

Tuning Machine Learning Algorithms with mlr3

mlr3tuning

Department of Statistics – LMU Munich



Intro

TUNING

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TUNING

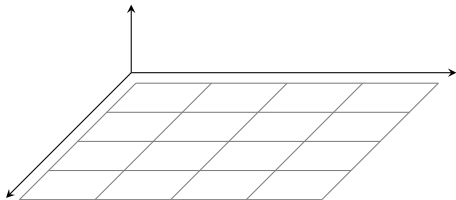
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Tuning toolbox for mlr3:

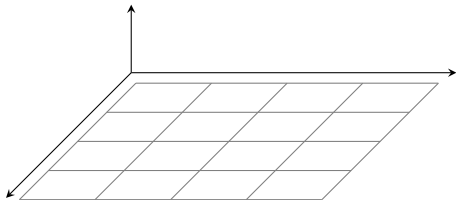
```
library("bbotk")  
library("mlr3tuning")
```

Tuning

TUNING

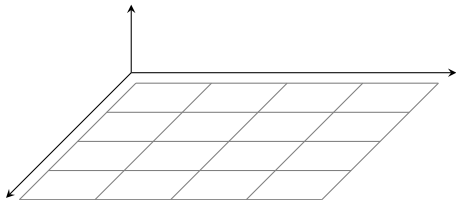


TUNING

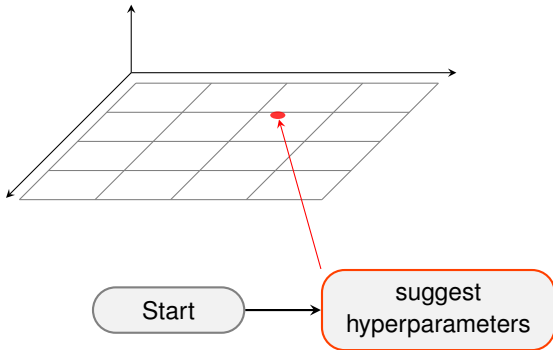


Start

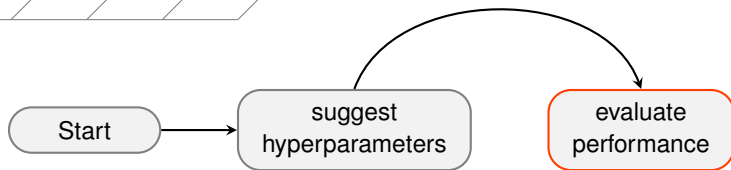
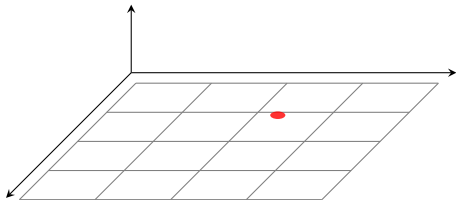
TUNING



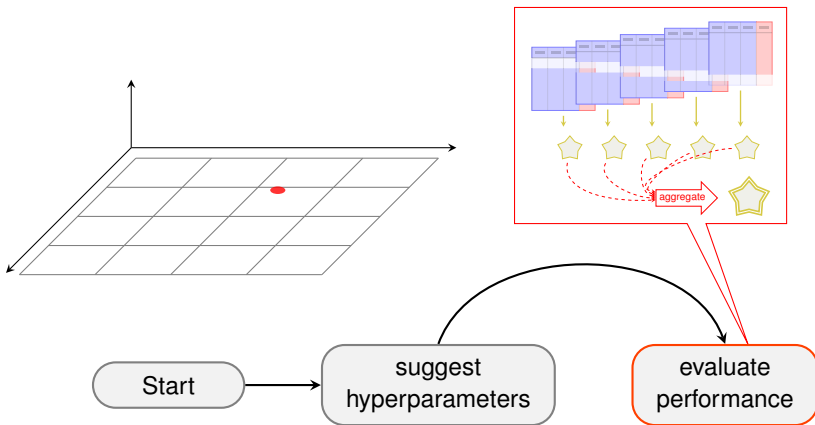
TUNING



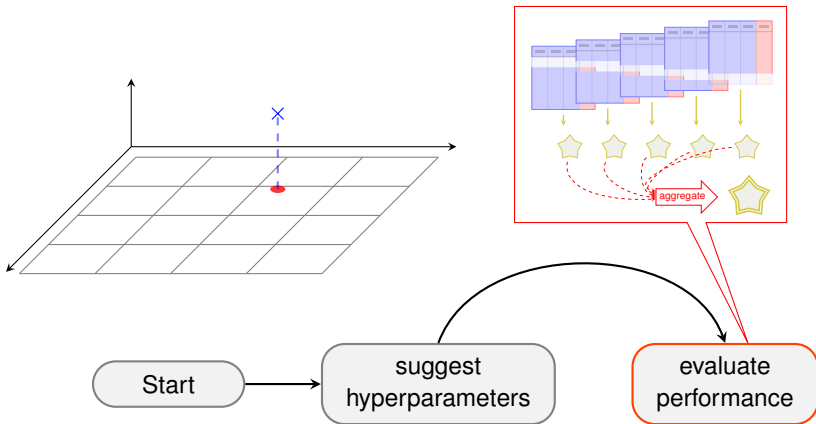
TUNING



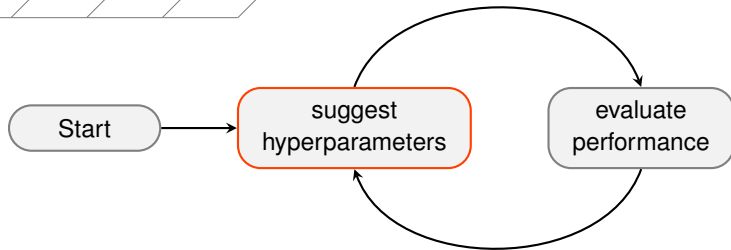
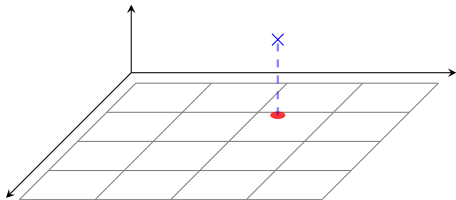
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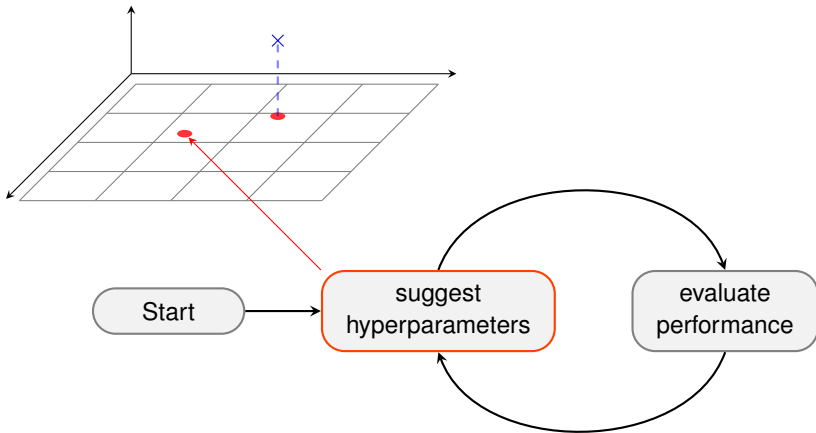
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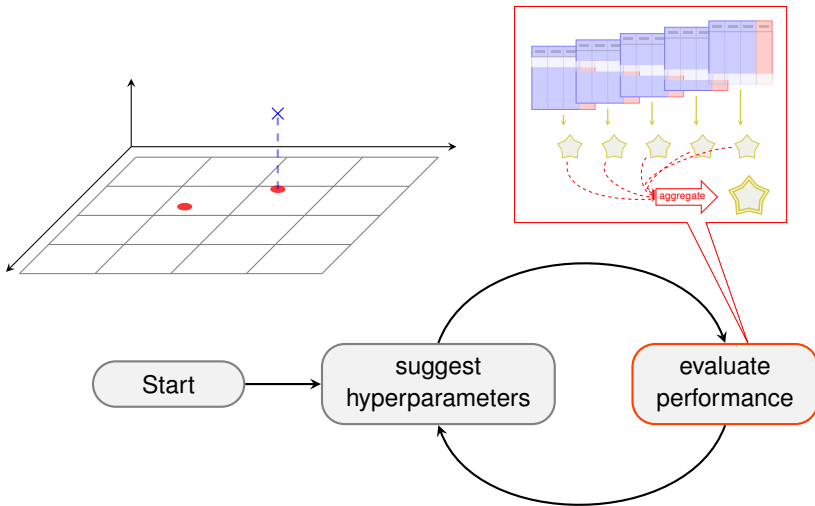
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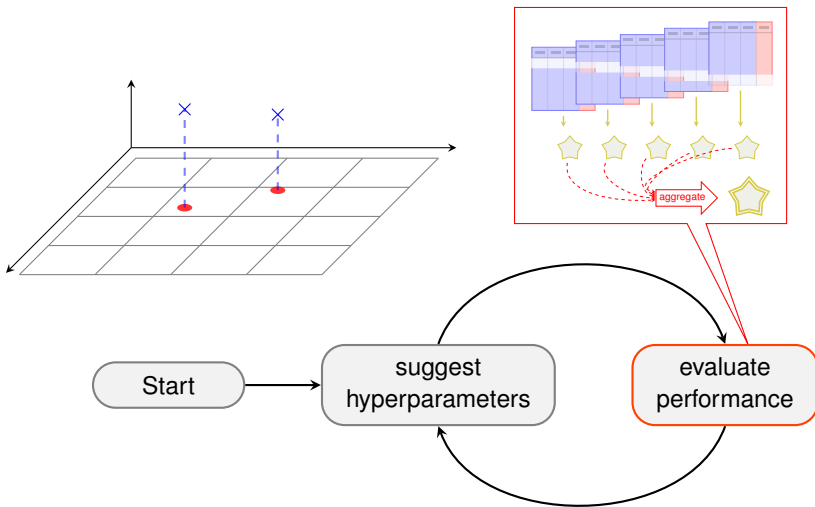
TUNING



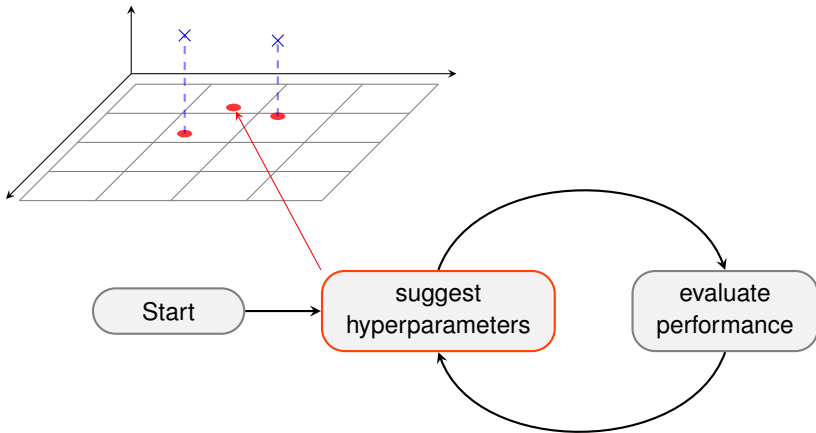
TUNING



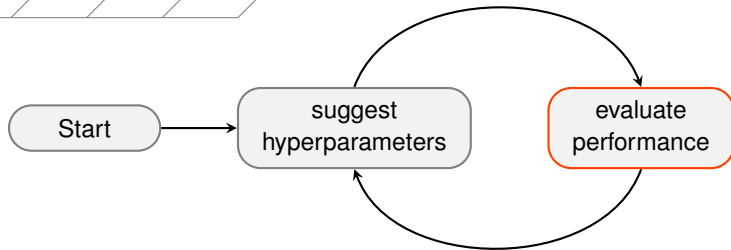
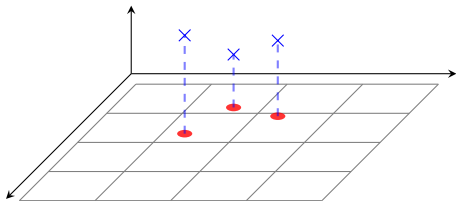
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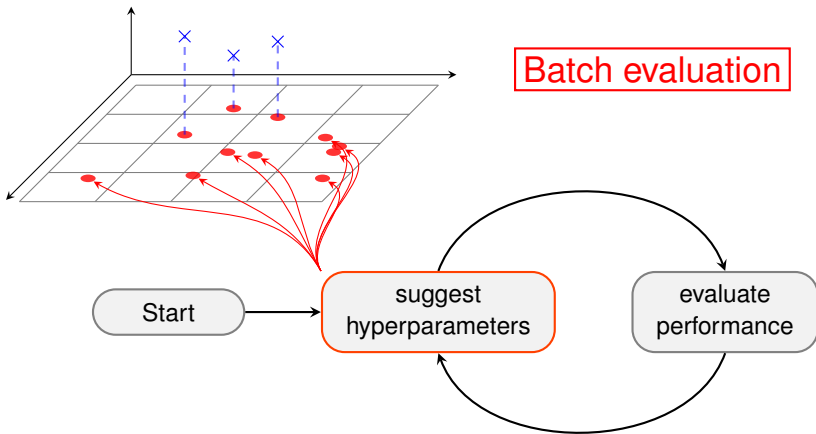
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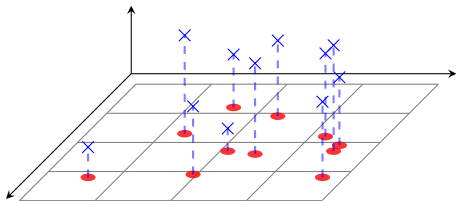
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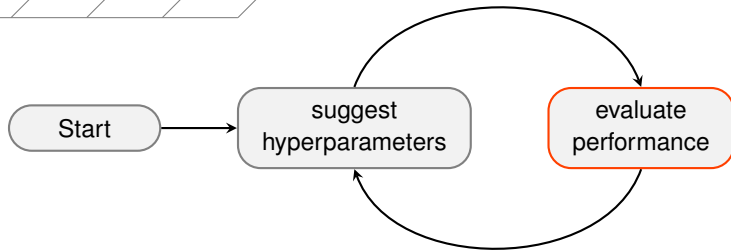
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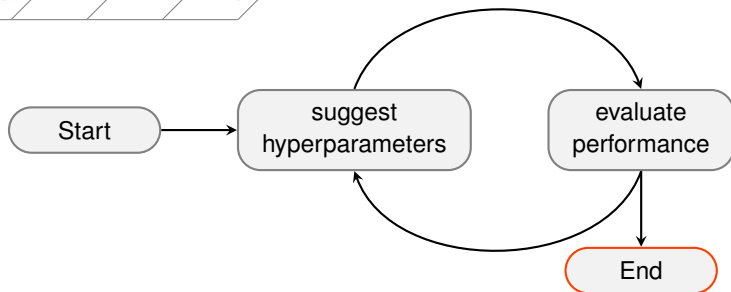
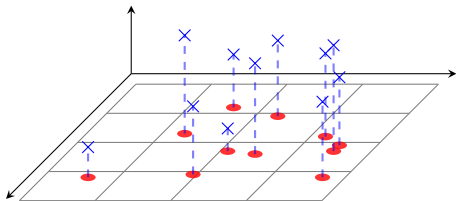
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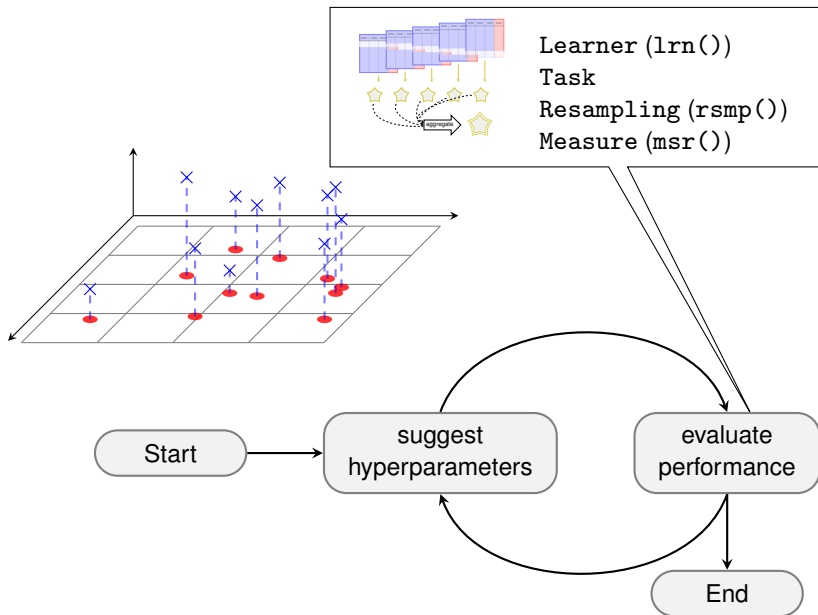
Batch evaluation



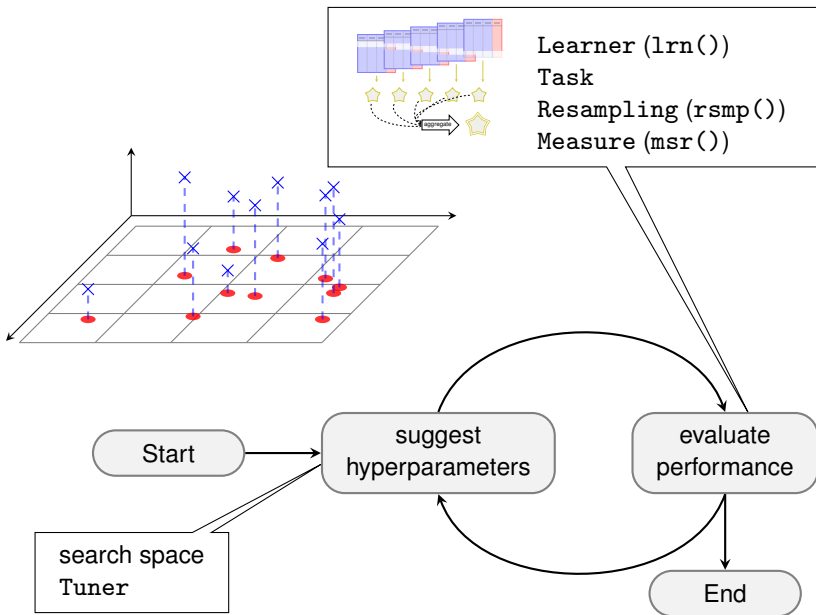
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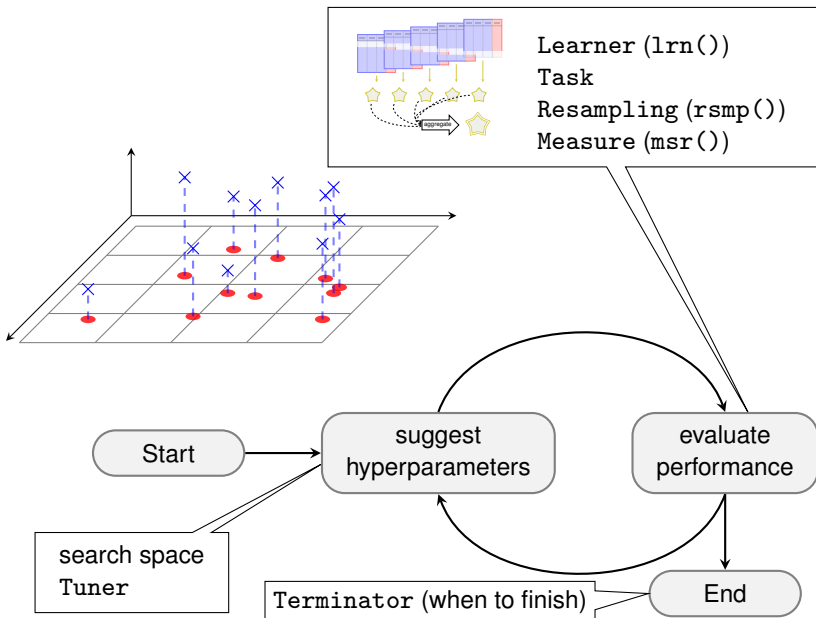
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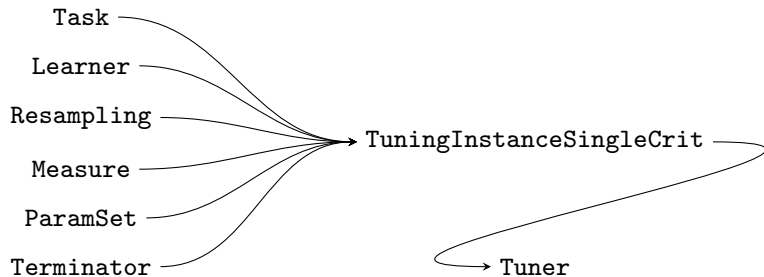


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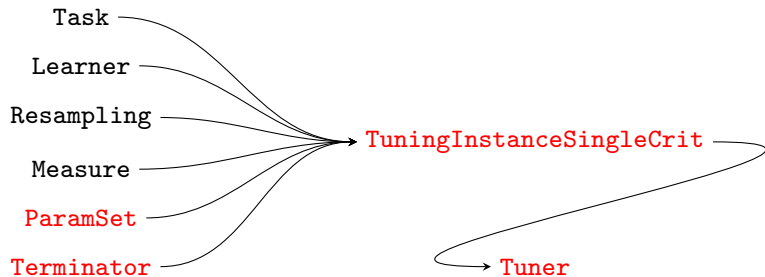


Tuning in mlr3

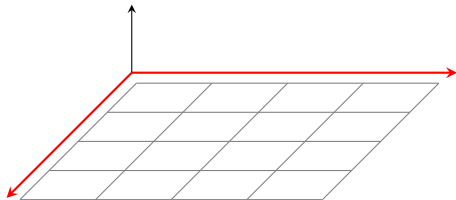
OBJECTS IN TUNING



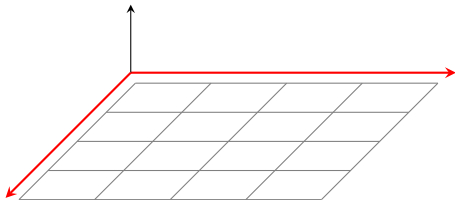
OBJECTS IN TUNING



SEARCH SPACE

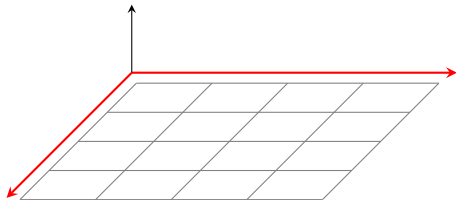


SEARCH SPACE



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


SEARCH SPACE



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```

Numerical parameter

```
ParamDbl$new(id, lower, upper)
```

Integer parameter

```
ParamInt$new(id, lower, upper)
```

Discrete parameter

```
ParamFct$new(id, levels)
```

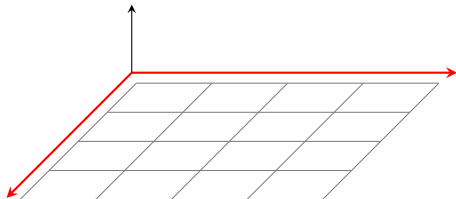
Logical parameter

```
ParamLgl$new(id)
```

Untyped parameter

```
ParamUty$new(id)
```

SEARCH SPACE



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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

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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
```

TUNING METHOD

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```
#>           key
#> 1: design_points
#> 2:         gensa
#> 3:   grid_search
#> 4:         nloptr
#> 5: random_search
```

TUNING METHOD

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

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- `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: -
```

TUNING METHOD

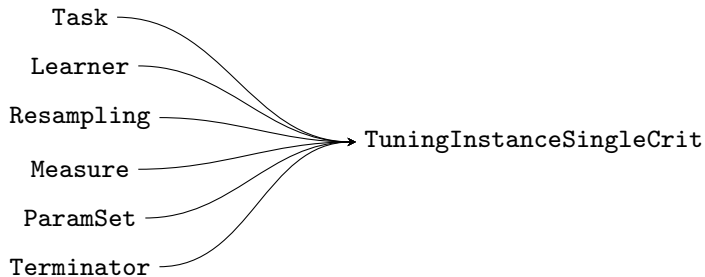
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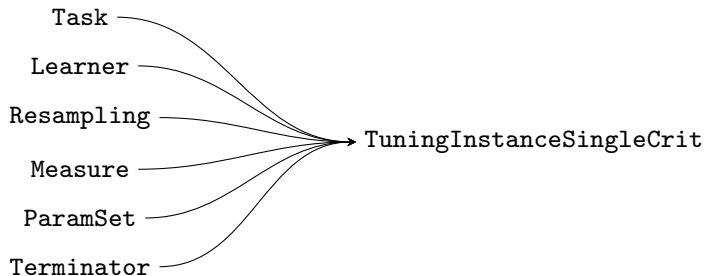
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print(gsearch)
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#> * Packages: -
```

- common parameter `batch_size` for parallelization

CALLING THE TUNER



CALLING THE TUNER



```
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 [15:39:33.347] Starting to optimize 1 parameter(s) with '<Optim
#> INFO [15:39:33.513] Evaluating 1 configuration(s)
#> INFO [15:39:37.078] Result of batch 1:
#> INFO [15:39:37.085] k classif.ce      resample_result
#> INFO [15:39:37.085] 10      0.04 <ResampleResult[18]>
#> INFO [15:39:37.089] Evaluating 1 configuration(s)
#> INFO [15:39:38.045] Result of batch 2:
#> INFO [15:39:38.054] k classif.ce      resample_result
#> INFO [15:39:38.054] 1      0.06 <ResampleResult[18]>
#> INFO [15:39:38.061] Evaluating 1 configuration(s)
#> INFO [15:39:38.262] Result of batch 3:
#> INFO [15:39:38.272] k classif.ce      resample_result
#> INFO [15:39:38.272] 20      0.08 <ResampleResult[18]>
#> INFO [15:39:38.302] Finished optimizing after 3 evaluation(s)
#> INFO [15:39:38.303] Result:
#> INFO [15:39:38.307] k learner_param_vals x_domain classif.ce
#> INFO [15:39:38.307] 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

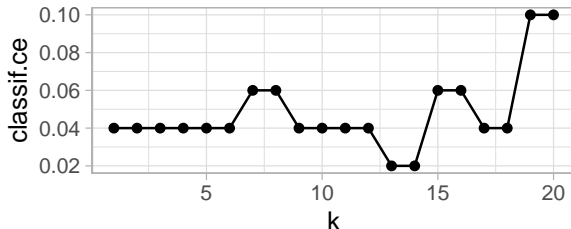
```
gsearch = tnr("grid_search", resolution = 20)

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
#> 1: 14          <list[2]> <list[1]>         0.02

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



RECAP

```
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  
#> 1: 1                <list[2]> <list[1]>      0.06
```

Parameter Transformation

PARAMETER TRANSFORMATION

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Example:

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Example:

- 1 sample from $\log(1) \dots \log(100)$ (`k_before_trafo`)

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Example:

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Example:

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- 2 transform by $\exp()$ in `trafo` function
- 3 don't forget to round (k must be integer)

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⇒ Transformations

- Part of ParamSet

Example:

- 1 sample from $\log(1) \dots \log(100)$ (`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?



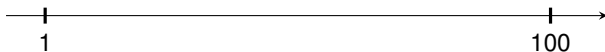
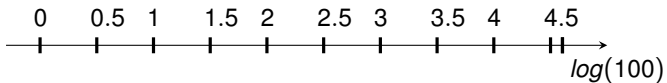
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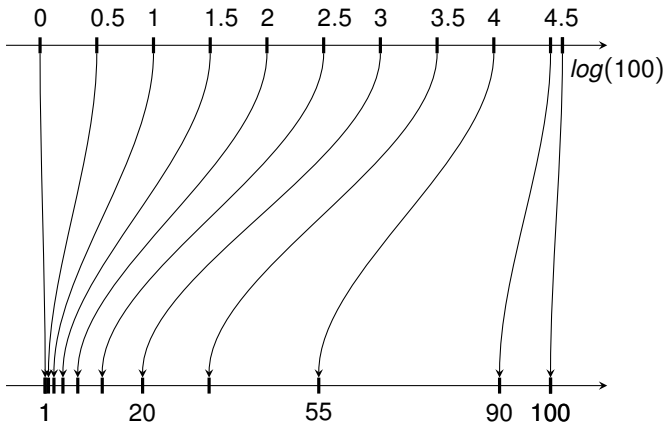
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PARAMETER TRANSFORMATION

Tuning again...

PARAMETER TRANSFORMATION

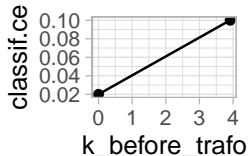
Tuning again...

```
inst$result
```

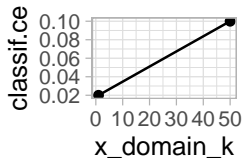
```
#>      k_before_trafo learner_param_vals  x_domain classif.ce  
#> 1:                0          <list[2]> <list[1]>        0.02
```

PARAMETER TRANSFORMATION

```
ggplot(inst$archive$data(),  
  aes(x = k_before_trafo, y = classif.ce)) + geom_line() + geom_point()
```



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



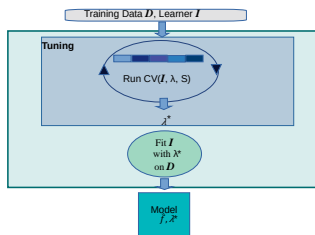
Nested Resampling

NESTED RESAMPLING

- Need to perform nested resampling to estimate tuned learner performance

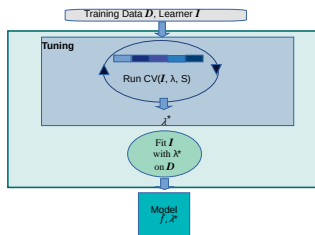
NESTED RESAMPLING

- 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
 - Predicting: Just use final model



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- Need to perform nested resampling to estimate tuned learner performance
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NESTED RESAMPLING

```
optlrn = AutoTuner$new(lrn("classif.kknn", kernel="rectangular"),  
  rsmp("holdout"), msr("classif.ce"), searchspace_knn,  
  trm("none"), tnr("grid_search", resolution = 10))
```

NESTED RESAMPLING

```
optltn = AutoTuner$new(lrn("classif.kknn", kernel="rectangular"),  
  rsmp("holdout"), msr("classif.ce"), searchspace_knn,  
  trm("none"), tnr("grid_search", resolution = 10))
```

```
optltn$train(tsk("iris"))
```

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optltn = AutoTuner$new(lrn("classif.kknn", kernel="rectangular"),  
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```

```
optltn$train(tsk("iris"))
```

```
optltn$model$learner
```

```
#> <LearnerClassifKKNN:classif.kknn>  
#> * Model: list  
#> * Parameters: kernel=rectangular, k=5  
#> * Packages: kknn  
#> * Predict Type: response  
#> * Feature types: logical, integer, numeric, factor, ordered  
#> * Properties: multiclass, twoclass
```

NESTED RESAMPLING

```
optltn = AutoTuner$new(lrn("classif.kknn", kernel="rectangular"),  
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```

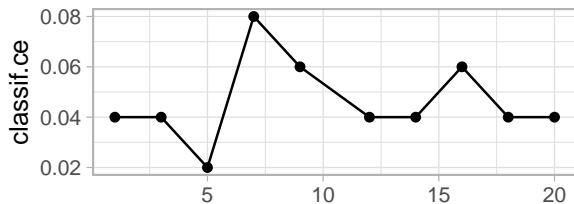
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#> * Predict Type: response  
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```

```
ggplot(optltn$model$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
```

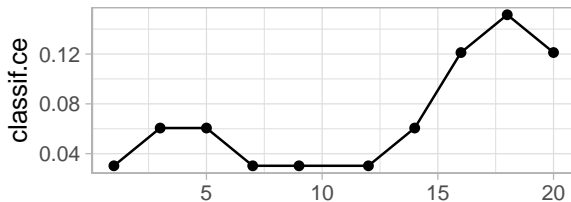
```
#> * Errors: 0 in 0 iterations
```

NESTED RESAMPLING

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

NESTED RESAMPLING

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



NESTED RESAMPLING

Aggregate performances of outer folds

```
result$aggregate()  
#> classif.ce  
#>      0.06
```

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  
#> 1: 7      <list[2]> <list[1]>          0.03
```

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()`