Tuning Machine Learning Algorithms with mlr3

https://mlr-org.com/

https://github.com/mlr-org
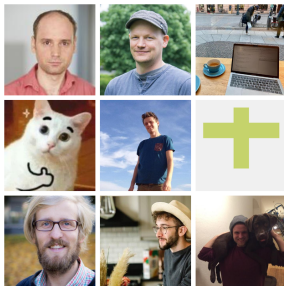
Bernd Bischl, Michel Lang, Martin Binder, Florian Pfisterer, Jakob Richter, Patrick Schratz, Lennart Schneider, Raphael Sonabend, Marc Becker, Giuseppe Casalicchio

February 18, 2021

Intro

TUNING

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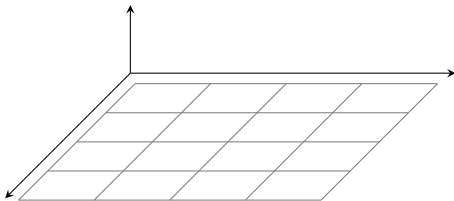
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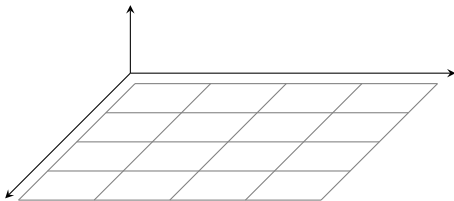
Tuning toolbox for `mlr3`:
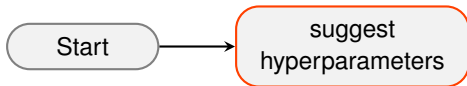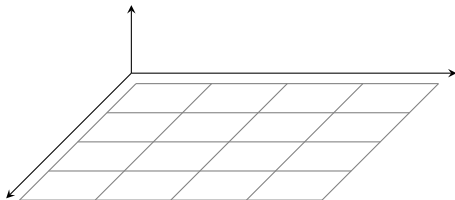
```
library("bbotk")
library("mlr3tuning")
```
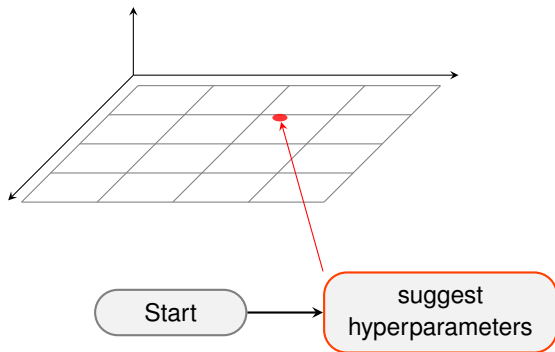
Tuning
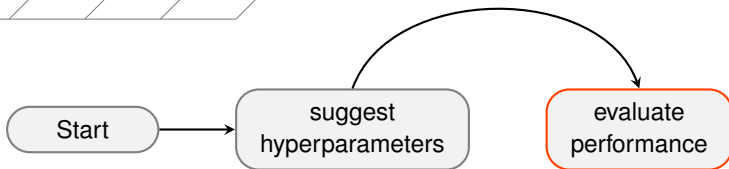
TUNING

TUNING

Start

TUNING

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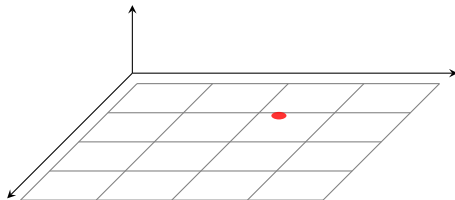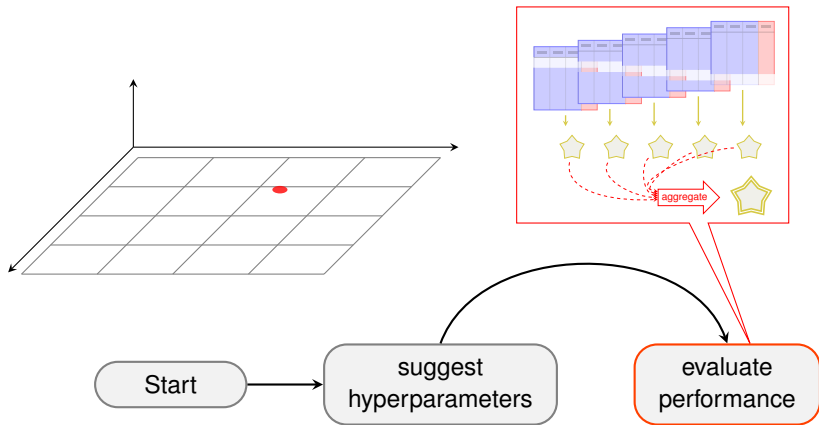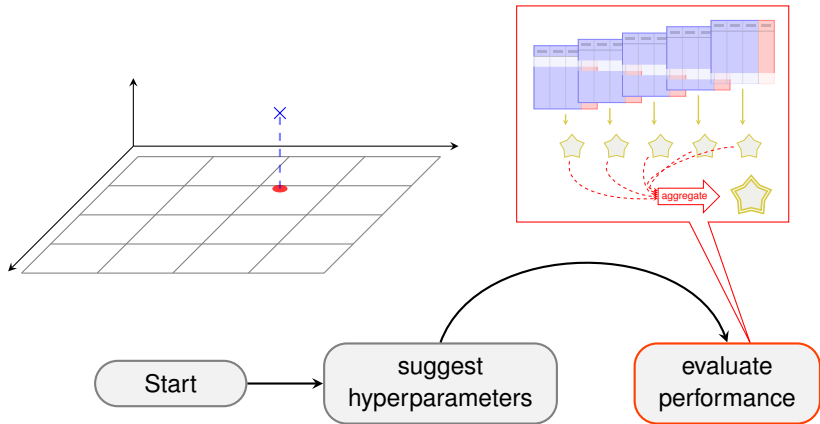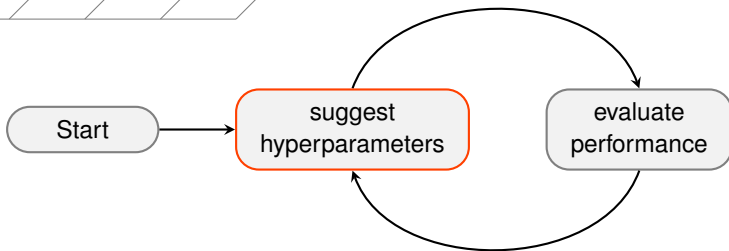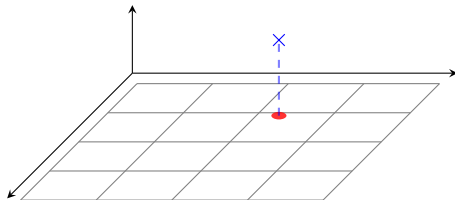
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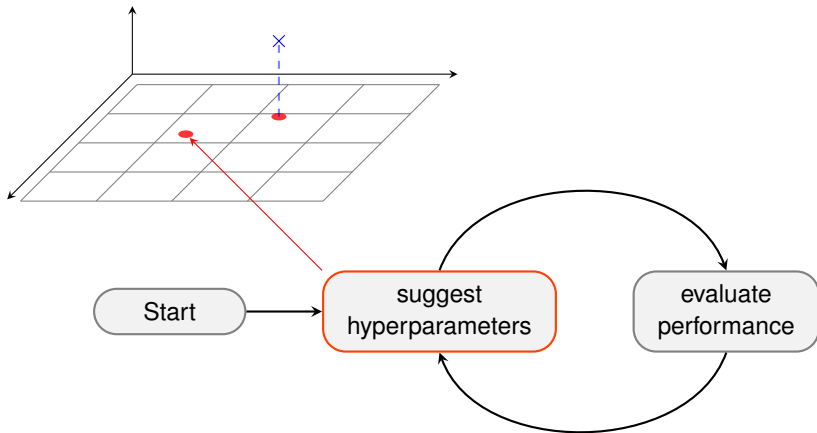
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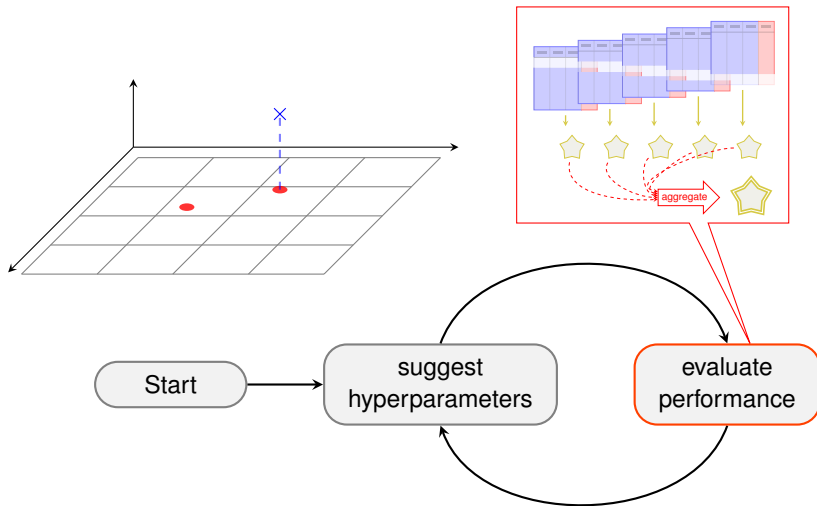
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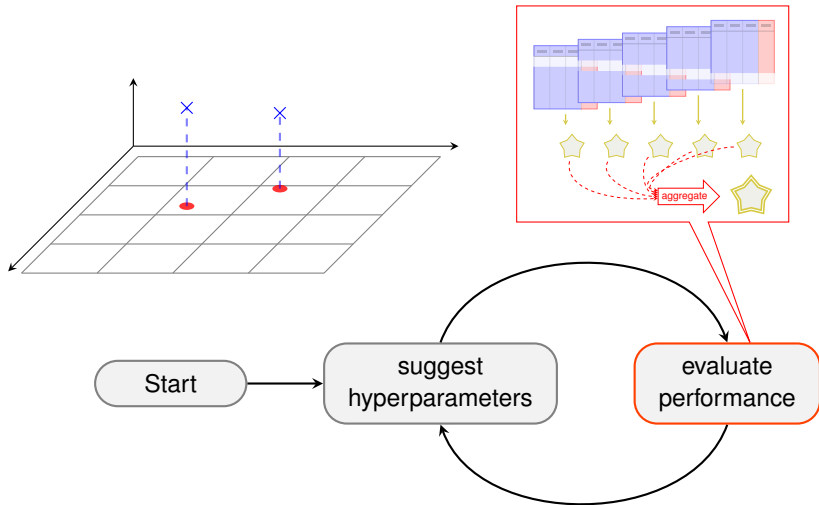
TUNING
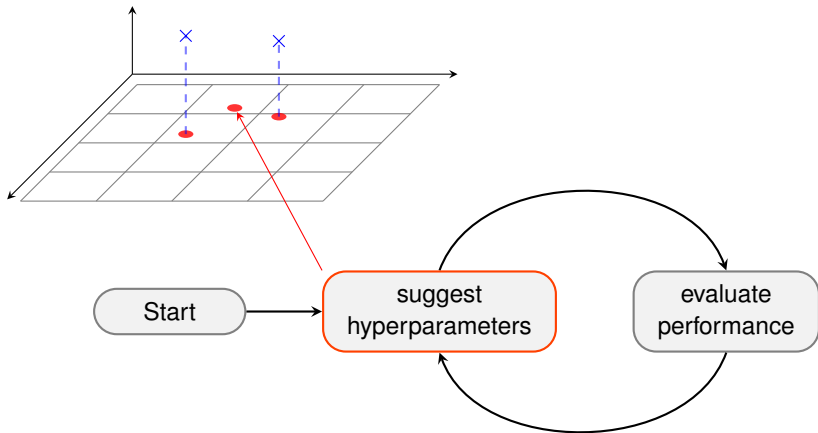
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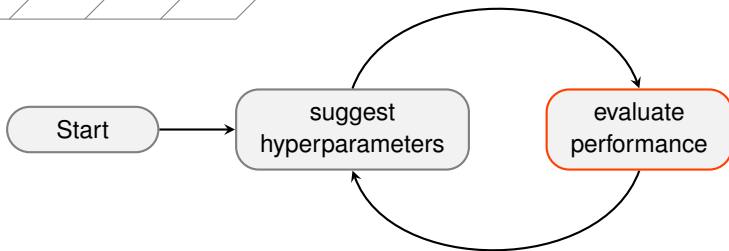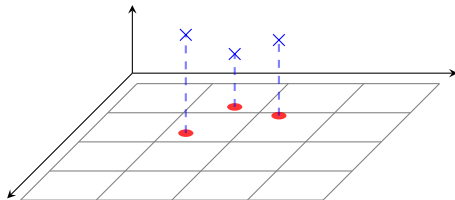
TUNING

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Batch evaluation

Start → suggest hyperparameters ↔ evaluate performance

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Start → suggest hyperparameters ⇄ evaluate performance

TUNING

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```
Learner (lrn())
Task
Resampling (rsmp())
Measure (msr())
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search space
`Tuner`

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Learner (`lrn()`)
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Measure (`msr()`)

Start → suggest hyperparameters ⇄ evaluate performance → End

search space
Tuner

Terminator (when to finish)
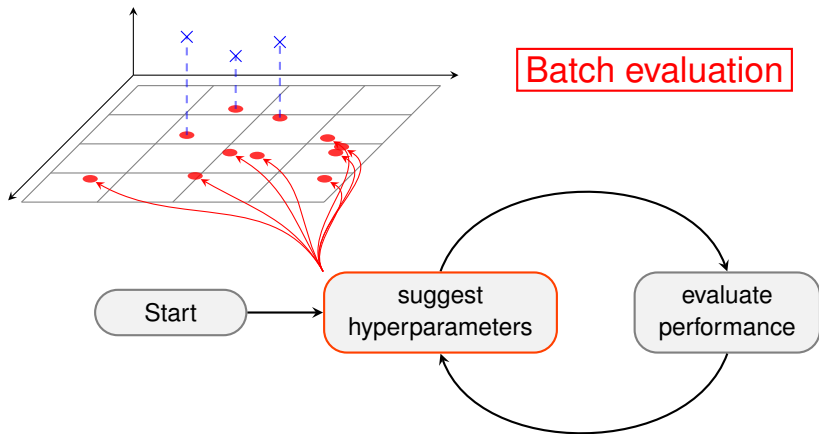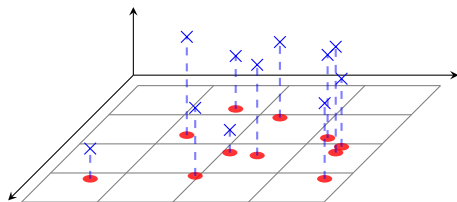
Tuning in mlr3

OBJECTS IN TUNING
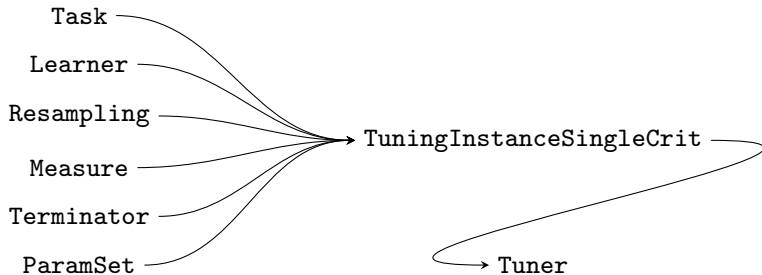
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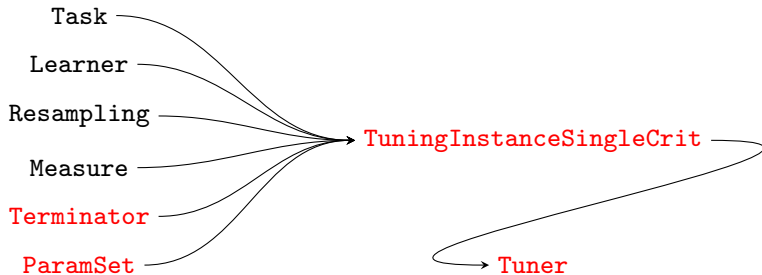
SEARCH SPACE
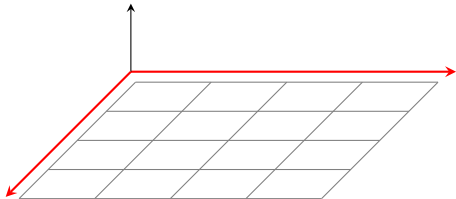
SEARCH SPACE
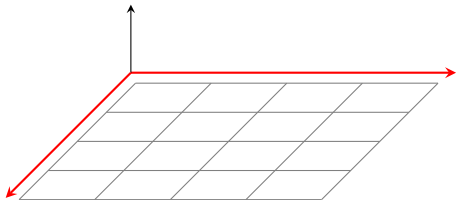

```
ParamSet$new(list(param1, param2, ...))
```

SEARCH SPACE
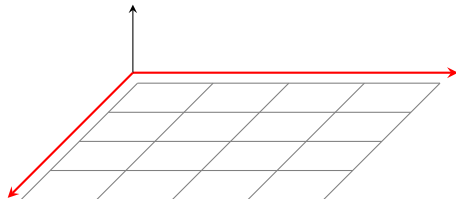

```
ParamSet$new(list(param1, param2, ...))
```

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)`

SEARCH SPACE
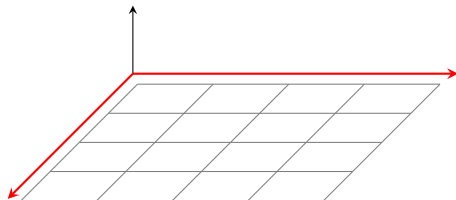

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```
library("paradox")
searchspace_knn = ParamSet$new(list(
  ParamInt$new("k", lower = 1, upper = 20)
))
```

SEARCH SPACE SHORT FORM
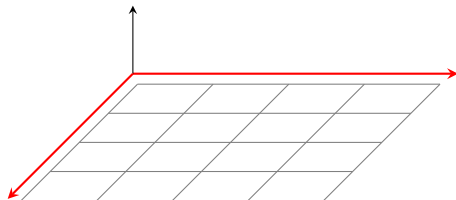

```
ps(id1 = domain1, id2 = domain2, ...)
```

Numerical parameter	`p_dbl(lower, upper)`
Integer parameter	`p_int(lower, upper)`
Discrete parameter	`p_fct(levels)`
Logical parameter	`p_lgl()`
Untyped parameter	`p_uty()`

```
library("paradox")
searchspace_knn = ps(
  "k" = p_int(lower = 1, upper = 20)
)
```

TERMINATION

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```
as.data.table(mlr_terminators)
#>                  key
#> 1:        clock_time
#> 2:            combo
#> 3:            evals
#> 4:             none
#> 5:      perf_reached
#> 6:         run_time
#> 7:       stagnation
#> 8: stagnation_batch
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```
trm("evals", n_evals = 20)
#> <TerminatorEvals>
#> * Parameters: n_evals=20
```

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```
as.data.table(mlr_tuners)
#>              key
#> 1:         cmaes
#> 2: design_points
#> 3:         gensa
#> 4:   grid_search
#> 5:        nloptr
#> 6: random_search
```

TUNING METHOD

- load Tuner with tnr(), set parameters

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- 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: -
  ```

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- load `Tuner` with `tnr()`, set parameters

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- common parameter `batch_size` for parallelization

CALLING THE TUNER
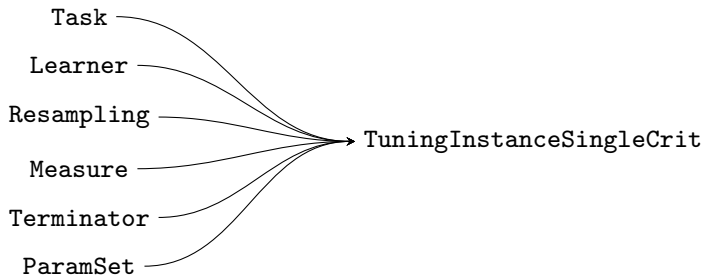
CALLING THE TUNER
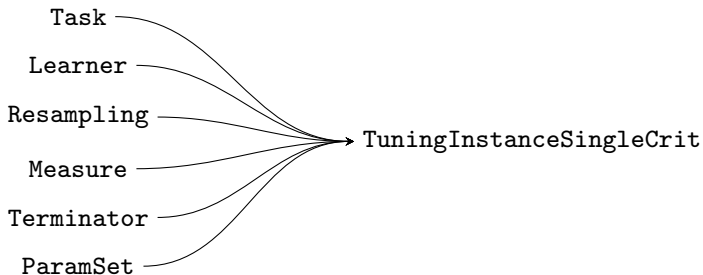
Task ⟶

Learner ⟶

Resampling ⟶   ⟶ TuningInstanceSingleCrit

Measure ⟶

Terminator ⟶

ParamSet ⟶

```
inst = TuningInstanceSingleCrit$new(task = tsk("iris"),
  learner = lrn("classif.kknn", kernel = "rectangular"),
  resampling = rsmp("holdout"), measure = msr("classif.ce"),
  terminator = trm("none"), search_space = searchspace_knn
)
```

CALLING THE TUNER

```
gsearch$optimize(inst)
#> INFO  [14:35:12.185] [bbotk] Starting to optimize 1 parameter(s) with '<OptimizerGridSea
#> INFO  [14:35:12.321] [bbotk] Evaluating 1 configuration(s)
#> INFO  [14:35:13.781] [bbotk] Result of batch 1:
#> INFO  [14:35:13.783] [bbotk]  k classif.ce                            uhash
#> INFO  [14:35:13.783] [bbotk]  10      0.04 f70af94d-3f75-4e31-8a3c-c23d36711d49
#> INFO  [14:35:13.785] [bbotk] Evaluating 1 configuration(s)
#> INFO  [14:35:13.948] [bbotk] Result of batch 2:
#> INFO  [14:35:13.951] [bbotk]  k classif.ce                            uhash
#> INFO  [14:35:13.951] [bbotk]  1       0.06 9e54838b-dea7-4d75-b1ce-57dba5d1e603
#> INFO  [14:35:13.953] [bbotk] Evaluating 1 configuration(s)
#> INFO  [14:35:14.108] [bbotk] Result of batch 3:
#> INFO  [14:35:14.111] [bbotk]  k classif.ce                            uhash
#> INFO  [14:35:14.111] [bbotk]  20      0.08 f53981d7-6028-4639-9cb1-763e98eb2f73
#> INFO  [14:35:14.120] [bbotk] Finished optimizing after 3 evaluation(s)
#> INFO  [14:35:14.122] [bbotk] Result:
#> INFO  [14:35:14.124] [bbotk]  k learner_param_vals  x_domain classif.ce
#> INFO  [14:35:14.124] [bbotk]  10         <list[2]> <list[1]>       0.04
#>     k learner_param_vals  x_domain classif.ce
#> 1: 10         <list[2]> <list[1]>       0.04
```

TUNING RESULTS

```r
inst = TuningInstanceSingleCrit$new(task = tsk("iris"),
  learner = lrn("classif.kknn", kernel = "rectangular"),
  resampling = rsmp("holdout"), measure = msr("classif.ce"),
  terminator = trm("none"), search_space = searchspace_knn)
gsearch = tnr("grid_search", resolution = 20)
gsearch$optimize(inst)

#>     k learner_param_vals  x_domain classif.ce
#> 1: 11          <list[2]>  <list[1]>       0.04

ggplot(as.data.table(inst$archive), aes(x = k, y = classif.ce)) +
  geom_line() + geom_point()
```
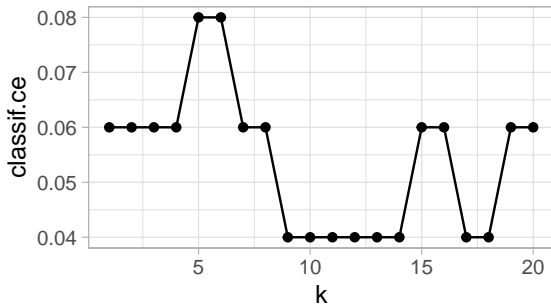
RECAP

1. Create a `Task`, `Learner`, `Resampling`, `Measure`, `Terminator` (defines when to stop), and a `ParamSet` (defines the search space):

```
task = tsk("iris")
learner = lrn("classif.kknn", kernel = "rectangular")
resampling = rsmp("holdout")
measure = msr("classif.ce")
terminator = trm("evals", n_evals = 2)
searchspace_knn = ParamSet$new(list(
  ParamInt$new("k", lower = 1, upper = 20)
))
```

2. Create the `TuningInstanceSingleCrit` object:

```
inst = TuningInstanceSingleCrit$new(task, learner,
  resampling, measure, terminator, searchspace_knn)
```

3. Create the `Tuner` (tuning method) and optimize the learner by passing over the previously created instance to the `$optimize` method:

```
gsearch = tnr("grid_search", resolution = 3)
gsearch$optimize(inst)
#>    k learner_param_vals  x_domain classif.ce
#> 1: 1          <list[2]> <list[1]>       0.04
```

Parameter Transformation

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Example:

1. optimize from $\log(1) \ldots \log(100)$

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Example:

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

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

PARAMETER TRANSFORMATION
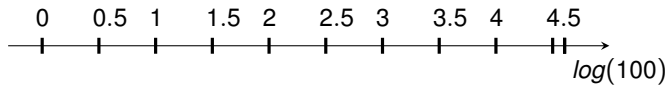
What is our transformation doing?

PARAMETER TRANSFORMATION
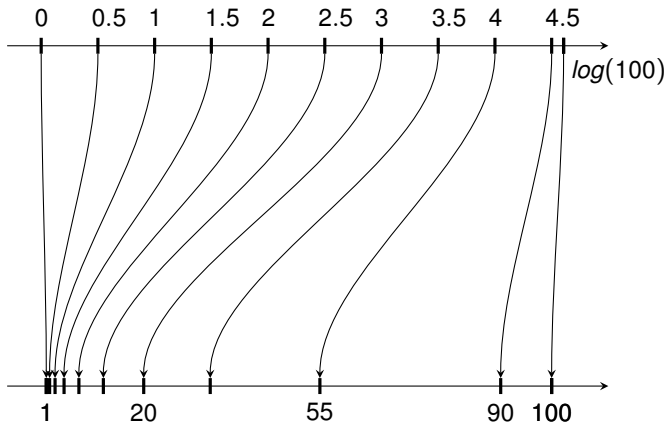
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Tuning again. . .
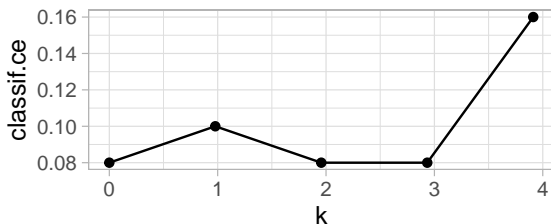
PARAMETER TRANSFORMATION

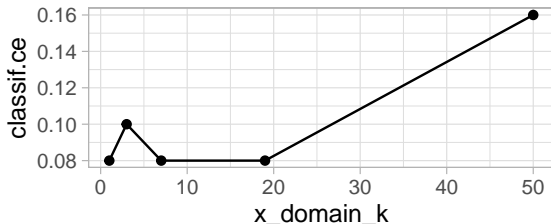Tuning again. . .

```
inst$result

#>      k learner_param_vals  x_domain classif.ce
#> 1: 2.9          <list[2]> <list[1]>       0.08

inst$result$x_domain

#> [[1]]
#> [[1]]$k
#> [1] 19
```

PARAMETER TRANSFORMATION

```r
ggplot(as.data.table(inst$archive), aes(x = k, y = classif.ce)) +
  geom_line() + geom_point()
```



```r
ggplot(as.data.table(inst$archive), aes(x = x_domain_k, y = classif.ce)) +
  geom_line() + geom_point()
```
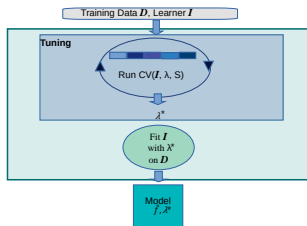
Nested Resampling

NESTED RESAMPLING

- Need to perform nested
  resampling to estimate tuned
  learner performance
$\Rightarrow$ 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
  - Predicting: Just use final
    model

NESTED RESAMPLING

```
optlrn = AutoTuner$new(
  learner = lrn("classif.kknn", kernel = "rectangular"),
  resampling = rsmp("holdout"), measure = msr("classif.ce"),
  terminator = trm("none"),
  tuner = tnr("grid_search", resolution = 10),
  search_space = searchspace_knn)
```
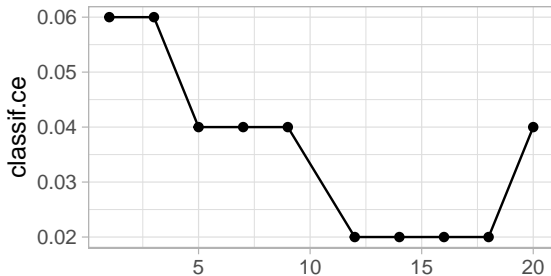
```
optlrn$train(tsk("iris"))
```

```
optlrn$model$learner

#> <LearnerClassifKKNN:classif.kknn>
#> * Model: list
#> * Parameters: kernel=rectangular, k=18
#> * Packages: kknn
#> * Predict Type: response
#> * Feature types: logical, integer, numeric, factor, ordered
#> * Properties: multiclass, twoclass
```

NESTED RESAMPLING

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

NESTED RESAMPLING

```
rr = resample(task = tsk("iris"), learner = optlrn,
  resampling = rsmp("holdout"), store_models = TRUE)
archive = as.data.table(rr$learners[[1]]$tuning_instance$archive)
ggplot(archive, aes(x = k, y = classif.ce)) +
  geom_line() + geom_point() + xlab("")
```