Tuning Machine Learning Algorithms with mlr3

mlr3tuning

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Intro

TUNING

- Behavior of most methods depends on *hyperparameters*
- We want to choose them so our algorithm performs well
- Good hyperparameters are data-dependent

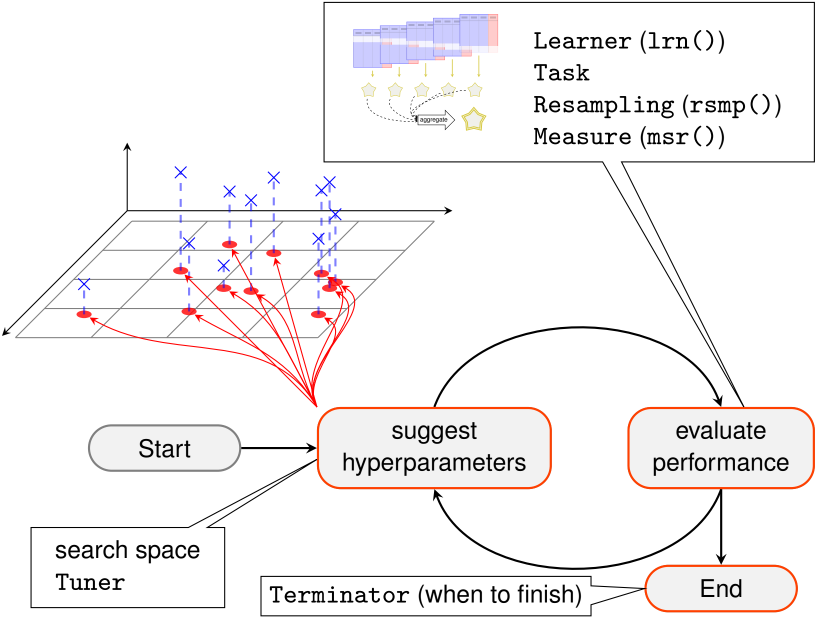
$\Rightarrow$ We do *black box optimization* (“Try stuff and see what works”)

Tuning toolbox for `mlr3`:

```r
library("bbotk")
library("mlr3tuning")
```

Tuning

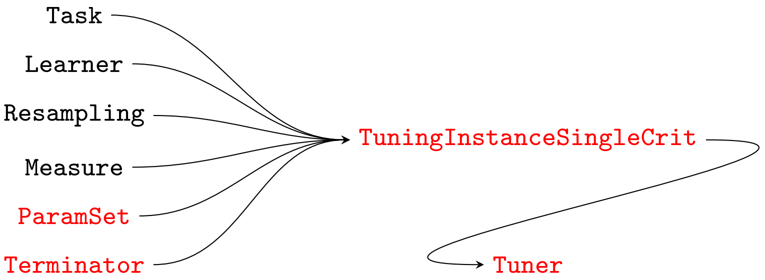
TUNING



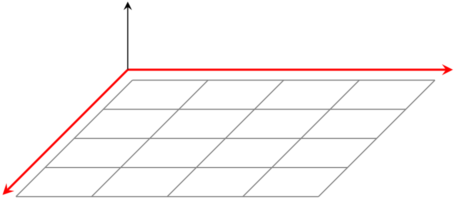
Learner (lrn())
Task
Resampling (rsmp())
Measure (msr())
aggregate
Start
suggest hyperparameters
evaluate performance
End
search space
Tuner
Terminator (when to finish)

Tuning in mlr3

OBJECTS IN TUNING



SEARCH SPACE



```
ParamSet$new(list(param1, param2, ...))
```

Numerical parameter	`ParamDbl$new(id, lower, upper)`
Integer parameter	`ParamInt$new(id, lower, upper)`
Discrete parameter	`ParamFct$new(id, levels)`
Logical parameter	`ParamLgl$new(id)`
Untyped parameter	`ParamUty$new(id)`

```
library("paradox")
searchspace_knn = ParamSet$new(list(
  ParamInt$new("k", 1, 20)
))
```

TERMINATION

- Tuning needs a *termination condition*: when to finish
- `Terminator` class
- `mlr_terminators` dictionary, `trm()` short form
- ```
  as.data.table(mlr_terminators)
  ```
  ```
  #> Key: <key>
  #>                   key
  #>                <char>
  #> 1:         clock_time
  #> 2:              combo
  #> 3:              evals
  #> 4:               none
  #> 5:       perf_reached
  #> 6:           run_time
  #> 7:         stagnation
  #> 8: stagnation_batch
  ```
- ```
  trm("evals", n_evals = 20)
  ```
  ```
  #> <TerminatorEvals>
  #> * Parameters: n_evals=20
  ```

TUNING METHOD

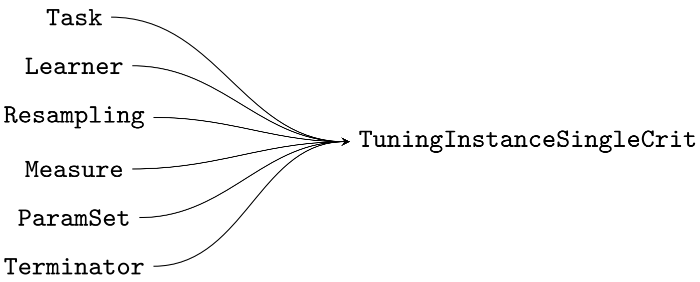
- need to choose a *tuning method*
- `Tuner` class
- `mlr_tuners` dictionary, `tnr()` short form
- ```
  as.data.table(mlr_tuners)
  ```
  ```
  #> Key: <key>
  #>                key
  #>             <char>
  #> 1: design_points
  #> 2:         gensa
  #> 3:   grid_search
  #> 4:        nloptr
  #> 5: random_search
  ```
  ```

TUNING METHOD

- load `Tuner` with `tnr()`, set parameters
- ```
  gsearch = tnr("grid_search", resolution = 3)

  print(gsearch)
  #> <TunerGridSearch>
  #> * Parameters: resolution=3, batch_size=1
  #> * Parameter classes: ParamLgl, ParamInt, ParamDbl, ParamFct
  #> * Properties: dependencies, single-crit, multi-crit
  #> * Packages: -
  ```
- common parameter `batch_size` for parallelization
  ```

CALLING THE TUNER




```r
inst = TuningInstanceSingleCrit$new(
  tsk("iris"), lrn("classif.kknn", kernel="rectangular"),
  rsmp("holdout"), msr("classif.ce"),
  searchspace_knn, trm("none")
)
```

CALLING THE TUNER

```
gsearch$optimize(inst)

#> INFO  [10:23:07.146] Starting to optimize 1 parameter(s) with '<Optim
#> INFO  [10:23:07.168] Evaluating 1 configuration(s)
#> INFO  [10:23:07.687] Result of batch 1:
#> INFO  [10:23:07.688]   k classif.ce      resample_result
#> INFO  [10:23:07.688]  10       0.04 <ResampleResult[18]>
#> INFO  [10:23:07.689] Evaluating 1 configuration(s)
#> INFO  [10:23:07.783] Result of batch 2:
#> INFO  [10:23:07.785]  k classif.ce      resample_result
#> INFO  [10:23:07.785]  1       0.06 <ResampleResult[18]>
#> INFO  [10:23:07.786] Evaluating 1 configuration(s)
#> INFO  [10:23:07.814] Result of batch 3:
#> INFO  [10:23:07.815]   k classif.ce      resample_result
#> INFO  [10:23:07.815]  20       0.08 <ResampleResult[18]>
#> INFO  [10:23:07.818] Finished optimizing after 3 evaluation(s)
#> INFO  [10:23:07.819] Result:
#> INFO  [10:23:07.819]      k learner_param_vals  x_domain classif.ce
#> INFO  [10:23:07.819]  <num>             <list>    <list>      <num>
#> INFO  [10:23:07.819]     10          <list[2]> <list[1]>       0.04
#>          k learner_param_vals  x_domain classif.ce
#>      <num>             <list>    <list>      <num>
#> 1:     10          <list[2]> <list[1]>       0.04
```

TUNING RESULTS

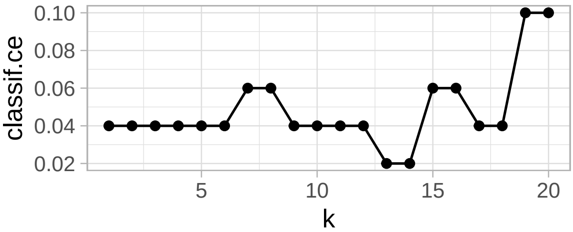
```
gsearch = tnr("grid_search", resolution = 20)

inst = TuningInstanceSingleCrit$new(
  tsk("iris"), lrn("classif.kknn", kernel="rectangular"), rsmp("holdout"),
  msr("classif.ce"),searchspace_knn, trm("none"))

gsearch$optimize(inst)

#>         k learner_param_vals  x_domain classif.ce
#>     <num>             <list>    <list>      <num>
#> 1:     14          <list[2]> <list[1]>       0.02

ggplot(inst$archive$data(unnest = "x_domain"),
  aes(x = k, y = classif.ce)) + geom_line() + geom_point()
```



RECAP

```r
inst = TuningInstanceSingleCrit$new(
  tsk("iris"), lrn("classif.kknn", kernel="rectangular"),
  rsmp("holdout"), msr("classif.ce"),
  searchspace_knn, trm("evals", n_evals = 2)
)

gsearch = tnr("grid_search", resolution = 3)

gsearch$optimize(inst)

#>        k learner_param_vals  x_domain classif.ce
#>    <num>             <list>    <list>      <num>
#> 1:     1          <list[2]> <list[1]>       0.06
```

Parameter Transformation

PARAMETER TRANSFORMATION

- Sometimes we do not want to sample evenly from a range
- $k = 1$ vs. $k = 2$ probably more interesting than $k = 101$ vs. $k = 102$

$\Rightarrow$ Transformations

- Part of `ParamSet`

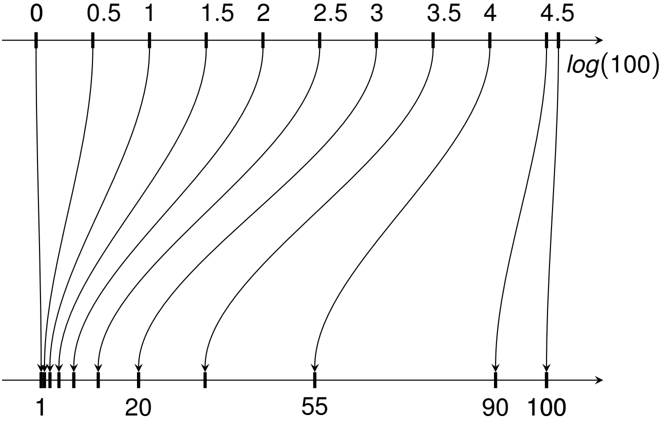
Example:

1. sample from $\log(1) \ldots \log(100)$ (`k_before_trafo`)
2. transform by $\exp()$ in `trafo` function
3. don't forget to `round` (k must be integer)

```
searchspace_knn_trafo = ParamSet$new(list(
  ParamDbl$new("k_before_trafo", log(1), log(50))
))
searchspace_knn_trafo$trafo = function(x, param_set) {
  return(list(k = round(exp(x$k_before_trafo))))
}
```

PARAMETER TRANSFORMATION

What is our transformation doing?



PARAMETER TRANSFORMATION

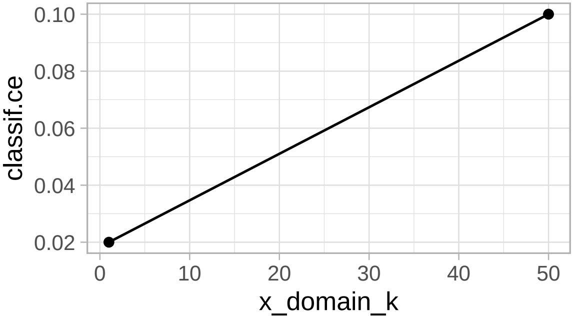
Tuning again…

```
inst$result

#>    k_before_trafo learner_param_vals  x_domain classif.ce
#>             <num>             <list>    <list>      <num>
#> 1:              0        <list[2]> <list[1]>       0.02
```

PARAMETER TRANSFORMATION

```
ggplot(inst$archive$data(unnest = "x_domain"),
  aes(x = x_domain_k, y = classif.ce)) + geom_line() + geom_point()
```



Nested Resampling

NESTED RESAMPLING

- Need to perform nested resampling to estimate tuned learner performance

⇒ Treat tuning as if it were a `Learner`!

  - Training:
    1. Tune model using (inner) resampling
    2. Train final model with best parameters on all (i.e. outer resampling) data
  - Predicing: Just use final model

- **AutoTuner**

```
optlrn = AutoTuner$new(lrn("classif.kknn", kernel="rectangular"),
  rsmp("holdout"), msr("classif.ce"), searchspace_knn,
  trm("none"), tnr("grid_search", resolution = 2))
```

NESTED RESAMPLING

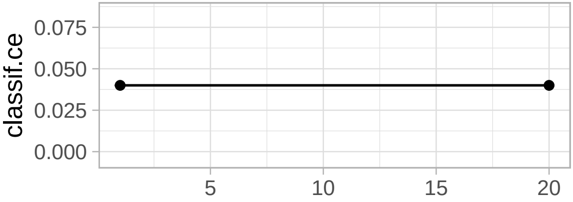
```r
optlrn$train(tsk("iris"))
```

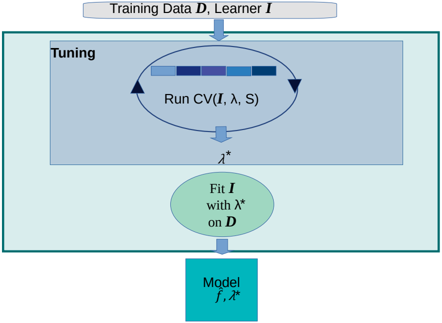
```r
optlrn$model$learner

#> <LearnerClassifKKNN:classif.kknn>
#> * Model: list
#> * Parameters: kernel=rectangular, k=1
#> * Packages: kknn
#> * Predict Type: response
#> * Feature types: logical, integer, numeric, factor, ordered
#> * Properties: multiclass, twoclass
```

```r
ggplot(optlrn$model$tuning_instance$archive$data(),
  aes(x = k, y = classif.ce)) + geom_line() + geom_point()
```

NESTED RESAMPLING





NESTED RESAMPLING

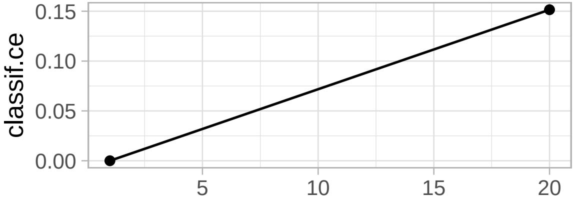
```
resample(tsk("iris"), optlrn, rsmp("holdout"))

#> <ResampleResult> of 1 iterations
#> * Task: iris
#> * Learner: classif.kknn.tuned
#> * Warnings: 0 in 0 iterations
#> * Errors: 0 in 0 iterations
```

NESTED RESAMPLING

```r
result = resample(tsk("iris"), optlrn, rsmp("holdout"),
  store_models = TRUE)
```

```r
ggplot(result$learners[[1]]$
       model$tuning_instance$archive$data(),
  aes(x = k, y = classif.ce)) + geom_line() + geom_point()
```



NESTED RESAMPLING

Aggregate performances of outer folds

```
result$aggregate()

#> classif.ce
#>       0.06
```

Retrieve inner tuning results

```
result$data$learner[[1]]$tuning_result

#>        k learner_param_vals  x_domain classif.ce
#>    <num>             <list>    <list>      <num>
#> 1:     1          <list[2]> <list[1]>          0
```

Outro

TUNING WITH MLR3TUNING

Tuning a `Learner`

1. Construct a `TuningInstanceSingleCrit`
   - `Task`—the Data to tune over
   - `Learner`—the algorithm to tune
   - `Resampling`—the resampling method to use
   - `Measure`—how to evaluate performance
   - `ParamSet`—the search space, possibly with `trafo`
   - `Terminator`—when to quit
2. Create a `Tuner`
   - Usually using `tnr()`
   - May have some parameters, e.g. `batch_size`
3. Call `tuner$optimize()`

Nested Resampling

1. Construct an `AutoTuner`
   - Constructor takes all arguments of a `TuningInstanceSingleCrit` *except* *`Task`*
   - Also takes the `Tuner` as an argument
2. Use like a normal `Learner` in `resample()` and `benchmark()`