Evaluating Hyperparameter Tuning

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Source: `vignettes/tutorial/hyperpar_tuning_effects.Rmd` (https://github.com/mlr-org/mlr/blob/master/vignettes/tutorial/hyperpar_tuning_effects.Rmd)

As mentioned on the tuning (tune.html) tutorial page, tuning a machine learning algorithm typically involves:

- the hyperparameter search space:

```
# ex: create a search space for the C hyperparameter from 0.01 to 0.1
ps = makeParamSet(
  makeNumericParam("C", lower = 0.01, upper = 0.1)
)
```

- the optimization algorithm (aka tuning method):

```
# ex: random search with 100 iterations
ctrl = makeTuneControlRandom (../../reference/makeTuneControlRandom.html)(maxit =
```

- an evaluation method, i.e., a resampling strategy and a performance measure:

```
# ex: 2-fold CV
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("CV", iters = 2L
```

After tuning, you may want to evaluate the tuning process in order to answer questions such as:

- How does varying the value of a hyperparameter change the performance of the machine learning algorithm?
- What's the relative importance of each hyperparameter?
- How did the optimization algorithm (prematurely) converge?

`mlr` provides methods to generate and plot the data in order to evaluate the effect of hyperparameter tuning.

Generating hyperparameter tuning data

`mlr` separates the generation of the data from the plotting of the data in case the user wishes to use the data in a custom way downstream.

The `generateHyperParsEffectData()` (`../../reference/generateHyperParsEffectData.html`) method takes the tuning result along with 2 additional arguments: `trafo` and `include.diagnostics`. The `trafo` argument will convert the hyperparameter data to be on the transformed scale in case a transformation was used when creating the parameter (as in the case below). The `include.diagnostics` argument will tell `mlr` whether to include the eol and any error messages from the learner.

Below we perform random search on the `C` parameter for SVM on the famous Pima Indians (`mlbench::PimaIndiansDiabetes()` (`http://www.rdocumentation.org/packages/mlbench/topics/PimaIndiansDiabetes`)) dataset. We generate the hyperparameter effect data so that the `C` parameter is on the transformed scale and we do not include diagnostic data:

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlRandom (../../reference/makeTuneControlRandom.html)(maxit =
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("CV", iters = 2I
res = tuneParams (../../reference/tuneParams.html)("classif.ksvm", task = pid.tas
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSE
generateHyperParsEffectData (../../reference/generateHyperParsEffectData.html)(re

## HyperParsEffectData:
## Hyperparameters: C
## Measures: acc.test.mean,mmce.test.mean
## Optimizer: TuneControlRandom
## Nested CV Used: FALSE
## Snapshot of data:
##            C acc.test.mean mmce.test.mean iteration exec.time
## 1 0.18477464     0.7317708      0.2682292         1     0.833
## 2 0.19252244     0.7304688      0.2695312         2     0.041
## 3 4.75219120     0.7200521      0.2799479         3     0.040
## 4 0.05567812     0.6536458      0.3463542         4     0.579
## 5 0.12179856     0.7161458      0.2838542         5     0.064
## 6 6.25359181     0.7239583      0.2760417         6     0.056
```

As a reminder from the resampling (resample.html) tutorial, if we wanted to generate data on the training set as well as the validation set, we only need to make a few minor changes:

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlRandom (../../reference/makeTuneControlRandom.html)(maxit =
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("CV", iters = 2L
res = tuneParams (../../reference/tuneParams.html)("classif.ksvm", task = pid.tas
  measures = list(acc, setAggregation (../../reference/setAggregation.html)(acc,
    train.mean)), resampling = rdesc, par.set = ps, show.info = FALSE)
generateHyperParsEffectData (../../reference/generateHyperParsEffectData.html)(re

## HyperParsEffectData:
## Hyperparameters: C
## Measures: acc.test.mean,acc.train.mean,mmce.test.mean,mmce.train.mean
## Optimizer: TuneControlRandom
## Nested CV Used: FALSE
## Snapshot of data:
##            C acc.test.mean acc.train.mean mmce.test.mean mmce.train.mean
## 1 0.07253028     0.6575521      0.6588542      0.3424479       0.3411458
## 2 4.09306975     0.7617188      0.8906250      0.2382812       0.1093750
## 3 2.23762232     0.7552083      0.8710938      0.2447917       0.1289062
## 4 0.11080224     0.6940104      0.7187500      0.3059896       0.2812500
## 5 3.37586150     0.7565104      0.8867188      0.2434896       0.1132812
## 6 1.77872565     0.7669271      0.8567708      0.2330729       0.1432292
##   iteration exec.time
## 1         1     0.095
## 2         2     0.079
## 3         3     0.102
## 4         4     0.092
## 5         5     0.071
## 6         6     0.088
```

In the example below, we perform grid search on the `C` parameter for SVM on the Pima Indians dataset using nested cross validation. We generate the hyperparameter effect data so that the `C` parameter is on the untransformed scale and we do not include diagnostic data. As you can see below, nested cross validation is supported without any extra work by the user, allowing the user to obtain an unbiased estimator for the performance.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlGrid (../../reference/makeTuneControlGrid.html)()
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("CV", iters = 2L
lrn = makeTuneWrapper (../../reference/makeTuneWrapper.html)("classif.ksvm", cont
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSE
res = resample (../../reference/resample.html)(lrn, task = pid.task, resampling =
generateHyperParsEffectData (../../reference/generateHyperParsEffectData.html)(re

## HyperParsEffectData:
## Hyperparameters: C
## Measures: acc.test.mean,mmce.test.mean
## Optimizer: TuneControlGrid
## Nested CV Used: TRUE
## Snapshot of data:
##            C acc.test.mean mmce.test.mean iteration exec.time
## 1 -5.0000000     0.6536458      0.3463542         1     0.064
## 2 -3.8888889     0.6536458      0.3463542         2     0.037
## 3 -2.7777778     0.6718750      0.3281250         3     0.036
## 4 -1.6666667     0.7291667      0.2708333         4     0.038
## 5 -0.5555556     0.7369792      0.2630208         5     0.037
## 6  0.5555556     0.7369792      0.2630208         6     0.051
##   nested_cv_run
## 1             1
## 2             1
## 3             1
## 4             1
## 5             1
## 6             1
```

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlGrid (../../reference/makeTuneControlGrid.html)()
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("CV", iters = 2L
lrn = makeTuneWrapper (../../reference/makeTuneWrapper.html)("classif.ksvm", cont
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSE
res = resample (../../reference/resample.html)(lrn, task = pid.task, resampling =
generateHyperParsEffectData (../../reference/generateHyperParsEffectData.html)(re

## HyperParsEffectData:
## Hyperparameters: C
## Measures: acc.test.mean,mmce.test.mean
## Optimizer: TuneControlGrid
## Nested CV Used: TRUE
## Snapshot of data:
##            C acc.test.mean mmce.test.mean iteration exec.time
## 1 -5.0000000     0.6718750      0.3281250         1     0.066
## 2 -3.8888889     0.6718750      0.3281250         2     0.077
## 3 -2.7777778     0.6744792      0.3255208         3     0.070
## 4 -1.6666667     0.7187500      0.2812500         4     0.049
## 5 -0.5555556     0.7526042      0.2473958         5     0.049
## 6  0.5555556     0.7630208      0.2369792         6     0.054
##   nested_cv_run
## 1             1
## 2             1
## 3             1
## 4             1
## 5             1
## 6             1
```

After generating the hyperparameter effect data, the next step is to visualize it. `mlr` has several methods built-in to visualize the data, meant to support the needs of the researcher and the engineer in industry. The next few sections will walk through the visualization support for several use-cases.

Visualizing the effect of a single hyperparameter

In a situation when the user is tuning a single hyperparameter for a learner, the user may wish to plot the performance of the learner against the values of the hyperparameter.

In the example below, we tune the number of clusters against the silhouette score on the mtcars dataset. We specify the x-axis with the `x` argument and the y-axis with the `y` argument. If the `plot.type` argument is not specified, `mlr` will attempt to plot a scatterplot

by default. Since `plotHyperParsEffect()` (../../reference/plotHyperParsEffect.html) returns a `ggplot2::ggplot()` (ggplot2.tidyverse.org/reference/ggplot.html) object, we can easily customize it to our liking!

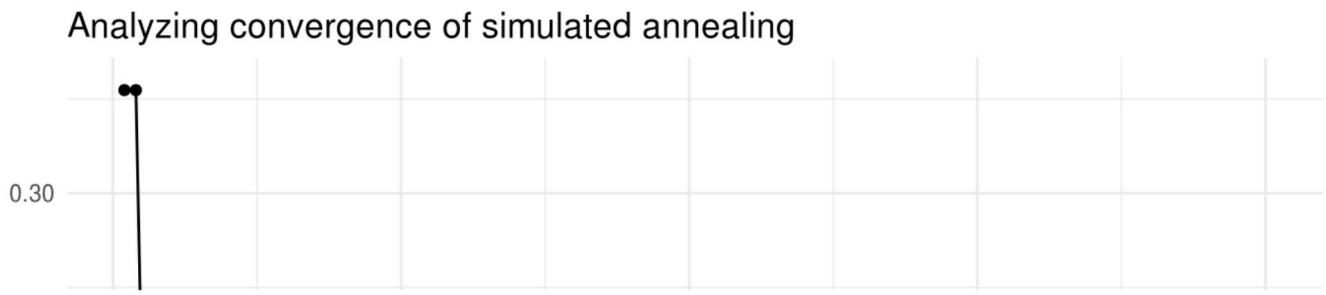
```
library("clusterSim")

ps = makeParamSet(
  makeDiscreteParam("centers", values = 3:10)
)
ctrl = makeTuneControlGrid (../../reference/makeTuneControlGrid.html)()
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("Holdout")
res = tuneParams (../../reference/tuneParams.html)("cluster.kmeans", task = mtca
  measures = silhouette, resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData (../../reference/generateHyperParsEffectData.h
plt = plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "

# add our own touches to the plot
plt + geom_point(colour = "red") +
  ggtitle("Evaluating Number of Cluster Centers on mtcars") +
  scale_x_continuous(breaks = 3:10) +
  theme_bw()
```

In the example below, we tune SVM with the `C` hyperparameter on the Pima dataset. We will use simulated annealing optimizer, so we are interested in seeing if the optimization algorithm actually improves with iterations. By default, `mlr` only plots improvements to the global optimum.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlGenSA (../../reference/makeTuneControlGenSA.html)(budget =
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("Holdout")
res = tuneParams (../../reference/tuneParams.html)("classif.ksvm", task = pid.tas
  resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData (../../reference/generateHyperParsEffectData.h
plt = plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "
  plot.type = "line")
plt + ggtitle("Analyzing convergence of simulated annealing") +
  theme_minimal()
```



In the case of a learner crash, `mlr` will impute the crash with the worst value graphically and indicate the point. In the example below, we give the `C` parameter negative values, which will result in a learner crash for SVM.

```
ps = makeParamSet(
  makeDiscreteParam("C", values = c(-1, -0.5, 0.5, 1, 1.5))
)
ctrl = makeTuneControlGrid (../../reference/makeTuneControlGrid.html)()
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("CV", iters = 2I
res = tuneParams (../../reference/tuneParams.html)("classif.ksvm", task = pid.tas
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSI
data = generateHyperParsEffectData (../../reference/generateHyperParsEffectData.h
plt = plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "C
plt + ggtitle("SVM learner crashes with negative C") +
  theme_bw()
```

The example below uses nested cross validation (nested_resampling.html) with an outer loop of 2 runs. `mlr` indicates each run within the visualization.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x)
)
ctrl = makeTuneControlGrid (../../reference/makeTuneControlGrid.html)()
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("Holdout")
lrn = makeTuneWrapper (../../reference/makeTuneWrapper.html)("classif.ksvm", cont
  measures = list(acc, mmce), resampling = rdesc, par.set = ps, show.info = FALSE
res = resample (../../reference/resample.html)(lrn, task = pid.task, resampling =
data = generateHyperParsEffectData (../../reference/generateHyperParsEffectData.h
plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "C", y =
```

Visualizing the effect of 2 hyperparameters

In the case of tuning 2 hyperparameters simultaneously, `mlr` provides the ability to plot a heatmap and contour plot in addition to a scatterplot or line.

In the example below, we tune the `C` and `sigma` parameters for SVM on the Pima dataset. We use interpolation to produce a regular grid for plotting the heatmap. The `interpolation` argument accepts any regression learner from `mlr` to perform the interpolation. The `z` argument will be used to fill the heatmap or color lines, depending on the `plot.type` used.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x),
  makeNumericParam("sigma", lower = -5, upper = 5, trafo = function(x) 2^x))
ctrl = makeTuneControlRandom (../../reference/makeTuneControlRandom.html)(maxit =
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("Holdout")
learn = makeLearner (../../reference/makeLearner.html)("classif.ksvm", par.vals =
res = tuneParams (../../reference/tuneParams.html)(learn, task = pid.task, contro
  resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData (../../reference/generateHyperParsEffectData.h
plt = plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "C
  plot.type = "heatmap", interpolate = "regr.earth")
min_plt = min(data$data$acc.test.mean, na.rm = TRUE)
max_plt = max(data$data$acc.test.mean, na.rm = TRUE)
med_plt = mean(c(min_plt, max_plt))
plt + scale_fill_gradient2(breaks = seq(min_plt, max_plt, length.out = 5),
  low = "blue", mid = "white", high = "red", midpoint = med_plt)
## Scale for 'fill' is already present. Adding another scale for 'fill',
## which will replace the existing scale.
```

We can use the `show.experiments` argument in order to visualize which points were specifically passed to the learner in the original experiment and which points were interpolated by `mlr`:

```
plt = plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "C
  plot.type = "heatmap", interpolate = "regr.earth", show.experiments = TRUE)
plt + scale_fill_gradient2(breaks = seq(min_plt, max_plt, length.out = 5),
  low = "blue", mid = "white", high = "red", midpoint = med_plt)
## Scale for 'fill' is already present. Adding another scale for 'fill',
## which will replace the existing scale.
```

We can also visualize how long the optimizer takes to reach an optima for the same example:

```
plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "iterat
  plot.type = "line")
```

In the case where we are tuning 2 hyperparameters and we have a learner crash, `mlr` will indicate the respective points and impute them with the worst value. In the example below, we tune `C` and `sigma`, forcing `C` to be negative for some instances which will crash SVM. We perform interpolation to get a regular grid in order to plot a heatmap. We can see that the interpolation creates axis parallel lines resulting from the learner crashes.

```
ps = makeParamSet(
  makeDiscreteParam("C", values = c(-1, 0.5, 1.5, 1, 0.2, 0.3, 0.4, 5)),
  makeDiscreteParam("sigma", values = c(-1, 0.5, 1.5, 1, 0.2, 0.3, 0.4, 5)))
ctrl = makeTuneControlGrid (../../reference/makeTuneControlGrid.html)()
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("Holdout")
learn = makeLearner (../../reference/makeLearner.html)("classif.ksvm", par.vals =
res = tuneParams (../../reference/tuneParams.html)(learn, task = pid.task, contro
  resampling = rdesc, par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData (../../reference/generateHyperParsEffectData.h
plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "C", y =
  plot.type = "heatmap", interpolate = "regr.earth")
```

A slightly more complicated example is using nested cross validation while simultaneously tuning 2 hyperparameters. In order to plot a heatmap in this case, `mlr` will aggregate each of the nested runs by a user-specified function. The default function is `mean`. As expected, we can still take advantage of interpolation.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x),
  makeNumericParam("sigma", lower = -5, upper = 5, trafo = function(x) 2^x))
ctrl = makeTuneControlRandom (../../reference/makeTuneControlRandom.html)(maxit =
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("Holdout")
learn = makeLearner (../../reference/makeLearner.html)("classif.ksvm", par.vals =
lrn = makeTuneWrapper (../../reference/makeTuneWrapper.html)(learn, control = ctr
  resampling = rdesc, par.set = ps, show.info = FALSE)
res = resample (../../reference/resample.html)(lrn, task = pid.task, resampling =
data = generateHyperParsEffectData (../../reference/generateHyperParsEffectData.h
plt = plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "C
  plot.type = "heatmap", interpolate = "regr.earth", show.experiments = TRUE,
  nested.agg = mean)
min_plt = min(plt$data$acc.test.mean, na.rm = TRUE)
max_plt = max(plt$data$acc.test.mean, na.rm = TRUE)
med_plt = mean(c(min_plt, max_plt))
plt + scale_fill_gradient2(breaks = seq(min_plt, max_plt, length.out = 5),
  low = "red", mid = "white", high = "blue", midpoint = med_plt)
## Scale for 'fill' is already present. Adding another scale for 'fill',
## which will replace the existing scale.
```

Visualizing the effects of more than 2 hyperparameters

In order to visualize the result when tuning 3 or more hyperparameters simultaneously we can take advantage of partial dependence plots (partial_dependence.html) to show how the performance depends on a one- or two-dimensional subset of the hyperparameters. Below we tune three hyperparameters `C`, `sigma`, and `degree` of an SVM with Bessel kernel and set the `partial.dep` flag to `TRUE` to indicate that we intend to calculate partial dependences.

```
ps = makeParamSet(
  makeNumericParam("C", lower = -5, upper = 5, trafo = function(x) 2^x),
  makeNumericParam("sigma", lower = -5, upper = 5, trafo = function(x) 2^x),
  makeDiscreteParam("degree", values = 2:5))
ctrl = makeTuneControlRandom (../../reference/makeTuneControlRandom.html)(maxit =
rdesc = makeResampleDesc (../../reference/makeResampleDesc.html)("Holdout", predi
learn = makeLearner (../../reference/makeLearner.html)("classif.ksvm", par.vals =
res = tuneParams (../../reference/tuneParams.html)(learn, task = pid.task, contro
  measures = list(acc, setAggregation (../../reference/setAggregation.html)(acc,
  par.set = ps, show.info = FALSE)
data = generateHyperParsEffectData (../../reference/generateHyperParsEffectData.h
```

You can generate a plot for a single hyperparameter like `C` as shown below. The `partial.dep.learn` can be any regression Learner (`makeLearner()` (../../reference/makeLearner.html)) in `mlr` and is used to regress the attained performance values on the values of the 3 hyperparameters visited during tuning. The fitted model serves as basis for calculating partial dependences.

```
plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "C", y =
  partial.dep.learn = "regr.randomForest")
## Loading required package: mmpf
```

We can also look at two hyperparameters simultaneously, for example `C` and `sigma`.

```
plotHyperParsEffect (../../reference/plotHyperParsEffect.html)(data, x = "C", y =
  plot.type = "heatmap", partial.dep.learn = "regr.randomForest")
```