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!

↳ unless you know the true model the data comes from (which you won't).

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

How to decide?

not like this.

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)*

Sometimes we talk about "root MSE"

$RMSE = \sqrt{MSE}$

(same scale as response).

$$\rightarrow MSE = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{f}(x_i)\right)^2$$

response for i^{th} obs.

prediction for i^{th} obs

Small if predictions are close to response.

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

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

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 for training data!
- Suppose we fit our learning method on our training data $\{(x_1,y_1),\dots,(x_n,y_n)\}$ and obtain estimate $\hat{f}$.

  $\hookrightarrow$ we can compute $\hat{f}(x_1),\dots,\hat{f}(x_n)$ if close to $y_1,\dots,y_n \Rightarrow$ small training MSE

But what 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 model that gives lowest test MSE

$\text{Ave}\left[\left(y_0 - \hat{f}(x_0)\right)^2\right]$ for 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 the scientific problem.

↳ access to set of observations that were not used to fit the model.

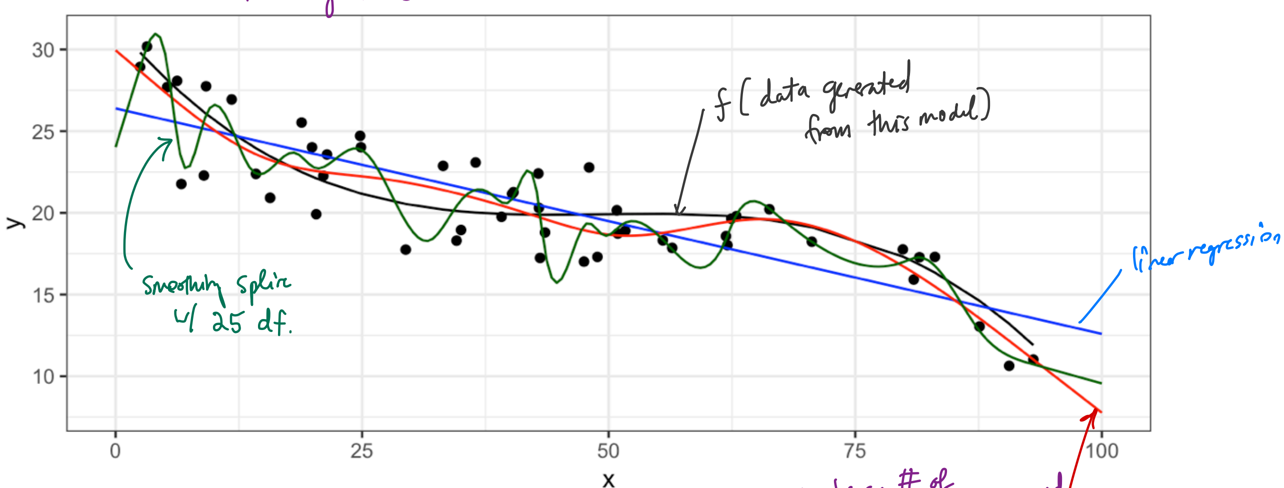
But what if we don't have a test set available?

Maybe we just minimize train MSE?

Problem: there is no guarantee that lowering training MSE lowers test MSE!

because many stat learning methods estimate coefs to lower training MSE

⇒ training MSE can be small but test MSE large!



smoothing spline w/ df=6 (ch. 7).

estimated using large # of draws from $f(x)+\varepsilon$ (not used to fit models)

model	df	Test MSE	Train MSE
Linear Regression	2	34.4168	4.9654
Smoothing Spline	6	38.9525	3.5248
Smoothing Spline	25	39.9288	2.3107

least flexible ↓ most flexible.

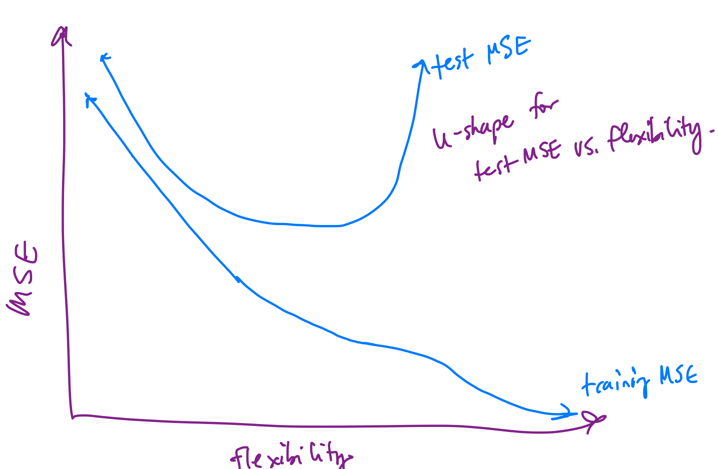
← linear regression has best test MSE!

worst test MSE

best training MSE

⇒ fits training data the best!

In general



How to choose model?

↳ need to estimate test MSE! (next).

1.1 Classification Setting

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.

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.

$$\frac{1}{n}\sum_{i=1}^{n} \mathbb{I}(\underbrace{y_i}_{\text{true label for } i^{th} \text{ obs.}} \neq \underbrace{\hat{y}_i}_{\text{predicted label for } i^{th} \text{ obs}}) \quad \text{where} \quad \mathbb{I}(y_i \neq \hat{y}_i) = \begin{cases} 1 & \text{if } y_i \neq \hat{y}_i \\ 0 & \text{o.w.} \end{cases}$$

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 mode interested in error rates for data *not* in our training data, i.e. test data (x_0, y_0)

The test error rate is

$$\text{Ave}\left(\mathbb{I}(y_0 \neq \underbrace{\hat{y}_0}_{\text{predicted class for test obs w/ predictor } x_0.})\right)$$

A good classifier is one for which the test error rate is small.

1.2 Bias-Variance Trade-off

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.

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

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

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

m

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 the data so closely $\Rightarrow$ new data means big changes in $\hat{f}$.

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

ex: linear regression assumes a linear form. It is unlikely that any real world problem is actually linear $\Rightarrow$ there will be some bias.

In general:

$\uparrow$ flexibility $\Rightarrow$ $\downarrow$ bias + $\uparrow$ variance.

how much these change determines 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, not usually the case.

In contrast, the training error can be easily calculated.

But training error can wildly under estimate 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?

> subset training data into 2 parts
>
> 1. (smaller) training data set
> 2. "test" data set.

> beg for money to create test data set.

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

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?

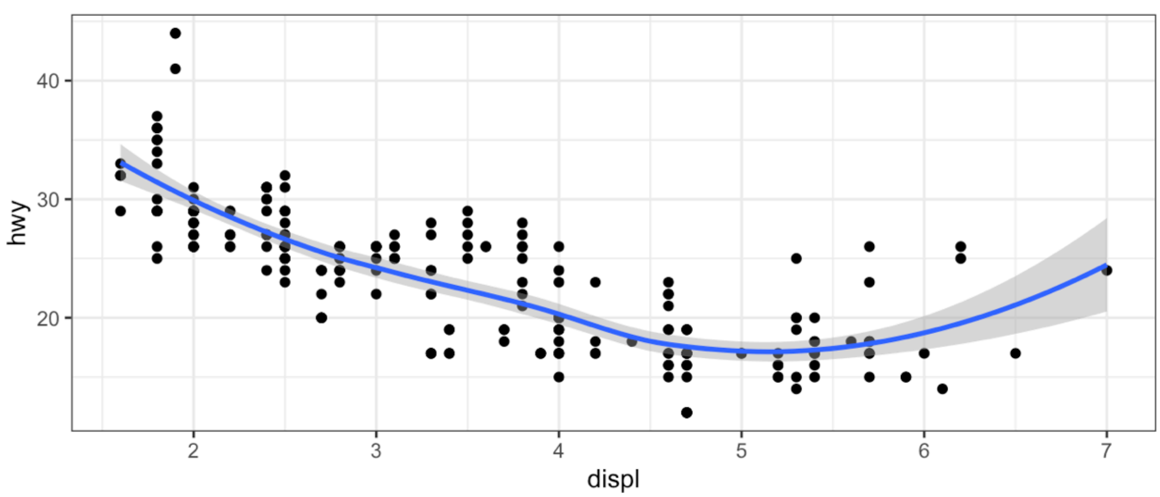
We could randomly divide our (training) data set into two parts: training & validation.

1 2 ... n original obs.

7 22 13 ... n*

fit model on these observations → 7 22 13 ... | 91 ... n* ← estimate test MSE on these observations

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!

$displ^3$, $displ^4$.

* library(rsample)

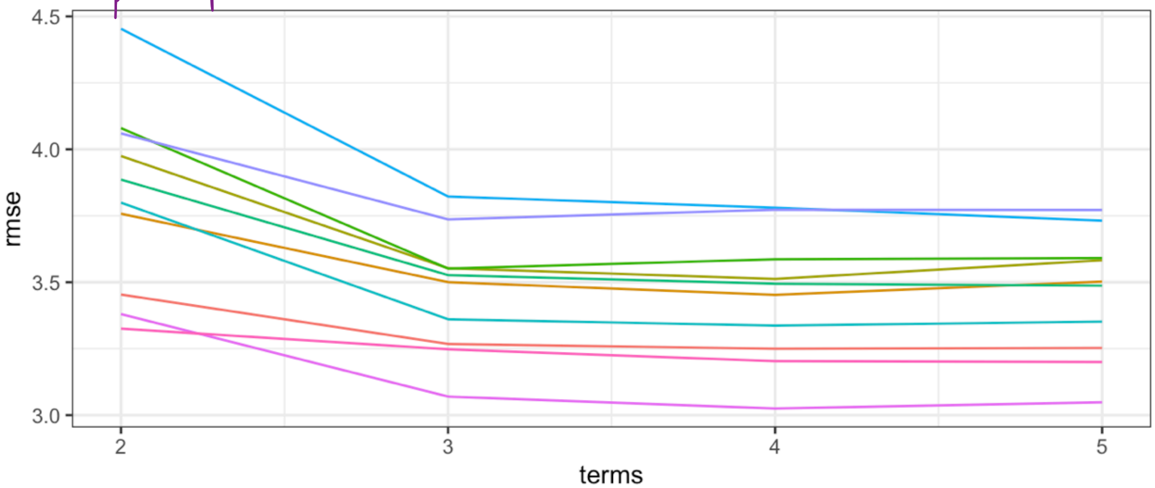
```r
## get index of training observations
# take 60% of observations as training and 40% for validation
mpg_val <- validation_split(mpg, prop = 0.6)

## models
lm_spec <- linear_reg()

linear_recipe <- recipe(hwy ~ displ, data = mpg)
quad_recipe <- linear_recipe |> step_mutate(displ2 = displ^2)
cubic_recipe <- quad_recipe |> step_mutate(displ3 = displ^3)
quart_recipe <- cubic_recipe |> step_mutate(displ4 = displ^4)

m0 <- workflow() |> add_model(lm_spec) |> add_recipe(linear_recipe) |>
         fit_resamples(resamples = mpg_val)
m1 <- workflow() |> add_model(lm_spec) |> add_recipe(quad_recipe) |>
         fit_resamples(resamples = mpg_val)
m2 <- workflow() |> add_model(lm_spec) |> add_recipe(cubic_recipe) |>
         fit_resamples(resamples = mpg_val)
m3 <- workflow() |> add_model(lm_spec) |> add_recipe(quart_recipe) |>
         fit_resamples(resamples = mpg_val)

## estimate test MSE
collect_metrics(m0) |> mutate(model = "linear") |>
  bind_rows(collect_metrics(m1) |> mutate(model = "quadratic")) |>
  bind_rows(collect_metrics(m2) |> mutate(model = "cubic")) |>
  bind_rows(collect_metrics(m3) |> mutate(model = "quartic")) |>
  select(model, .metric, mean) |>
  pivot_wider(names_from = .metric, values_from = mean) |>
  select(-rsq) |>
  kable()
```

test root MSE $= \sqrt{\text{test MSE}}$

model	rmse
linear	4.318968
quadratic	3.882112
cubic	3.866194
quartic	3.860612

← looks like best model!

Repeated process 10 times.



lot of variability here
→ sometimes we choose squared model!

- The validation estimate of the test error is highly variable
  depends on which observations were held out!

- Only a subset used to fit the model. Since statical models tend to better with more data.

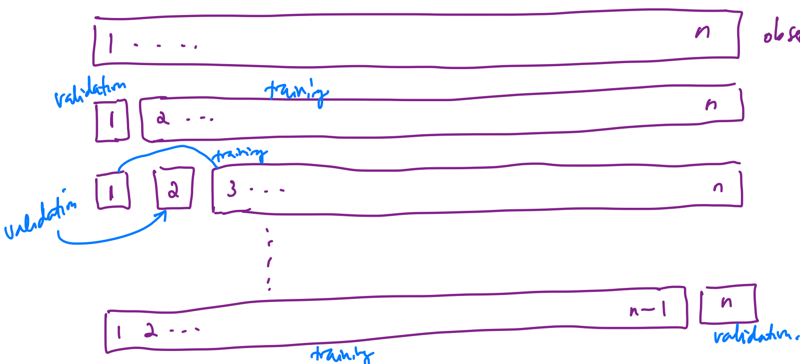
  The validation set error can overestimate the test error.

⇒ 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) $\hat{y}$ prediction made for held out observation.

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

low bias, 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 validation method).

Advantages

- less bias in estimate of error.
- since we fit with $n-1$ observations (instead $\approx \frac{n}{2}$ for validation approach).
  - $\Rightarrow$ LOOCV does not overestimate the test error as much.
- No randomness in this approach. $\Rightarrow$ will get the same result every time.

Disadvantages

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

LOO CV requires us to fit the model n times

$\Rightarrow$ could be very very slow.

n splits.

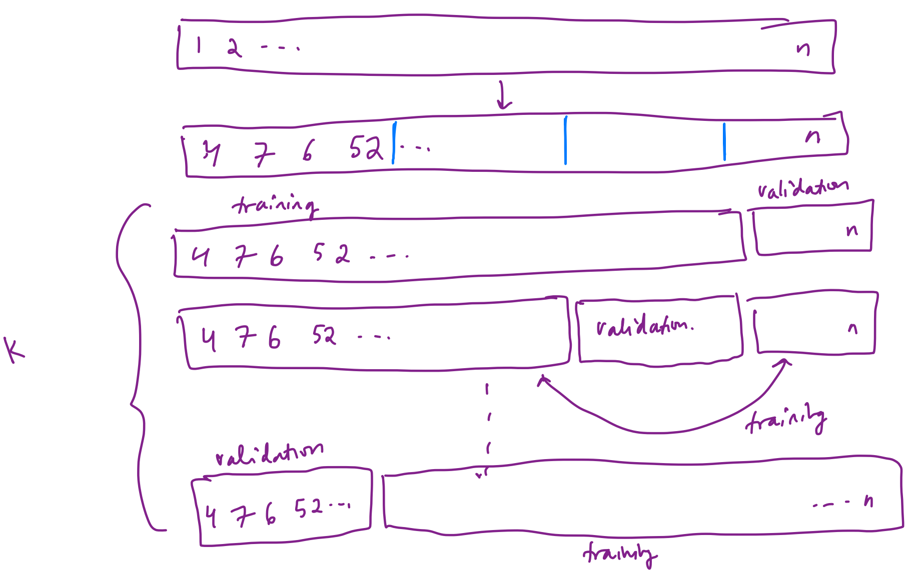
```r
## perform LOOCV on the mpg dataset
mpg_loocv <- vfold_cv(mpg, v = nrow(mpg))

## models
m0 <- workflow() |> add_model(lm_spec) |> add_recipe(linear_recipe) |>
        fit_resamples(resamples = mpg_loocv)
m1 <- workflow() |> add_model(lm_spec) |> add_recipe(quad_recipe) |>
        fit_resamples(resamples = mpg_loocv)
m2 <- workflow() |> add_model(lm_spec) |> add_recipe(cubic_recipe) |>
        fit_resamples(resamples = mpg_loocv)
m3 <- workflow() |> add_model(lm_spec) |> add_recipe(quart_recipe) |>
        fit_resamples(resamples = mpg_loocv)

## estimate test MSE
collect_metrics(m0) |> mutate(model = "linear") |>
  bind_rows(collect_metrics(m1) |> mutate(model = "quadratic")) |>
  bind_rows(collect_metrics(m2) |> mutate(model = "cubic")) |>
  bind_rows(collect_metrics(m3) |> mutate(model = "quartic")) |>
  select(model, .metric, mean) |>
  pivot_wider(names_from = .metric, values_from = mean) |>
  select(-rsq) |>
  kable()
```

model	rmse
linear	2.808356
quadratic	2.675896
cubic	2.615363
quartic	2.643536

we would choose level of flexibility w/ lowest $CV_{(n)}$ estimate of test MSE.

2.3 k-Fold Cross Validation

An alternative to LOOCV is *k*-fold CV. → randomly divide the set of 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.

The k-fold CV estimate is computed by averaging

$$CV_{(k)} = \frac{1}{K}\sum_{i=1}^{K} MSE_i = \frac{1}{K}\sum_{i=1}^{K}\frac{1}{|F_k|}\sum_{\underbrace{j\in F_k}_{\text{fold } k.}}(y_i - \hat{y}_i)^2$$

Usually use $k=5$ or 10

Why k-fold over LOOCV?

LOOCV is a special case of k-fold CV in which $k=n$.

Computational advantage! Now fit model k times (not n) can be huge!

Also other advantages due to bias-variance trade off. (more later).

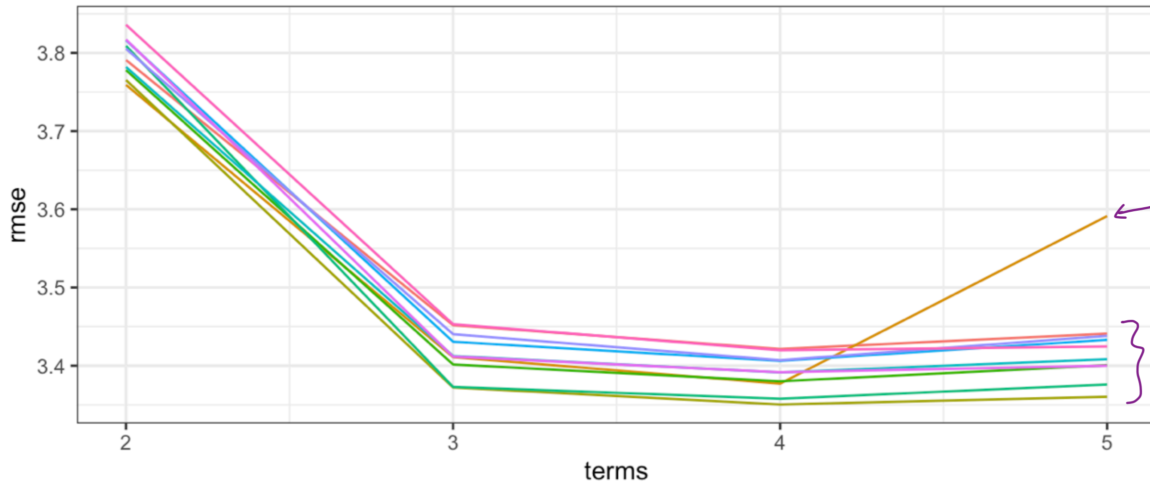
```
## perform k-fold on the mpg dataset
mpg_10foldcv <- vfold_cv(mpg, v = 10)

## models
m0 <- workflow() |> add_model(lm_spec) |> add_recipe(linear_recipe) |>
        fit_resamples(resamples = mpg_10foldcv)
m1 <- workflow() |> add_model(lm_spec) |> add_recipe(quad_recipe) |>
        fit_resamples(resamples = mpg_10foldcv)
m2 <- workflow() |> add_model(lm_spec) |> add_recipe(cubic_recipe) |>
        fit_resamples(resamples = mpg_10foldcv)
m3 <- workflow() |> add_model(lm_spec) |> add_recipe(quart_recipe) |>
        fit_resamples(resamples = mpg_10foldcv)

## estimate test MSE
collect_metrics(m0) |> mutate(model = "linear") |>
  bind_rows(collect_metrics(m1) |> mutate(model = "quadratic")) |>
  bind_rows(collect_metrics(m2) |> mutate(model = "cubic")) |>
  bind_rows(collect_metrics(m3) |> mutate(model = "quartic")) |>
  select(model, .metric, mean) |>
  pivot_wider(names_from = .metric, values_from = mean) |>
  select(-rsq) |>
  kable()
```

k=10.

model	rmse
linear	3.805566
quadratic	3.432052
cubic	3.409391
quartic	3.408420

close.

Now there is some randomness in how we assign obs to folds.



much tighter than validation approach.

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

Most often we use it to find the minimum CV error to help us pick a model (or model 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 advantage to LOOCV.

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

- Often k-fold CV gives a more accurate estimate of the test error 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 levels of bias
(use $\frac{(K-1)}{K} n$ obs to fit).

$\Rightarrow$ LOOCV gives lowest bias.

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

LOOCV has higher variance then k-fold CV w/ $k<n$.

Why?

LOOCV fits n models on almost identical data points $\Rightarrow$ averages outputs highly correlated w/ each other.

mean of highly correlated quantities has higher variance than mean of less correlated quantities.

k-fold average K outputs w/ more different observations than LOOCV (overlap smaller). $\Rightarrow$ LOOCV has higher variance than k-fold CV!

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.

in numerical experiments (simulations).

2.5 Cross-Validation for Classification Problems

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

MSE to quantify test error.

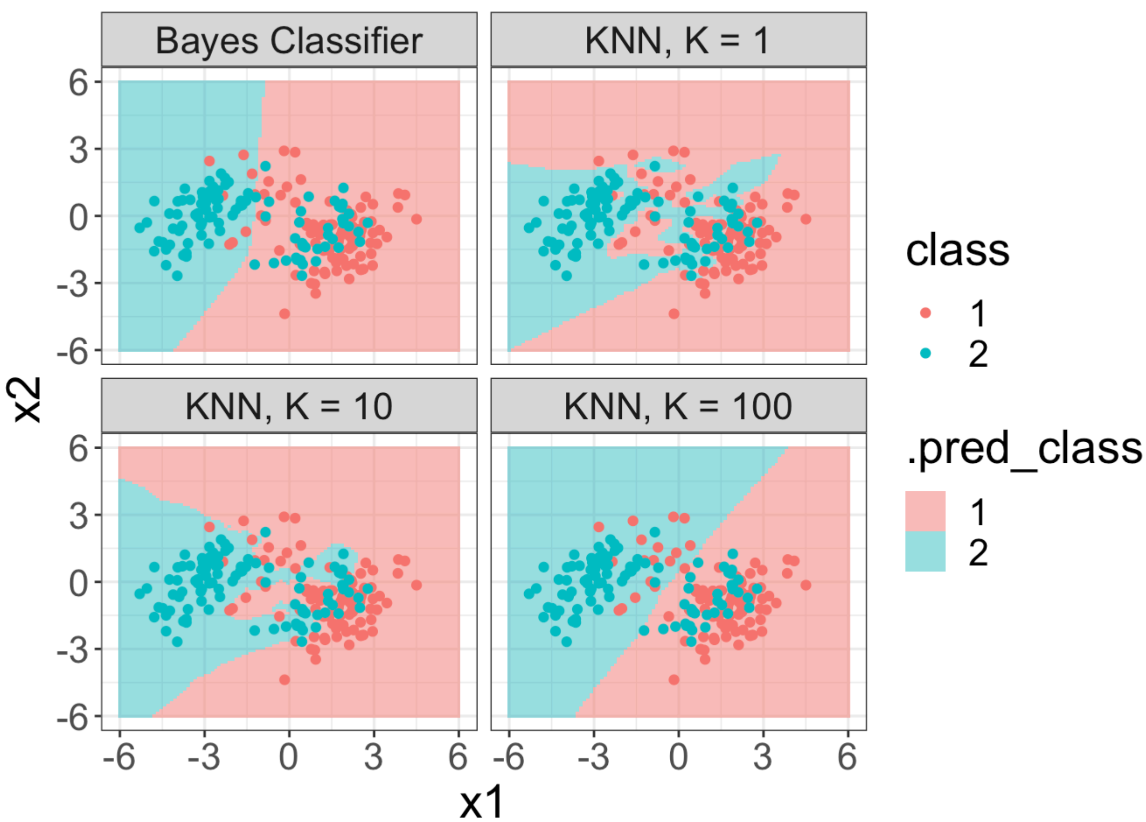
→ categorical response.

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

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

where $Err_i = \mathbb{I}(y_i \neq \hat{y}_i) = \begin{cases} 1 & y_i \neq \hat{y}_i \\ 0 & \text{o.w.} \end{cases}$

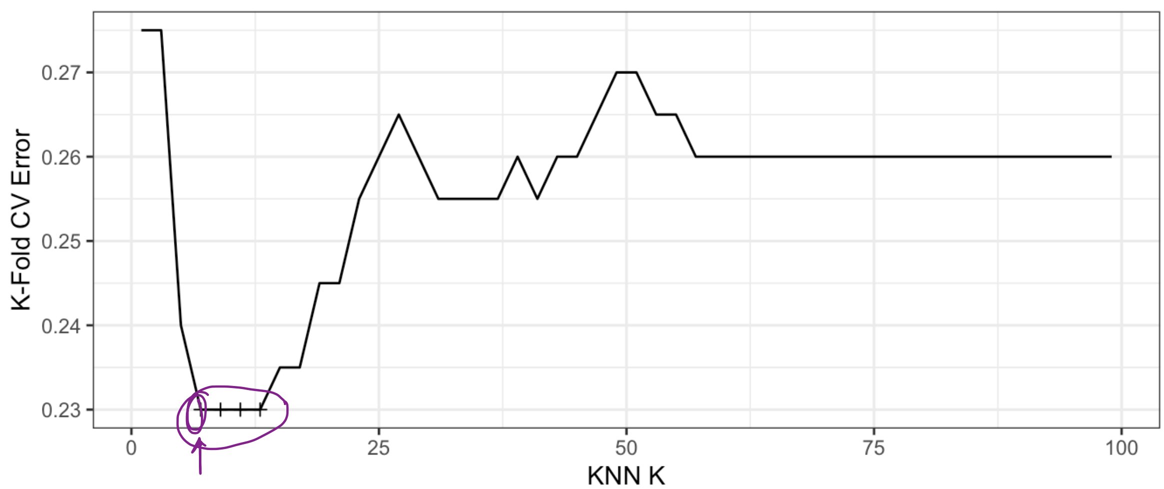
K-fold and validation errors estimated accordingly.



recall this simulated example.

Can we choose K using CV approach?
"tune" K

```
k_fold <- 10
train_cv <- vfold_cv(train, v = k_fold)

grid_large <- tibble(neighbors = seq(1, 100, by = 2))

knn_spec <- nearest_neighbor(mode = "classification", neighbors =
        tune("neighbors"))
knn_spec |>
  tune_grid(class ~ x1 + x2, resamples = train_cv, grid = grid_large)
        |>
  collect_metrics() |>
  filter(.metric == "accuracy") |>
  mutate(error = 1 - mean) -> knn_err
```



Minimum CV error of 0.23 found at $K = 7$.

So we might choose $K=7$,
and fit KNN classification model w/ $K=7$ on entire training data set