LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Tuning Machine Learning Algorithms with mlr3

mlr3tuning

Department of Statistics – LMU Munich

Intro

TUNING

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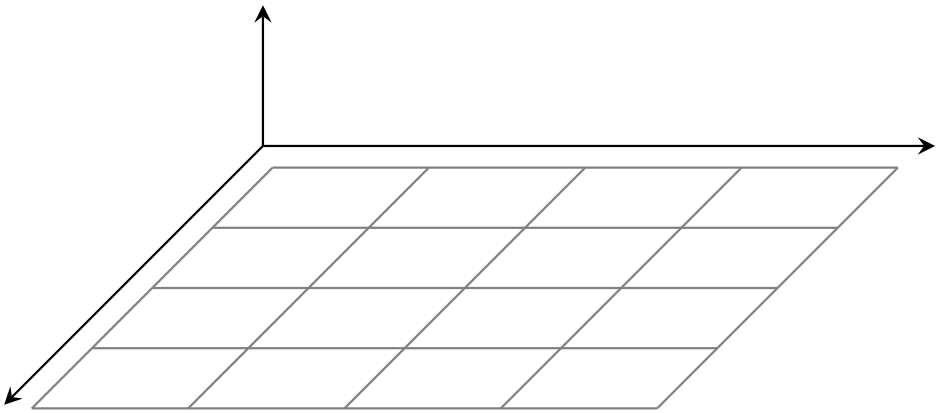
Tuning toolbox for `mlr3`:

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

Tuning

TUNING



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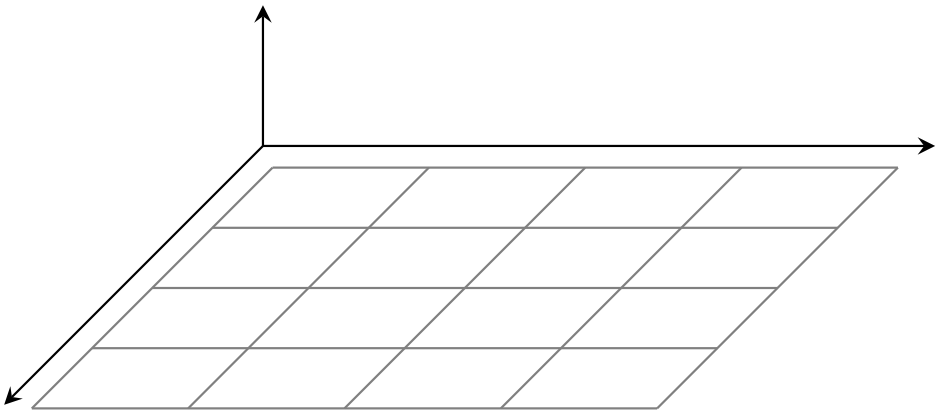

Start

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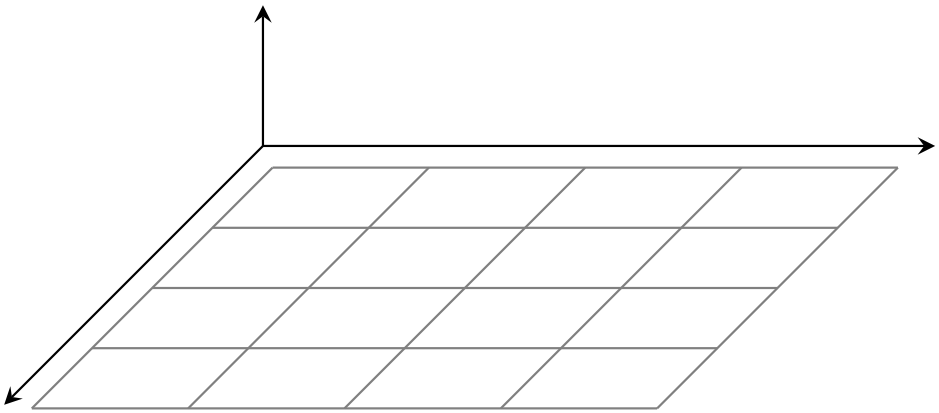

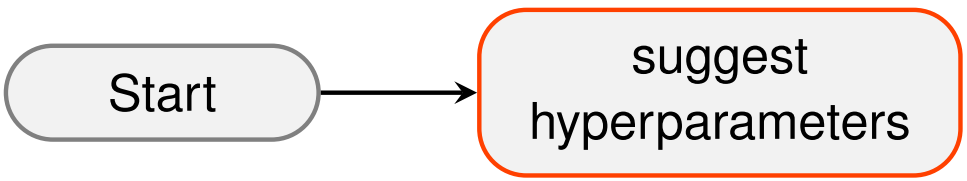

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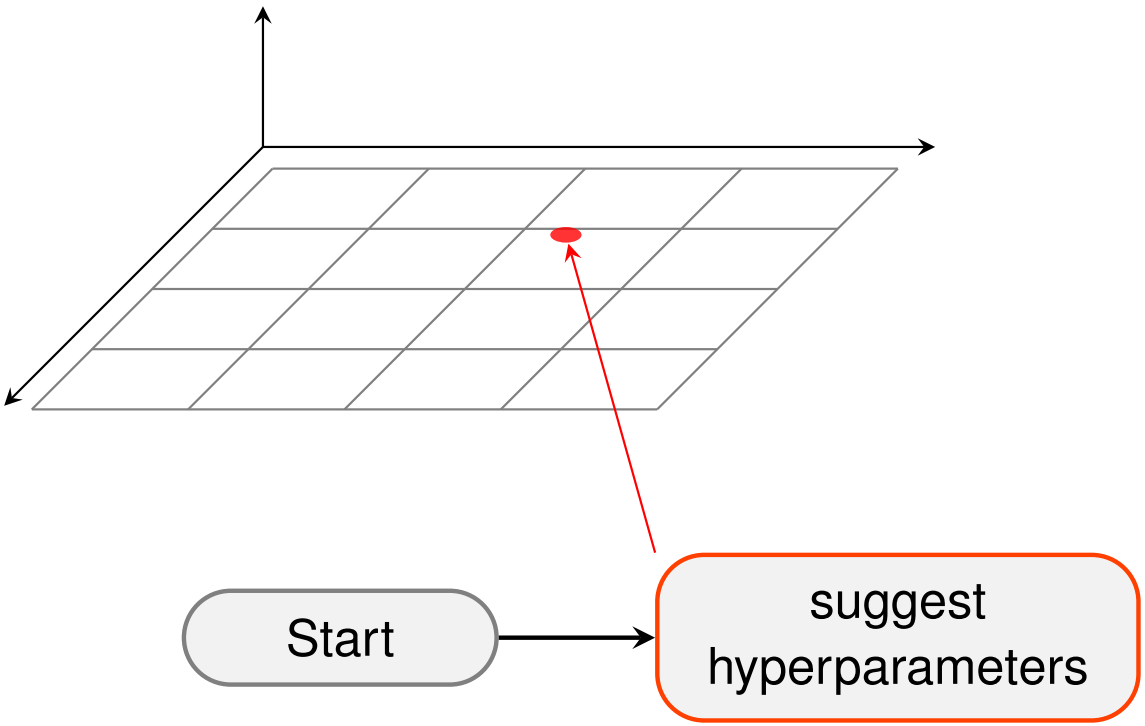

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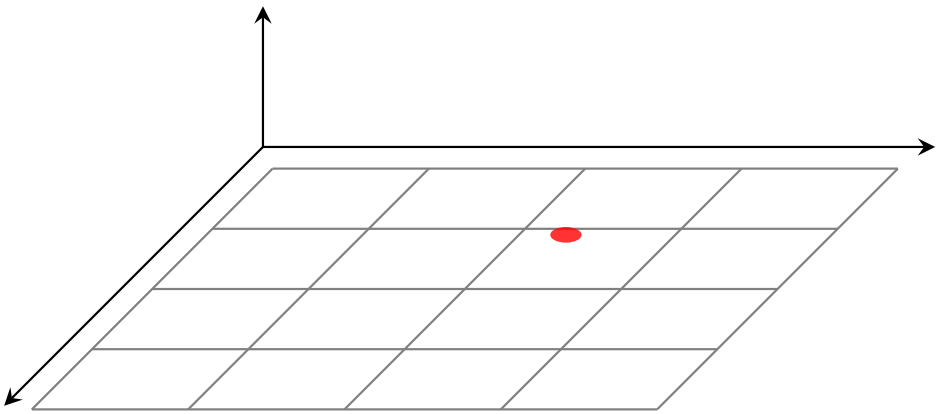

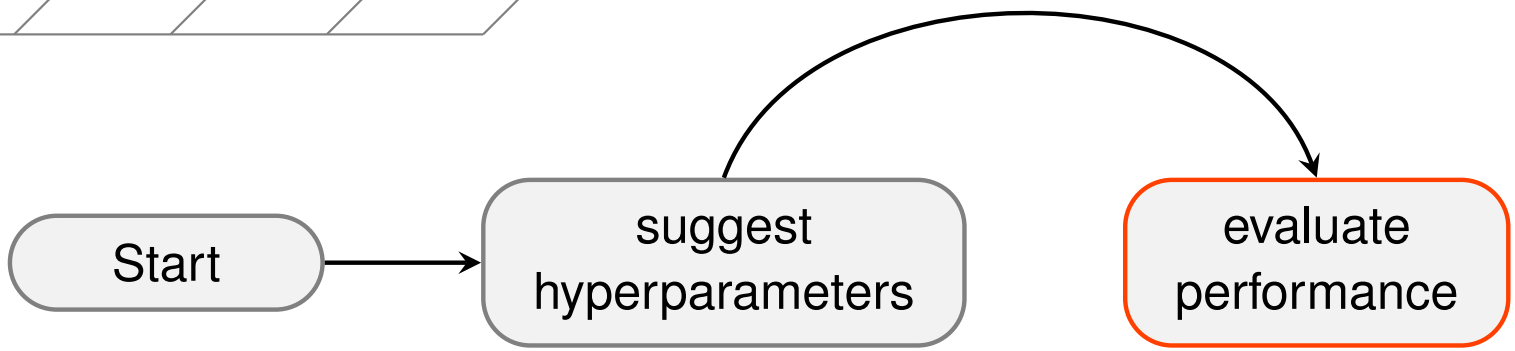

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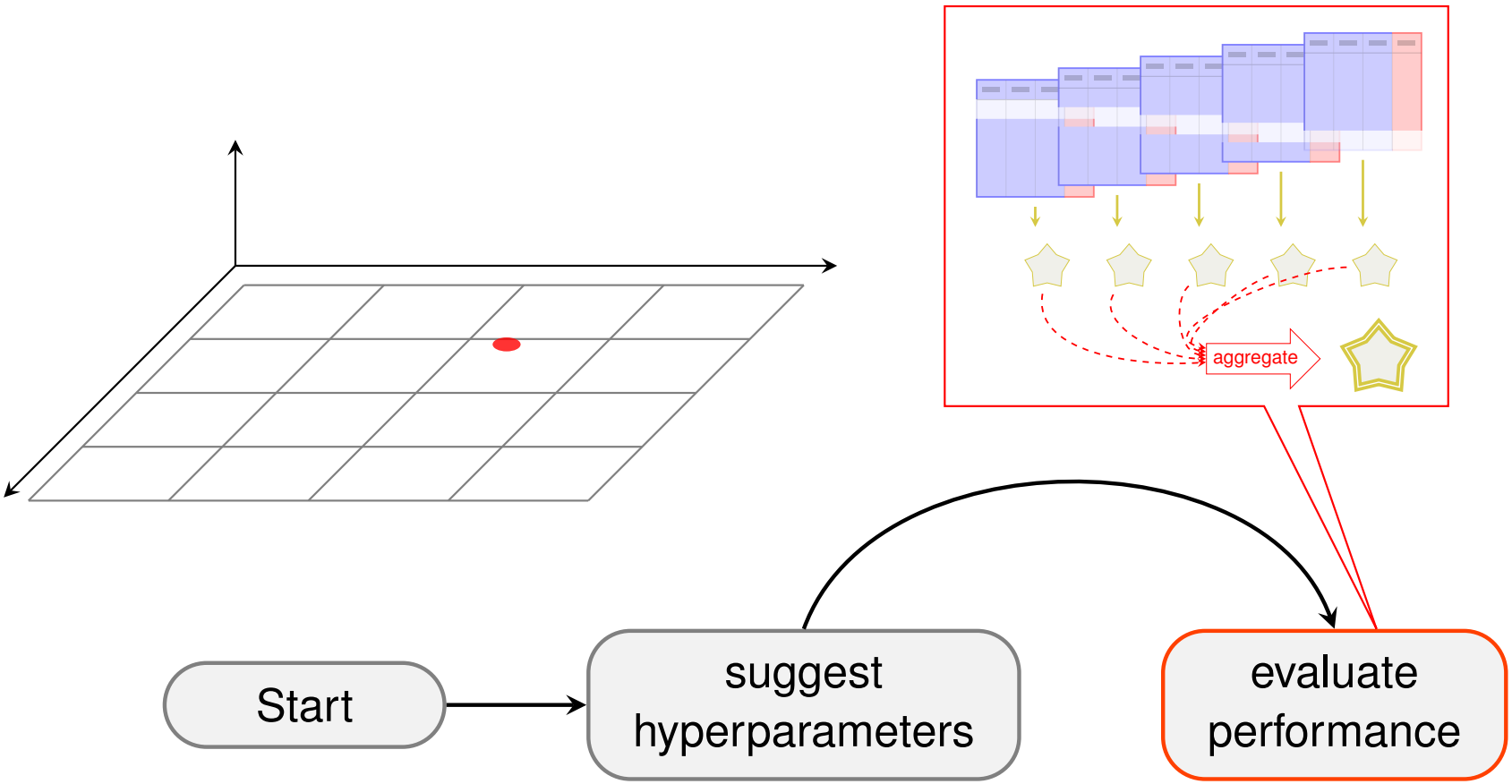
aggregate
Start
suggest hyperparameters
evaluate performance

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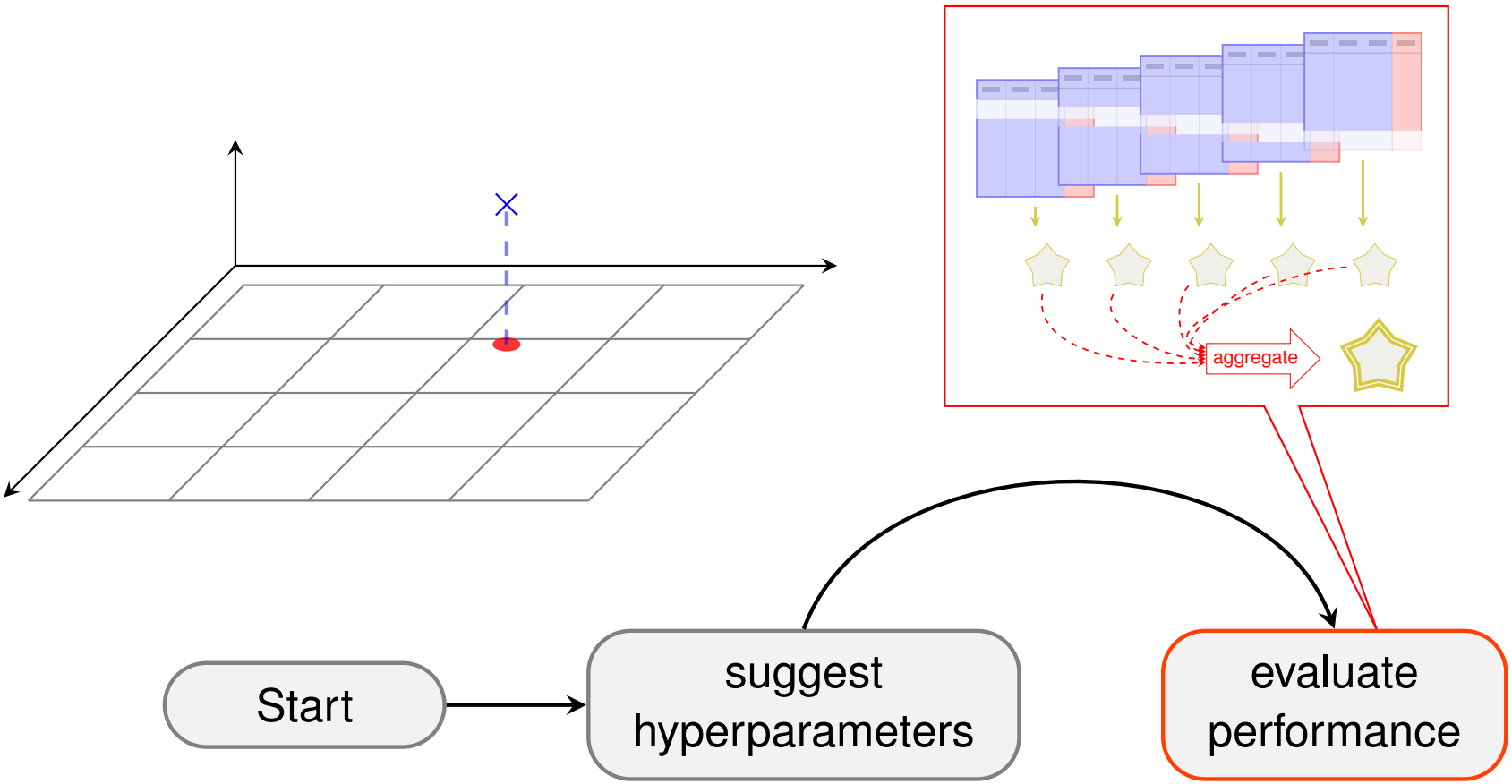
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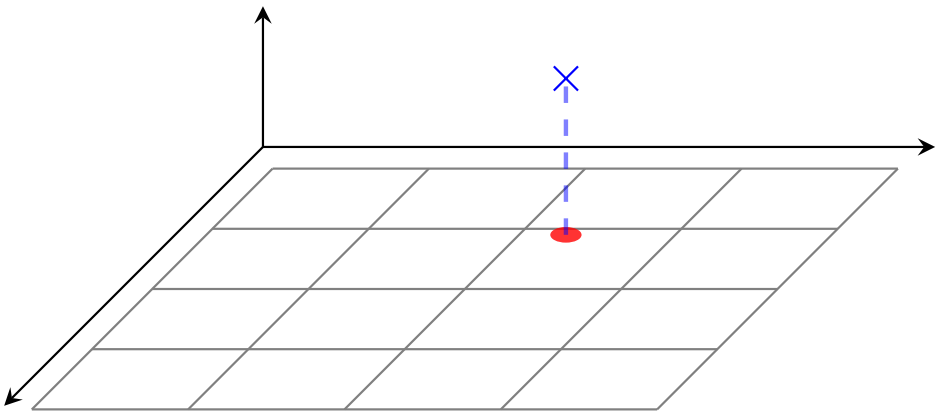

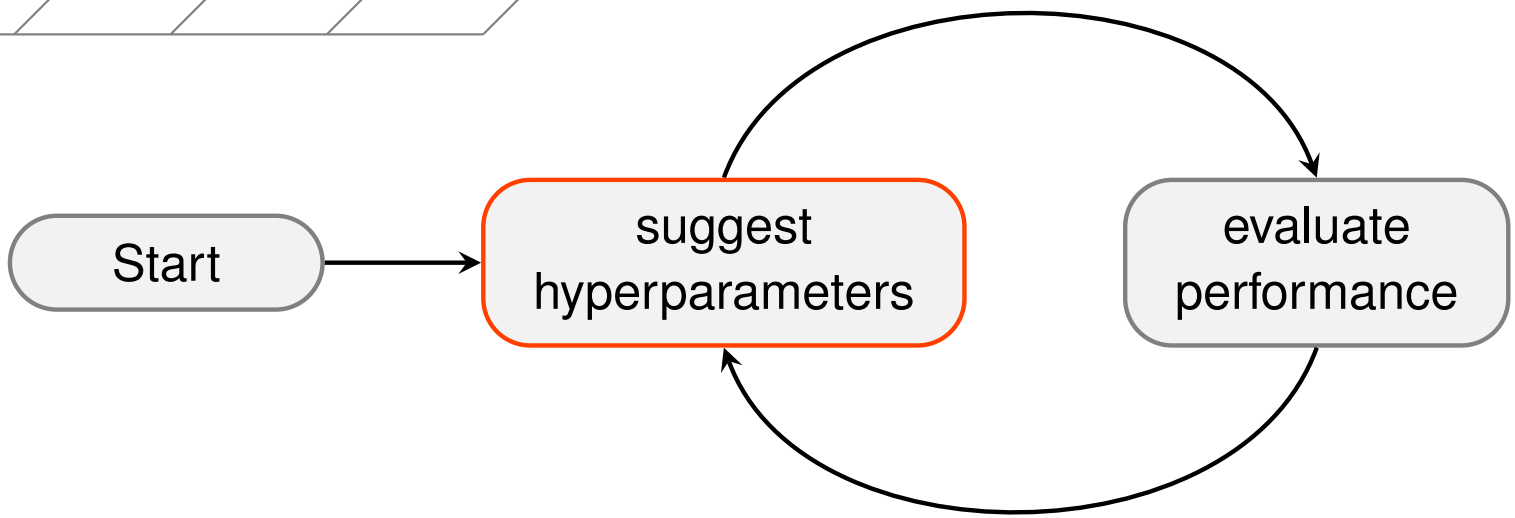

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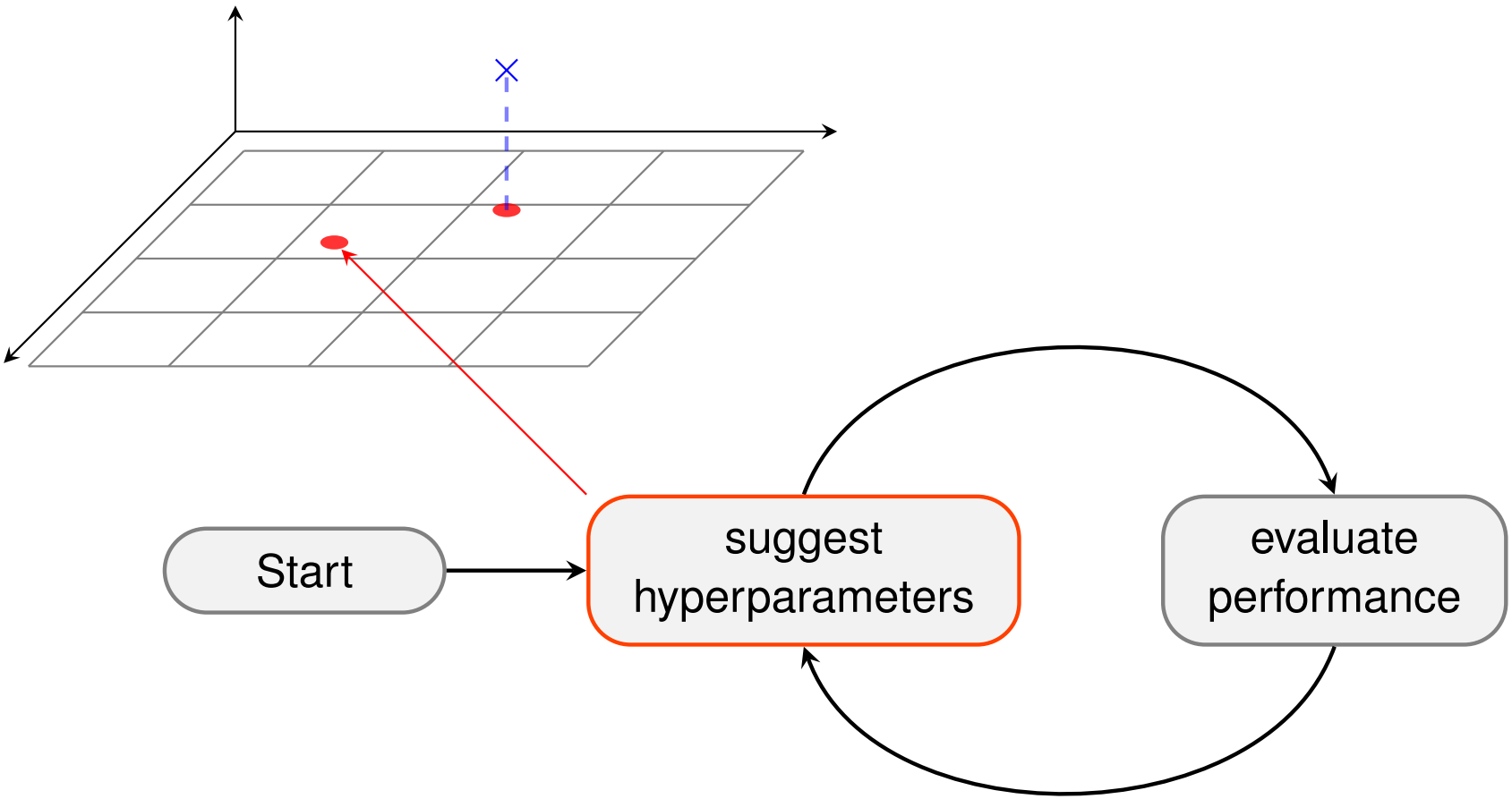

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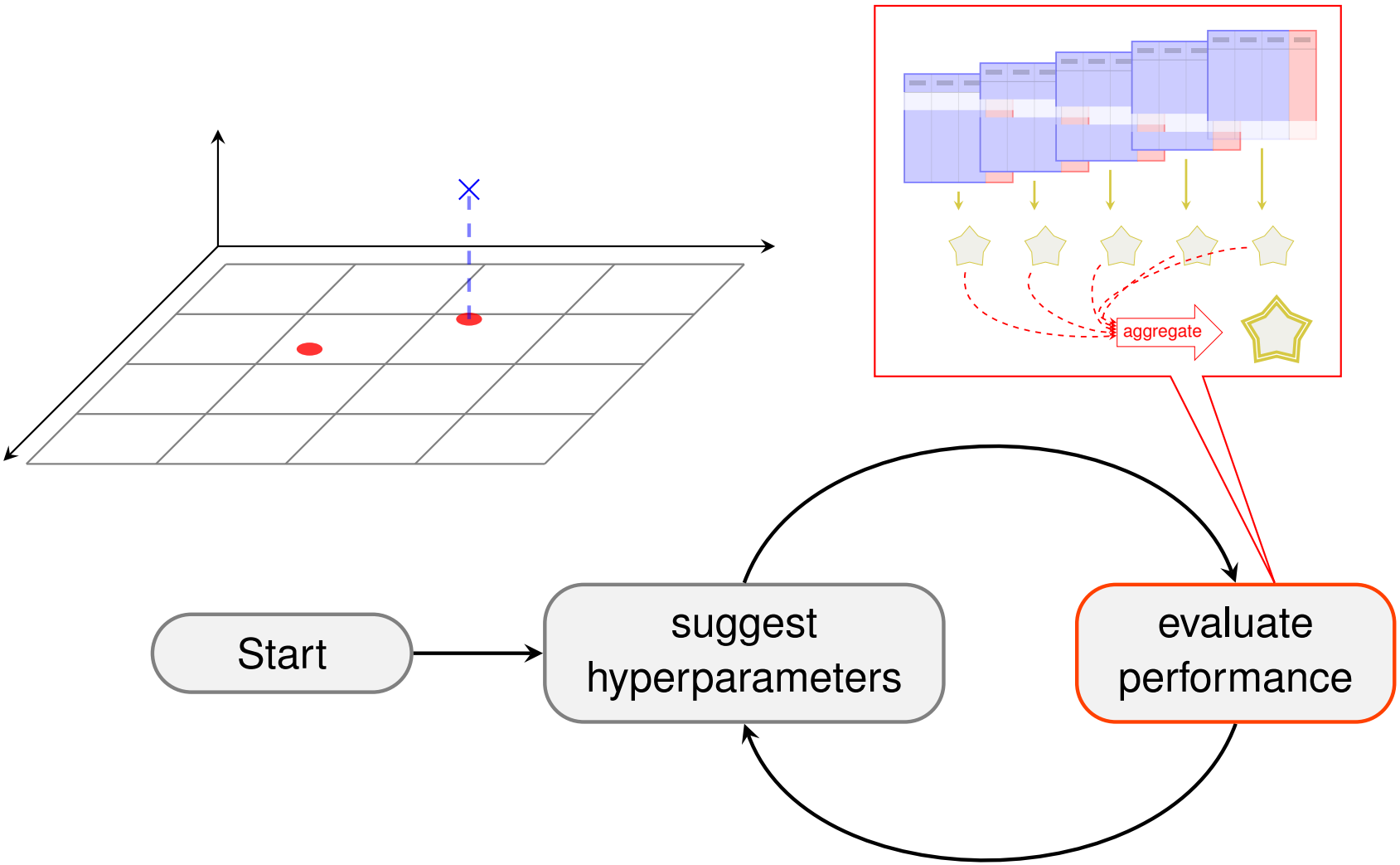
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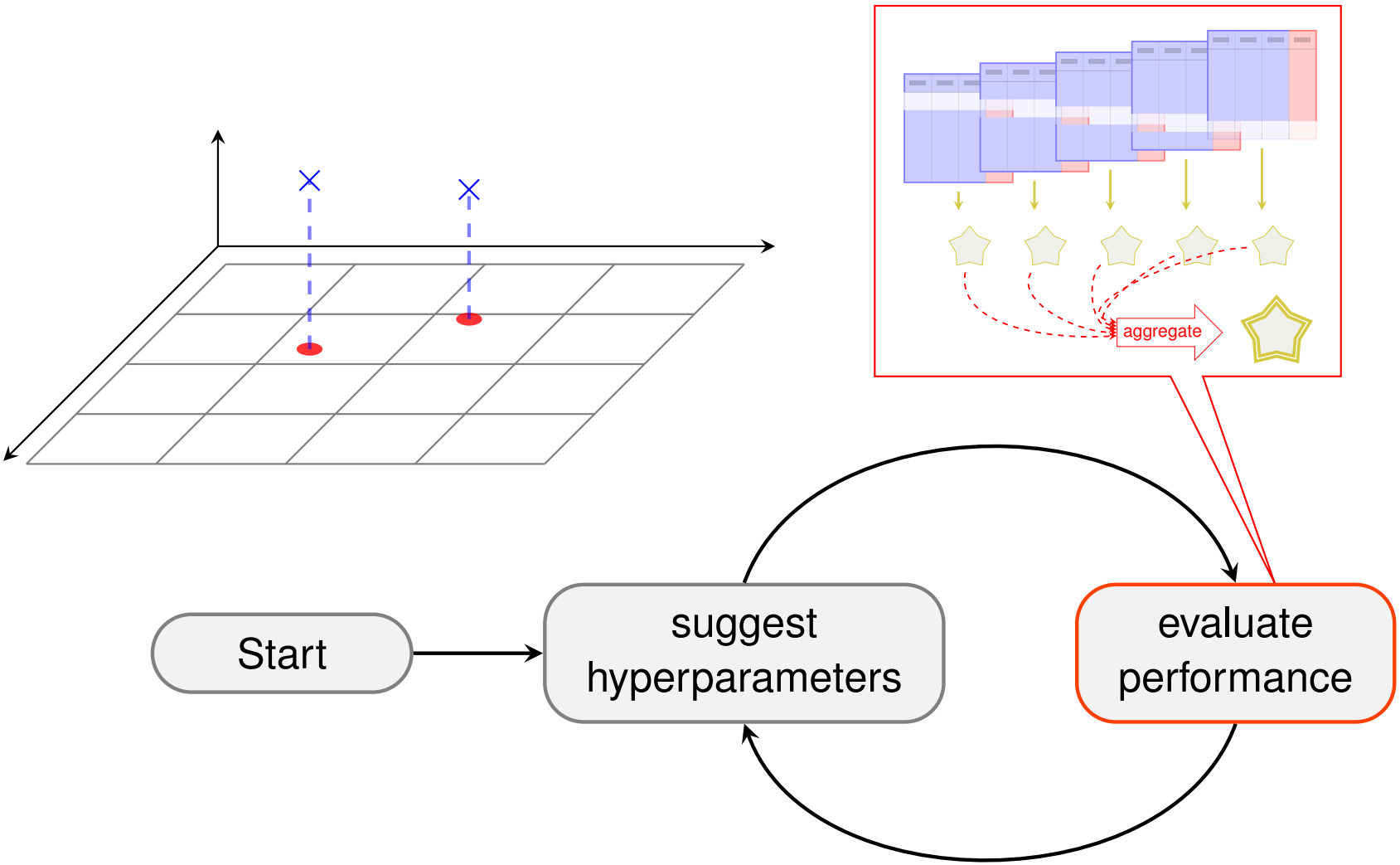
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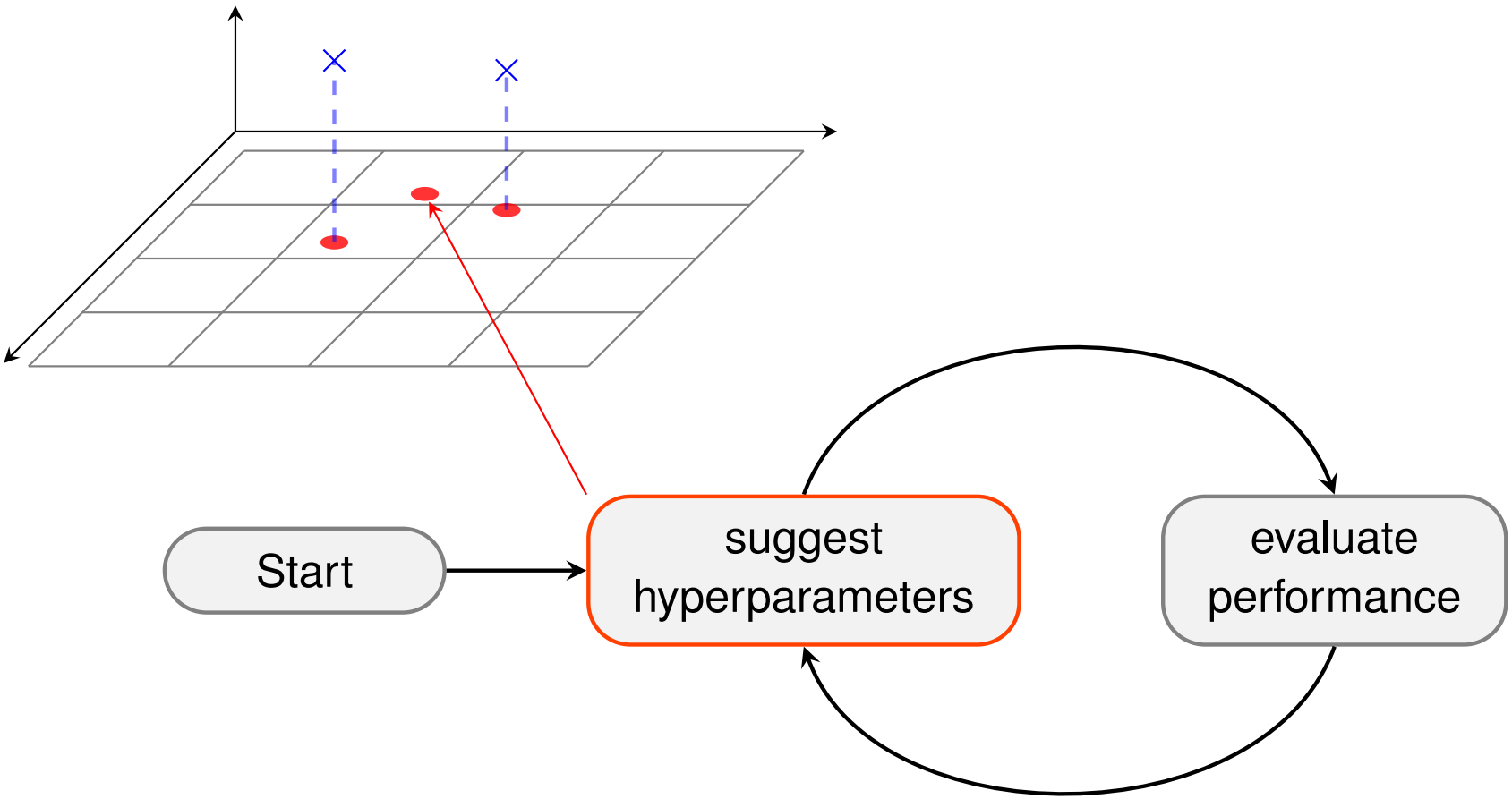

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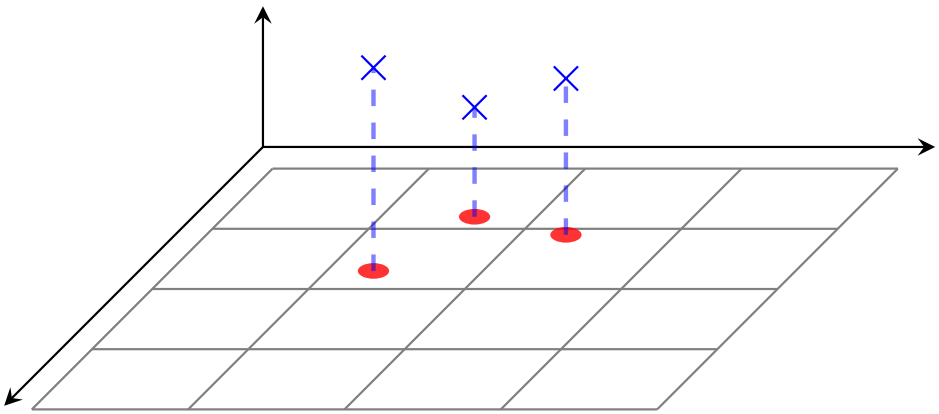

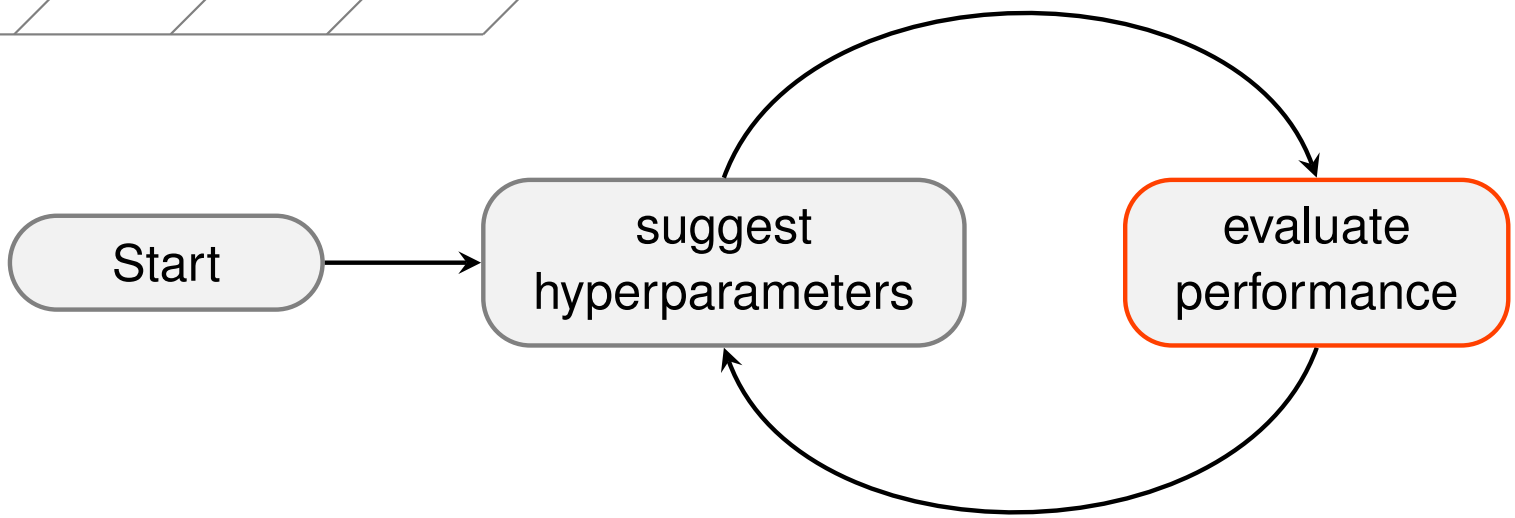

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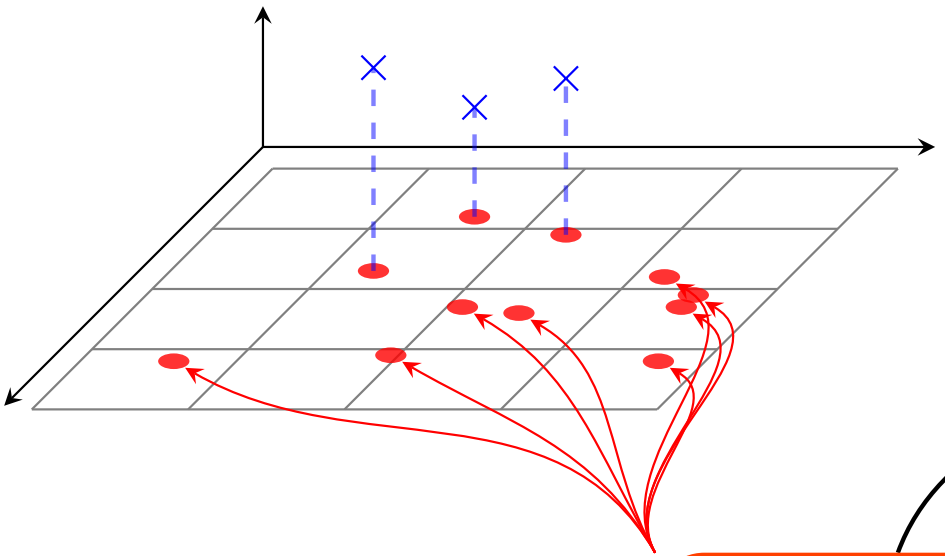
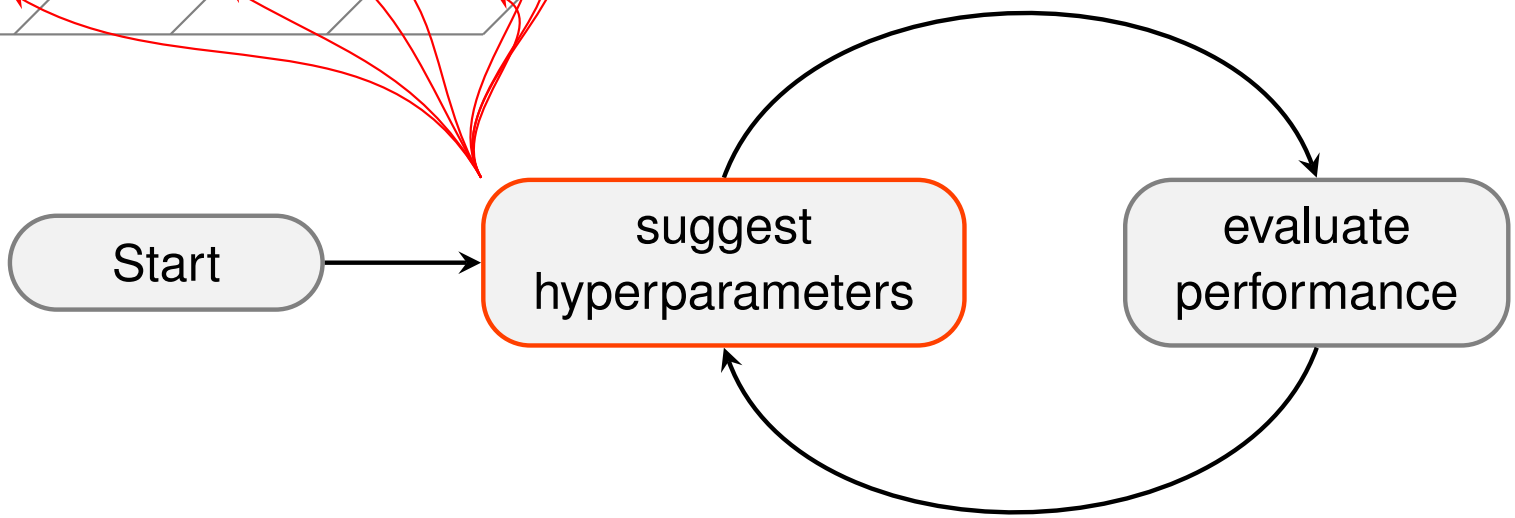


Batch evaluation



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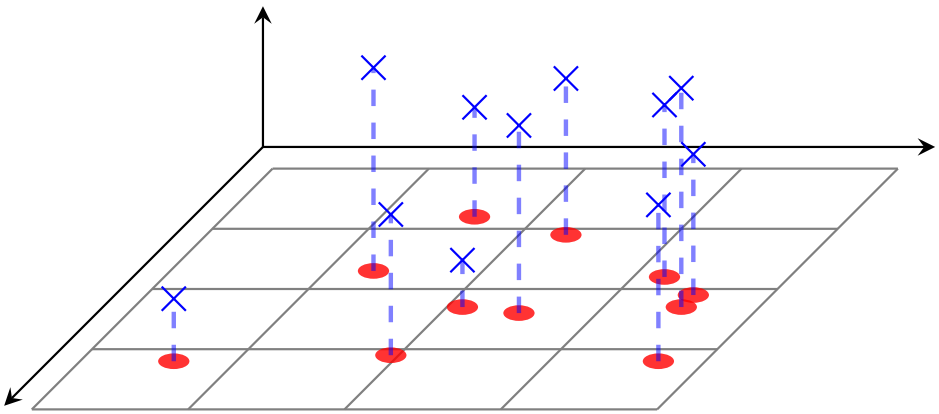

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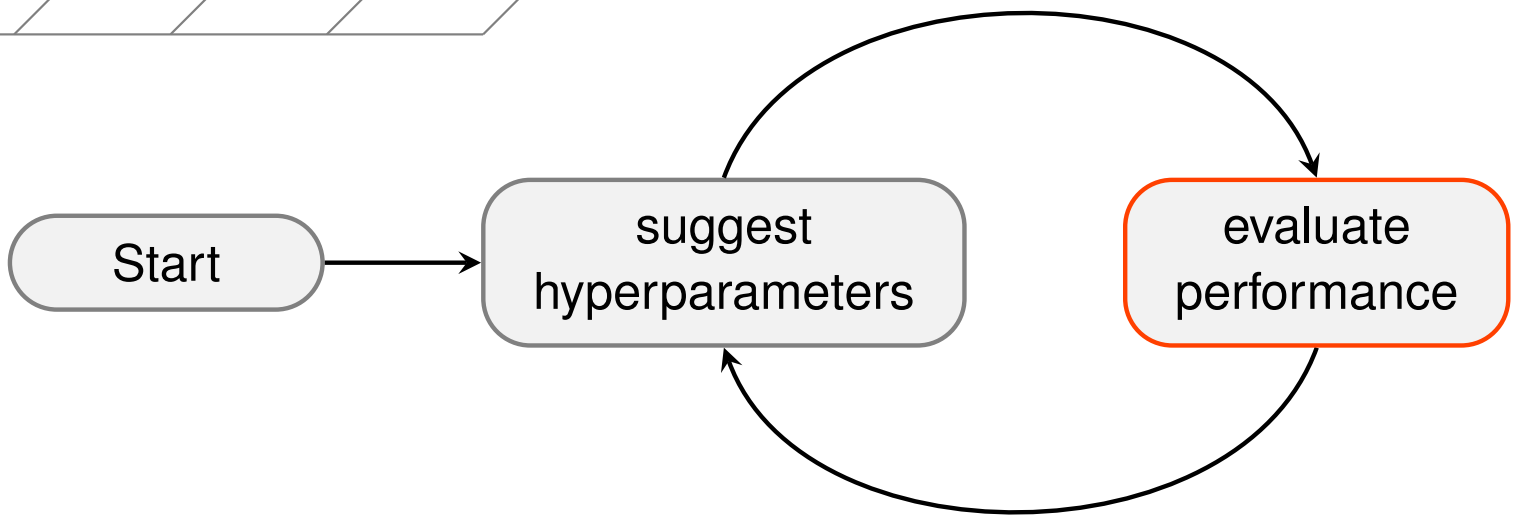

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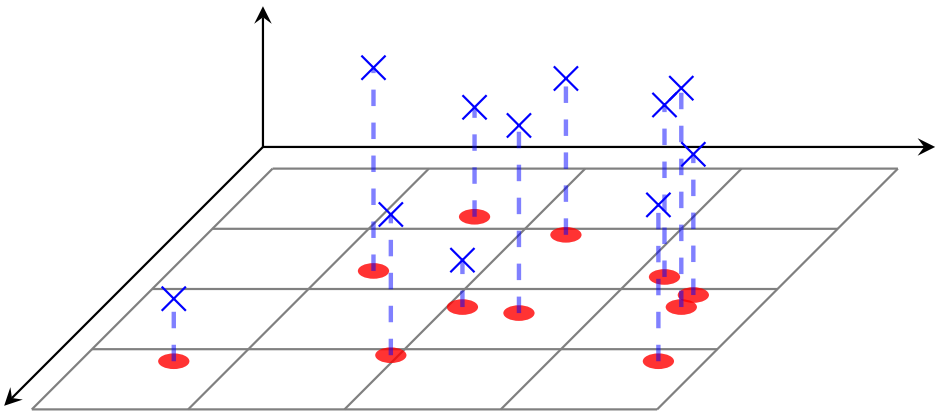

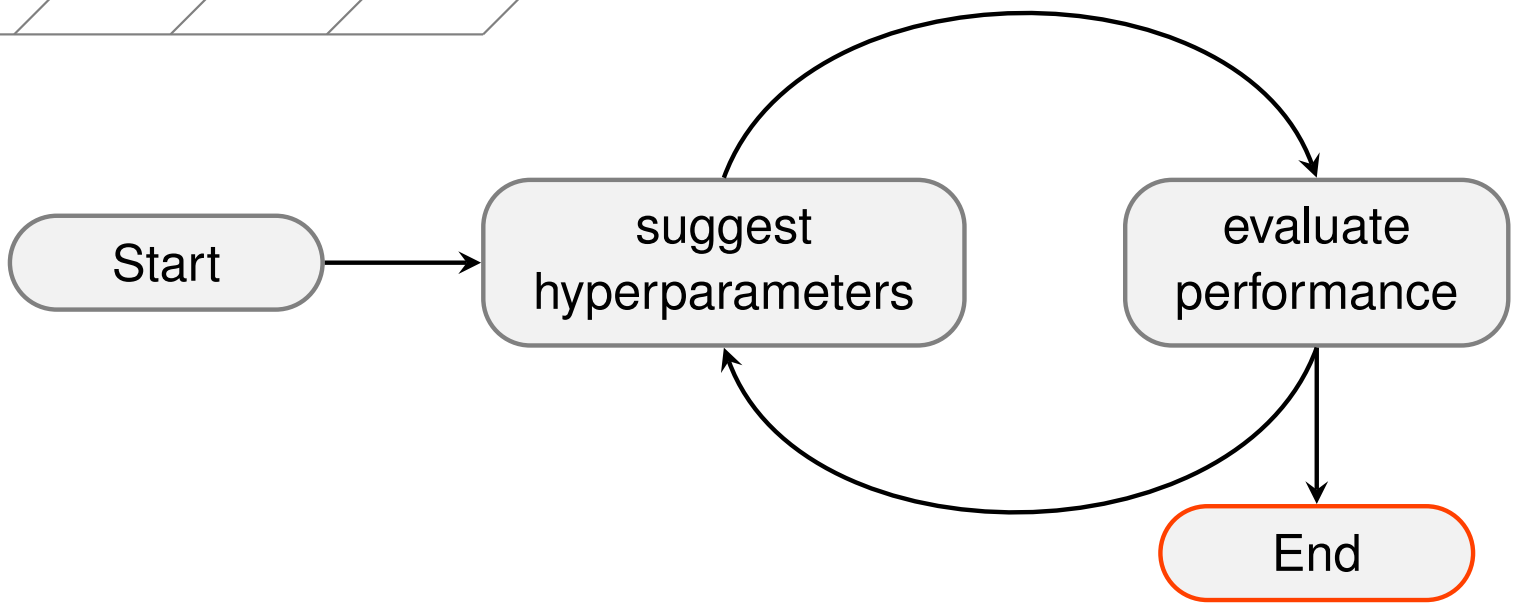

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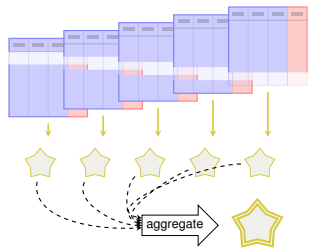
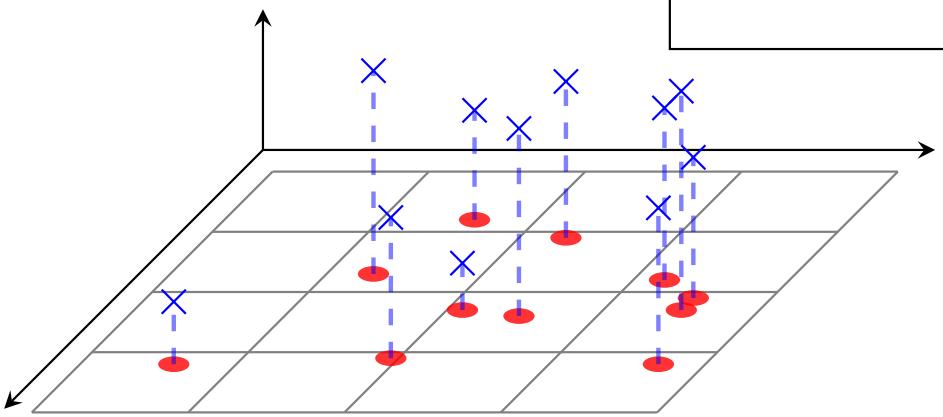
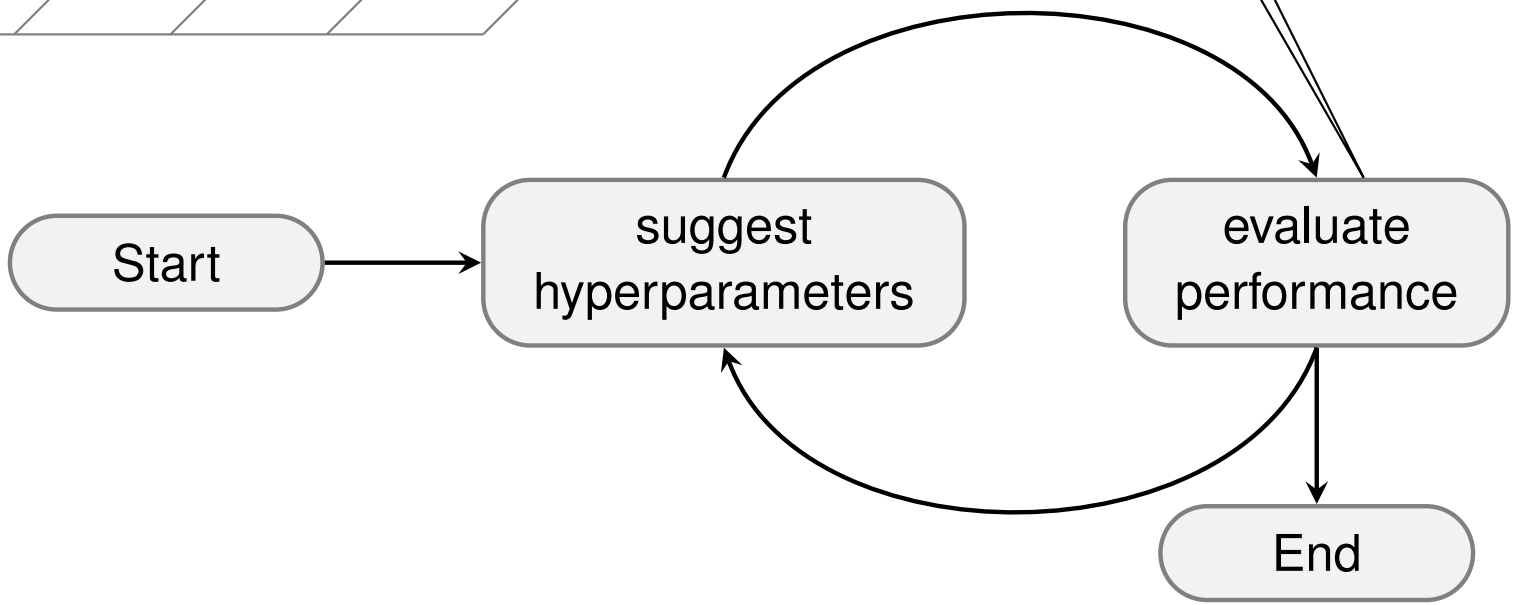


`Learner (lrn())`
`Task`
`Resampling (rsmp())`
`Measure (msr())`





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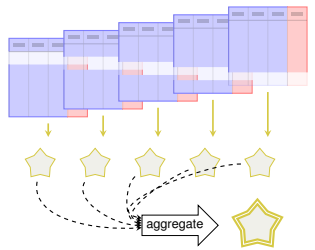

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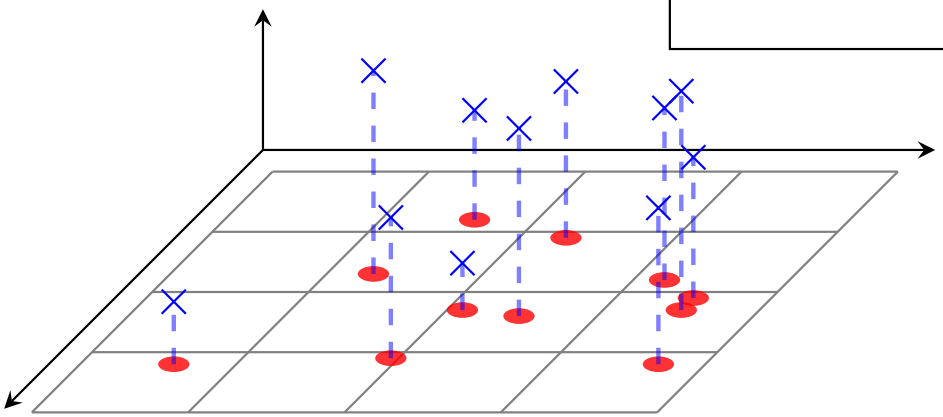


Start

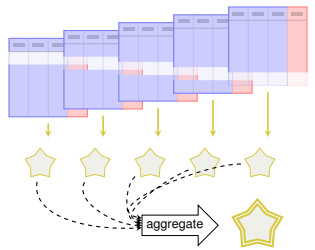
suggest hyperparameters

evaluate performance

End

search space
`Tuner`

TUNING



`Learner` (`lrn()`)
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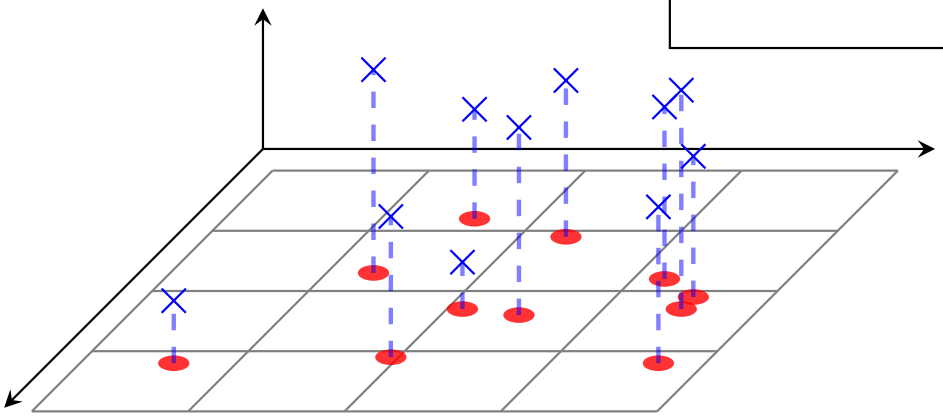

Start

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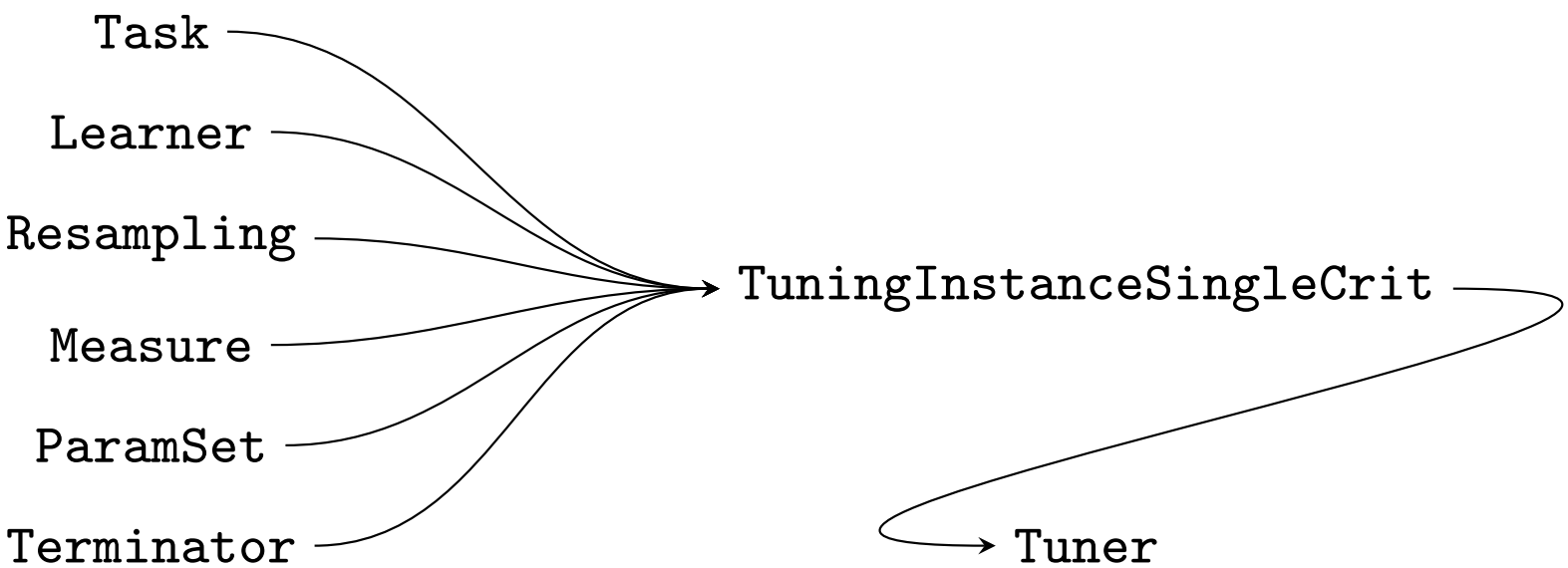
search space
`Tuner`

`Terminator` (when to finish)

End

Tuning in mlr3

OBJECTS IN TUNING



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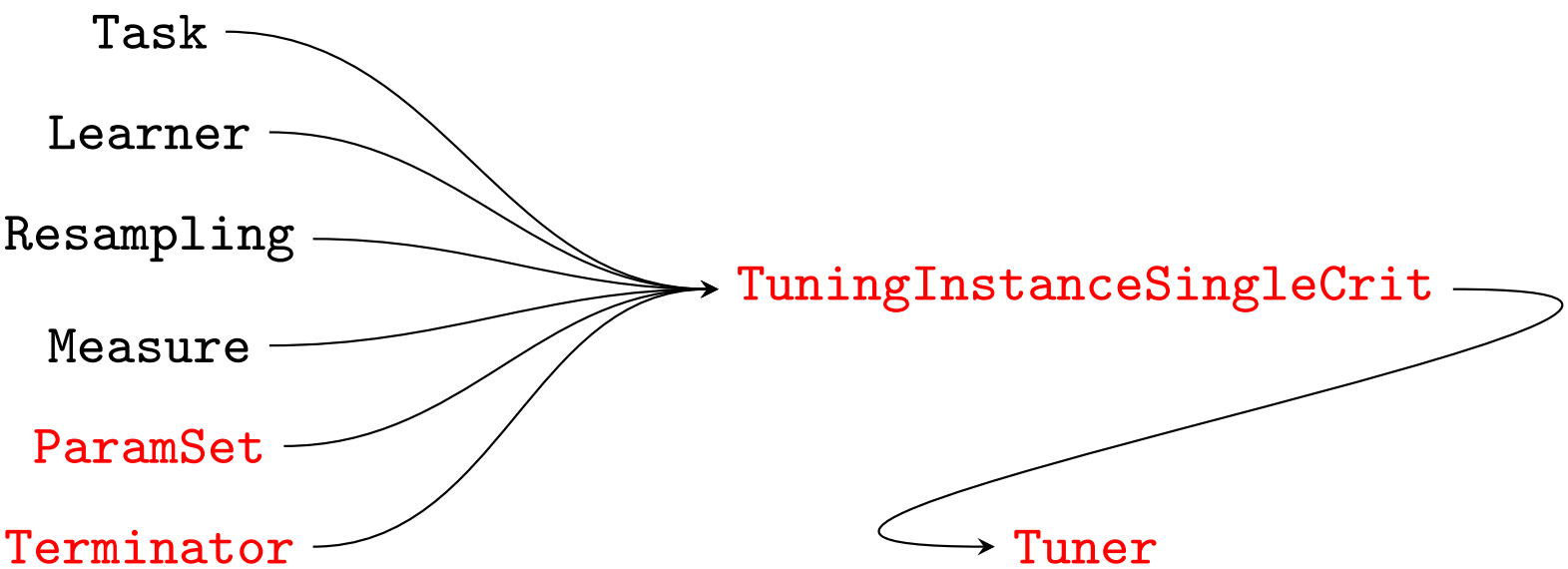
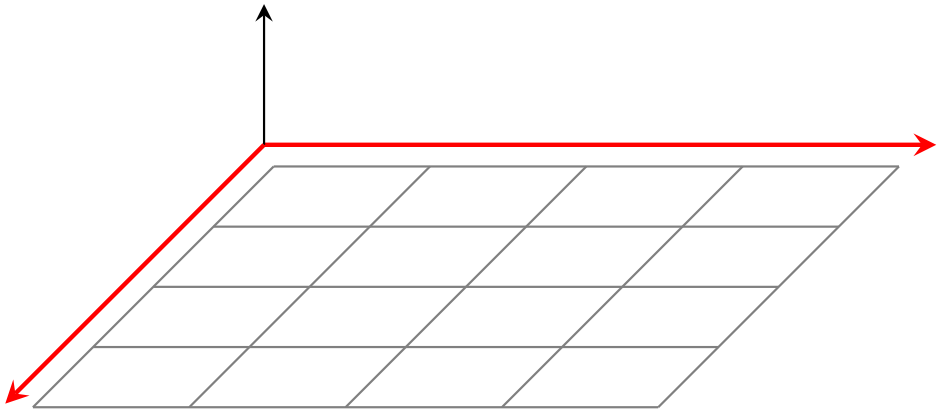


SEARCH SPACE



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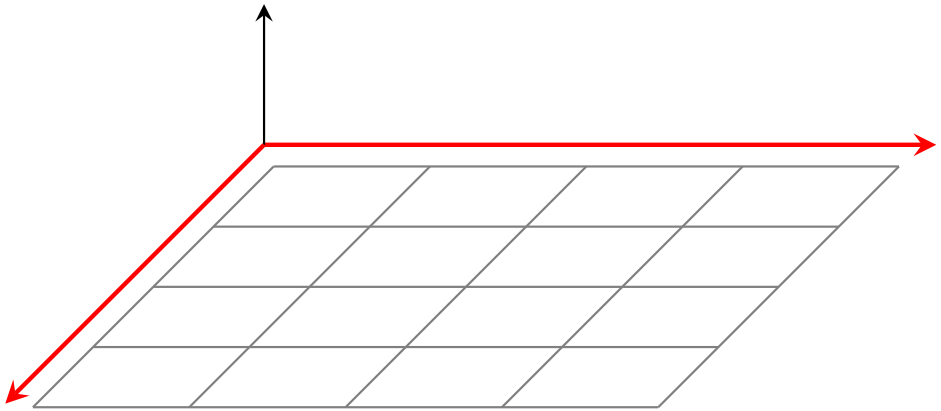
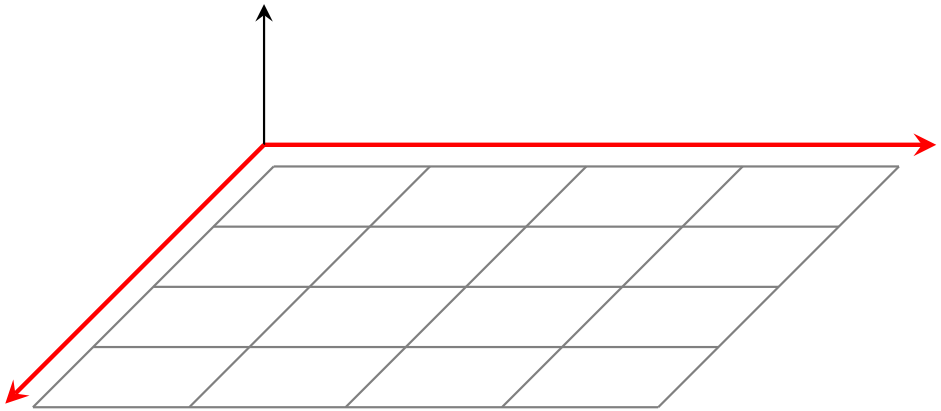


```
ParamSet$new(list(param1, param2, ...))
```

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)`

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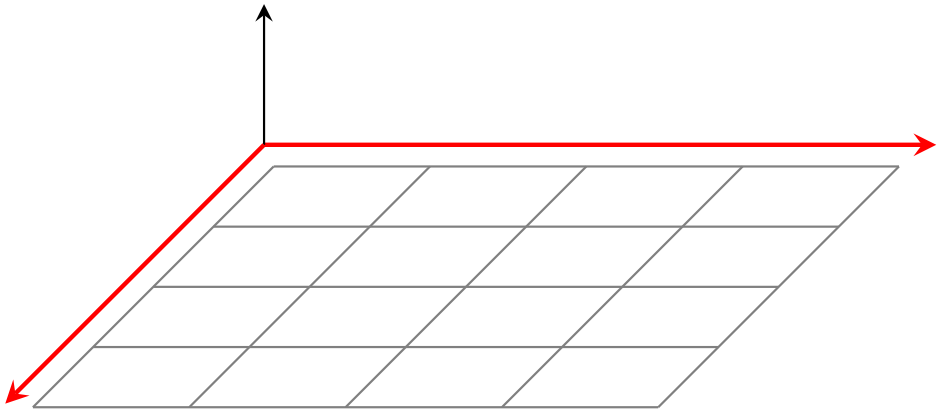

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Untyped parameter	`ParamUty$new(id)`

```
library("paradox")
searchspace_knn = ParamSet$new(list(
  ParamInt$new("k", 1, 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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#> 8: stagnation_batch
```

```
trm("evals", n_evals = 20)
#> <TerminatorEvals>
#> * Parameters: n_evals=20
```

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

TUNING METHOD

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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: -
  ```
  ```

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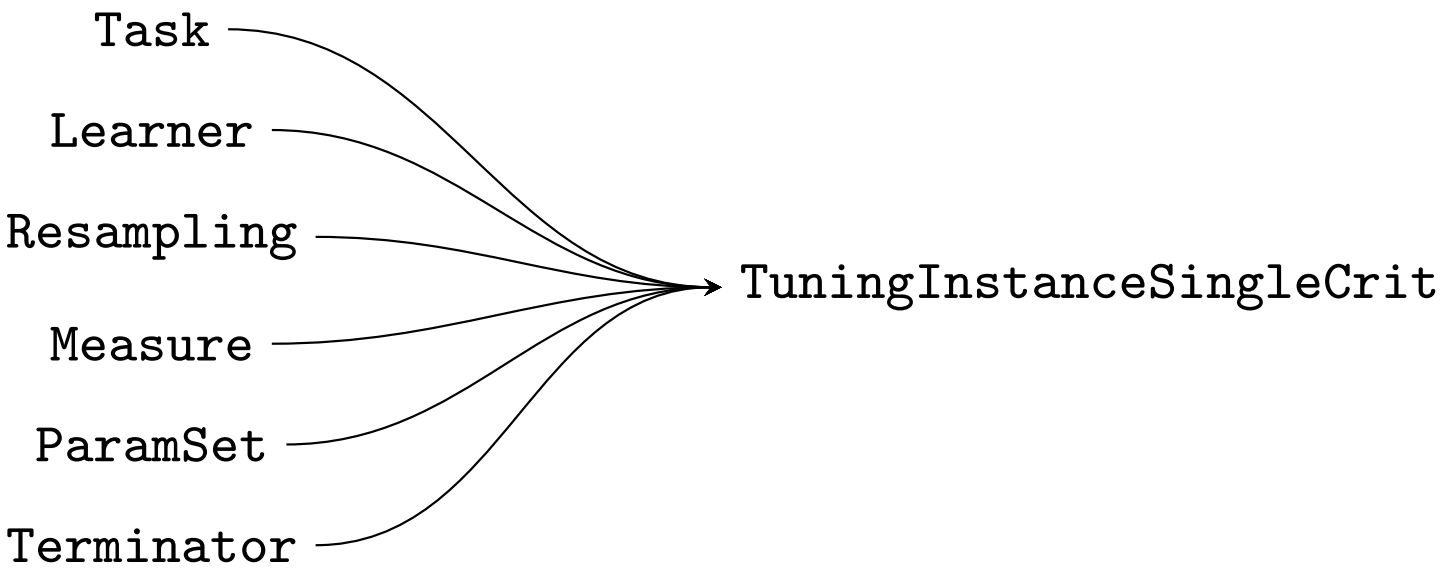
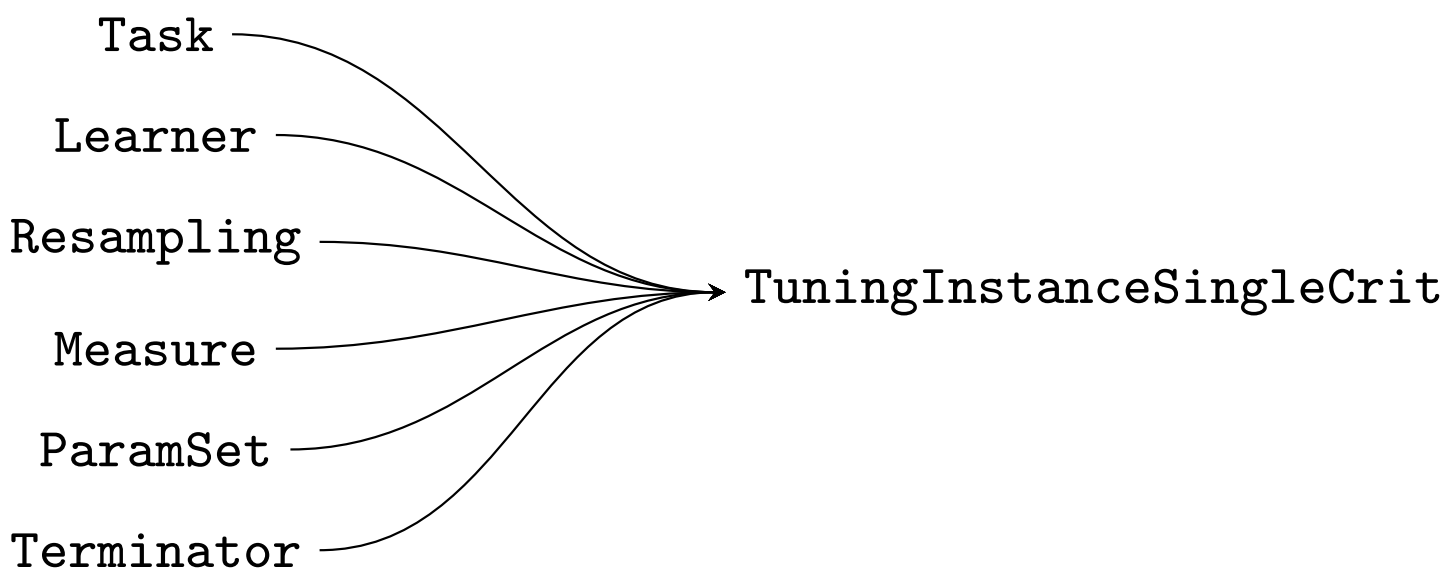
  #> * Packages: -
  ```
- common parameter `batch_size` for parallelization
  ```

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)

#>     k learner_param_vals  x_domain classif.ce
#> 1: 10          <list[2]> <list[1]>       0.04
```

TUNING RESULTS

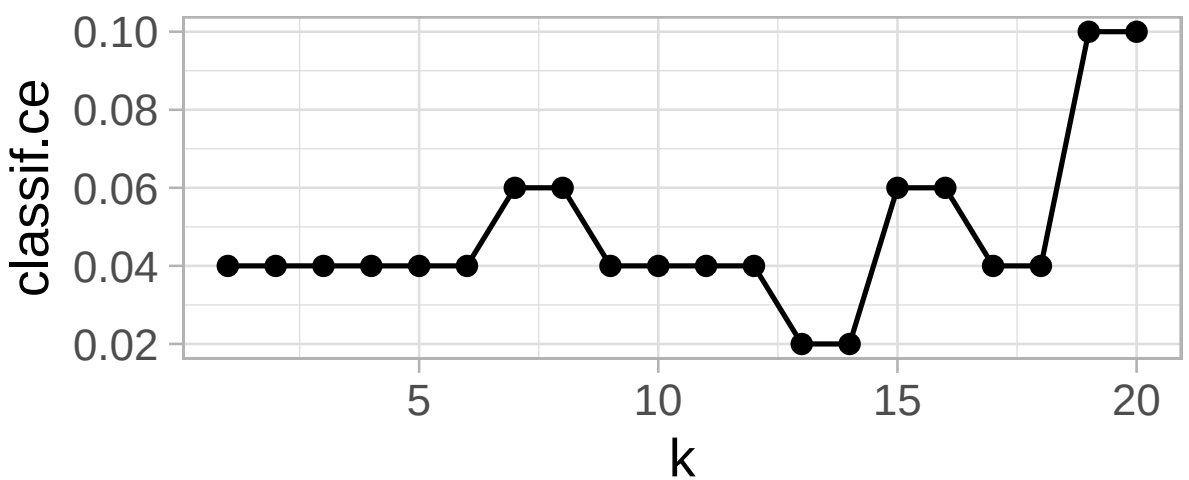
```
gsearch = tnr("grid_search", resolution = 20)

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

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Example:

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

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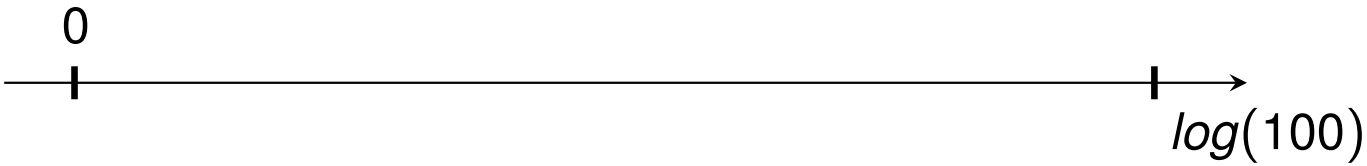
2. transform by $\exp()$ in `trafo` function
3. don't forget to `round` (k must be integer)

```
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

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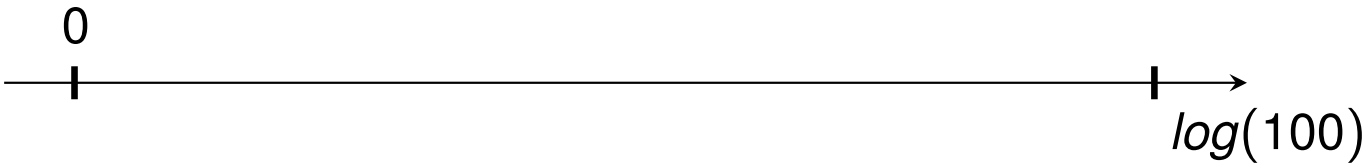

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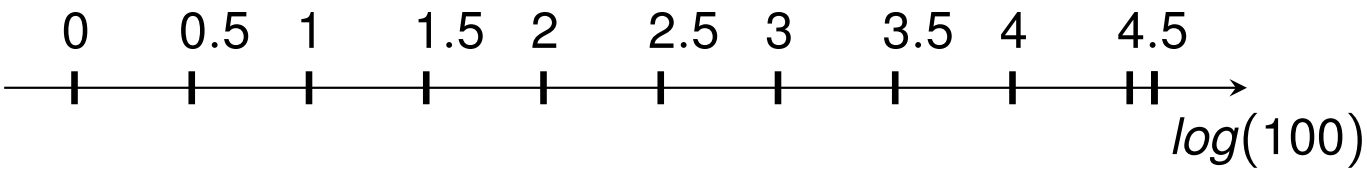

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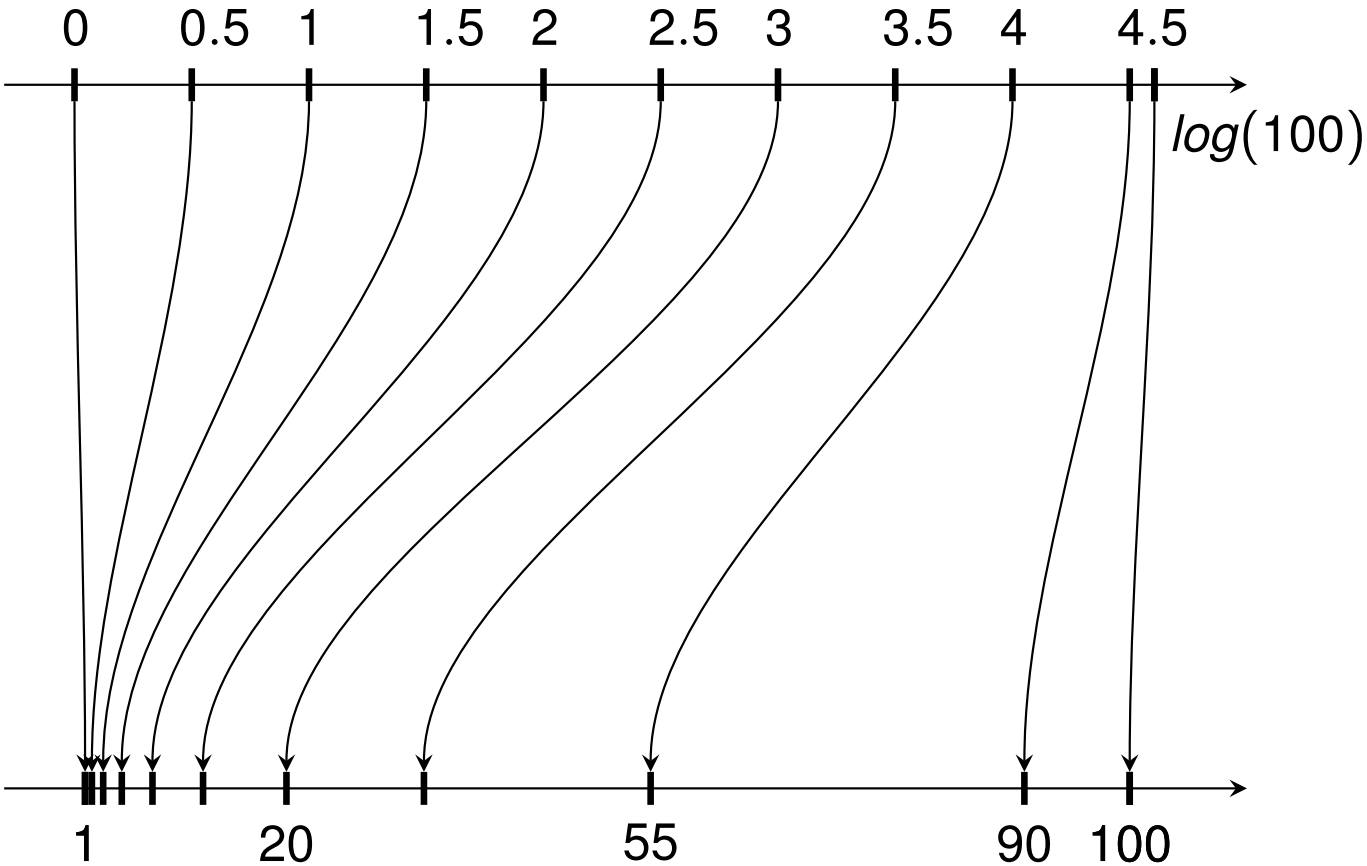


PARAMETER TRANSFORMATION

Tuning again. . .

PARAMETER TRANSFORMATION

Tuning again...

```
inst$result

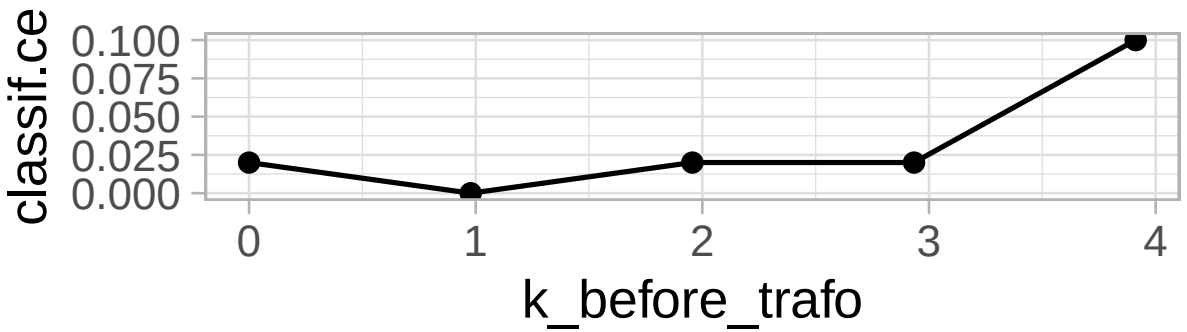
#>    k_before_trafo learner_param_vals  x_domain classif.ce
#> 1:           0.98          <list[2]> <list[1]>          0

inst$result$x_domain

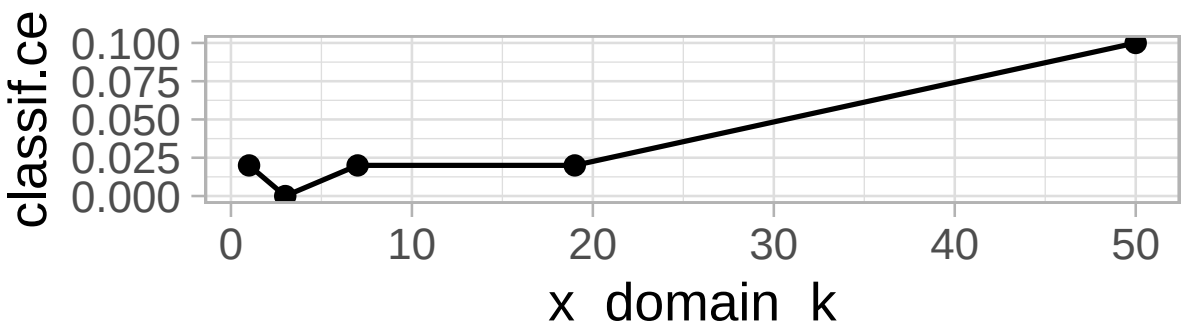
#> [[1]]
#> [[1]]$k
#> [1] 3
```

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()
```



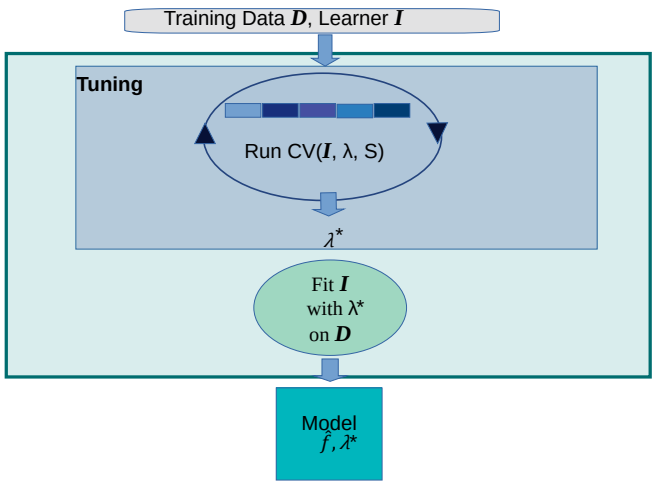
Nested Resampling

NESTED RESAMPLING

- Need to perform nested resampling to estimate tuned learner performance

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

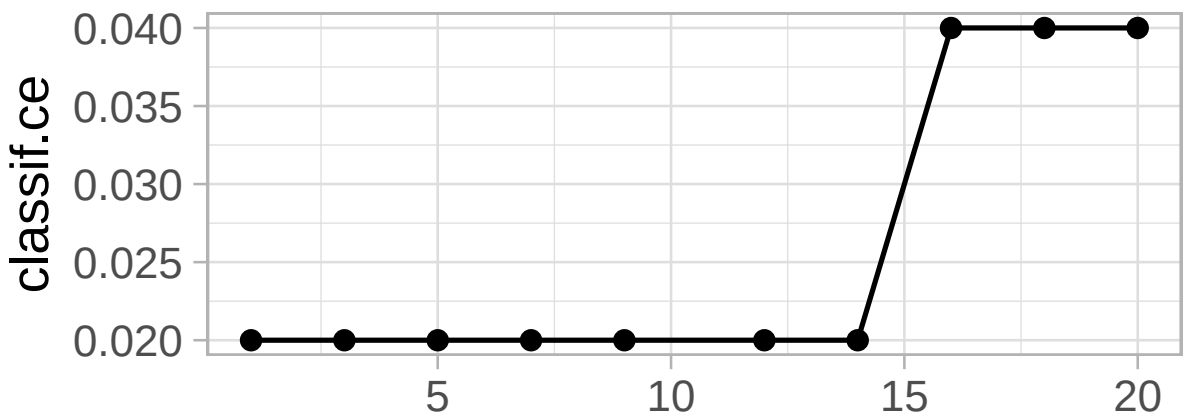
```
optlrn$train(tsk("iris"))
```

```
optlrn$model$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

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



NESTED RESAMPLING

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