

Resampling Methods

AU STAT-427/627

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Motivation

We are already familiar with train-test splits

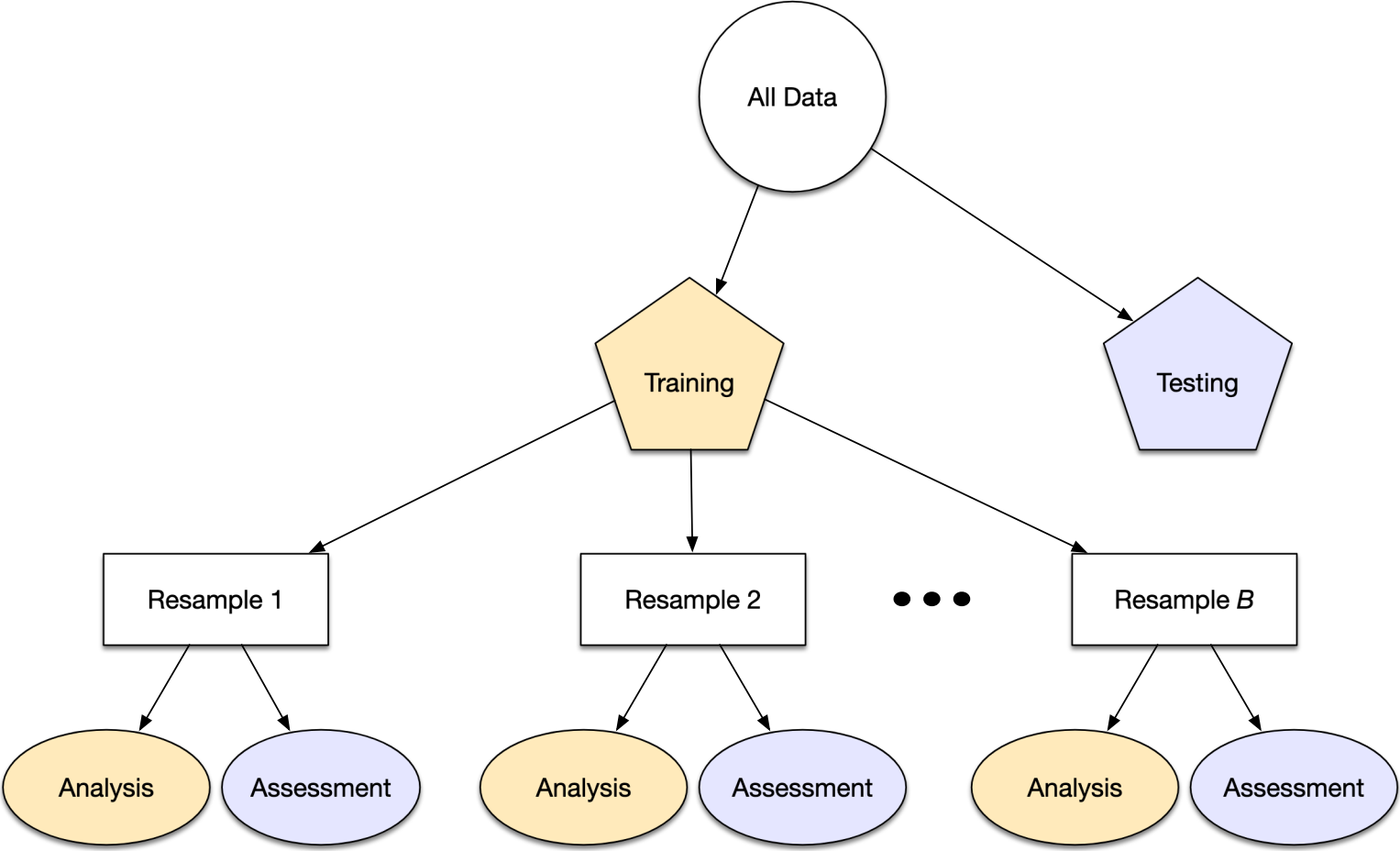
The main downside to to train-test splits so far is that we can only use them once

This means we effectively can't make any decisions about the models we are using

Resampling

Resampling estimates of performance can generalize to new data

Resampling Workflow



Resampling Workflow

The resampling is only conducted on the training set

We are still keeping the test set. The test set is not involved.

For each iteration of resampling, the data are partitioned into two subsamples:

- The model is fit with the **analysis set**
- The model is evaluated with the **assessment set**

Resampling Workflow

We have effectively created many train-test split out of our training data set.

The [challenge](#) here now becomes how we are creating these resample sets

Resampling Workflow

Suppose we generate 10 different resamples

This mean that we will be:

- Fitting 10 different models
- Perform predictions 10 times
- Prodice 10 sets of performance statistics

The final estimate of the **performance** of the model will be the average of these 10 models

Resampling Workflow

If the resampling is done in an appropriate way then this average has very good generalization properties

Leave-One-Out Cross Validation

- 1 observation is used as the **assessment set**
- The remaining observations make up the **analysis set**

Notes:

We are fitting the model on $n - 1$ observations and a prediction \hat{y}_1 is made on the **assessment set** using the value x_1

Leave-One-Out Cross Validation

Since (x_1, y_1) is not used in the fitting process, then $MSE_1 = (y_1 - \hat{y}_1)^2$ provides an approximately unbiased estimate for the test error.

While this estimate is approximately unbiased, it is quite poor since it is highly variable

Leave-One-Out Cross Validation

We can repeat this for

- $MSE_2 = (y_2 - \hat{y}_2)^2$

- $MSE_3 = (y_3 - \hat{y}_3)^2$

- ...

-

$$MSE_n = (y_n - \hat{y}_n)^2$$

to get n estimates of the test error

Leave-One-Out Cross Validation

The LOOCV estimate of the test MSE is

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

Leave-One-Out Cross Validation

Pros

The LOOCV estimate of the test MSE is going to have low bias

There is no randomness in the LOOCV estimate

Cons

You need a lot of computational power even for modest data sets

(Some models don't need to be repeatedly refit)

K-Fold Cross Validation

Could we think of a compromise between fitting 1 model and n models?

K-Fold Cross Validation has an answer:

Randomly divide the observations into k groups (or **folders**) of approximately equal size

K-Fold Cross Validation

Randomly divide the observations into k groups (or **fold**s) or approximately equal size

- 1 **fold** is used as the **assessment set**
- The remaining **fold**s make up the **analysis set**

Everything else happens as before.

We now get fewer performance metrics, BUT they are each less variable

Training
Data



Training
Data

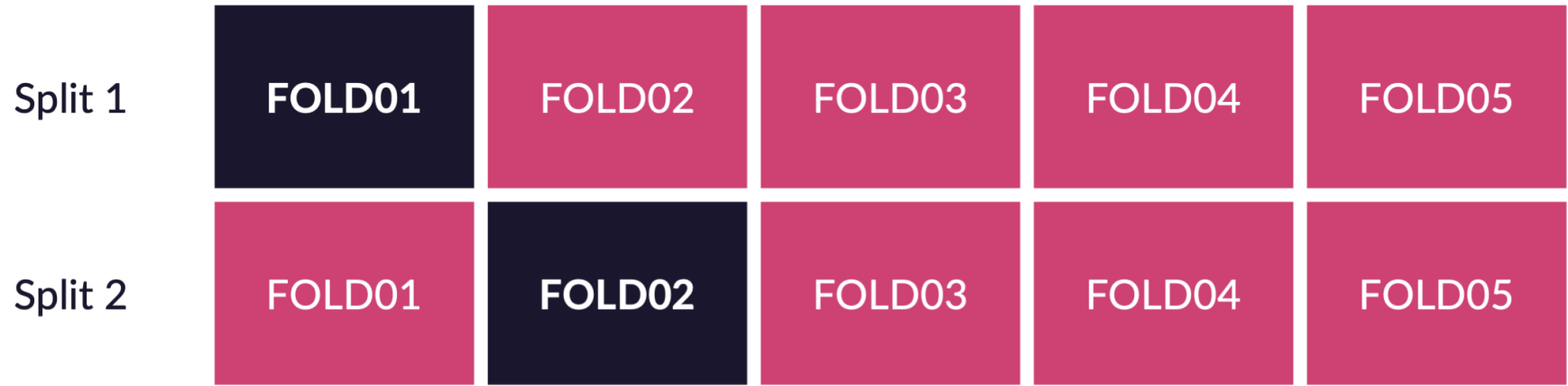


Training
Data



Split 1

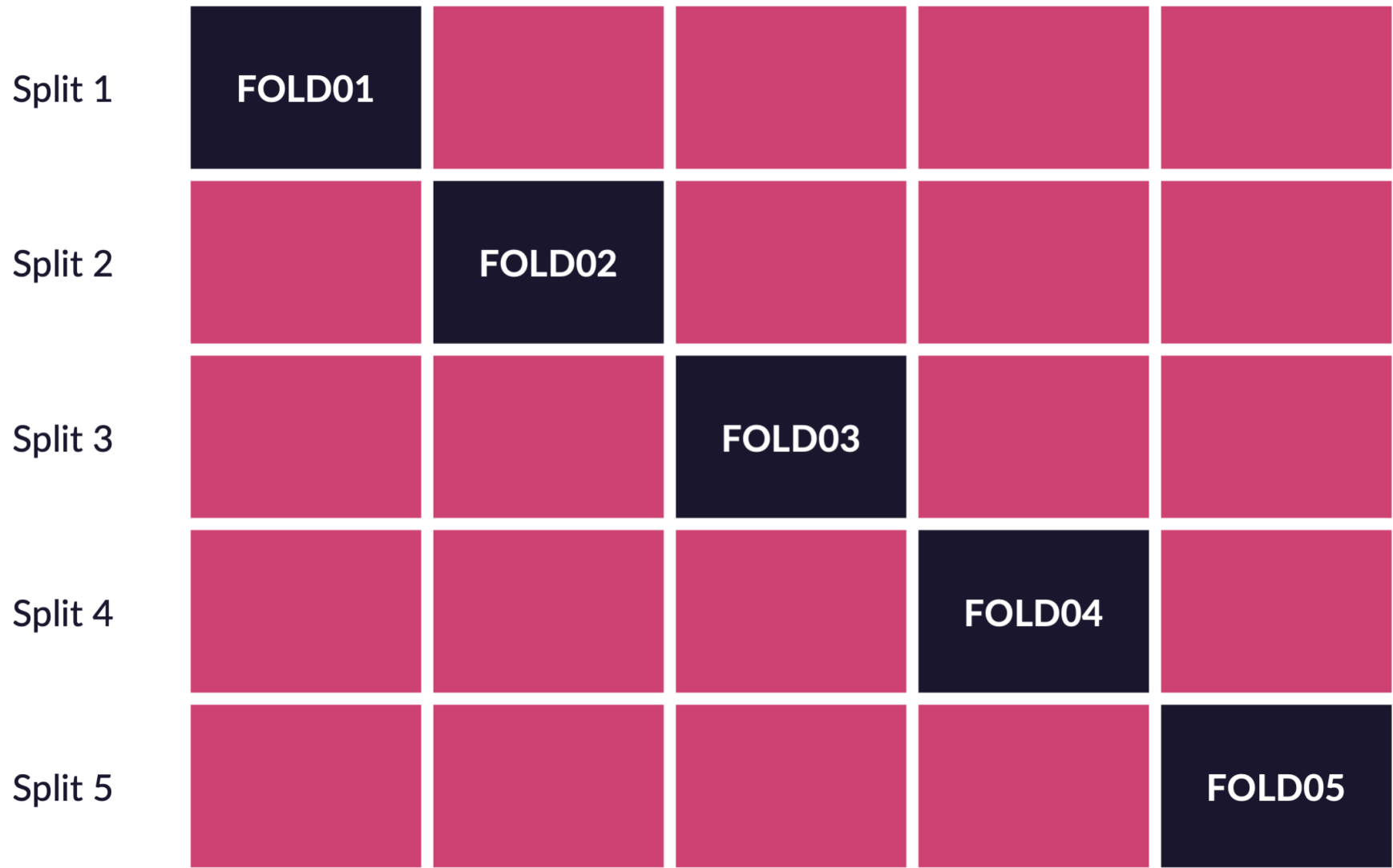


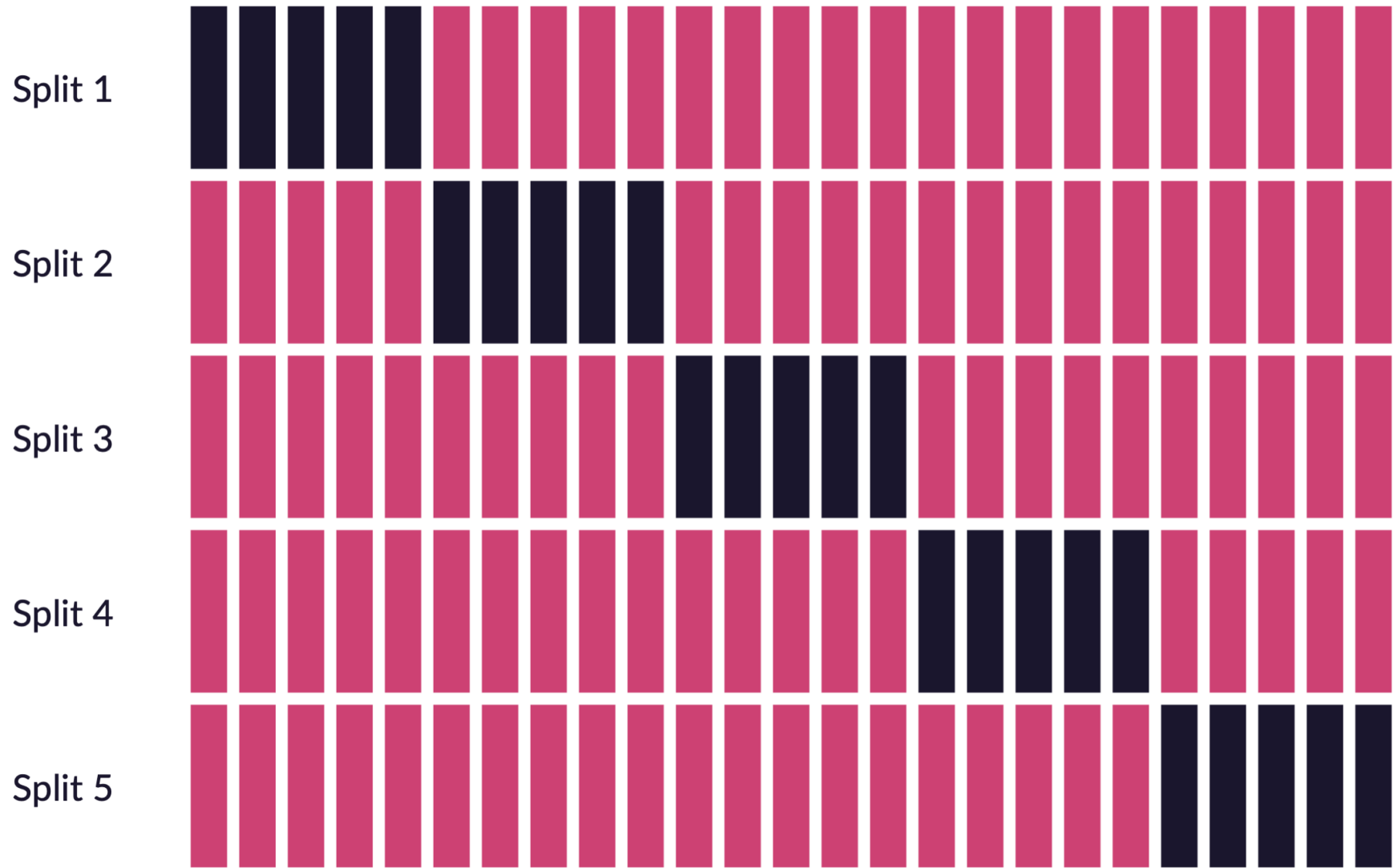


Split 1	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 2	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 3	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05

Split 1	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 2	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 3	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 4	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05

Split 1	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 2	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 3	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 4	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05
Split 5	FOLD01	FOLD02	FOLD03	FOLD04	FOLD05





Cross validation

When we perform cross-validation our goal might be to determine how well a given model is expected to perform on new data

Other times we are using cross-validation to find the best model/hyperparameters

Bias-Variance tradeoff of LOOCV and k-fold Cross Validation

LOOCV has a lower bias than k-fold CV

However since the mean of many highly correlated quantities has higher variance than the mean of many not correlated quantities, we have that LOOCV has a higher variance than k-fold CV

Rsample

We are back with `rsample`

```
library(rsample)
```

```
mtcars
```

```
##           mpg cyl  disp  hp drat   wt  qsec vs am gear carb
## Mazda RX4      21.0   6 160.0 110 3.90 2.620 16.46 0  1   4    4
## Mazda RX4 Wag  21.0   6 160.0 110 3.90 2.875 17.02 0  1   4    4
## Datsun 710     22.8   4 108.0  93 3.85 2.320 18.61 1  1   4    1
## Hornet 4 Drive 21.4   6 258.0 110 3.08 3.215 19.44 1  0   3    1
## Hornet Sportabout 18.7   8 360.0 175 3.15 3.440 17.02 0  0   3    2
## Valiant        18.1   6 225.0 105 2.76 3.460 20.22 1  0   3    1
## Duster 360     14.3   8 360.0 245 3.21 3.570 15.84 0  0   3    4
## Merc 240D      24.4   4 146.7  62 3.69 3.190 20.00 1  0   4    2
## Merc 230       22.8   4 140.8  95 3.92 3.150 22.90 1  0   4    2
## Merc 280       19.2   6 167.6 123 3.92 3.440 18.30 1  0   4    4
## Merc 280C      17.8   6 167.6 123 3.92 3.440 18.90 1  0   4    4
## Merc 450SE     16.4   8 275.8 180 3.07 4.070 17.40 0  0   3    3
## Merc 450SL     17.3   8 275.8 180 3.07 3.730 17.60 0  0   3    3
## Merc 450SLC    15.2   8 275.8 180 3.07 3.780 18.00 0  0   3    3
```

Rsample

We can use the `vfold_cv()` function on a `data.frame` to create a `vfold_cv` object

```
mtcars_folds <- vfold_cv(mtcars, v = 4)
mtcars_folds
```

```
## # 4-fold cross-validation
## # A tibble: 4 x 2
##   splits          id
##   <list>         <chr>
## 1 <split [24/8]> Fold1
## 2 <split [24/8]> Fold2
## 3 <split [24/8]> Fold3
## 4 <split [24/8]> Fold4
```

Rsample

An under the hood, we have 4 analysis/assessment splits similar to `initial_split()`

```
mtcars_folds <- vfold_cv(mtcars, v = 4)
mtcars_folds$splits
```

```
## [[1]]
## <Analysis/Assess/Total>
## <24/8/32>
##
## [[2]]
## <Analysis/Assess/Total>
## <24/8/32>
##
## [[3]]
## <Analysis/Assess/Total>
## <24/8/32>
##
## [[4]]
## <Analysis/Assess/Total>
## <24/8/32>
```

Using resamples in action

We start by creating a linear regression sepecification

```
library(parsnip)
linear_spec <- linear_reg() %>%
  set_mode("regression") %>%
  set_engine("lm")
```

Workflows

Simple package that helps us formulate more about what happens to our model.

Main functions are `workflow()`, `add_model()`, `add_formula()` or `add_variables()` (we will see `add_recipe()` later in the course)

```
library(workflows)
```

```
linear_wf <- workflow() %>%  
  add_model(linear_spec) %>%  
  add_formula(mpg ~ disp + hp + wt)
```


Workflows

This allows up to combine the model with what variables it should expect

```
library(workflows)

linear_wf <- workflow() %>%
  add_model(linear_spec) %>%
  add_formula(mpg ~ disp + hp + wt)
linear_wf
```

```
## — Workflow —————
## Preprocessor: Formula
## Model: linear_reg()
##
## — Preprocessor —————
## mpg ~ disp + hp + wt
##
## — Model —————
## Linear Regression Model Specification (regression)
##
## Computational engine: lm
```

`add_variables()` allows for a different way of specifying the the response and predictors in our model

Workflows

```
library(workflows)

linear_wf <- workflow() %>%
  add_model(linear_spec) %>%
  add_variables(outcomes = mpg,
               predictors = c(displ, hp, wt))

linear_wf
```

```
## — Workflow —————
## Preprocessor: Variables
## Model: linear_reg()
##
## — Preprocessor —————
## Outcomes: mpg
## Predictors: c(displ, hp, wt)
##
## — Model —————
## Linear Regression Model Specification (regression)
##
## Computational engine: lm
```

Workflows

You can use a `workflow` just like a `parsnip` object and fit it directly

```
fit(linear_wf, data = mtcars)
```

```
## — Workflow [trained] —————  
## Preprocessor: Variables  
## Model: linear_reg()  
##  
## — Preprocessor —————  
## Outcomes: mpg  
## Predictors: c(displ, hp, wt)  
##  
## — Model —————  
##  
## Call:  
## stats::lm(formula = ..y ~ ., data = data)  
##  
## Coefficients:  
## (Intercept)          displ           hp           wt  
##  37.105505    -0.000937    -0.031157    -3.800891
```

Tune

We introduce the **tune** package. This package helps us fit many models in a controlled manner in the tidymodels framework. It relies heavily on parsnip and rsample

Tune

We can use `fit_resamples()` to fit the workflow we created within each resample

```
library(tune)

linear_fold_fits <- fit_resamples(
  linear_wf,
  resamples = mtcars_folds
)
```

Tune

The results of this resampling comes as a data.frame

```
linear_fold_fits
```

```
## # Resampling results
## # 4-fold cross-validation
## # A tibble: 4 x 4
##   splits          id    .metrics          .notes
##   <list>         <chr> <list>          <list>
## 1 <split [24/8]> Fold1 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 2 <split [24/8]> Fold2 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 3 <split [24/8]> Fold3 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 4 <split [24/8]> Fold4 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
```

Tune

`collect_metrics()` can be used to extract the CV estimate

```
library(tune)

linear_fold_fits <- fit_resamples(
  linear_wf,
  resamples = mtcars_folds
)

collect_metrics(linear_fold_fits)

## # A tibble: 2 x 6
##   .metric .estimator  mean     n std_err .config
##   <chr>   <chr>      <dbl> <int>  <dbl> <chr>
## 1 rmse    standard    3.54     4  0.529 Preprocessor1_Model1
## 2 rsq     standard    0.778     4  0.0793 Preprocessor1_Model1
```

Tune

Setting `summarize = FALSE` in `collect_metrics()` Allows us to see the individual performance metrics for each fold

```
collect_metrics(linear_fold_fits, summarize = FALSE)
```

```
## # A tibble: 8 x 5
##   id      .metric .estimator .estimate .config
##   <chr> <chr>    <chr>         <dbl> <chr>
## 1 Fold1 rmse     standard     3.50  Preprocessor1_Model1
## 2 Fold1 rsq     standard     0.836 Preprocessor1_Model1
## 3 Fold2 rmse     standard     2.25  Preprocessor1_Model1
## 4 Fold2 rsq     standard     0.796 Preprocessor1_Model1
## 5 Fold3 rmse     standard     3.56  Preprocessor1_Model1
## 6 Fold3 rsq     standard     0.555 Preprocessor1_Model1
## 7 Fold4 rmse     standard     4.84  Preprocessor1_Model1
## 8 Fold4 rsq     standard     0.926 Preprocessor1_Model1
```


Tune

There are some settings we can set with `control_resamples()`.

One of the most handy ones (IMO) is `verbose = TRUE`

```
library(tune)
```

```
linear_fold_fits <- fit_resamples(  
  linear_wf,  
  resamples = mtcars_folds,  
  control = control_resamples(verbose = TRUE)  
)
```

```
i Fold1: preprocessor 1/1  
✓ Fold1: preprocessor 1/1  
i Fold1: preprocessor 1/1, model 1/1  
✓ Fold1: preprocessor 1/1, model 1/1  
i Fold1: preprocessor 1/1, model 1/1 (predictions)  
i Fold2: preprocessor 1/1  
✓ Fold2: preprocessor 1/1  
i Fold2: preprocessor 1/1, model 1/1  
✓ Fold2: preprocessor 1/1, model 1/1  
i Fold2: preprocessor 1/1, model 1/1 (predictions)  
i Fold3: preprocessor 1/1  
✓ Fold3: preprocessor 1/1  
i Fold3: preprocessor 1/1, model 1/1  
✓ Fold3: preprocessor 1/1, model 1/1  
i Fold3: preprocessor 1/1, model 1/1 (predictions)  
i Fold4: preprocessor 1/1  
✓ Fold4: preprocessor 1/1  
i Fold4: preprocessor 1/1, model 1/1  
✓ Fold4: preprocessor 1/1, model 1/1  
i Fold4: preprocessor 1/1, model 1/1 (predictions)  
i Fold5: preprocessor 1/1  
✓ Fold5: preprocessor 1/1  
i Fold5: preprocessor 1/1, model 1/1  
✓ Fold5: preprocessor 1/1, model 1/1  
i Fold5: preprocessor 1/1, model 1/1 (predictions)
```

Tune

We can also directly specify the metrics that are calculated within each resample

```
library(tune)

linear_fold_fits <- fit_resamples(
  linear_wf,
  resamples = mtcars_folds,
  metrics = metric_set(rmse, rsq, mase)
)

collect_metrics(linear_fold_fits)

## # A tibble: 3 x 6
##   .metric .estimator  mean      n std_err .config
##   <chr>   <chr>      <dbl> <int>  <dbl> <chr>
## 1 mase    standard    0.519     4  0.0634 Preprocessor1_Model1
## 2 rmse    standard    3.54      4  0.529  Preprocessor1_Model1
## 3 rsq     standard    0.778     4  0.0793 Preprocessor1_Model1
```

Bootstrapping

Last week we looked at a couple of different Cross-Validation methods

- Leave-One-Out Cross-Validation (LOOCV)
- K-fold Cross-Validation

Bootstrapping

This week we will look at **Bootstrapping**

This is a technique that uses resampling with replacement to estimate the uncertainty with a given estimator or statistical learning method

It is a powerful and general statistical tool, and can be used with most estimators/methods

Bootstrapping VS Cross-Validation

- **Cross-Validation**: provide estimates of the test error.
- **Bootstrap**: provides the standard error of the estimates.

Motivation

Suppose We have an estimate we want to find out how variable it is.

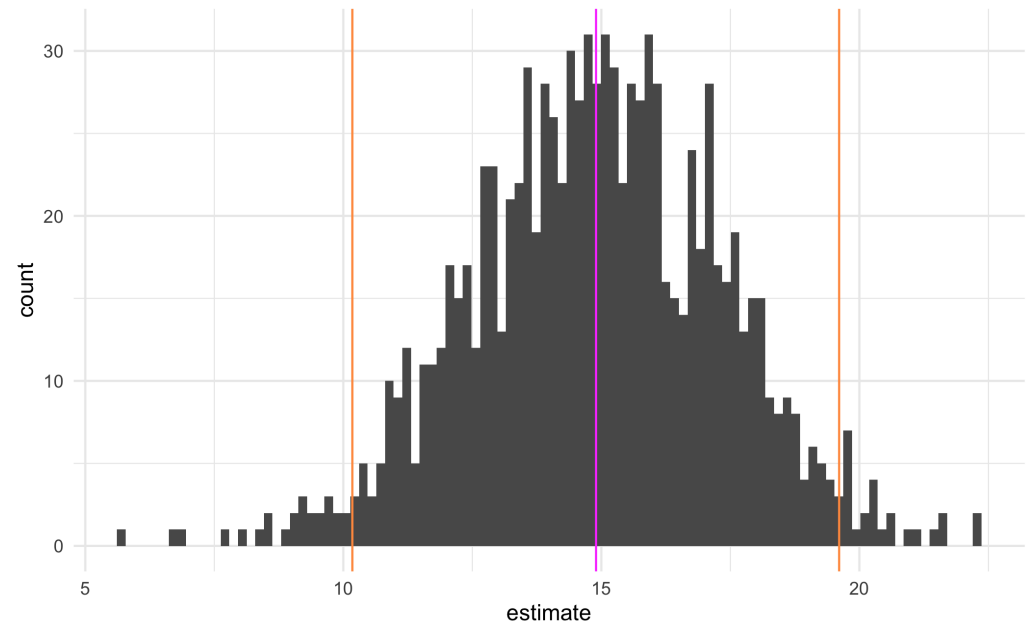
We could collect data n times and calculate the estimates.

We then have a distribution of and can see the how well it is doing

1000 realizations

pink line is the mean

orange lines 95% percent quantiles



Motivation

The Problem

We are not always able to conduct multiple data collections at will

Sometimes for resource issues or time-sensitive data

We need the different samples to come from the same underlying distribution

Motivation

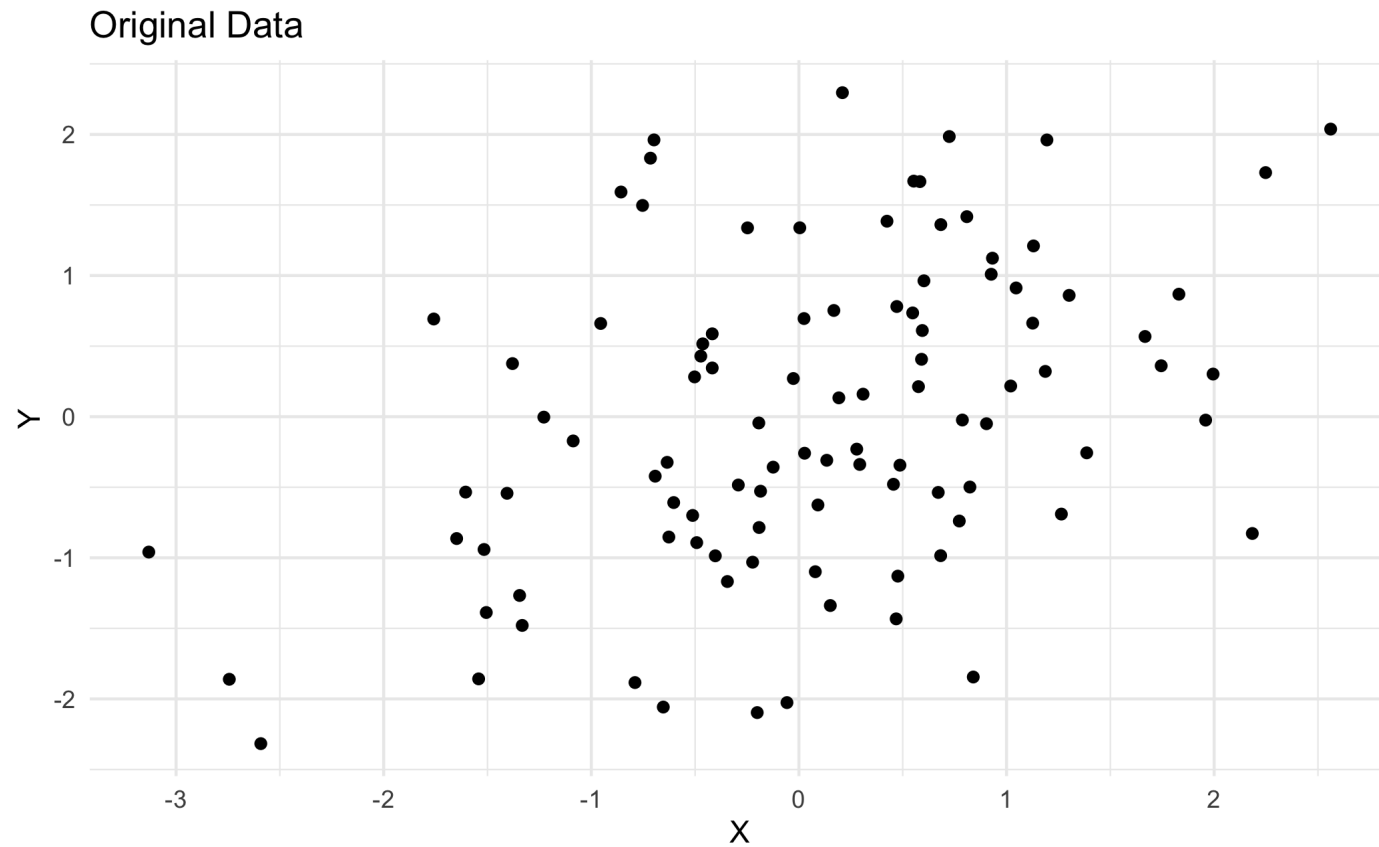
The Solution

We take our one data set and resample the rows with replacement. This allows us to get new data sets that approximate the original data set

If the original data set is close to the underlying true distribution then the resampled data sets are also approximations of the true underlying distribution

Example

From "An Introduction to Statistical Learning"

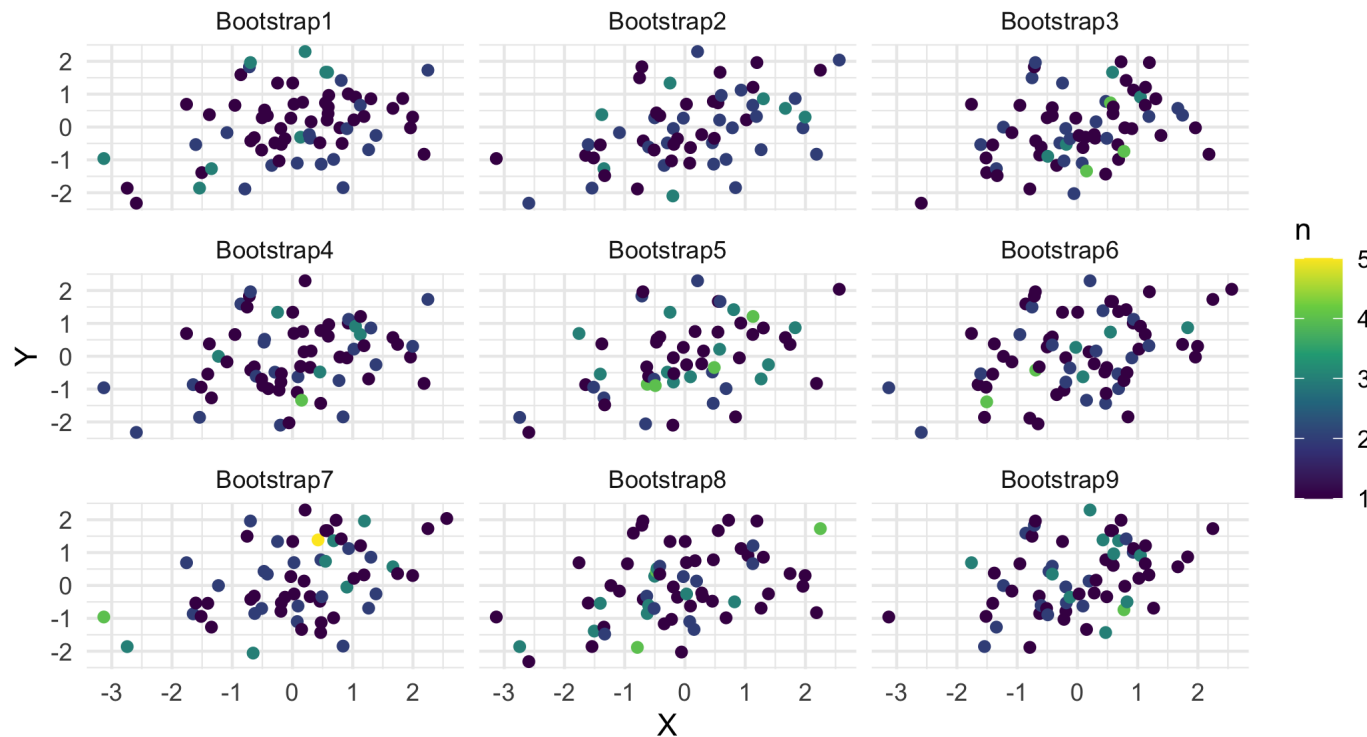


Example

Visualizing multiple bootstrappings

9 realizations of Bootstrapping

Color indicates the number of times the observation is sampled



Example

We want to minimize

$$\alpha = \frac{\sigma_Y^2 - \sigma_{XY}}{\sigma_X^2 + \sigma_Y^2 - 2\sigma_{XY}}$$

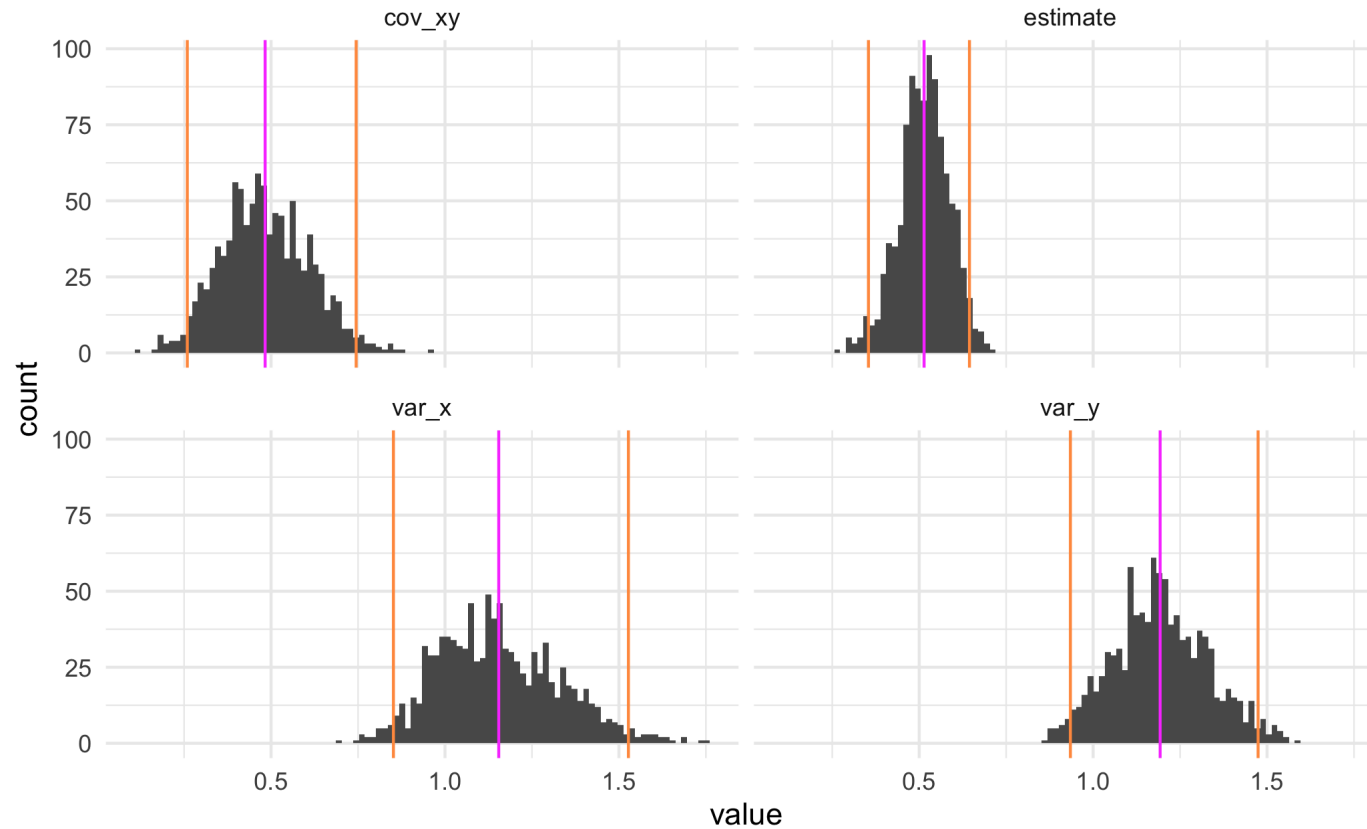
Where $\sigma_X^2 = \text{Var}(X)$, $\sigma_Y^2 = \text{Var}(Y)$, and $\sigma_{XY} = \text{Cov}(X, Y)$

Bootstrapping results

```
## # A tibble: 1,000 x 5
##   id          var_x var_y cov_xy estimate
##   <chr>        <dbl> <dbl> <dbl>    <dbl>
## 1 Bootstrap0001 0.972  1.09  0.472    0.555
## 2 Bootstrap0002 1.29   1.52  0.806    0.593
## 3 Bootstrap0003 1.10   1.25  0.481    0.554
## 4 Bootstrap0004 1.38   1.33  0.514    0.485
## 5 Bootstrap0005 1.44   1.22  0.603    0.424
## 6 Bootstrap0006 0.919  1.01  0.269    0.533
## 7 Bootstrap0007 1.26   1.18  0.409    0.475
## 8 Bootstrap0008 1.16   1.21  0.457    0.520
## 9 Bootstrap0009 1.29   1.19  0.505    0.468
## 10 Bootstrap0010 1.53   1.33  0.699    0.431
## # ... with 990 more rows
```

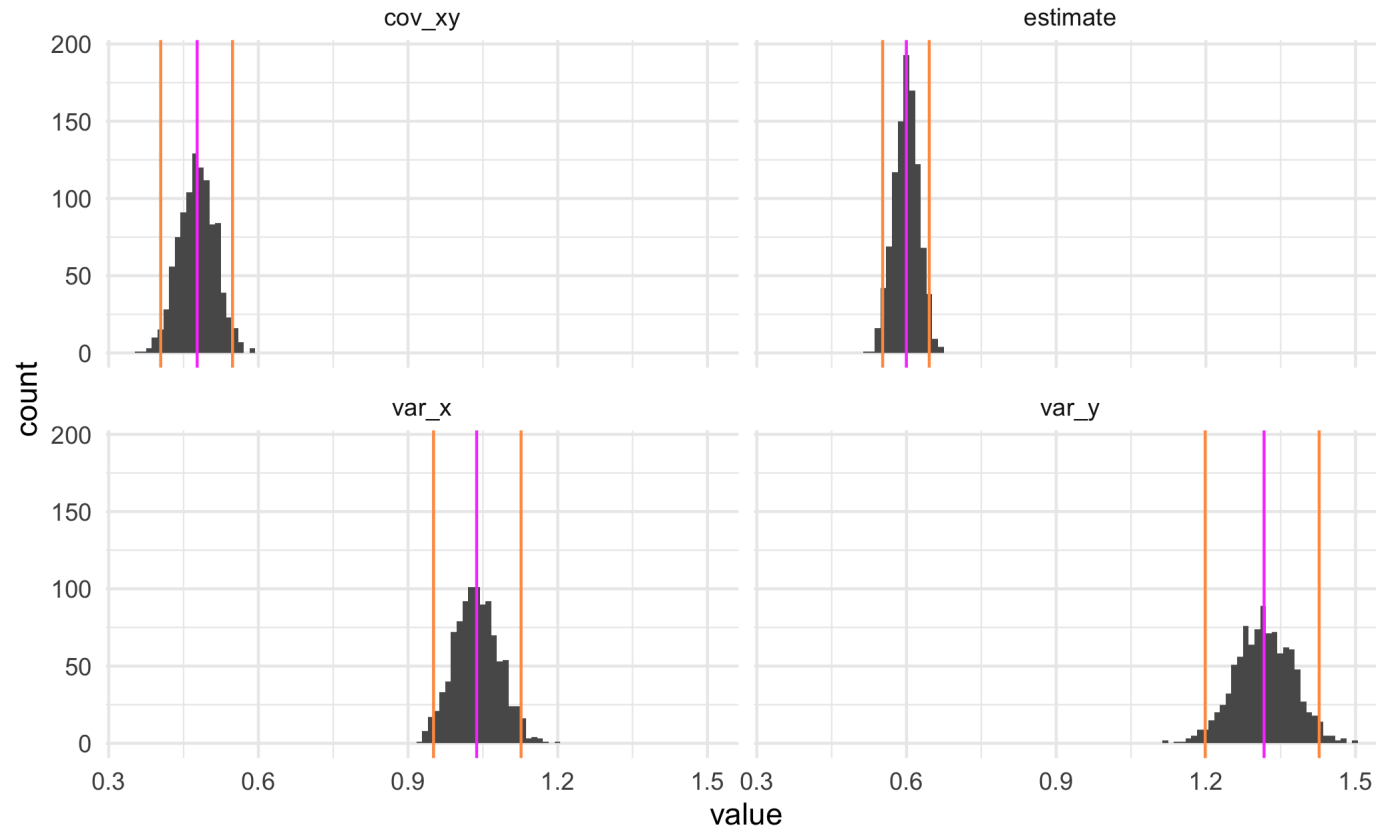
Bootstrapping results

With $n = 100$ in original data set



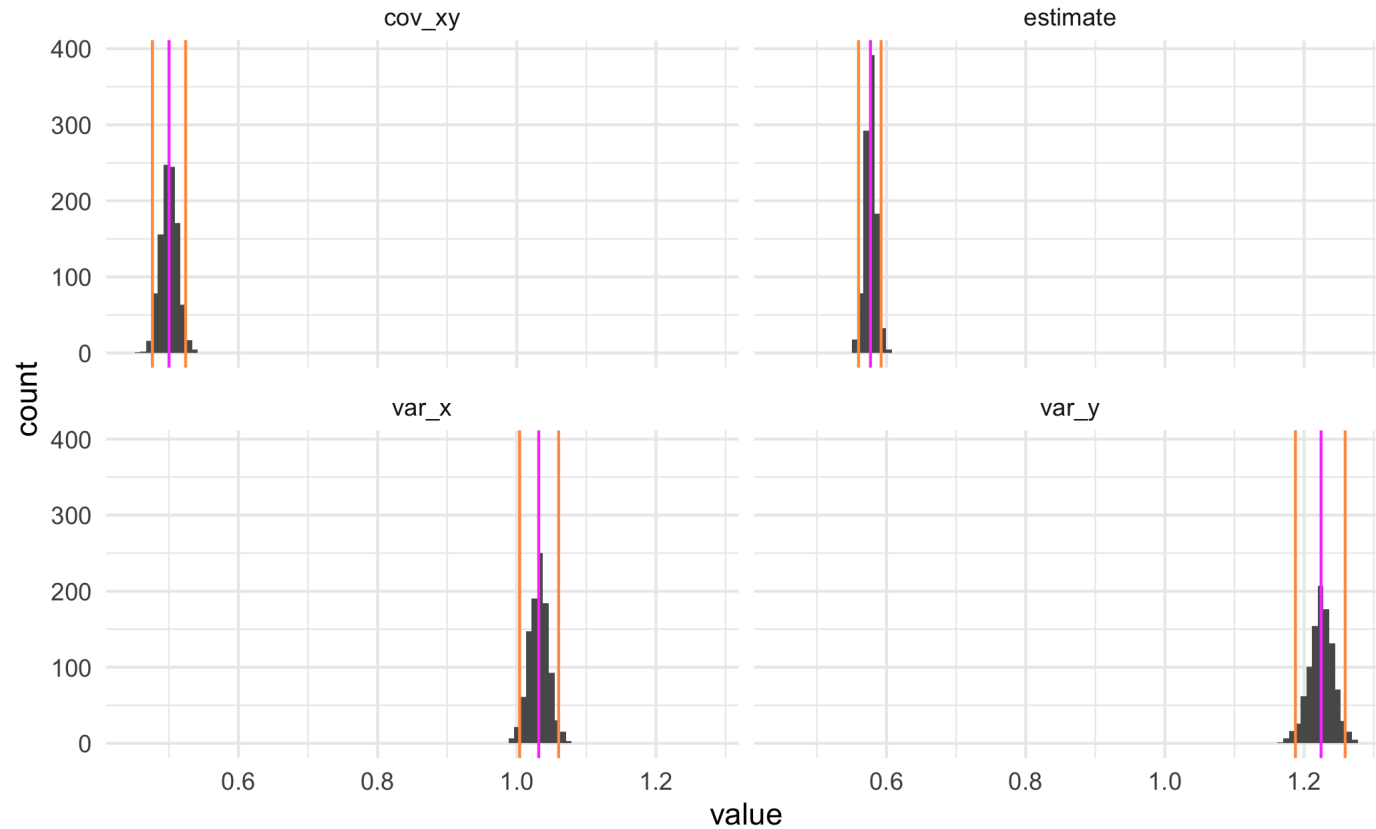
Bootstrapping results

With $n = 1000$ in original data set



Bootstrapping results

With $n = 10000$ in original data set



What size of bootstrappings are we looking for?

We are using bootstrapping sizes to be the same size of to get a comparatively estimate of the variation

Rsample

We are back with `rsample` and the `mtcars` data set

```
library(rsample)
```

```
mtcars
```

```
##           mpg  cyl  disp  hp  drat    wt    qsec vs  am  gear  carb
## Mazda RX4      21.0    6 160.0 110  3.90  2.620 16.46 0  1    4    4
## Mazda RX4 Wag  21.0    6 160.0 110  3.90  2.875 17.02 0  1    4    4
## Datsun 710     22.8    4 108.0  93  3.85  2.320 18.61 1  1    4    1
## Hornet 4 Drive  21.4    6 258.0 110  3.08  3.215 19.44 1  0    3    1
## Hornet Sportabout 18.7    8 360.0 175  3.15  3.440 17.02 0  0    3    2
## Valiant        18.1    6 225.0 105  2.76  3.460 20.22 1  0    3    1
## Duster 360     14.3    8 360.0 245  3.21  3.570 15.84 0  0    3    4
## Merc 240D      24.4    4 146.7  62  3.69  3.190 20.00 1  0    4    2
## Merc 230       22.8    4 140.8  95  3.92  3.150 22.90 1  0    4    2
## Merc 280       19.2    6 167.6 123  3.92  3.440 18.30 1  0    4    4
## Merc 280C      17.8    6 167.6 123  3.92  3.440 18.90 1  0    4    4
## Merc 450SE     16.4    8 275.8 180  3.07  4.070 17.40 0  0    3    3
## Merc 450SL     17.3    8 275.8 180  3.07  3.730 17.60 0  0    3    3
## Merc 450SLC    15.2    8 275.8 180  3.07  3.780 18.00 0  0    3    3
```

Rsample

We can use the `bootstraps()` function on a `data.frame` to create a `bootstraps` object

```
mtcars_boots <- bootstraps(mtcars, times = 10)
mtcars_boots
```

```
## # Bootstrap sampling
## # A tibble: 100 x 2
##   splits          id
##   <list>         <chr>
## 1 <split [32/13]> Bootstrap001
## 2 <split [32/13]> Bootstrap002
## 3 <split [32/11]> Bootstrap003
## 4 <split [32/11]> Bootstrap004
## 5 <split [32/10]> Bootstrap005
## 6 <split [32/11]> Bootstrap006
## 7 <split [32/13]> Bootstrap007
## 8 <split [32/13]> Bootstrap008
## 9 <split [32/13]> Bootstrap009
## 10 <split [32/10]> Bootstrap010
## # ... with 90 more rows
```

Rsample

An under the hood, we have 100 analysis/assessment splits similar to `initial_split()` and `vfold_cv()`

```
mtcars_boots <- bootstraps(mtcars, times = 10)
mtcars_boots$splits
```

```
## [[1]]
## <Analysis/Assess/Total>
## <32/12/32>
##
## [[2]]
## <Analysis/Assess/Total>
## <32/14/32>
##
## [[3]]
## <Analysis/Assess/Total>
## <32/15/32>
##
## [[4]]
## <Analysis/Assess/Total>
## <32/11/32>
##
## [[5]]
```

Using resamples in action

We start by creating a linear regression specification and create a `workflow` object with `workflows()`

```
library(parsnip)
linear_spec <- linear_reg() %>%
  set_mode("regression") %>%
  set_engine("lm")

library(workflows)

linear_wf <- workflow() %>%
  add_model(linear_spec) %>%
  add_formula(mpg ~ disp + hp + wt)
```

Tune

We can use `fit_resamples()` to fit the workflow we created within each bootstrap

```
library(tune)

linear_fold_fits <- fit_resamples(
  linear_wf,
  resamples = mtcars_boots
)
```

Tune

The results of this resampling comes as a data.frame

```
linear_fold_fits
```

```
## # Resampling results
## # Bootstrap sampling
## # A tibble: 100 x 4
##   splits          id      .metrics          .notes
##   <list>         <chr>    <list>          <list>
## 1 <split [32/12]> Bootstrap001 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 2 <split [32/14]> Bootstrap002 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 3 <split [32/15]> Bootstrap003 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 4 <split [32/11]> Bootstrap004 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 5 <split [32/12]> Bootstrap005 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 6 <split [32/8]>  Bootstrap006 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 7 <split [32/11]> Bootstrap007 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 8 <split [32/11]> Bootstrap008 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 9 <split [32/15]> Bootstrap009 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## 10 <split [32/12]> Bootstrap010 <tibble[,4] [2 x 4]> <tibble[,1] [0 x 1]>
## # ... with 90 more rows
```

Tune

`collect_metrics()` can be used to extract the CV estimate

```
library(tune)
```

```
collect_metrics(linear_fold_fits)
```

```
## # A tibble: 2 x 6
##   .metric .estimator  mean     n std_err .config
##   <chr>   <chr>      <dbl> <int>  <dbl> <chr>
## 1 rmse    standard    3.00   100  0.0585 Preprocessor1_Model1
## 2 rsq     standard    0.816  100  0.00635 Preprocessor1_Model1
```

Tune

Setting `summarize = FALSE` in `collect_metrics()` Allows us to see the individual performance metrics for each fold

```
collect_metrics(linear_fold_fits, summarize = FALSE)
```

```
## # A tibble: 200 x 5
##   id          .metric .estimator .estimate .config
##   <chr>      <chr>    <chr>      <dbl> <chr>
## 1 Bootstrap001 rmse     standard    3.84 Preprocessor1_Model1
## 2 Bootstrap001 rsq      standard    0.851 Preprocessor1_Model1
## 3 Bootstrap002 rmse     standard    2.94 Preprocessor1_Model1
## 4 Bootstrap002 rsq      standard    0.726 Preprocessor1_Model1
## 5 Bootstrap003 rmse     standard    4.15 Preprocessor1_Model1
## 6 Bootstrap003 rsq      standard    0.822 Preprocessor1_Model1
## 7 Bootstrap004 rmse     standard    2.88 Preprocessor1_Model1
## 8 Bootstrap004 rsq      standard    0.794 Preprocessor1_Model1
## 9 Bootstrap005 rmse     standard    2.66 Preprocessor1_Model1
## 10 Bootstrap005 rsq      standard    0.866 Preprocessor1_Model1
## # ... with 190 more rows
```