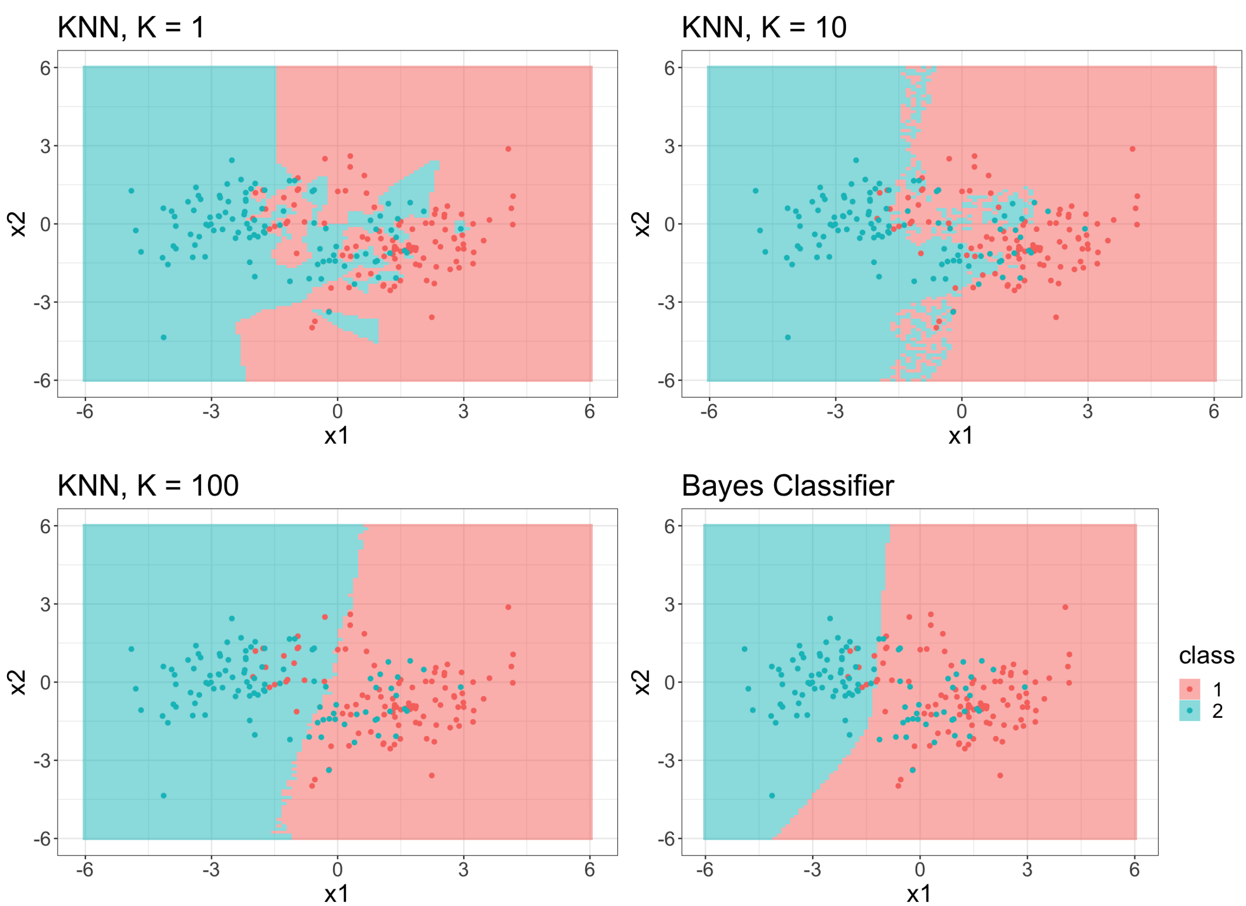
Why?

To summarise, there is a bias-variance trade-off associated with the choice of k in k-fold CV. Typically we use $k = 5$ or $k = 10$ because these have been shown empirically to yield test error rates closest to the truth.

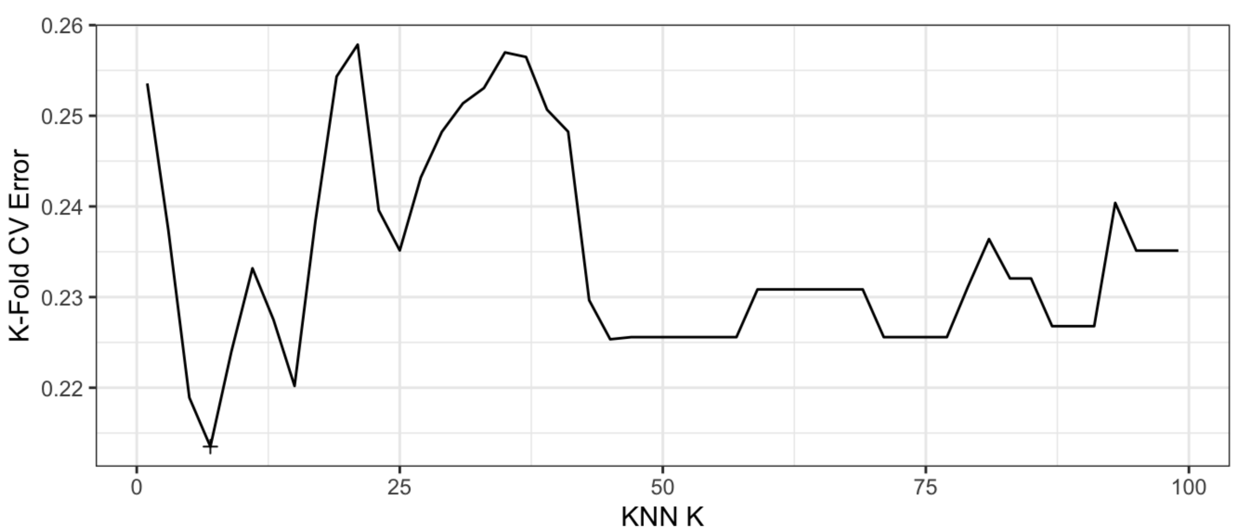
2.5 Cross-Validation for Classification Problems

So far we have talked only about CV for regression problems.

But CV can also be very useful for classification problems! For example, the LOOCV error rate for classification problems takes the form



```
k_fold <- 10
cv_label <- sample(seq_len(k_fold), nrow(train), replace = TRUE)
err <- rep(NA, k) # store errors for each flexibility level

for(k in seq(1, 100, by = 2)) {
  err_cv <- rep(NA, k_fold) # store error rates for each fold
  for(ell in seq_len(k_fold)) {
    trn_vec <- cv_label != ell # fit model on these
    tst_vec <- cv_label == ell # estimate error on these

    ## fit knn
    knn_fit <- knn(train[trn_vec, -1], train[tst_vec, -1],
  train[trn_vec, ]$class, k = k)
    ## error rate
    err_cv[ell] <- mean(knn_fit != train[tst_vec, ]$class)
  }
  err[k] <- mean(err_cv)
}
err <- na.omit(err)
```



Minimum CV error of 0.2135 found at $K = 7$.