

Tuning Machine Learning Algorithms with mlr3

mlr3tuning

Department of Statistics – LMU Munich

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Intro

TUNING

- Behaviour of most methods depends on *hyperparameters*

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- We want to choose them so our algorithm performs well

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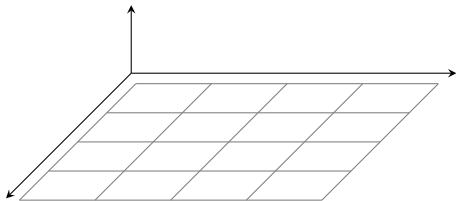
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- Good hyperparameters are data-dependent

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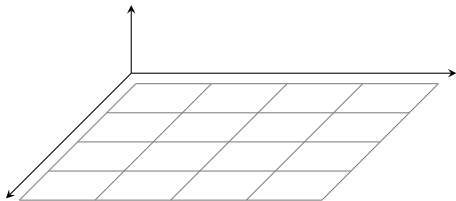
- Behaviour of most methods depends on *hyperparameters*
 - We want to choose them so our algorithm performs well
 - Good hyperparameters are data-dependent
- ⇒ We do *black box optimization* (“Try stuff and see what works”)

Tuning

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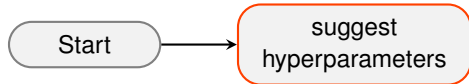
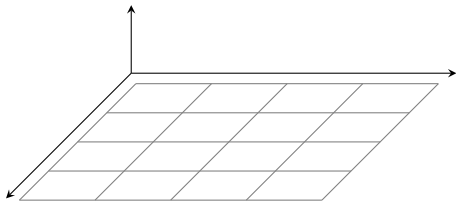


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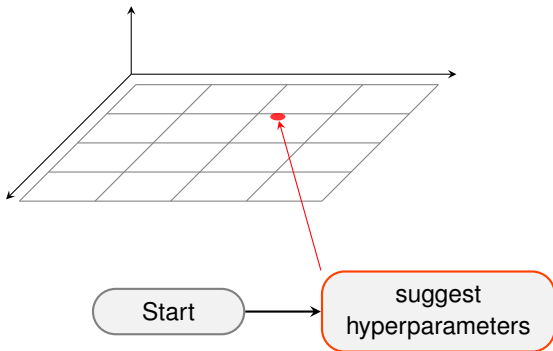


Start

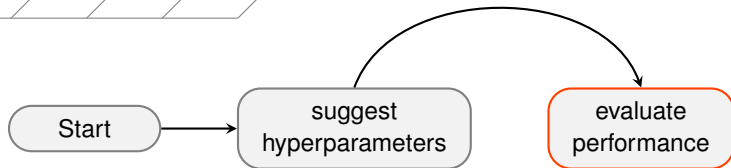
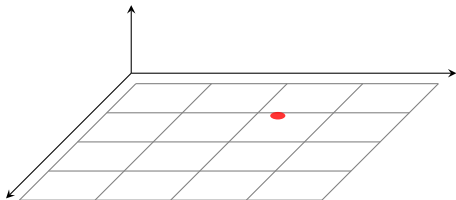
TUNING



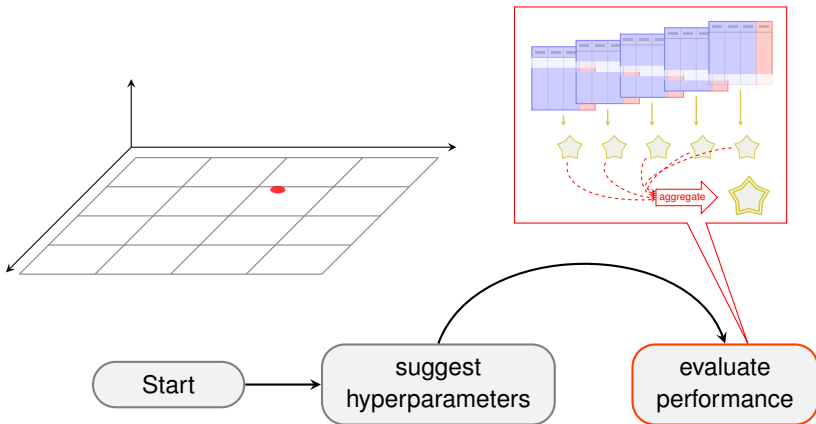
TUNING



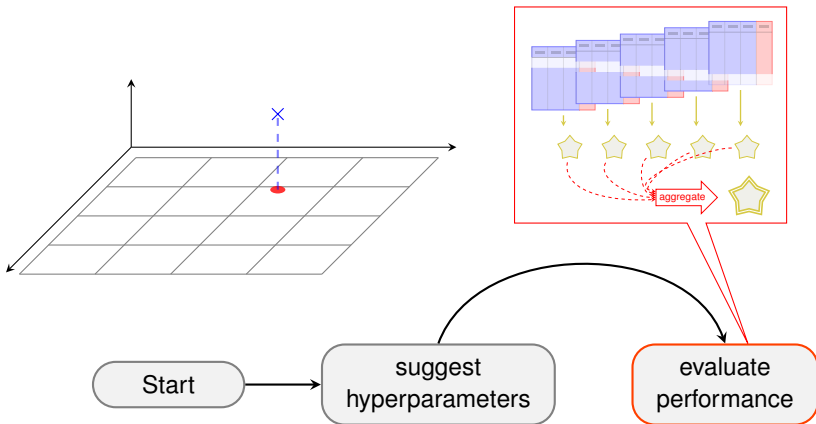
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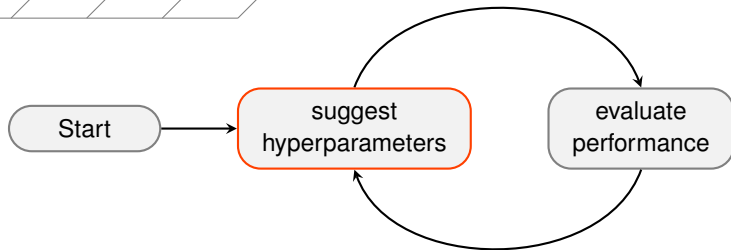
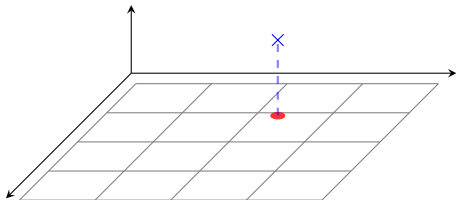
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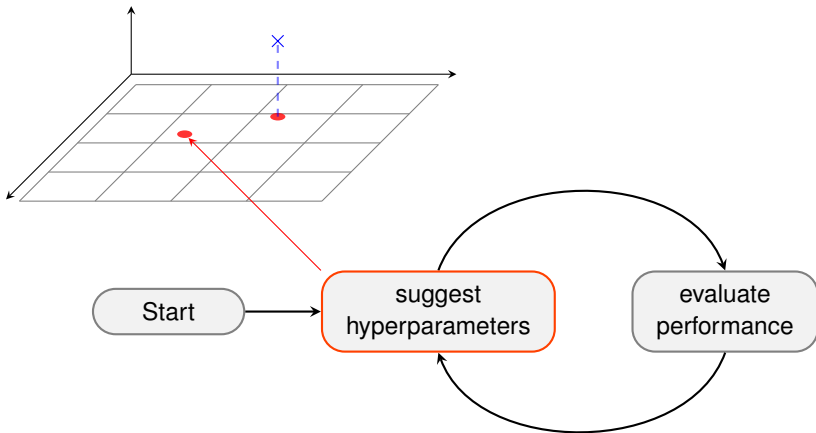
TUNING



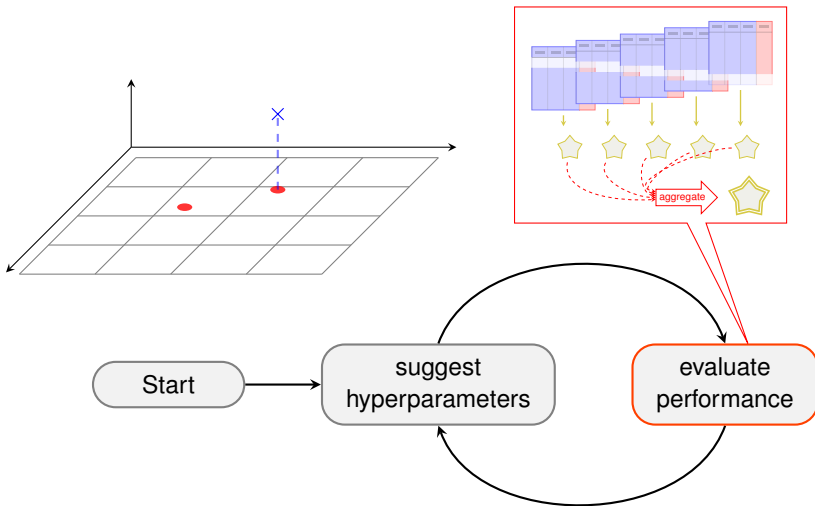
TUNING



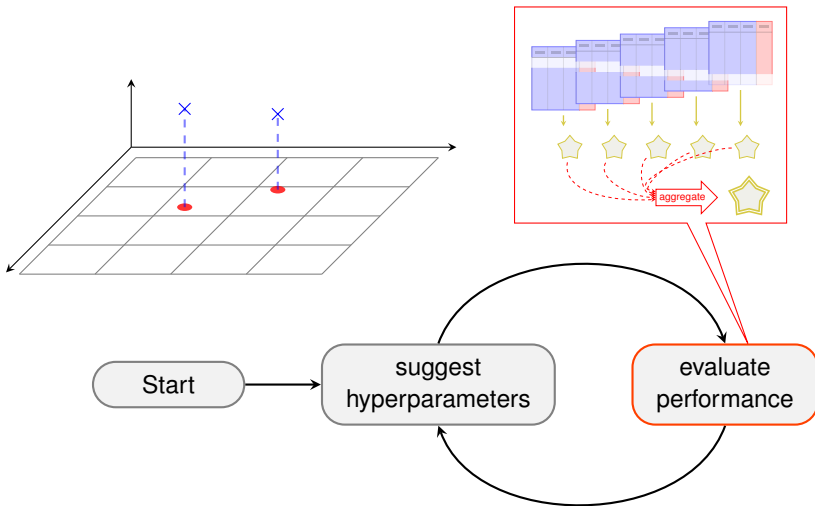
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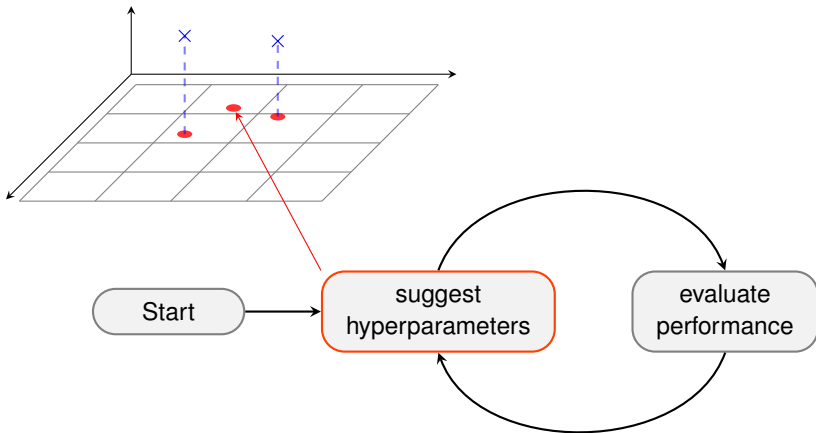
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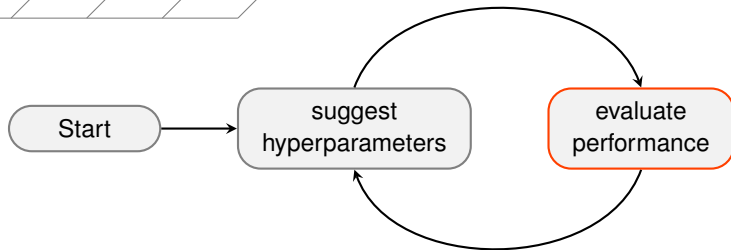
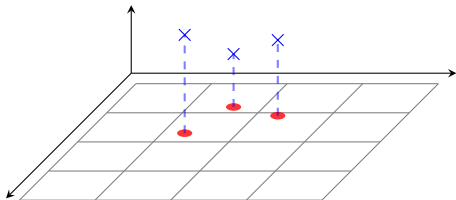
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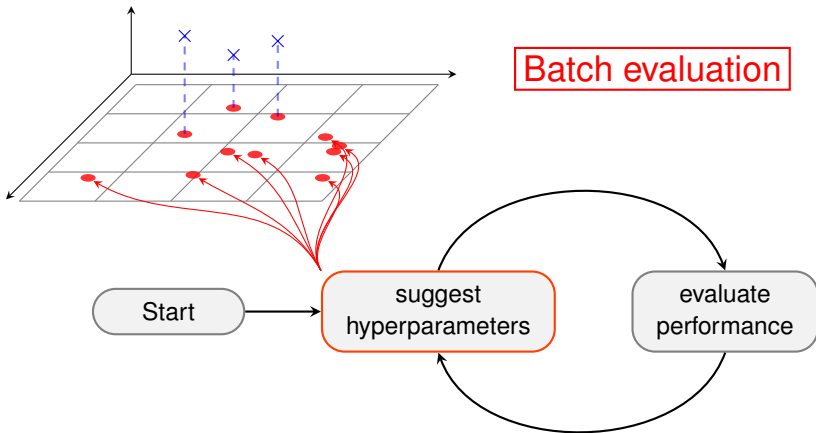
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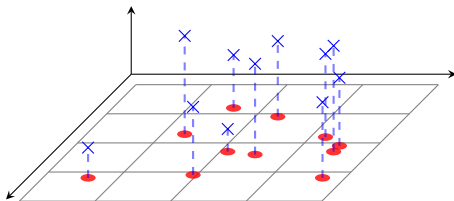
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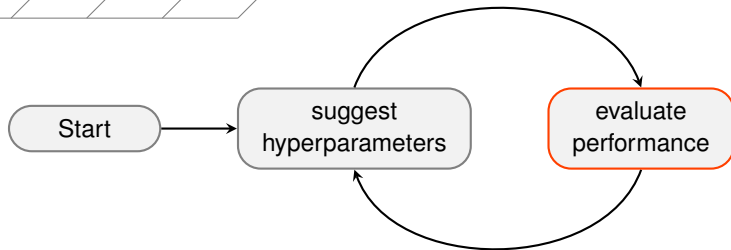
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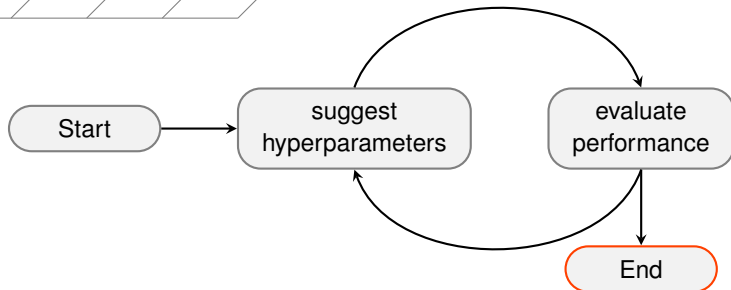
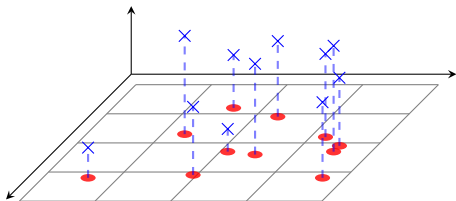
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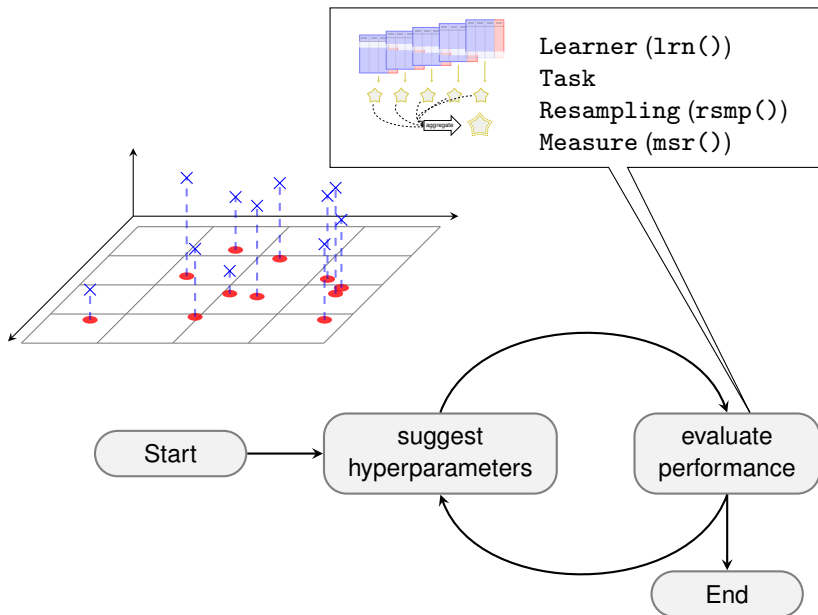
Batch evaluation



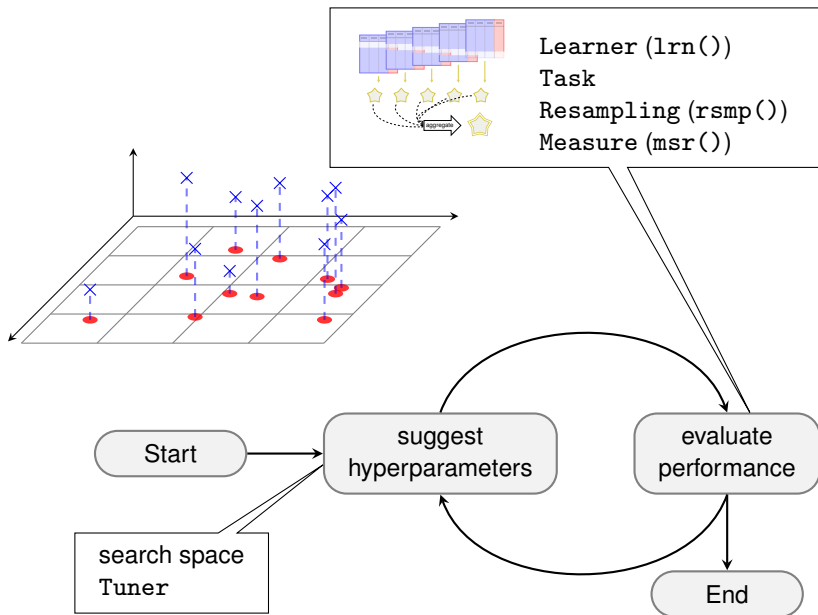
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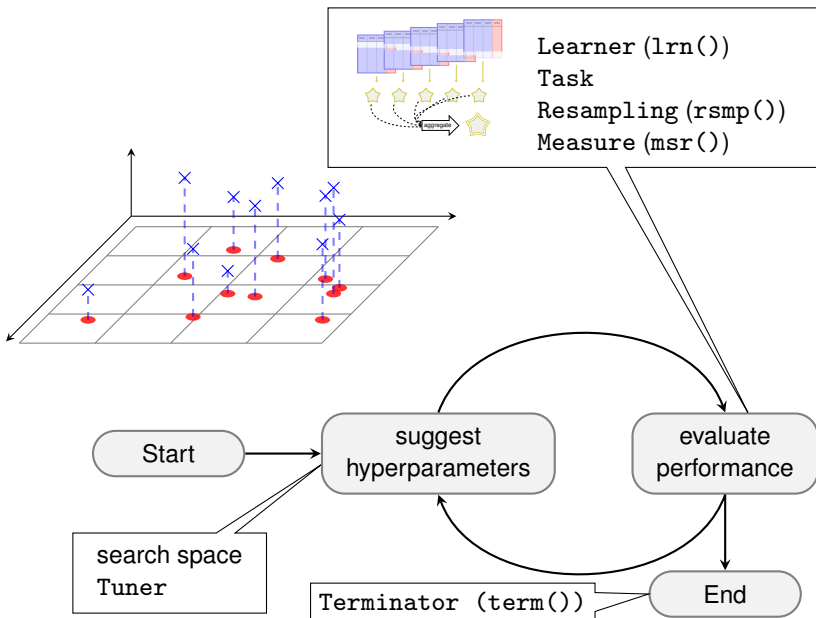
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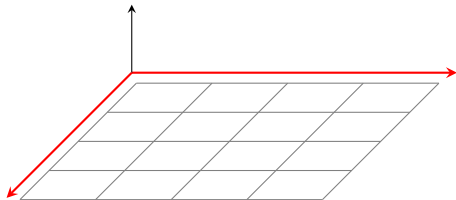


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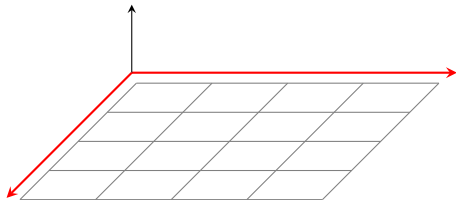


Search Space

SEARCH SPACE

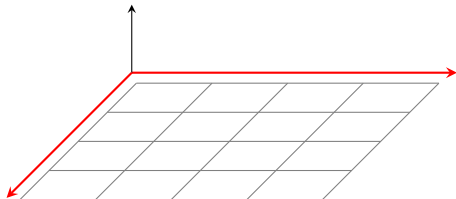


SEARCH SPACE



```
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)
```

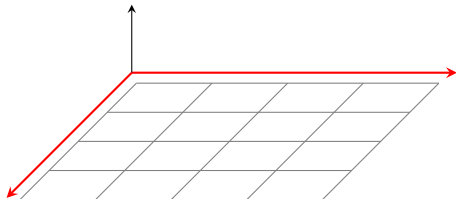
Logical parameter

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

Untyped parameter

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

SEARCH SPACE



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

Numerical parameter ParamDbl\$new(id, lower, upper)

Integer parameter ParamInt\$new(id, lower, upper)

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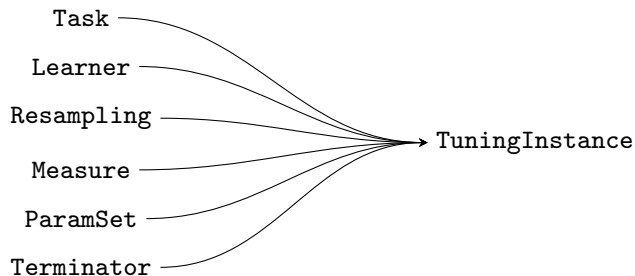
Logical parameter ParamLgl\$new(id)

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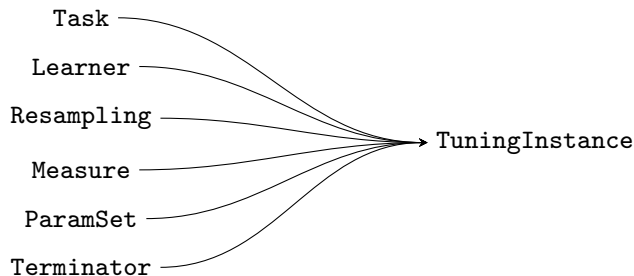
```
library("paradox")
searchspace_knn = ParamSet$new(list(
  ParamInt$new("k", 1, 20)
))
```

Tuning with mlr3tuning

OBJECTS IN TUNING



OBJECTS IN TUNING



```
library("mlr3tuning")

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

TUNING METHOD

- need to choose a *tuning method*

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

```
print(gsearch)

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

TUNING METHOD

- need to choose a *tuning method*
- Tuner class, load with `tnr()`, set parameters
- `gsearch = tnr("grid_search", resolution = 20)`

```
print(gsearch)

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

- common parameter `batch_size` for parallelization

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
```

```
#>
```

```
#>
```

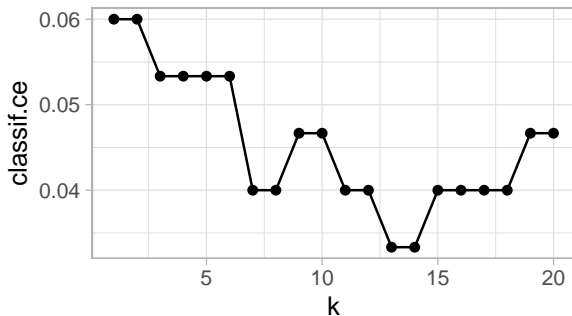
```
#> $perf
```

```
#> 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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Example:

- 1 sample from $\log(1) \dots \log(100)$ (`k_before_trafo`)
- 2 transform by $\exp()$ in `trafo` function

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- 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)

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

⇒ 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))))  
}
```

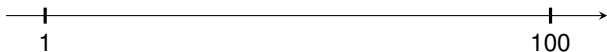
PARAMETER TRANSFORMATION

What is our transformation doing?



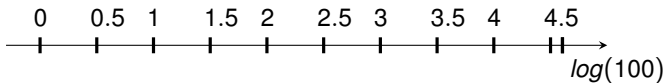
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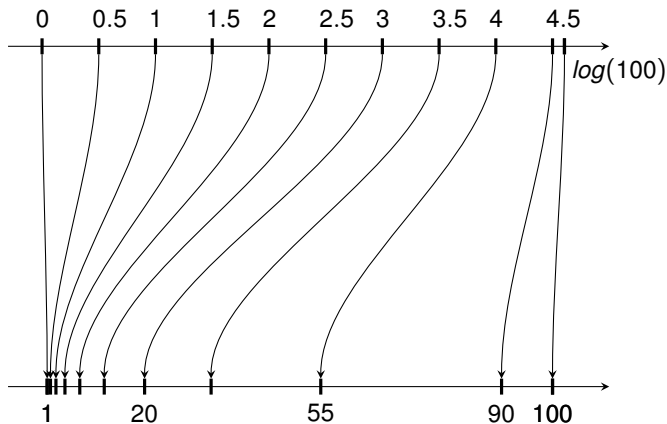
PARAMETER TRANSFORMATION

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PARAMETER TRANSFORMATION

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PARAMETER TRANSFORMATION

Tuning again...

PARAMETER TRANSFORMATION

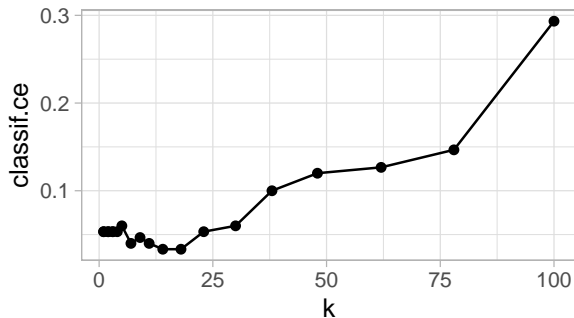
Tuning again...

```
inst$result

#> $tune_x
#> $tune_x$k_before_trafo
#> [1] 2.7
#>
#>
#> $params
#> $params$kernel
#> [1] "rectangular"
#>
#> $params$k
#> [1] 14
#>
#>
#> $perf
#> classif.ce
#>          0.033
```

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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⇒ 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

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

NESTED RESAMPLING

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

```
optlrn$model$learner
```

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

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

```
#> * Parameters: kernel=rectangular, k=13
```

```
#> * 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=13
```

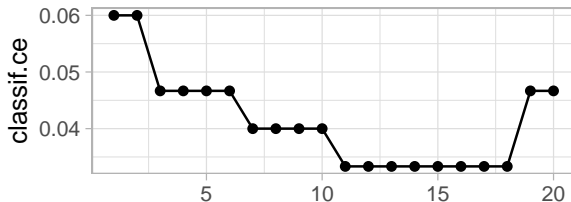
```
#> * Packages: withr, kknn
```

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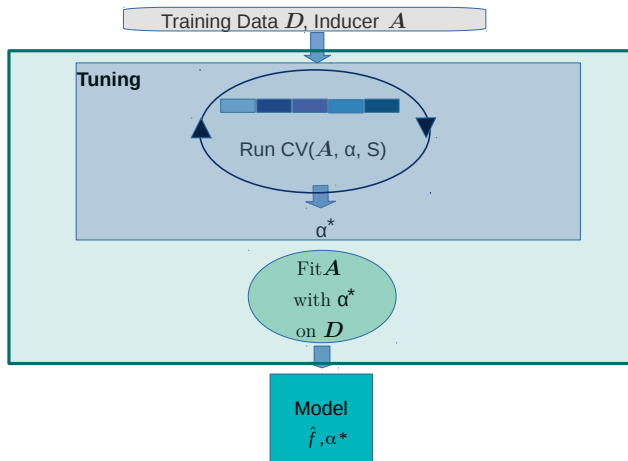
```
#> * Feature types: logical, integer, numeric, factor, ordered
```

```
#> * 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
```

```
#> * Performance: 0.067 [classif.ce]
```

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

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

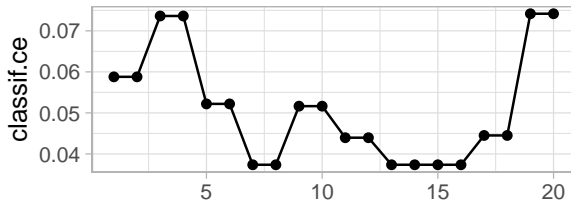
NESTED RESAMPLING

```
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

- ❶ 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
- ❷ Create a Tuner
 - Usually using `tnr()`
 - May have some parameters, e.g. `batch_size`
- ❸ Call `tuner$tune()`

Nested Resampling

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