Solution 1: Tuning Principles

a) Benchmark result:

(i) Total number of models trained:

$$\underbrace{4 \cdot 10}_{\text{outer resampling}} + \underbrace{2 \cdot \underbrace{10 \cdot \underbrace{5 \cdot 200}_{\text{one tuning iteration}}}_{\text{all outer folds in one tuning procedure}}}_{\text{all tuning procedures}} = 20,040.$$

(ii) Since we evaluate on AUC, we select k-NN with the best average result in that respect.

b) Less data for training leads to higher bias, less data for evaluation leads to higher variance.

c) Statements:

i) True – 3-CV leads to smaller train sets, therefore we are not able to learn as well as in, e.g., 10-CV.

ii) False – we are relatively flexible in choosing the outer loss, but the inner loss needs to be suitable for empirical risk minimization, which encompasses differentiability in most cases (i.e., whenever optimization employs derivatives).

Solution 2: AutoML with `mlr3`

This exercise is a compact version of a tutorial on mlr3gallery. Feel free to explore the additional steps and explanations featured in the original (there is also a bunch of other useful code demos).

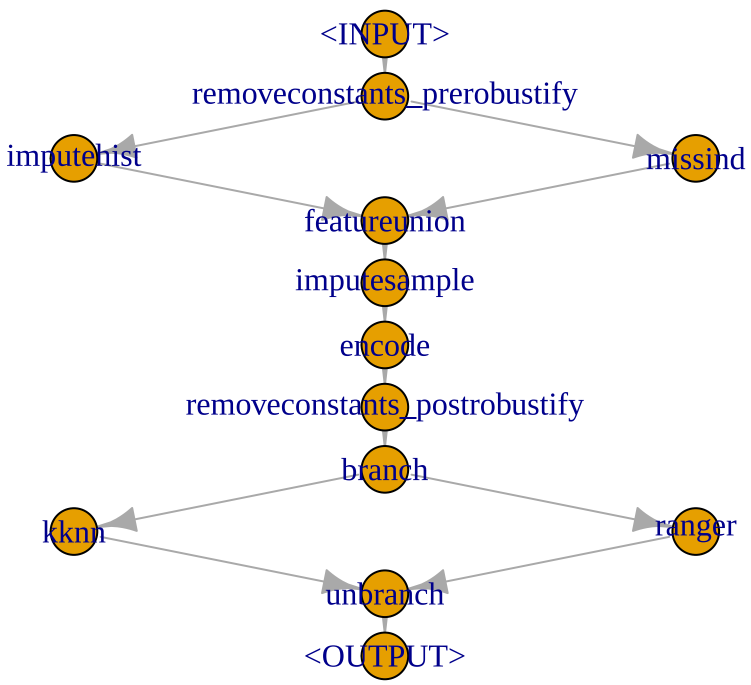
a)
```r
library(mlr3verse)

## Loading required package:  mlr3

library(mlr3tuning)

## Loading required package:  paradox

(task <- tsk("pima"))

## <TaskClassif:pima> (768 x 9): Pima Indian Diabetes
## * Target: diabetes
## * Properties: twoclass
## * Features (8):
##   - dbl (8): age, glucose, insulin, mass, pedigree, pregnant, pressure,
##     triceps
```

b)
```r
learners <- list(
  po(lrn("classif.kknn", id = "kknn")),
  po(lrn("classif.ranger", id = "ranger")))
```

c)
```r
ppl_preproc <- ppl("robustify", task = task, factors_to_numeric = TRUE)
```

d)
```r
ppl_learners <- ppl("branch", learners)
```

e)
```r
ppl_combined <- ppl_preproc %>>% ppl_learners
plot(ppl_combined)
```



```r
graph_learner <- as_learner(ppl_combined)
```

f)
```r
# check available hyperparameters for tuning (converting to data.table for
# better readability)
tail(as.data.table(graph_learner$param_set), 10)

##                                      id    class lower upper
##  1:               ranger.sample.fraction ParamDbl     0     1
##  2:                   ranger.save.memory ParamLgl    NA    NA
##  3: ranger.scale.permutation.importance ParamLgl    NA    NA
##  4:                     ranger.se.method ParamFct    NA    NA
##  5:                          ranger.seed ParamInt  -Inf   Inf
##  6:          ranger.split.select.weights ParamUty    NA    NA
##  7:                     ranger.splitrule ParamFct    NA    NA
##  8:                       ranger.verbose ParamLgl    NA    NA
##  9:                  ranger.write.forest ParamLgl    NA    NA
## 10:                     branch.selection ParamInt     1     2
##                       levels nlevels is_bounded special_vals        default
##  1:                              Inf       TRUE    <list[0]> <NoDefault[3]>
##  2:               TRUE,FALSE       2       TRUE    <list[0]>          FALSE
##  3:               TRUE,FALSE       2       TRUE    <list[0]>          FALSE
##  4:             jack,infjack       2       TRUE    <list[0]>        infjack
##  5:                              Inf      FALSE    <list[1]>
##  6:                              Inf      FALSE    <list[0]>
##  7: gini,extratrees,hellinger       3       TRUE    <list[0]>           gini
##  8:               TRUE,FALSE       2       TRUE    <list[0]>           TRUE
##  9:               TRUE,FALSE       2       TRUE    <list[0]>           TRUE
## 10:                                2       TRUE    <list[0]> <NoDefault[3]>
##     storage_type                   tags
##  1:      numeric                  train
##  2:      logical                  train
##  3:      logical                  train
##  4:    character                predict
##  5:      integer          train,predict
##  6:         list                  train
##  7:    character                  train
##  8:      logical          train,predict
##  9:      logical                  train
## 10:      integer train,predict,required

# seeing all our hyperparameters of interest are of type int, we specify the
# tuning objects accordingly, and dependencies for k and mtry
graph_learner$param_set$values$branch.selection <-
  to_tune(p_int(1, 2))
graph_learner$param_set$values$kknn.k <-
  to_tune(p_int(3, 10, depends = branch.selection == 1))
graph_learner$param_set$values$ranger.mtry <-
  to_tune(p_int(1, 5, depends = branch.selection == 2))

# rename learner (otherwise, mlr3 will display a lengthy chain of operations
# in result tables)
graph_learner$id <- "graph_learner"
```

g)
```r
# make sure to set a seed for reproducible results
set.seed(123)
```

```r
# perform nested resampling, terminating after 3 evaluations
rr <- tune_nested(
  method = "random_search",
  task = task,
  learner = graph_learner,
  inner_resampling = rsmp ("cv", folds = 3),
  outer_resampling = rsmp("cv", folds = 3),
  measure = msr("classif.ce"),
  term_evals = 3)
```

h)
```r
rr$score()

##                  task task_id         learner          learner_id
## 1: <TaskClassif[50]>    pima <AutoTuner[46]> graph_learner.tuned
## 2: <TaskClassif[50]>    pima <AutoTuner[46]> graph_learner.tuned
## 3: <TaskClassif[50]>    pima <AutoTuner[46]> graph_learner.tuned
##            resampling resampling_id iteration              prediction
## 1: <ResamplingCV[20]>            cv         1 <PredictionClassif[20]>
## 2: <ResamplingCV[20]>            cv         2 <PredictionClassif[20]>
## 3: <ResamplingCV[20]>            cv         3 <PredictionClassif[20]>
##    classif.ce
## 1:  0.2460938
## 2:  0.2421875
## 3:  0.2109375

rr$aggregate()

## classif.ce
##  0.2330729
```

The performance estimate for our tuned learner then amounts to an MCE of around 0.23.

Solution 3: Kaggle Challenge

We do not provide an explicit solution here, but have a look at the tuning code demo, which covers some parts, and take inspiration from the public contributions on Kaggle.