HYPERPARAMETER TUNING IN R

Machine learning with mlr

Dr. Shirin Elsinghorst
Data Scientist

The mlr package

- `mlr` is another framework for **machine learning** in R.

Model training follows **three steps**:

1. Define the **task**
2. Define the **learner**
3. Fit the **model**

https://mlr-org.github.io/mlr

New dataset: User Knowledge Data

```
library(tidyverse)
glimpse(knowledge_data)

Observations: 150
Variables: 6
$ STG <dbl> 0.080, 0.000, 0.180, 0.100, 0.120, 0.090, 0.080, 0.150, ...
$ SCG <dbl> 0.080, 0.000, 0.180, 0.100, 0.120, 0.300, 0.325, 0.275, ...
$ STR <dbl> 0.100, 0.500, 0.550, 0.700, 0.750, 0.680, 0.620, 0.800, ...
$ LPR <dbl> 0.24, 0.20, 0.30, 0.15, 0.35, 0.18, 0.94, 0.21, 0.19, ...
$ PEG <dbl> 0.90, 0.85, 0.81, 0.90, 0.80, 0.85, 0.56, 0.81, 0.82, ...
$ UNS <chr> "High", "High", "High", "High", "High", "High", ...

knowledge_data %>%
  count(UNS)

# A tibble: 3 x 2
  UNS         n
  <chr>   <int>
1 High       50
2 Low        50
3 Middle     50
```

Tasks in mlr for supervised learning

- `RegrTask()` for regression
- `ClassifTask()` for binary and multi-class classification
- `MultilabelTask()` for multi-label classification problems
- `CostSensTask()` for general cost-sensitive classification

With our student knowledge dataset we can build a classifier:

```
task <- makeClassifTask(data = knowledge_train_data,
                        target = "UNS")
```

Learners in mlr

```
listLearners()

                     class                package
1              classif.ada             ada,rpart
2       classif.adaboostm1                 RWeka
3      classif.bartMachine           bartMachine
4         classif.binomial                 stats
5         classif.boosting          adabag,rpart
6              classif.bst             bst,rpart
7              classif.C50                   C50
8          classif.cforest                 party
9       classif.clusterSVM     SwarmSVM,LiblineaR
10           classif.ctree                 party
...

# Define learner
lrn <- makeLearner("classif.h2o.deeplearning",
                   fix.factors.prediction = TRUE,
                   predict.type = "prob")
```

Model fitting in mlr

```
tic()
# Define task
task <- makeClassifTask(data = knowledge_train_data,
                        target = "UNS")

# Define learner
lrn <- makeLearner("classif.h2o.deeplearning",
                   fix.factors.prediction = TRUE)

# Fit model
model <- train(lrn,
               task)
toc()

3.782 sec elapsed
```

HYPERPARAMETER TUNING IN R

Let's practice!

HYPERPARAMETER TUNING IN R

Hyperparameter tuning with mlr - grid and random search

Dr. Shirin Glander
Data Scientist

Hyperparameter tuning with mlr

In `mlr` you have to define

1. the **search space** for every hyperparameter
2. the **tuning method** (e.g. grid or random search)
3. the **resampling method**

Defining the search space

```
makeParamSet(
  makeNumericParam(),
  makeIntegerParam(),
  makeDiscreteParam(),
  makeLogicalParam(),
  makeDiscreteVectorParam()
)

getParamSet("classif.h2o.deeplearning")

                                       Type  len          Def
autoencoder                         logical    -        FALSE
use_all_factor_level                logical    -         TRUE
activation                         discrete    -    Rectifier
hidden                        integervector <NA>      200,200
epochs                              numeric    -           10
train_samples_per_iteration         numeric    -           -2
seed                                integer    -            -
adaptive_rate                       logical    -         TRUE
rho                                 numeric    -         0.99
epsilon                             numeric    -        1e-08
rate                                numeric    -        0.005
```

Defining the search space

```
getParamSet("classif.h2o.deeplearning")

                                        Type  len               Def
autoencoder                          logical    -             FALSE
use_all_factor_level                 logical    -              TRUE
activation                          discrete    -         Rectifier
hidden                         integervector <NA>           200,200
epochs                               numeric    -                10
train_samples_per_iteration          numeric    -                -2
seed                                 integer    -                 -
adaptive_rate                        logical    -              TRUE
rho                                  numeric    -              0.99
epsilon                              numeric    -             1e-08
rate                                 numeric    -             0.005

param_set <- makeParamSet(
  makeDiscreteParam("hidden", values = list(one = 10, two = c(10, 5, 10))),
  makeDiscreteParam("activation", values = c("Rectifier", "Tanh")),
  makeNumericParam("l1", lower = 0.0001, upper = 1),
  makeNumericParam("l2", lower = 0.0001, upper = 1)
)
```

Defining the tuning method

- Grid search

```
ctrl_grid <- makeTuneControlGrid()
ctrl_grid

Tune control: TuneControlGrid
Same resampling instance: TRUE
Imputation value: <worst>
Start: <NULL>

Tune threshold: FALSE
Further arguments: resolution=10
```

- Random search

```
ctrl_random <- makeTuneControlRandom()
ctrl_random

Tune control: TuneControlRandom
Same resampling instance: TRUE
Imputation value: <worst>
Start: <NULL>
Budget: 100
Tune threshold: FALSE
Further arguments: maxit=100
```

Can only deal with **discrete** parameter sets!

Define resampling strategy

```
cross_val <- makeResampleDesc("RepCV",
                              predict = "both",
                              folds = 5 * 3)

param_set <- makeParamSet(
  ...
)

ctrl_grid <- makeTuneControlGrid()

task <- makeClassifTask(data = knowledge_train_data,
                        target = "UNS")

lrn <- makeLearner("classif.h2o.deeplearning",
                   predict.type = "prob",
                   fix.factors.prediction = TRUE)

lrn_tune <- tuneParams(lrn,
                       task,
                       resampling = cross_val,
                       control = ctrl_grid,
                       par.set = param_set)
```

Tuning hyperparameters

```
lrn_tune <- tuneParams(lrn,
                       task,
                       resampling = cross_val,
                       control = ctrl_grid,
                       par.set = param_set)

[Tune-y] 27: mmce.test.mean=0.6200000; time: 0.0 min
[Tune-x] 28: hidden=two; activation=Rectifier; l1=0.578; l2=1
[Tune-y] 28: mmce.test.mean=0.6800000; time: 0.0 min
[Tune-x] 29: hidden=one; activation=Rectifier; l1=0.156; l2=0.68
[Tune-y] 29: mmce.test.mean=0.4400000; time: 0.0 min
[Tune-x] 30: hidden=one; activation=Rectifier; l1=0.717; l2=0.427
[Tune-y] 30: mmce.test.mean=0.6600000; time: 0.0 min

[Tune] Result: hidden=two; activation=Tanh; l1=0.113;
l2=0.0973 : mmce.test.mean=0.2000000

# tictoc
26.13 sec elapsed
```

HYPERPARAMETER TUNING IN R

Let's practice!

HYPERPARAMETER TUNING IN R

Evaluating tuned hyperparameters with mlr

Dr. Shirin Glander
Data Scientist

Evaluation of our results can tell us:

- How different hyperparameters **affect the performance** of our model.
- Which hyperparameters have a particularly strong or weak **impact** on our model performance.
- Whether our hyperparameter search **converged**, i.e. whether we can be reasonably confident that we found the most **optimal hyperparameter combination** (or close to it).

Recap

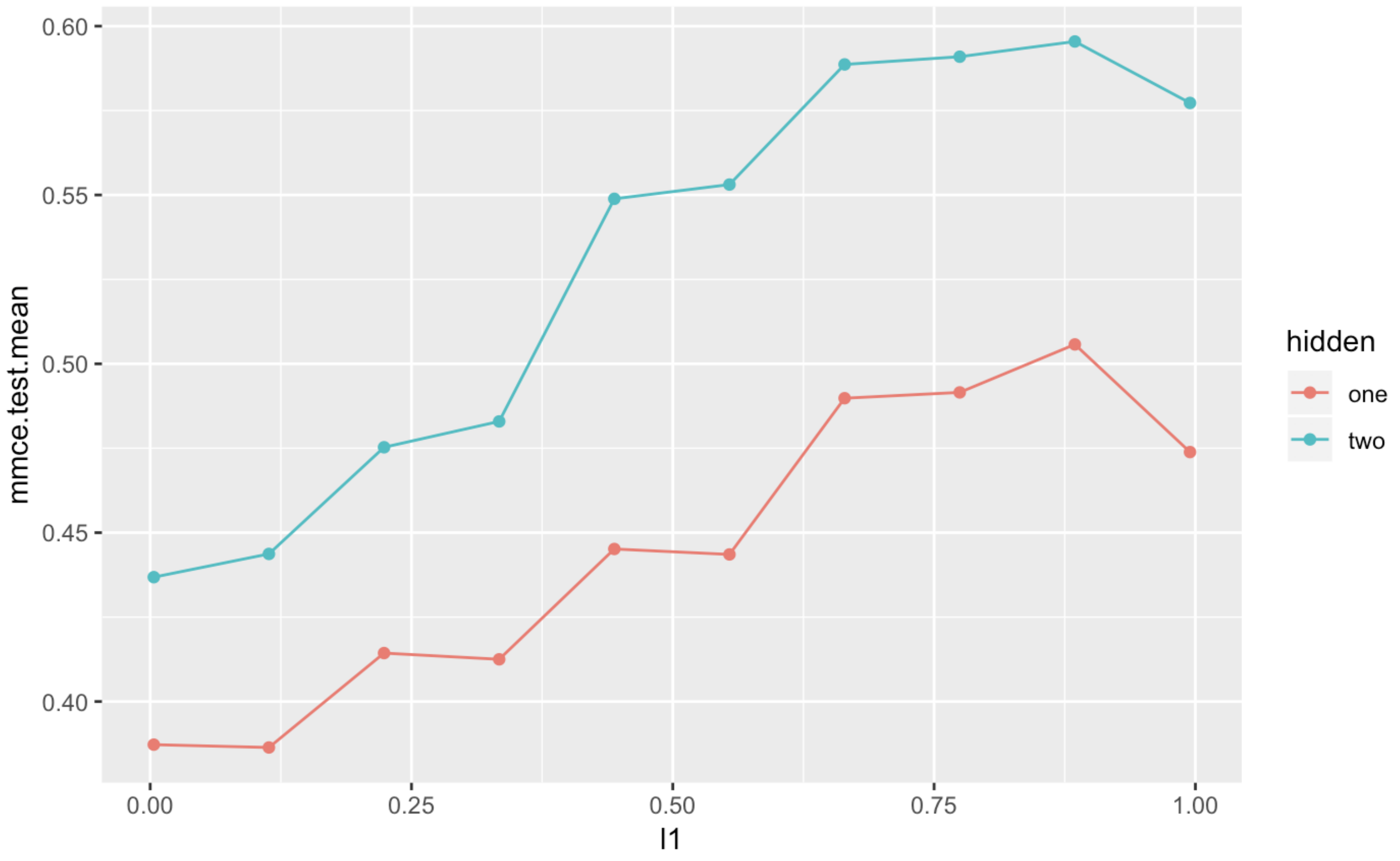
```
getParamSet("classif.h2o.deeplearning")

param_set <- makeParamSet(
  makeDiscreteParam("hidden", values = list(one = 10, two = c(10, 5, 10))),
  makeDiscreteParam("activation", values = c("Rectifier", "Tanh")),
  makeNumericParam("l1", lower = 0.0001, upper = 1),
  makeNumericParam("l2", lower = 0.0001, upper = 1)
)

ctrl_random <- makeTuneControlRandom(maxit = 50)

holdout <- makeResampleDesc("Holdout")

task <- makeClassifTask(data = knowledge_train_data, target = "UNS")

lrn <- makeLearner("classif.h2o.deeplearning", predict.type = "prob",
                   fix.factors.prediction = TRUE)

lrn_tune <- tuneParams(lrn,
                       task,
                       resampling = holdout,
                       control = ctrl_random,
                       par.set = param_set)
```

Evaluating the tuning results

```
lrn_tune

Tune result:
Op. pars: hidden=one; activation=Rectifier; l1=0.541; l2=0.229
mmce.test.mean=0.160000

generateHyperParsEffectData(lrn_tune, partial.dep = TRUE)

HyperParsEffectData:
Hyperparameters: hidden,activation,l1,l2
Measures: mmce.test.mean
Optimizer: TuneControlRandom
Nested CV Used: FALSE
[1] "Partial dependence requested"
Snapshot of data:
  hidden activation         l1        l2 mmce.test.mean iteration exec.time
1    one  Rectifier 0.75940339 0.9956819           0.40         1     0.883
2    one  Rectifier 0.16701526 0.2948697           0.40         2     0.836
3    one  Rectifier 0.88458832 0.9228281           0.70         3     0.830
4    two  Rectifier 0.48840740 0.7276899           0.70         4     0.820
5    one       Tanh 0.87114452 0.9971268           0.40         5     0.835
6    two       Tanh 0.07412213 0.3841913           0.44         6     0.830
```

Plotting hyperparameter tuning results

```
hyperpar_effects <- generateHyperParsEffectData(lrn_tune, partial.dep = TRUE)
plotHyperParsEffect(hyperpar_effects, partial.dep.learn = "regr.randomForest",
                    x = "l1", y = "mmce.test.mean", z = "hidden",
                    plot.type = "line")
```



HYPERPARAMETER TUNING IN R

Now it's your turn!

HYPERPARAMETER TUNING IN R

Advanced tuning with mlr

Dr. Shirin Glander
Data Scientist

Advanced tuning controls

- `makeTuneControlCMAES`: CMA Evolution Strategy
- `makeTuneControlDesign`: Predefined data frame of hyperparameters
- `makeTuneControlGenSA`: Generalized simulated annealing
- `makeTuneControlIrace`: Tuning with iterated F-Racing
- `makeTuneControlMBO`: Model-based / Bayesian optimization

Choosing evaluation metrics

```
# Generalized simulated annealing
ctrl_gensa <- makeTuneControlGenSA()

# Create holdout sampling
bootstrap <- makeResampleDesc("Bootstrap", predict = "both")

# Perform tuning
lrn_tune <- tuneParams(learner = lrn,
                       task = task,
                       resampling = bootstrap,
                       control = ctrl_gensa,
                       par.set = param_set,
                       measures = list(acc, mmce))

[Tune-x] 2170: eta=0.0771; max_depth=4
[Tune-y] 2170: acc.test.mean=0.9317275,mmce.test.mean=0.0682725; time: 0.0 m
[Tune-x] 2171: eta=0.822; max_depth=8
[Tune-y] 2171: acc.test.mean=0.9276912,mmce.test.mean=0.0723088; time: 0.0 m
[Tune-x] 2172: eta=0.498; max_depth=4
[Tune-y] 2172: acc.test.mean=0.9311626,mmce.test.mean=0.0688374; time: 0.0 m
[Tune-x] 2173: eta=0.365; max_depth=4
[Tune-y] 2173: acc.test.mean=0.9288406,mmce.test.mean=0.0711594; time: 0.0 m
```

Choosing evaluation metrics

```
# Create holdout sampling
bootstrap <- makeResampleDesc("Bootstrap", predict = "both")

# Perform tuning
lrn_tune <- tuneParams(learner = lrn,
                       task = task,
                       resampling = bootstrap,
                       control = ctrl_gensa,
                       par.set = param_set,
                       measures = list(acc,
                                       setAggregation(acc, train.mean),
                                       mmce,
                                       setAggregation(mmce, train.mean)))

[Tune-x] 3920: eta=0.294; max_depth=8
[Tune-y] 3920: acc.test.mean=0.9250118,
               acc.train.mean=0.9740000,
               mmce.test.mean=0.0749882,
               mmce.train.mean=0.0260000;
               time: 0.0 min
```

Nested cross-validation & nested resampling

```
lrn_wrapper <- makeTuneWrapper(learner = lrn,
                               resampling = bootstrap,
                               control = ctrl_gensa,
                               par.set = param_set,
                               measures = list(acc, mmce))
```

- Either train **directly**

```
model_nested <-  train(lrn_wrapper, task)
getTuneResult(model_nested)
```

- Or add 2x **nested** cross-validation

```
cv2 <- makeResampleDesc("CV", iters = 2)
res <- resample(lrn_wrapper,
                task,
                resampling = cv2,
                extract = getTuneResult)
generateHyperParsEffectData(res)
```

Choose hyperparameters from a tuning set

```
lrn_best <- setHyperPars(lrn, par.vals = list(minsplit = 4,
                                               minbucket = 3,
                                               maxdepth = 6))

model_best <- train(lrn_best, task)

predict(model_best, newdata = knowledge_test_data)

Prediction: 30 observations
predict.type: response
threshold:
time: 0.00
  truth response
1  High     High
2  High     High
3  High     High
4  High     High
5  High     High
6  High     High
... (#rows: 30, #cols: 2)
```

HYPERPARAMETER TUNING IN R

It's your turn!