Exercise 1: Tuning Principles

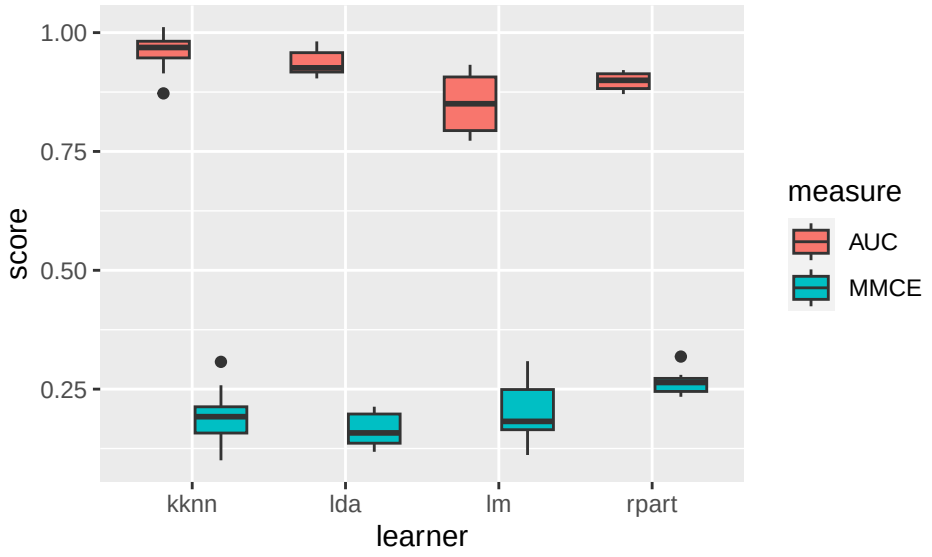
a) Suppose that we want to compare four different learners:

Learner	Tuning required
Logistic regression (`lm`)	no
CART (`rpart`)	yes
k-NN (`kknn`)	yes
LDA (`lda`)	no

For performance evaluation and subsequent comparison, we use 10-CV as outer resampling strategy. Within the inner tuning loop, applicable to CART and k-NN, we use 5-CV in combination with random search, drawing 200 hyperparameter configurations for each model. Our measure of interest is the AUC.

i) How many models need to be fitted in total to conduct the final benchmark?

ii) Giving the following benchmark result, which learner performs best? Explain your decision.



b) Recap briefly 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 estimate for 3-CV is higher than for 10-CV.

ii) Every outer loss can also be used as inner loss, assuming standard gradient-based optimization.

Exercise 2: AutoML

In this exercise, we build a simple automated machine learning (AutoML) system that will make data-driven choices on which learner/estimator to use and also conduct the necessary tuning.

`R` **Exercise**:

`mlr3pipelines` make this endeavor easy, modular and guarded against many common modeling errors.

We work on the `pima` data to classify patients as diabetic and design a system that is able to choose between k-NN and a random forest, both with tuned hyperparameters.

To this end, we will use a graph learner, a "single unit of data operation" that can be trained, resampled, evaluated, ... as a whole – in other words, treated as any other learner.

a) Create a task object in `mlr3` (the problem is pre-specified under the ID "pima").

b) Specify the above learners, where you need to give each learner a name as input to the `id` argument. Convert each learner to a pipe operator by wrapping them in the sugar function `po()`, and store them in a `list`.

c) Before starting the actual learning pipeline, take care of pre-processing. While this step is highly customizable, you can use an existing sequence to impute missing values, encode categorical features, and remove variables with constant value across all observations. For this, specify a pipeline (`ppl()`) of type `"robustify"` (setting `factors_to_numeric` to `TRUE`).

d) Create another `ppl`, of type `"branch"` this time, to enable selection between your learners.

e) Chain both pipelines using the double pipe and plot the resulting graph. Next, convert it into a graph learner with `as_learner()`.

f) Now you have a learner object just like any other. Take a look at its tunable hyperparameters. You will optimize the learner selection, the number of neighbors in k-NN (between 3 and 10), and the number of split candidates to try in the random forest (between 1 and 5). Define the search range for each like so:

```
<learner>$param_set$values$<hyperparameter> <- to_tune(p_int(lower, upper))
```

`p_int` marks an integer hyperparameter with lower and upper bounds as defined; similar objects exist for other data types. With `to_tune()`, you signal that the hyperparameter shall be optimized in the given range.

Hint: You need to define dependencies, since the tuning process is defined by which learner is selected in the first place (no need to tune k in a random forest).

g) Conveniently, there is a sugar function, `tune_nested()`, that takes care of nested resampling in one step. Use it to evaluate your tuned graph learner with

- mean classification error as inner loss,
- random search as tuning algorithm (allowing for 3 evaluations), and
- 3-CV in both inner and outer loop.

h) Lastly, extract performance estimates per outer fold (`score()`) and overall (`aggregate()`). If you want to risk a look under the hood, try `extract_inner_tuning_archives()`.

`Python` **Exercise**:

`sklearn.pipeline.Pipeline` makes this endeavor easy, modular and guarded against many common modeling errors.

We work on the `pima` data to classify patients as diabetic and design a system that is able to choose between k-NN and a random forest, both with tuned hyperparameters.

The purpose of the pipeline is to assemble several steps of transformation and a final estimator that can be cross-validated together while setting different parameters. So to speak, the pipeline estimator can be treated as any other estimator.

a) Load the data set `pima`, encode the target `"diabetes"` as 0-1-vector and perform a stratified `train_test_split`.

b) As part of our modeling process, we want to perform certain preprocessing steps. While this step is highly customizable, we want to include at least One-Hot-Encoding of categorical features, and imputing of missing values.
Instance a `ColumnTransformer` object and include these two steps for a dynamic choice of columns.
(Hint: Strings are considered as `dtype = object`)

c) Next, both pipelines for the k-NN and random forest are created. Like this you can create estimators with highly individual preprocessing steps. Include the previously created `ColumnTransformer`, a `VarianceThreshold` to remove constant columns and the corresponding estimator as a final step. Additionally, scale the columns for the k-NN estimator.

d) A very common ensembling technique is to predict according to the decisions of numerous estimators. This is refered to as `VotingClassifier` and enables you to predict the class label based on the argmax of the sums of the predicted probabilities. Instanciate a `VotingClassifier` with the two classifier pipelines for k-NN and random forest.
(Hint: set the parameters `voting = "soft"` and `n_jobs = -1` for parallel computation.)

e) Now you have an estimator object just like any other. Take a look at its tunable hyperparameters. You will optimize the number of neighbors in k-NN (between 3 and 10), and the number of split candidates to try in the random forest (between 1 and 5). Define the search range for each like so:

```
param_grid_voting = [{"<voting_estimator1>__<pipelie1_estimator>__<hyperparameter>":
                          list(<parameter_range>)},
                     {"<voting_estimator2>__<pipelie2_estimator>__<hyperparameter>":
                          list(<parameter_range>)}]
```

Please note, that the estimator names should be on par with the labels given in the `VotingClassifier`, the `Pipeline` and, of course, the hyperparameter of the used estimator in the pipeline. Each level of hyperparameters of our created ensemble estimator is accessable through the seperation "__" (double underscore).

f) Nested Resampling is a method to avoid the so called *optimization bias* by tuning parameters and evaluation performance on different subsets of your training data. Use

- Stratified 3-CV in both inner and outer loop.
- accuracy as inner performance measure,
- grid search as tuning algorithm.

You may use the following, incomplete code to compute the nested resampling:

```
NUM_OUTER_FOLDS = <...>
nested_scores_voting = np.zeros(NUM_OUTER_FOLDS) # initalize scores with 0
# Choose cross-validation techniques for the inner and outer loops,
# independently of the dataset.
# E.g "GroupKFold", "LeaveOneOut", "LeaveOneGroupOut", etc.
inner_cv = <...>(n_splits=<...>, shuffle=True, random_state=42)
outer_cv = <...>(n_splits=<...>, shuffle=True, random_state=42)
```

```
for i, (train_index, val_index) in enumerate(outer_cv.split(X_train, y_train)):
  # Nested CV with parameter optimization for ensemble pipeline
  clf_gs_voting = <...>(
      estimator=<...>,
      param_grid=<...>,
      cv=<...>,
      n_jobs=-1
  )
  clf_gs_voting.fit(X_train.iloc[<...>], y_train[<...>])
  nested_scores_voting[i] = clf_gs_voting.score(X_train.iloc[<...>], y_train[<...>])
```

g) Extract performance estimates per outer fold and overall (as mean). According to your results, determin the best classifier object.

h) Lastly, evaluate the performance on the test set. Think about the imbalance of your data set and how this is affecting the performance measurement accuracy. Try to find a better metric and compare these two.

Congrats, you just designed a turn-key AutoML system that does (nearly) all the work with a few lines of code!

Exercise 3: Kaggle Challenge

Make yourself familiar with the Titanic Kaggle challenge (`https://www.kaggle.com/c/titanic`).

Based on everything you have learned in this course, do your best to achieve a good performance in the survival challenge.

- Try out different classifiers you have encountered during the course (or maybe even something new?)
- Improve the prediction by creating new features (feature engineering).
- Tune your parameters (see: `https://mlr3book.mlr-org.com/tuning.html` or `https://scikit-learn.org/stable/modules/grid_search.html`).
- How do you fare compared to the public leaderboard?

`mlr3` **Hint:** Use the `titanic` package to directly access the data. Use `titanic::titanic_train` for training and `titanic::titanic_test` for your final prediction.