Exercise Collection – Tuning & Resampling

Contents

Lecture exercises

Exercise 1: benchmark experiment – CART vs k-NN

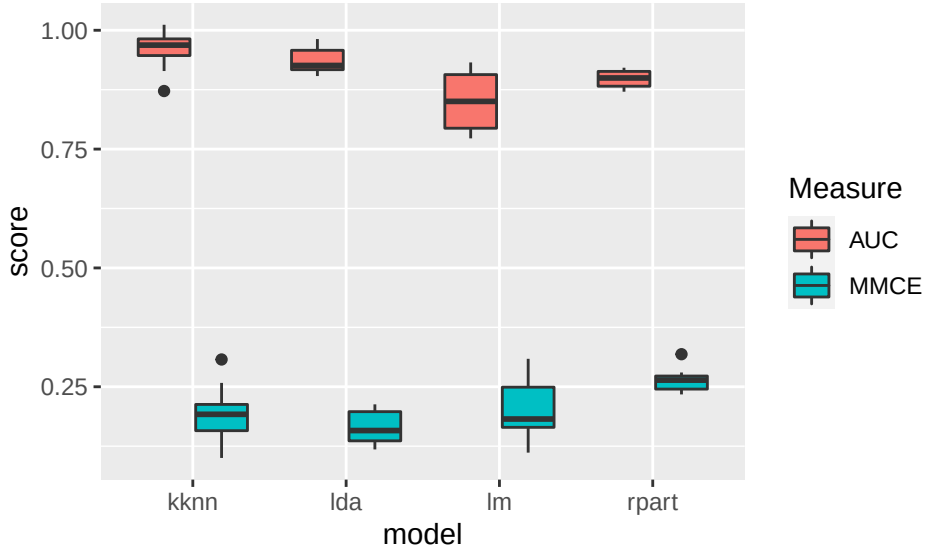
(a) Suppose that we want to compare four different models:

Model	Needs Tuning
Logit Model (lm)	No
CART (rpart)	Yes
k-NN (kknn)	Yes
LDA (lda)	No

To be able to compare the different models we use a 10-fold cross-validation as outer resampling strategy. Within the tuning of CART and k-NN we use a 5-fold cross-validation in combination with random search by drawing 200 hyperparameter configurations for each model. Our measure of interest is the AUC.

(i) To conduct the final benchmark to compare the models, how many models need to be fitted in total?

(ii) Giving the following benchmark result, which model is best? Explain your decision in one sentence.



(b) Explain in two sentences what is meant by the *bias - variance trade-off in resampling*.

(c) Are the following statements true or not, explain your answer in one sentence.

(i) The bias of the generalization error for 3-fold cross-validation is higher than for 10-fold cross-validation.

(ii) Every outer loss can also be used as inner loss. Assume any gradient descent based model.

Solution 1:

(a) (i) Important parts:

- Correct number of models for tuning
- Correctly multiplying tuning models times the two learners that need tuning
- Correctly adding $4 \cdot 10$ for learner comparison ()

$$\#\text{models} = \underbrace{4 \cdot 10}_{\#\text{ models outer resampling}} + 2 \cdot \underbrace{\underbrace{10 \cdot \underbrace{5 \cdot 200}_{\#\text{ models for one tuning}}}_{\#\text{ models for all outer folds for one tuning}}}_{\#\text{ models for both tunings}} = 20040$$

(ii) We would select the k-NN (k-Nearest Neighbors) learner since it achieves the best values for the AUC.

(b)

- Less data for training leads to higher bias
- More data for training and less data for evaluation lead to higher variance

(c) Are the following statements true or not, explain your answer in one sentence.

(i) True, using 3-fold cross-validation leads to smaller train sets and therefore we are not able to learn as much as for, e.g., 10-fold cross-validation.

(ii) False, the outer loss doesn't has as much restrictions as the inner loss, e.g. the outer loss doesn't has to be differentiable.

Exercise 2: benchmark study for classification

We want to conduct a small benchmark study:

(a) Set up at least two datasets with a discrete target of your choice and save them in a list.

(b) Set up at least three classifiers of your choice (that you are familiar with) and save them in a second list.

(c) Create a resample description. Use an adequate method, depending on the size of your datasets and the complexity of the learners, so that the benchmark doesn't need hours to compute.

(d) Run and visualize your benchmark study.

Solution 2:

See R code

Exercise 3: cross validation for k-NN

Use the `bodyfat` dataset from the package `TH.data` for this exercise.

(a) Create a `mlr` regression task for the `bodyfat` data with `DEXfat` as target variable.

(b) Fit a K-Nearest-Neighbor regression model

(c) Visualize the predictions for the features `waistcirc` and `anthro3c` seperately as well as together in one plot.

(d) Resample the bodyfat dataset with 10-fold crossvalidation and calculate the mean squared error and the median absolute error.

Solution 3:

See R code

Exercise 4: leave-one-out estimator

In this exercise we take a look at the leave-one-out-estimator. We will use a data independent model, so our data are all i.i.d. bernoulli(0.5) distributed labels, $\{0, 1\}$, $Y_1, \ldots, Y_n$. Our (a bit strange) rule results after looking at the training data always in a constant estimation. It works like that: If the training data consists of an odd number of 1s it will estimate a 1, otherwise a 0.

(a) What is the expected error of this rule?

(b) Now we estimate this expected error on the training data with the leave-one-out-estimator. What expected value and variance has the result? How would you interpret this result?

Solution 4:

(a) Let $Y_1, \ldots, Y_n, Y$ all be i.i.d and Bernloulli-($\frac{1}{2}$) distributed. $Y_1, \ldots, Y_n$ is the training data, Y is a new test observation and $\hat{Y}$ the prediction of our data independent rule for Y.

It follows:

$$P(\hat{Y} \neq Y) = P(\hat{Y} = 1)(1 - 0.5) + (1 - P(\hat{Y} = 1))0.5$$

and (this is not really required but will be useful later)

$$P(\hat{Y} = 1) = \frac{1}{2}.$$

This is the case because in the product space for $Y_1, \ldots, Y_n$ all events $Y_1 = y_1, \ldots, Y_n = y_n$ have the same probability (0.5^n) and exactly half of the events have an even number of 1s, the other half an odd number.

So it follows that:

$$P(\hat{Y} \neq Y) = 0.5$$

(b) Let $\hat{L}$ be the leave-one-out (LOO) estimator of $Y_1, \ldots, Y_n$ and $\hat{Y}_i$ the prediction of our data independent rule for Y_i with LOO. This means the estimation is based on $Y_1, \ldots, Y_n$ without Y_i.

It follows:

$$\hat{L} = \frac{1}{n} \sum_{i=1}^{n} I(\hat{Y}_i \neq Y_i).$$

$\hat{L}$ can only have the value 1 or 0. Which can be explained like this:

Assume that $Y_1(\omega), \ldots, Y_n(\omega)$ have an even number of 1s. Now drop one $Y_i(\omega)$. If it was a 0, the remaining observations still have an even number of 1s, a 0 will be predicted and $\hat{Y}_j(\omega) = 0 = Y_j(\omega)$. If it is a 1, it results in an odd number of 1s, a 1 will be predicted and $\hat{Y}_j(\omega) = 1 = Y_j(\omega)$. So, $\hat{L}(\omega) = 0$.

Now assume that $Y_1(\omega), \ldots, Y_n(\omega)$ have an odd number of 1s. Again, drop one $Y_i(\omega)$. If it was a 0, the remaining observations still have an odd number of 1s, a 1 is predicted and $\hat{Y}_j(\omega) \neq Y_j(\omega)$. If it is a 1, it results in an even number of 1s, a 0 will be predicted and $\hat{Y}_j(\omega) \neq Y_j(\omega)$. So, $\hat{L}(\omega) = 1$.

This means that $\hat{L}$ is a Bernoulli distributed random variable. An even number of 1s in $Y_1, \ldots, Y_n$ has the same probability as an odd number, so $\hat{L} \sim$ Bernoulli-(0.5) and consequently $E(\hat{L}) = 1/2$ and $Var(\hat{L}) = 1/4$.

The expected value is also correct like in a). But the variance is very high. The LOO can only be calculated once and it behaves like a fair coin toss. It will produce an error of 0% or an error of 100%. The example is rather theoretical but shows the disadvantageous property of a high variance in the LOO estimator.

Questions from past exams

Exercise 5: WS2020/21, main exam, question 6

Assume a polynomial regression model with a continuous target variable y and a continuous, p-dimensional feature vector $\mathbf{x}$ and polynomials of degree d, i.e.,
$f\left(\mathbf{x}^{(i)}\right) = \sum_{j=1}^{p} \sum_{k=0}^{d} \theta_{j,k} (\mathbf{x}_j^{(i)})^k$ and $y^{(i)} = f\left(\mathbf{x}^{(i)}\right) + \epsilon^{(i)}$ where the $\epsilon^{(i)}$ are iid with $\mathsf{Var}(\epsilon^{(i)}) = \sigma^2 \; \forall i \in \{1, \ldots, n\}$.

(a) For each of the following situations, indicate whether we would generally expect the performance of a flexible polynomial learner (high d) to be better or worse than an inflexible polynomial learner (low d). Justify your answer.

(i) The sample size n is extremely large, and the number of features p is small.

(ii) The number of features p is extremely large, and the number of observations n is small.

(iii) The true relationship between the features and the response is highly non-linear.

(iv) The variance of the error terms, σ^2, is extremely high.

(b) On a given data set with sample size $n = 1000$, $p = 1$ feature and degree $d = 1$ we want to estimate the generalization error. Describe the advantages and disadvantages of the following three resampling strategies. Additionally, state which strategy you would use here.

(i) hold-out sampling, i.e., a single train-test split

(ii) leave-one-out cross-validation, i.e., n-fold cross-validation

(iii) 5-fold cross-validation

Solution 5:

(a)
- (i): flexible: because it covers a larger Hypothesis space and we have enough data
- (ii): inflexible: to prevent overfitting
- (iii): flexible: because it covers a larger Hypothesis space and we have enough data, an inflexible approach would be too restrictive
- (iv): inflexible: to prevent overfitting

(b)
- (i): fastest, but very dependent on the given split, i.e., can vary quite a lot with varying seed
- (ii): slow, very robust - does not depend on seed $\Rightarrow$ Perhaps best in that case, because linear model is fast
- (iii): trade-off: higher bias as loocv but not that dependent on the seed $\Rightarrow$ Depending on computation time perhaps better than loocv

Ideas & exercises from other sources