Resampling methods

02-14-2020

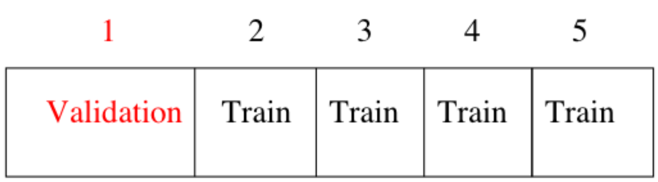
```r
library(tidyverse)
library(rsample)
```

Resampling methods

- we discuss two resampling methods: cross-validation and the bootstrap.
- these methods refit a model of interest to samples formed from the training set, in order to obtain additional information about the fitted model.
- For example, they provide estimates of test-set prediction error, and the standard deviation and bias of our parameter estimates

K-fold Cross-validation

- Widely used approach for estimating test error.
- Estimates can be used to select best model, and to give an idea of the test error of the final chosen model.
- Idea is to randomly divide the data into K equal-sized parts. We leave out part k, fit the model to the other $K-1$ parts (combined), and then obtain predictions for the left-out kth part.
- This is done in turn for each part k and then the results are combined.



Details

- Let the K parts be $C_1, \ldots, C_k$, where C_k denotes the indices of the observations in part k. There are n_k observations in part k.

- the cross-validation error is
$$CV_K = \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in C_k} (y_i - \hat{f}_{-k}(x_i))^2$$
where $\hat{f}_{-k}(x_i)$ is the prediction of y_i based on the data with part k removed.

- if $K = 2$: split-sample cross-validation. Our CV error estimates are going to be biased upwards, because we are only training on half the data each time

- Setting $K = n$ yields n-fold or leave-one out cross-validation (LOOCV).

How to choose K

- This is a hard quesiton.
- The choices $K = 5$ or $K = 10$ are pretty much the standards, and people believe that these give good estimates of prediction error, but there is not really any theory supporting this

A example

```r
folds <- vfold_cv(mtcars, 5)
folds %>% pull(splits) %>%
  map_dbl(
  ~ {
    train_data <- analysis(.)
    fit <- lm(mpg ~ wt, data = train_data)
    test_data <- assessment(.)
    sqrt(mean((test_data$mpg - predict(fit, test_data))^2))
  }
  ) %>%
  mean()
```

```
## [1] 3.165513
```

The Bootstrap

- The bootstrap is a flexible and powerful statistical tool that can be used to quantify the uncertainty associated with a given estimator or statistical learning method.
- It can provide an estimate of the standard error of a coefficient, or a confidence interval for that coefficient.

In the ideal world

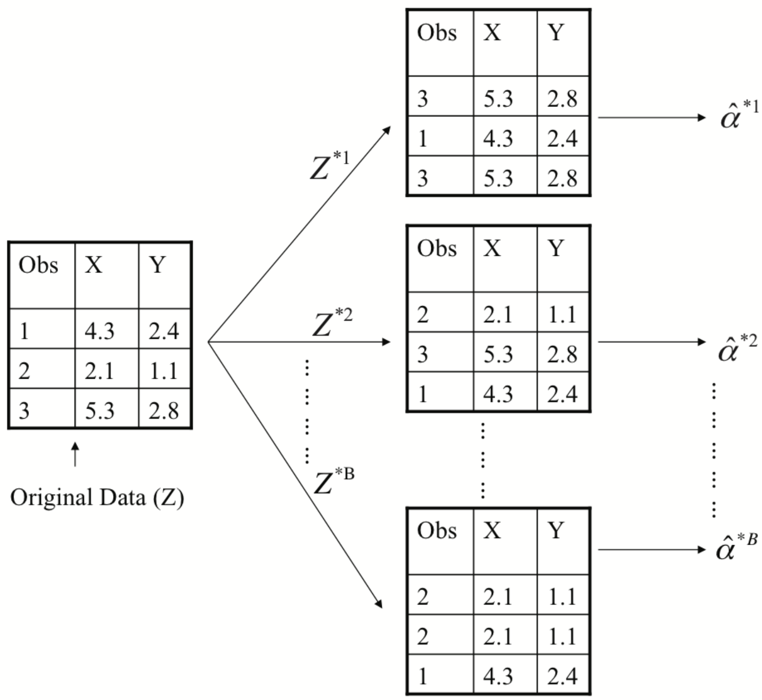
- For example, we have an estimator $\hat{\alpha}$ of α and we are interested in its s.d. (to construct confidence interval)
  - $\hat{\alpha}$ is a function of the observations (x_i, y_i), $i = 1, \ldots, n$
  - To estimate the standard deviation of $\hat{\alpha}$, we could simulate observations $(\tilde{x}_i, \tilde{y}_i)$, $i = 1, \ldots, n$ which have the same distribution as (x_i, y_i).
  - A new estimate of α is obtained, called it $\tilde{\alpha}$
  - repeat the process 1000 times, we have 1000 $\tilde{\alpha}$'s and the sample deviations of those 1000 $\tilde{\alpha}$'s can be used to estimate the s.d. of $\hat{\alpha}$.
- The procedure outlined above cannot be applied, because for real data we cannot generate new samples from the original population.

Now back to the real world

- However, the bootstrap approach allows us to use a computer to mimic the process of obtaining new data sets, so that we can estimate the variability of our estimate without generating additional samples.
- Rather than repeatedly obtaining independent data sets from the population, we instead obtain distinct data sets by repeatedly sampling observations from the original data set *with replacement*.

- Each of these 'bootstrap data sets' is created by sampling with replacement, and is the same size as our original dataset. As a result some observations may appear more than once in a given bootstrap data set and some not at all.

Example with just 3 observations



Notations

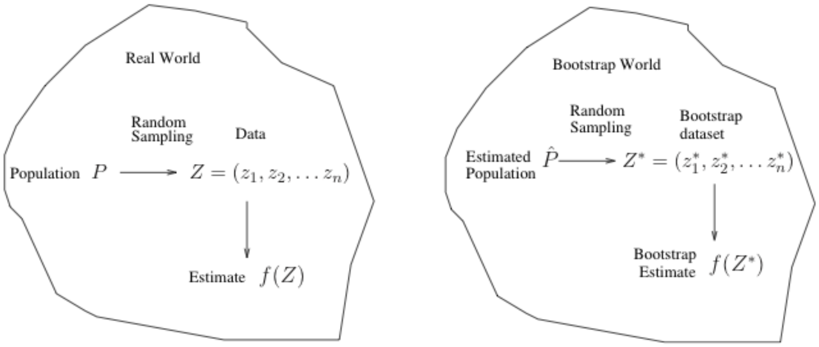
- Denoting the first bootstrap data set by Z^{*1}, we use Z^{*1} to produce a new bootstrap estimate for α, which we call $\hat{\alpha}^{*1}$
- this procedure is repeated B times for some large value of B (say 100 or 1000)
- we have B different bootstrap data sets, $Z^{*1}, \ldots, Z^{*B}$, and B corresponding α estimates, $\hat{\alpha}^{*1}, \ldots, \hat{\alpha}^{*B}$
- We estimate the standard error of these bootstrap estimates using the formula

$$SE_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1} \sum_{r=1}^{B} (\hat{\alpha}^{*r} - \bar{\hat{\alpha}}^{*})}$$

  where $\bar{\hat{\alpha}}^{*}$ is the average of $\hat{\alpha}^{*r}$'s.

- This serves as an estimate of the standard error of $\hat{\alpha}$ estimated from the original data set.

A general picture for the bootstrap



A example

```r
mtcars %>%
  summarize(r = cor(mpg, hp)) %>%
  pull(r)
```

```
## [1] -0.7761684
```

To get the "classical" confidence interval

```r
with(mtcars, cor.test(mpg, hp)) %>%
  tidy()
```

```
## # A tibble: 1 x 8
##   estimate statistic  p.value parameter conf.low conf.high method    alternative
##      <dbl>     <dbl>    <dbl>     <int>    <dbl>     <dbl> <chr>     <chr>
## 1   -0.776     -6.74  1.79e-7        30   -0.885    -0.586 Pearson'~ two.sided
```

Use bootstrap to obtain a confidence interval

```r
boots <- bootstraps(mtcars, times = 1000)
se <- boots %>% pull(splits) %>%
  map_dbl(
  ~ {
    train_data <- analysis(.)
    with(train_data, cor(mpg, hp))
  }
  ) %>%
  sd()

with(mtcars, cor(mpg, hp)) + c(-1, 1) * se
```

```
## [1] -0.8207580 -0.7315787
```

Other uses of the bootstrap

- Primarily used to obtain standard errors of an estimate.
- Also provides approximate confidence intervals for a population parameter.
- Consider the 2.5th and 97.5 percentile of $\hat{\alpha}^{*1}, \ldots, \hat{\alpha}^{*B}$
- The above interval is called a Bootstrap Percentile confidence interval. It is the simplest method (among many approaches) for obtaining a confidence interval from the bootstrap.

Reference

- rsample: https://tidymodels.github.io/rsample/
- Chapter 5 of An Introduction to Statistical Learning http://faculty.marshall.usc.edu/gareth-james/ISL/