

Tuning Machine Learning Algorithms with mlr3

mlr3tuning

Department of Statistics – LMU Munich

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Intro

TUNING

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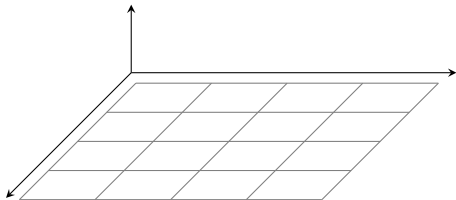
⇒ We do *black box optimization* (“Try stuff and see what works”)

Tuning toolbox for `mlr3`:

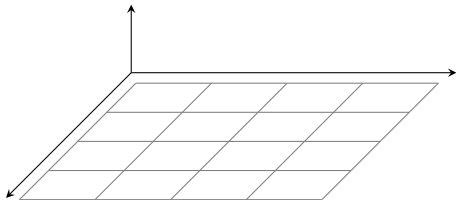
```
library("mlr3tuning")
```

Tuning

TUNING

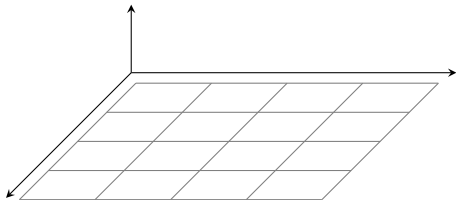


TUNING

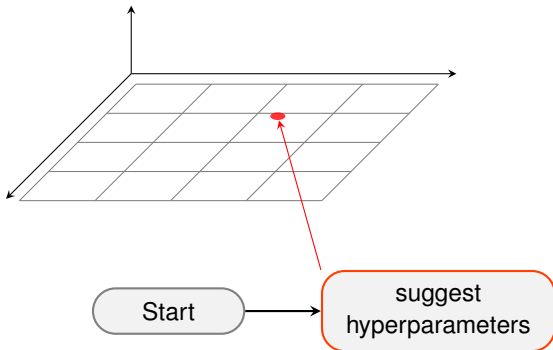


Start

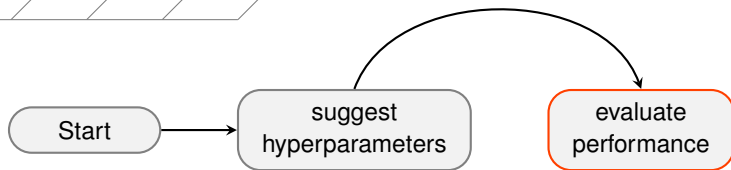
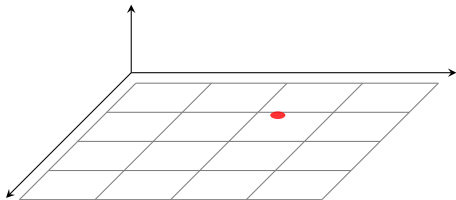
TUNING



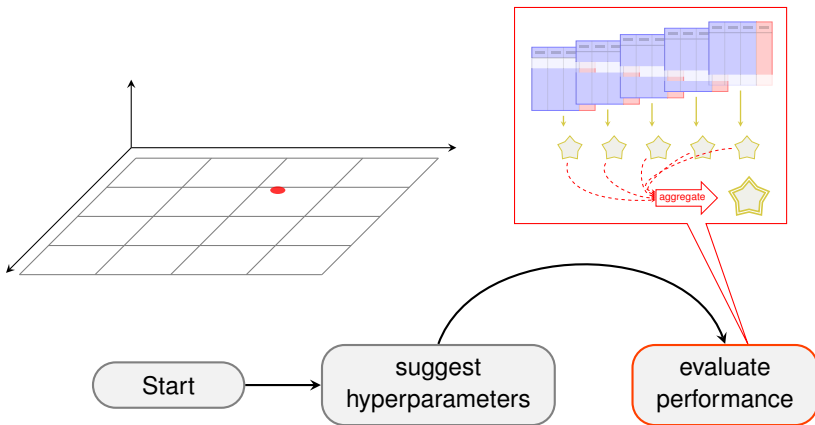
TUNING



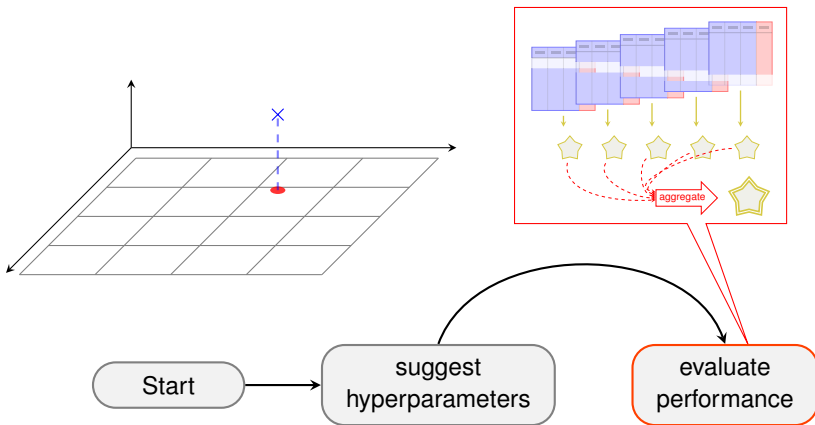
TUNING



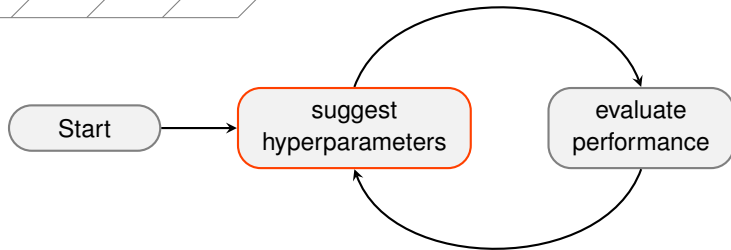
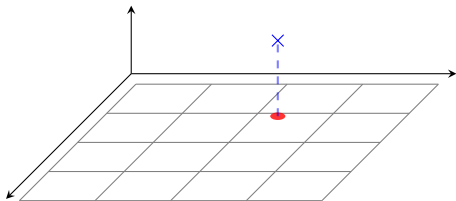
TUNING



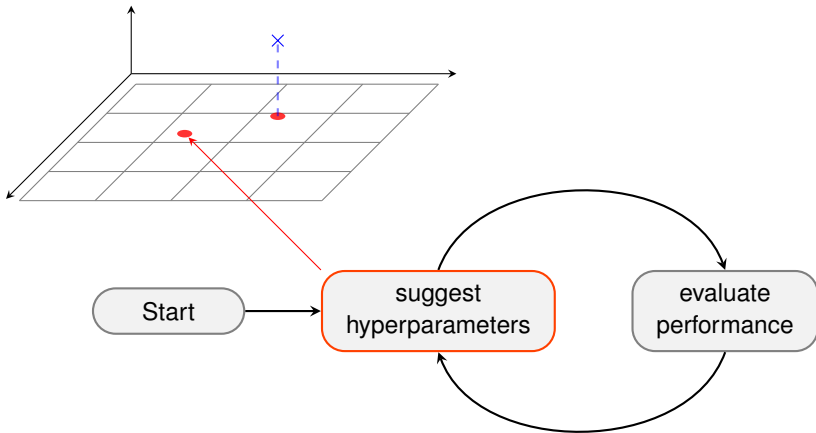
TUNING



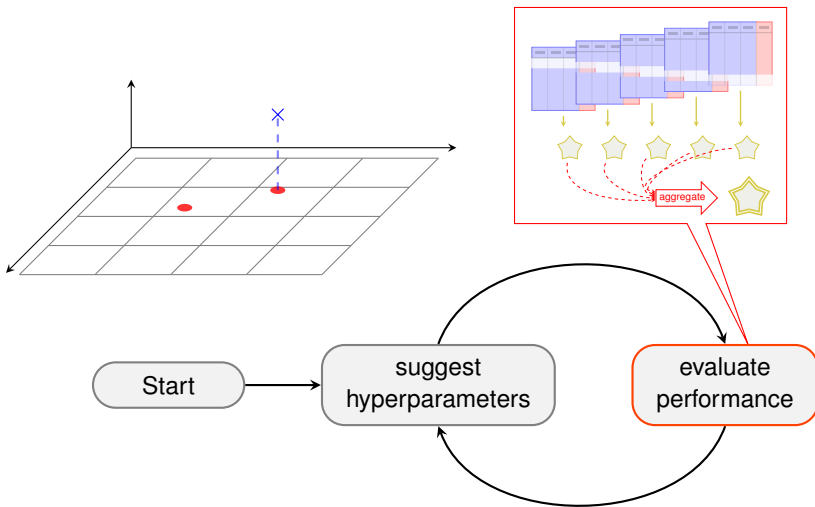
TUNING



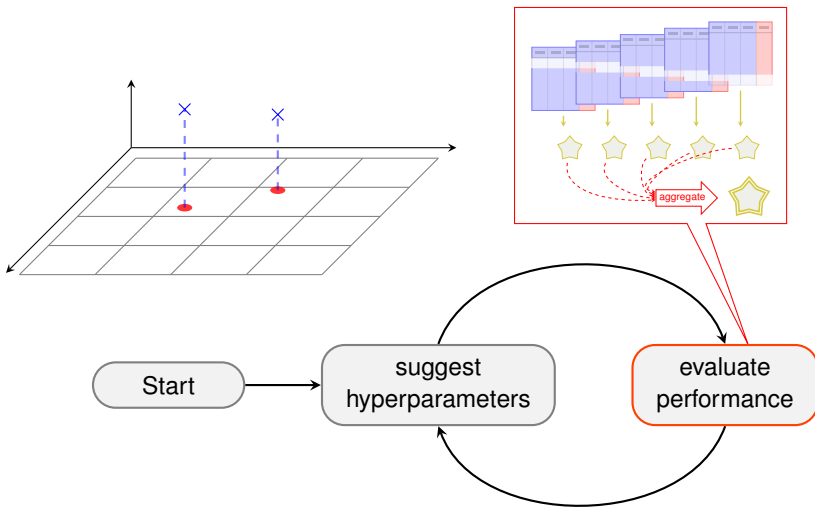
TUNING



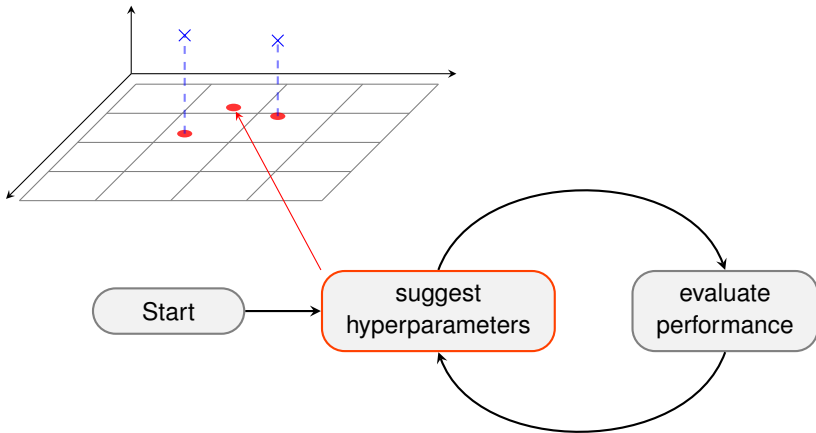
TUNING



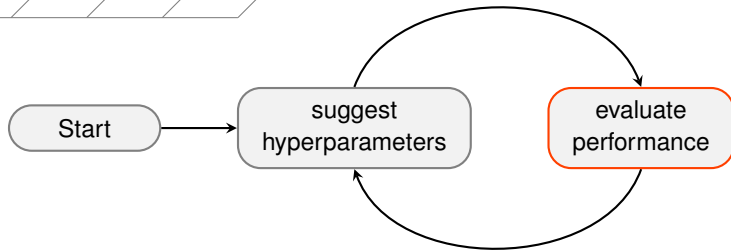
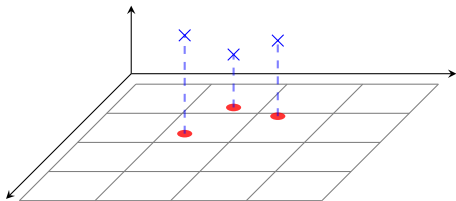
TUNING



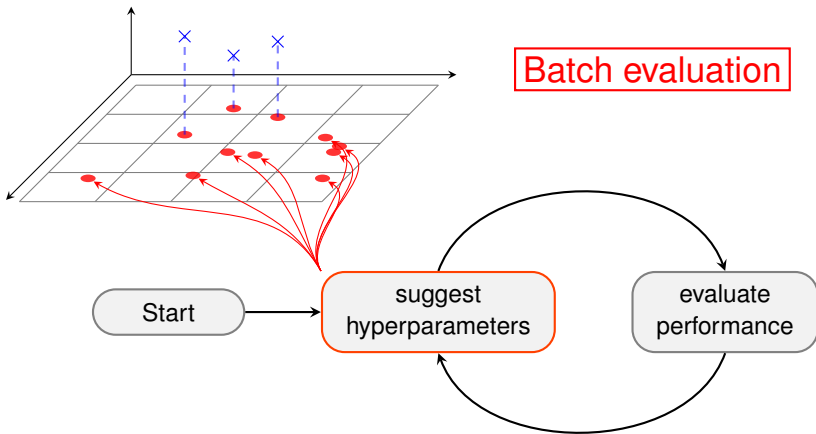
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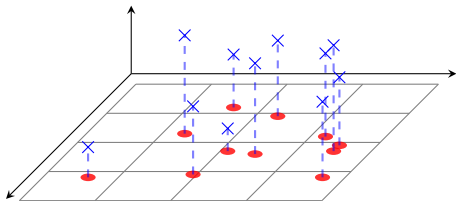
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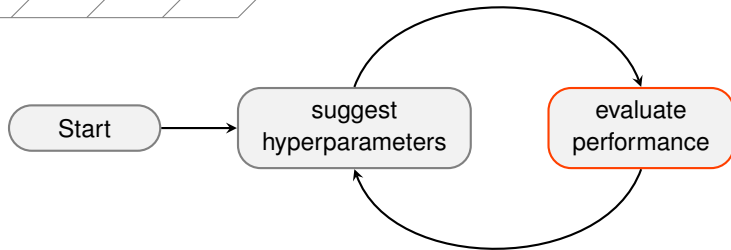
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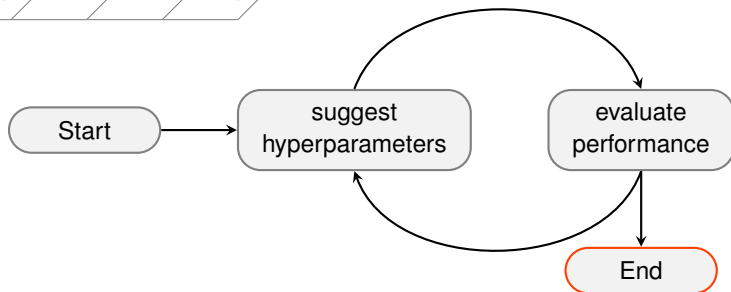
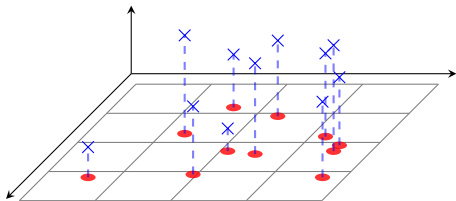
TUNING



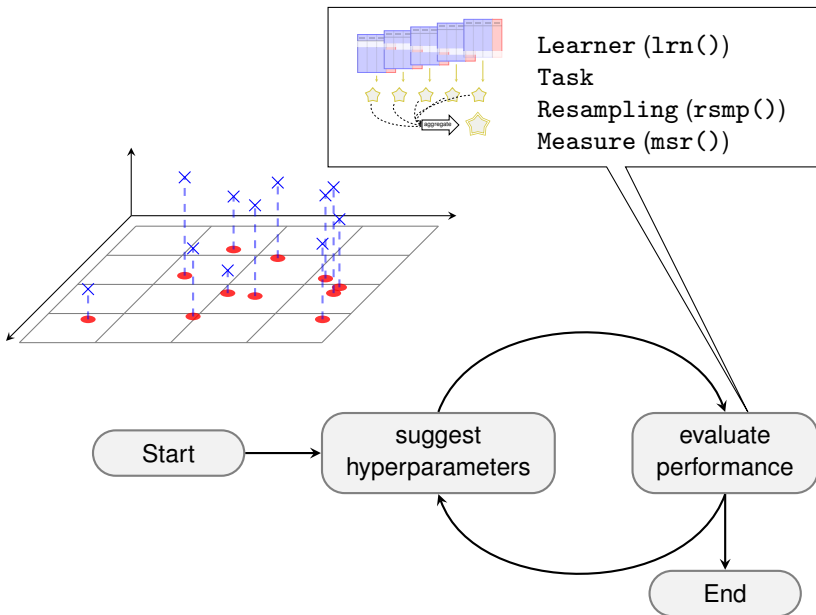
Batch evaluation



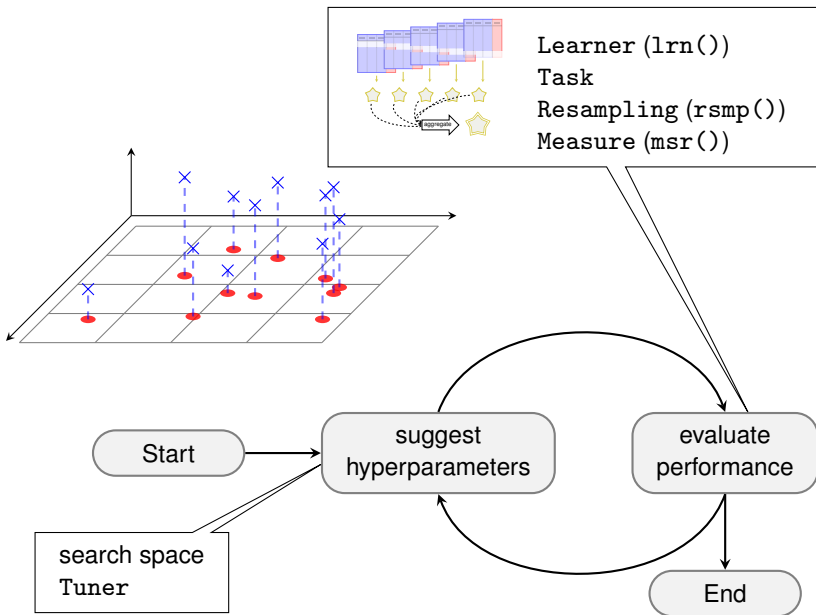
TUNING



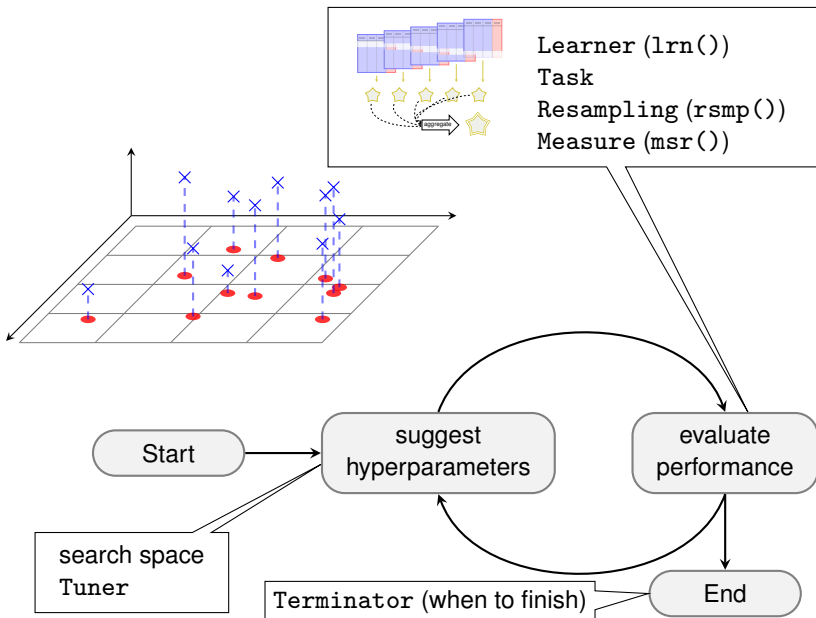
TUNING



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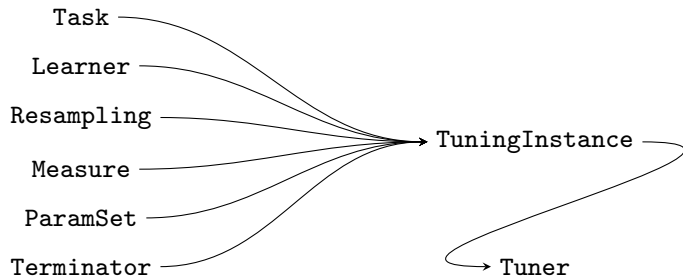


TUNING

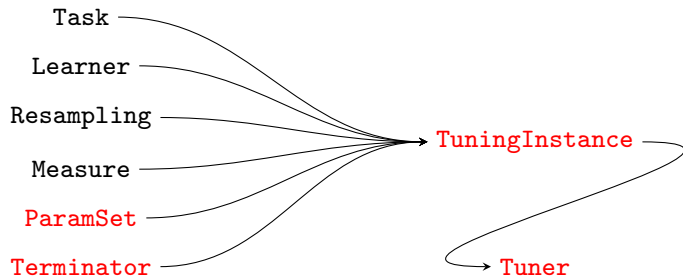


Tuning in mlr3

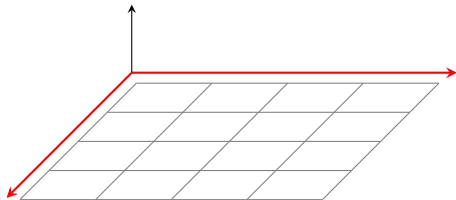
OBJECTS IN TUNING



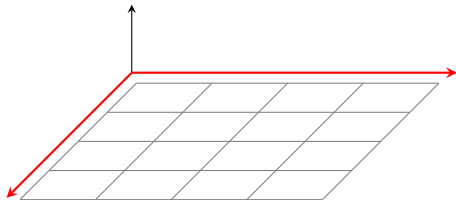
OBJECTS IN TUNING



SEARCH SPACE

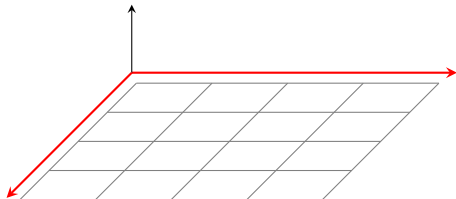


SEARCH SPACE



```
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)
```

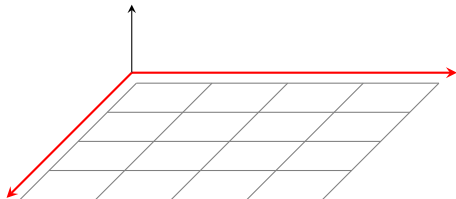
Logical parameter

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

Untyped parameter

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

SEARCH SPACE



```
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```

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: model_time
#> 5:      none
#> 6: perf_reached
#> 7:  stagnation
```

TERMINATION

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#> 4: model_time
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#> 7:  stagnation
```

- `term("evals", n_evals = 20)`

```
#> <TerminatorEvals>
#> * Parameters: n_evals=20
```

TUNING METHOD

- need to choose a *tuning method*

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- `as.data.table(mlr_tuners)`

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

TUNING METHOD

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

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

```
print(gsearch)
```

```
#> <TunerGridSearch>
```

```
#> * Parameters: resolution=20, batch_size=1
```

```
#> * Packages: -
```

```
#> * Properties: dependencies
```

TUNING METHOD

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

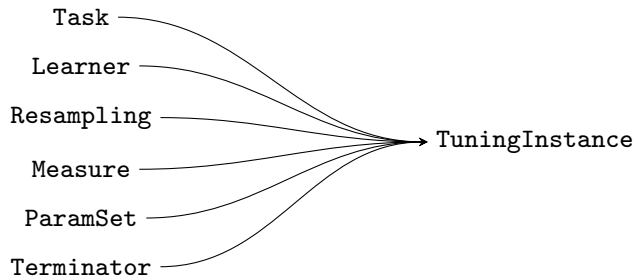
- `gsearch = tnr("grid_search", resolution = 20)`

```
print(gsearch)

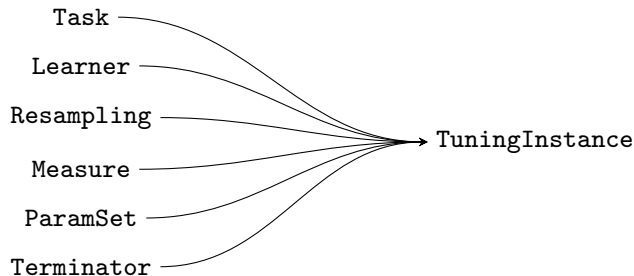
#> <TunerGridSearch>
#> * Parameters: resolution=20, batch_size=1
#> * Packages: -
#> * Properties: dependencies
```

- common parameter `batch_size` for parallelization

CALLING THE TUNER



CALLING THE TUNER



```
inst = TuningInstance$new(  
  tsk("iris"), lrn("classif.kknn", kernel="rectangular"),  
  rsmp("cv"), msr("classif.ce"),  
  searchspace_knn, term("none")  
)
```


CALLING THE TUNER

```
gsearch$tune(inst)
```

CALLING THE TUNER

```
gsearch$tune(inst)
```

```
inst$result
```

```
#> $tune_x
```

```
#> $tune_x$k
```

```
#> [1] 13
```

```
#>
```

```
#>
```

```
#> $params
```

```
#> $params$kernel
```

```
#> [1] "rectangular"
```

```
#>
```

```
#> $params$k
```

```
#> [1] 13
```

```
#>
```

```
#>
```

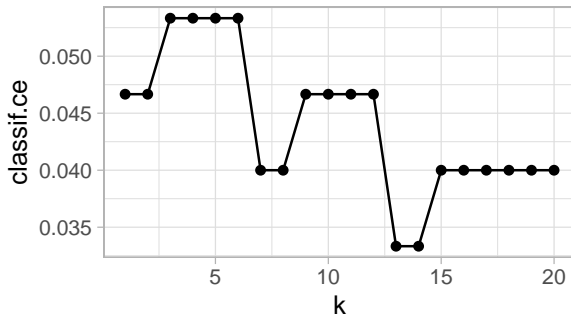
```
#> $perf
```

```
#> classif.ce
```

```
#>          0.033
```

TUNING RESULTS

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



RECAP

```
inst = TuningInstance$new(  
  tsk("iris"), lrn("classif.kknn", kernel="rectangular"),  
  rsmp("cv"), msr("classif.ce"),  
  searchspace_knn, term("evals", n_evals = 20)  
)  
  
gsearch = tnr("grid_search", resolution = 20)  
  
gsearch$tune(inst)
```

Parameter Transformation

PARAMETER TRANSFORMATION

- Sometimes we do not want to sample evenly from a range

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Example:

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Example:

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

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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

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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)

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- $k = 1$ vs. $k = 2$ probably more interesting than $k = 101$ vs. $k = 102$

⇒ 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(100))  
)  
)  
searchspace_knn_trafo$trafo = function(x, param_set) {  
  return(list(k = round(exp(x$k_before_trafo))))  
}
```

PARAMETER TRANSFORMATION

What is our transformation doing?



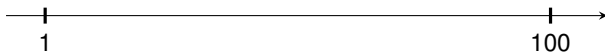
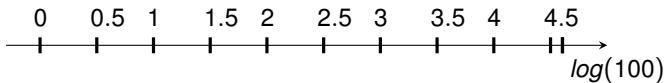
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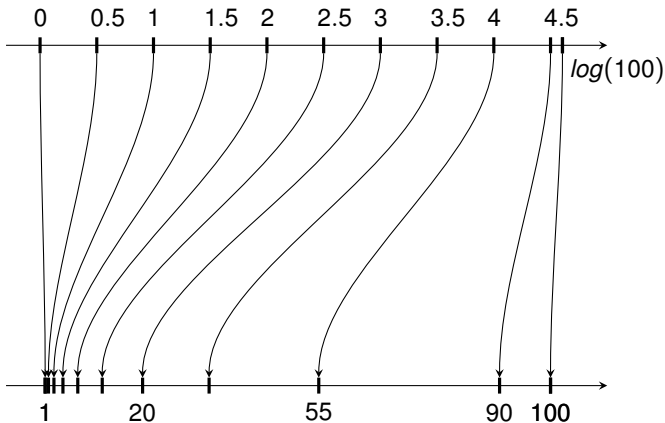
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PARAMETER TRANSFORMATION

Tuning again...

PARAMETER TRANSFORMATION

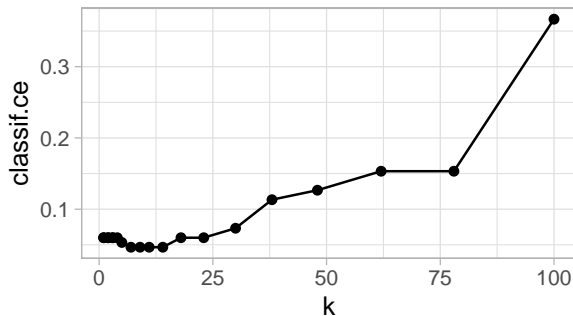
Tuning again...

```
inst$result

#> $tune_x
#> $tune_x$k_before_trafo
#> [1] 2.7
#>
#>
#> $params
#> $params$kernel
#> [1] "rectangular"
#>
#> $params$k
#> [1] 14
#>
#>
#> $perf
#> classif.ce
#>          0.047
```

PARAMETER TRANSFORMATION

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



Nested Resampling

NESTED RESAMPLING

- Need to perform nested resampling to estimate tuned learner performance

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- 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

NESTED RESAMPLING

- Need to perform nested resampling to estimate tuned learner performance

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

- Training:

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- Predicting: Just use final model

- **AutoTuner**

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

- **AutoTuner**

```
optlrn = AutoTuner$new(lrn("classif.kknn", kernel="rectangular"),  
  rsmp("cv"), msr("classif.ce"), searchspace_knn,  
  term("none"), tnr("grid_search", resolution = 20))
```

NESTED RESAMPLING

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

NESTED RESAMPLING

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

```
optlrn$model$learner
```

```
#> <LearnerClassifKKNN:classifier.kknn>
```

```
#> * Model: data.table
```

```
#> * Parameters: kernel=rectangular, k=18
```

```
#> * Packages: withr, kknn
```

```
#> * Predict Type: response
```

```
#> * Feature types: logical, integer, numeric, factor, ordered
```

```
#> * Properties: multiclass, twoclass
```

NESTED RESAMPLING

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

```
optlrn$model$learner
```

```
#> <LearnerClassifKKNN:classif.kknn>
```

```
#> * Model: data.table
```

```
#> * Parameters: kernel=rectangular, k=18
```

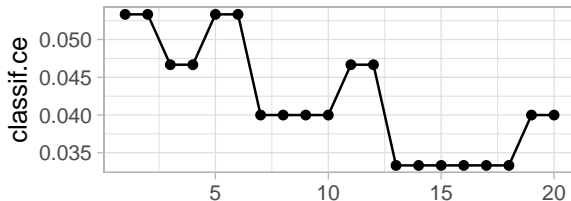
```
#> * Packages: withr, kknn
```

```
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```

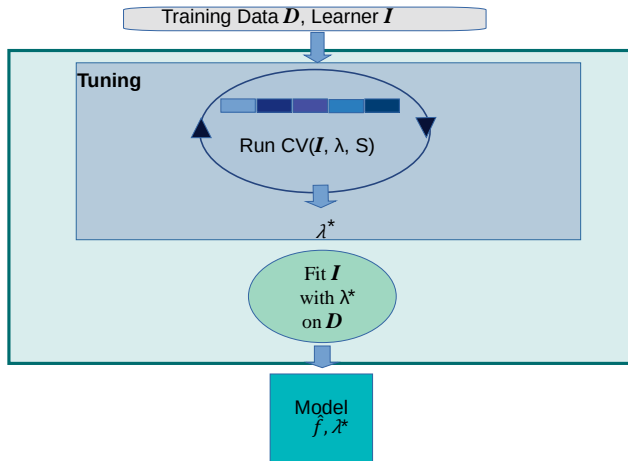
```
#> * Feature types: logical, integer, numeric, factor, ordered
```

```
#> * Properties: multiclass, twoclass
```

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



NESTED RESAMPLING



NESTED RESAMPLING

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

```
#> <ResampleResult> of 10 iterations
```

```
#> * Task: iris
```

```
#> * Learner: classif.kknn.tuned
```

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

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

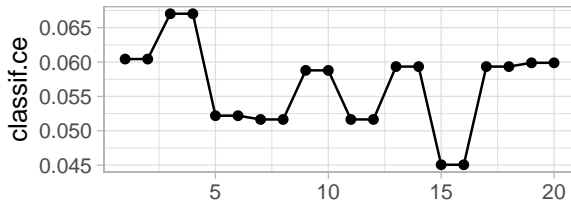
NESTED RESAMPLING

```
result = resample(tsk("iris"), optlrn, rsmp("cv"),  
  store_model = TRUE)
```


NESTED RESAMPLING

```
result = resample(tsk("iris"), optlrn, rsmp("cv"),  
  store_model = TRUE)
```

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



Outro

TUNING WITH MLR3TUNING

Tuning a Learner

- 1 Construct a `TuningInstance`
 - `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$tune()`

Nested Resampling

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