Module 5: Solutions to Recommended Exercises

TMA4268 Statistical Learning V2021

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February 9, 2021

Recommended exercises on cross-validation

Problem 1: Explain how k-fold cross-validation is implemented

a) See Figure 1

validate	train	train	train	train
train	validate	train	train	train
train	train	validate	train	train
train	train	train	validate	train
train	train	train	train	validate

b) In run 1 fold 1 is kept aside and folds 2 - 5 are used to train the method. The error is calculated on fold 1 (MSE_1). We do this for the remaining 4 runs. The cross-validation error is given by

$$CV_5 = \frac{1}{n}\sum_{j=1}^{5} n_j \cdot \text{MSE}_j \ ,$$

where n_j is the size of the j^{th} fold.

For a regression problem $\text{MSE}_j = \frac{1}{n_j}\sum_{i \in V_j}(y_i - \hat{y}_i)^2$ for all i in the validation set V_j. For a binary classification problem the error might be the average of correctly classified observations.

c) Find the optimal number of neighbours k in KNN or the optimal polynoimial degree in polynomial regression.

d) For a calssification problem we can use CV to choose between QDA or LDA.

Problem 2: Advantages and disadvantages of k-fold Cross-Validation

a) The validation set approach:

D: The k-fold cross validation is computationally more expensive, and has more bias.

A: The advandge is that it has less variance

b) In LOOCV there is no radomness in the splits.

A: k-fold-CV is computationally less expensive, as we run the model k times where $k \ll n$

A: k-fold-CV has less variance, because in LOOCV we are averaging from n fitted models that are trained on nearly the same data, therefore we have positively correlated data.

D: k-fold-CV has more bias, as in LOOCV we use a larger data set to fit the model, which gives a less biased version of the test error.

c) We know that if $k = n =$ LOOCV the estimator of test error will have small bias but high variance and it is computationally expensive.

If k is too small (for example 2), the estimator will have larger bias but lower variance.

Experimental research (simulations) has found that $k = 5$ or $k = 10$ to be good choice.

Problem 3: Selection bias and the "wrong way to do CV".

No solution is provided on top of the guidelines in the exercise sheet.

Recommended exercises on bootstrapping

Problem 4: Probability of being part of a bootstrap sample

a) $P(\text{draw } X_i) = \frac{1}{n}$ and $P(\text{not draw } X_i) = 1 - P(\text{draw } X_i) = 1 - \frac{1}{n}$

b) $P(\text{not draw any } X_i) = (1 - \frac{1}{n})^n$ and $P(\text{draw at least one } X_i) = 1 - (1 - \frac{1}{n})^n$

c) $P(X_i \text{ in bootstrap sample}) = 1 - (1 - \frac{1}{n})^n \approx 1 - \exp(-1) = 0.632$

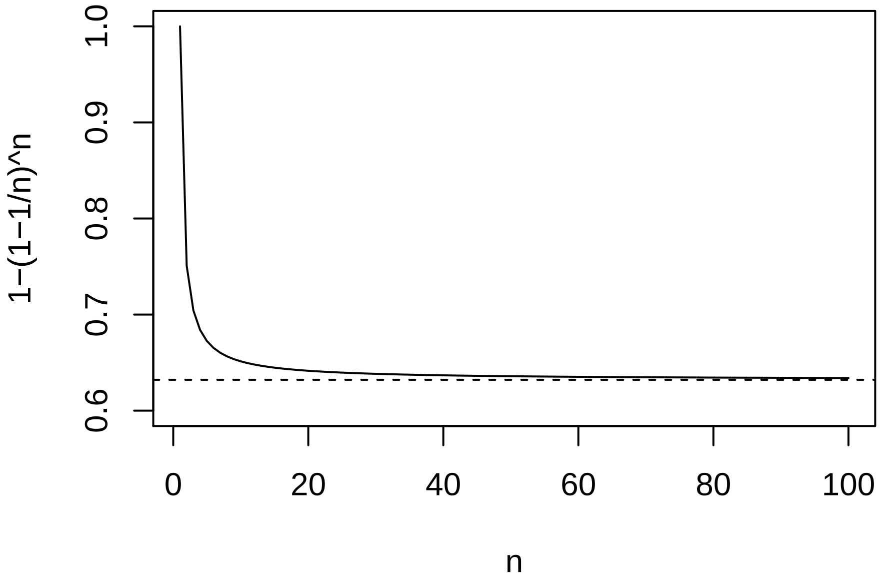
d)

```
n = 100
B = 10000
j = 1
res = rep(NA, B)
for (b in 1:B) res[b] = (sum(sample(1:n, replace = TRUE) == j) > 0)
mean(res)
```

```
## [1] 0.6261
```

The approximation becomes quickly very good as n increases, as the following graph shows:

```
curve(1 - (1 - 1/x)^x, 1, 100, ylim = c(0.6, 1), xlab = "n", ylab = "1-(1-1/n)^n")
abline(h = 1 - 1/exp(1), lty = 2)
```



Problem 5: Estimate standard deviation and confidence intervals with bootstrapping

We repeat the following for $b = 1, \cdots, B$:

- Draw with replacement a bootstrap sample
- Fit the model
- Store $\hat{\beta}_b$

Calculate $\hat{SD}(\hat{\beta}) = \sum_{b=1}^{B} \sqrt{\frac{1}{B-1} \sum_{b=1}^{B} (\hat{\beta}_b - \frac{1}{B} \sum_{b=1}^{B} \hat{\beta}_b)}$.

For the 95% CI, we can calculate the 0.025 and 0.975 quantiles of the sample $\hat{\beta}_b$, $b = 1, \cdots, B$.

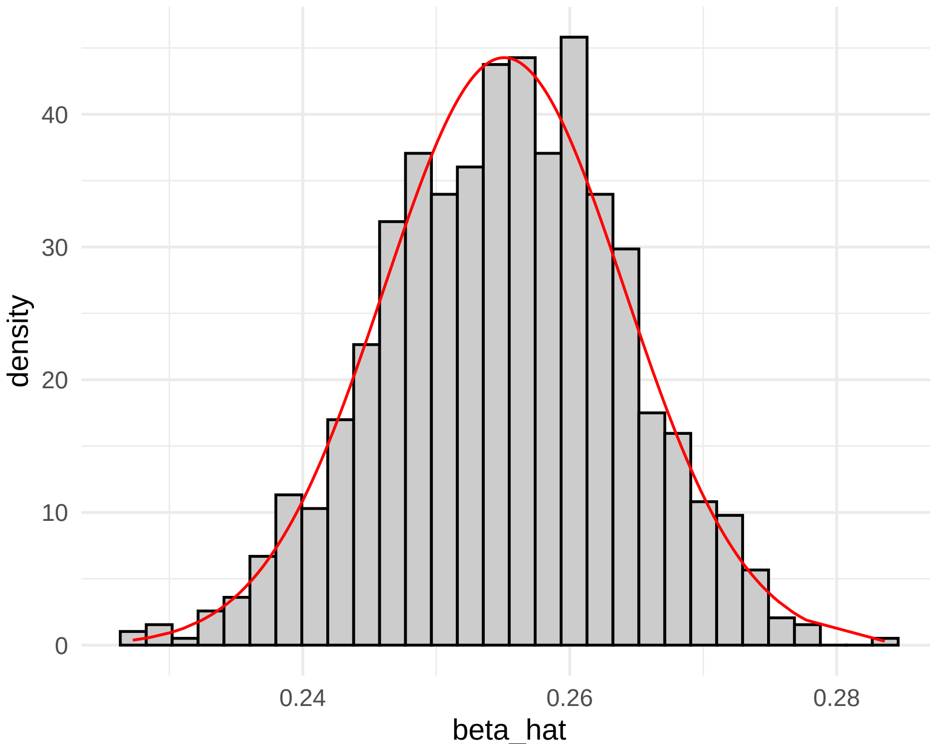
Problem 6: Implement problem 5

```r
library(carData)
boot.fn = function(data, index) {
    return(coef(lm(wages ~ ., data = SLID, subset = index)))
}

beta_hat = c()
B = 1000
for (i in 1:B) {
    beta_hat[i] = boot.fn(SLID, sample(nrow(SLID), nrow(SLID), replace = T))["age"]
}
```

We can for example look at the histogram of the samples of $\hat{\beta}$ to get an idea of the distribution:

```r
library(ggplot2)
data = data.frame(beta_hat = beta_hat, norm_den = dnorm(beta_hat, mean(beta_hat),
    sd(beta_hat)))
ggplot(data) + geom_histogram(aes(x = beta_hat, y = ..density..), fill = "grey80",
    color = "black") + geom_line(aes(x = beta_hat, y = norm_den), color = "red") +
    theme_minimal()
```



The 95% CI for $\hat{\beta}_{age}$ can now be derived by either using the 2.5% and 97.5% quantiles of the samples, or by using the $\hat{\beta} \pm 1.96 \cdot \mathrm{SD}(\hat{\beta})$ idea:

```
sd(beta_hat)
```

```
## [1] 0.009011869
```

```
quantile(beta_hat, c(0.025, 0.975))
```

```
##      2.5%     97.5%
## 0.2370727 0.2722128
```

```
c(mean(beta_hat) - 1.96 * sd(beta_hat), mean(beta_hat) + 1.96 * sd(beta_hat))
```

```
## [1] 0.2374249 0.2727514
```

We can compare these results to what we would obtain directly from fitting the model and calcualating the confidence interval

```
SLID.lm = lm(wages ~ ., data = SLID)
confint(SLID.lm)
```

```
##                      2.5 %     97.5 %
## (Intercept)    -9.0891576 -6.6884008
## education       0.8484610  0.9847670
## age             0.2380522  0.2722214
## sexMale         3.0452719  3.8655493
## languageFrench -0.8518577  0.8214111
## languageOther  -0.4946904  0.7798996
```

As expected, the 95% CI for `age` is essentially the same as the one we obtained from bootstrapping.

If you prefer to use the built in function `boot()`

```r
library(boot)
bo = boot(SLID, boot.fn, 1000)
bo
```

```
##
## ORDINARY NONPARAMETRIC BOOTSTRAP
##
##
## Call:
## boot(data = SLID, statistic = boot.fn, R = 1000)
##
##
## Bootstrap Statistics :
##        original        bias    std. error
## t1* -7.88877921 -0.0054150827 0.666660984
## t2*  0.91661398  0.0008918457 0.040321320
## t3*  0.25513680 -0.0001890008 0.008975787
## t4*  3.45541061  0.0074509980 0.206354231
## t5* -0.01522333  0.0046192348 0.428076432
## t6*  0.14260463 -0.0111938153 0.312171855
```

Summing up

Take home messages

- Use $k = 5$ or 10 fold cross-validation for model selection or assessment.
- Use bootstrapping to estimate the standard deviation of an estimator, and understand how it is performed before module 8 on trees.

Further reading

- Videoes on YouTube by the authors of ISL, Chapter 5, and corresponding slides
- Solutions to exercises in the book, chapter 5