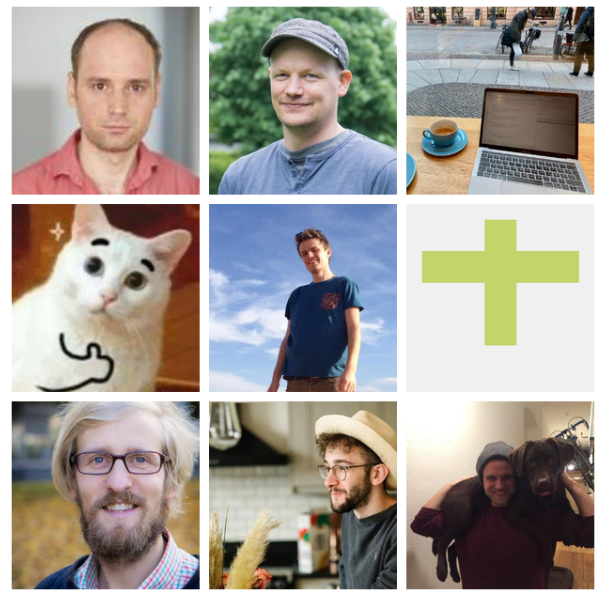
Tuning Machine Learning Algorithms with mlr3

https://mlr-org.com/

https://github.com/mlr-org



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February 11, 2021

Intro

TUNING

- Behavior of most methods depends on *hyperparameters*

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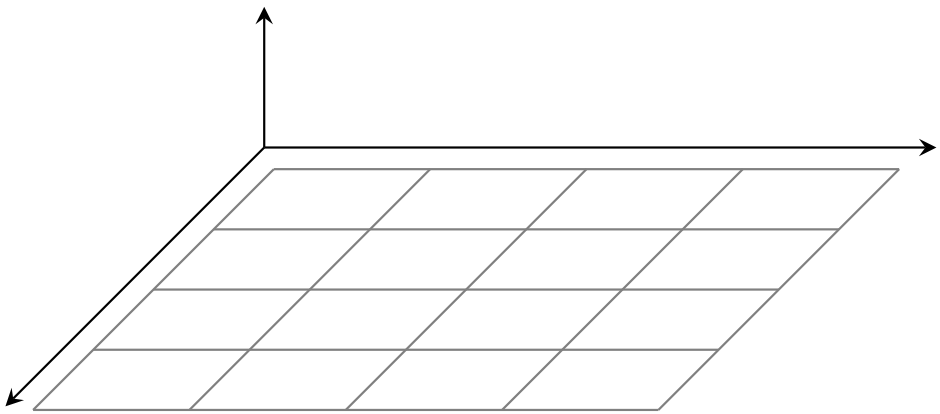
Tuning toolbox for `mlr3`:

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

Tuning

TUNING



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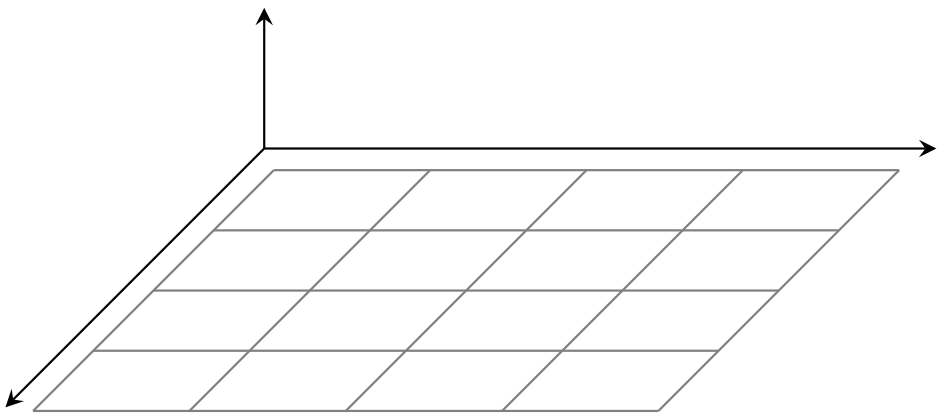
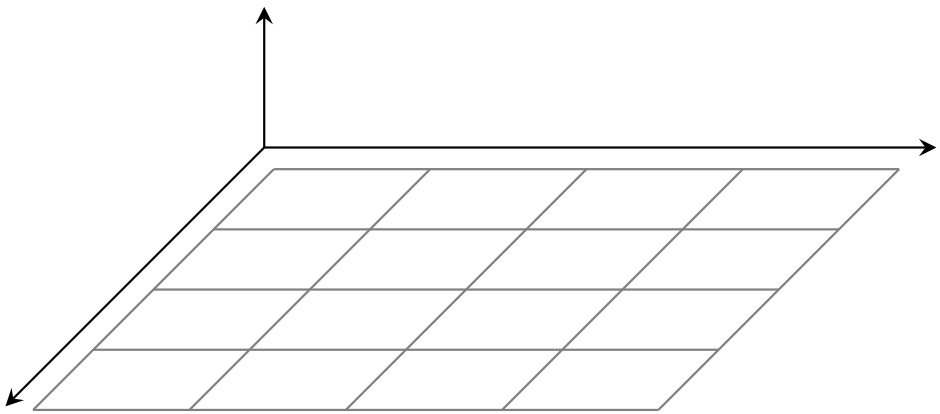
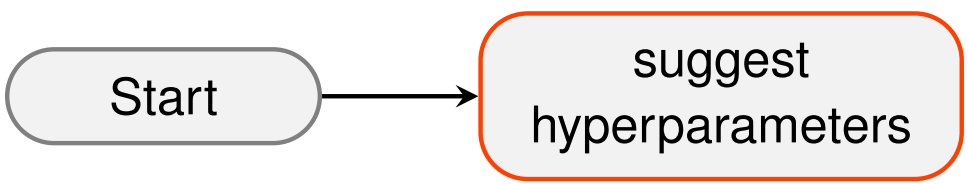


Start

TUNING





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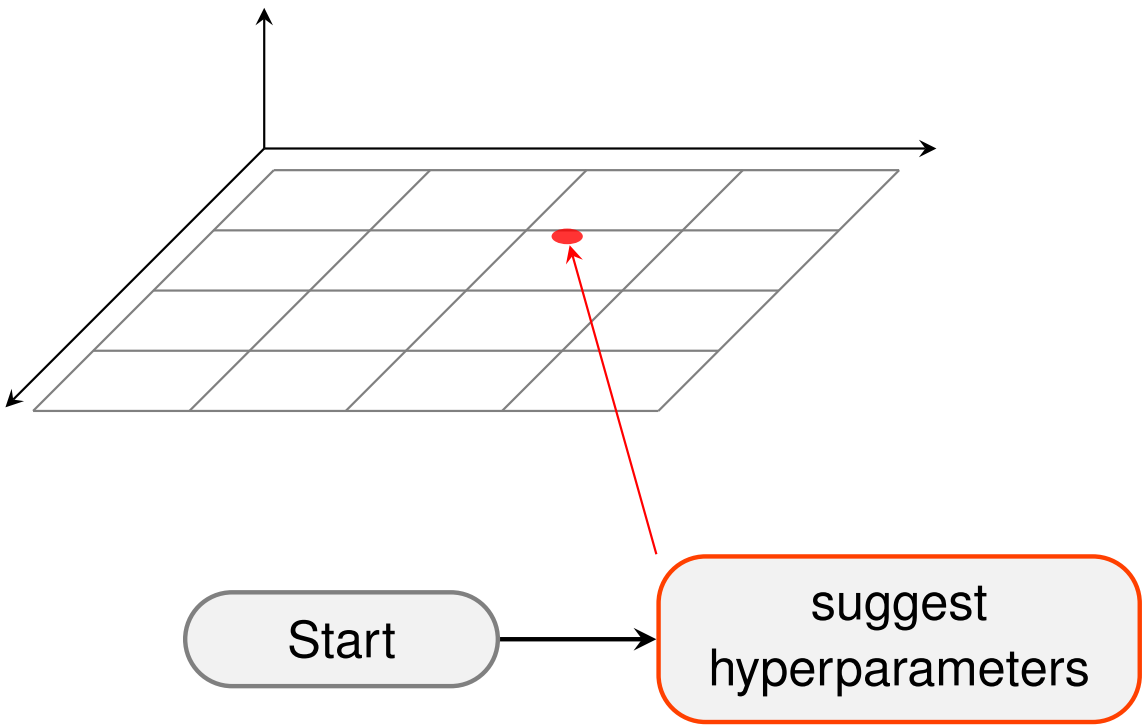

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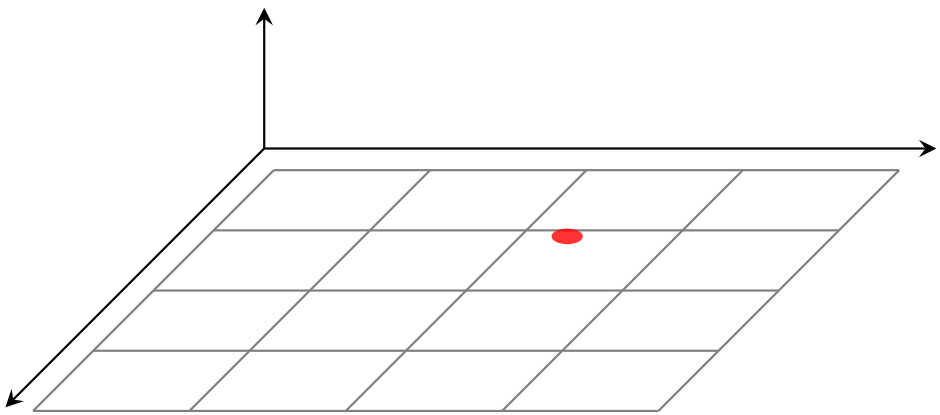

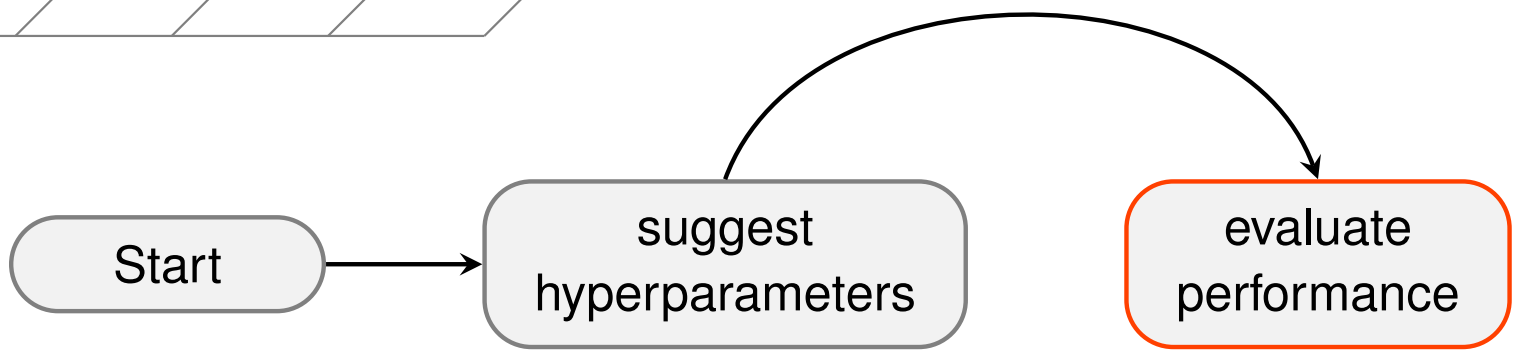

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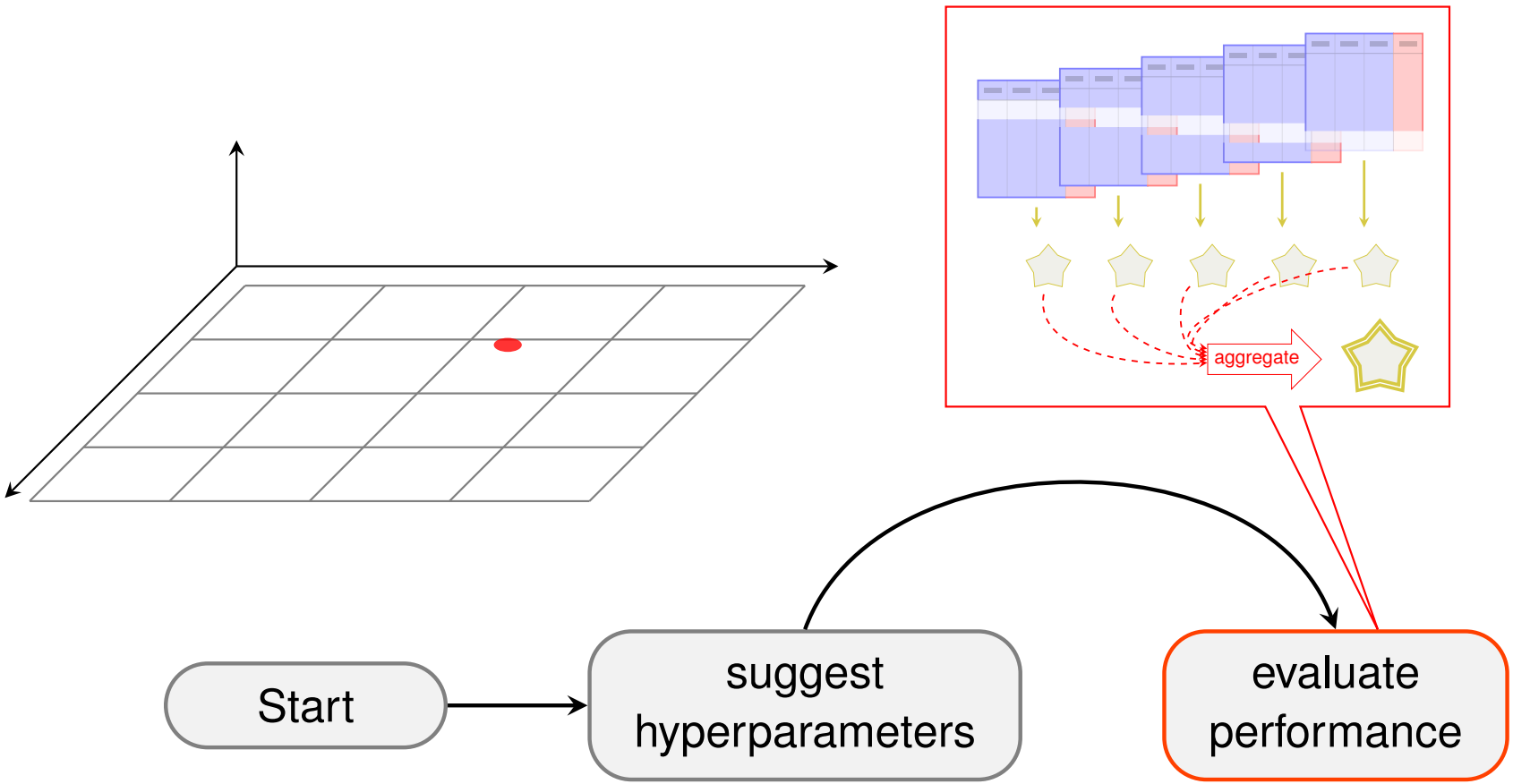
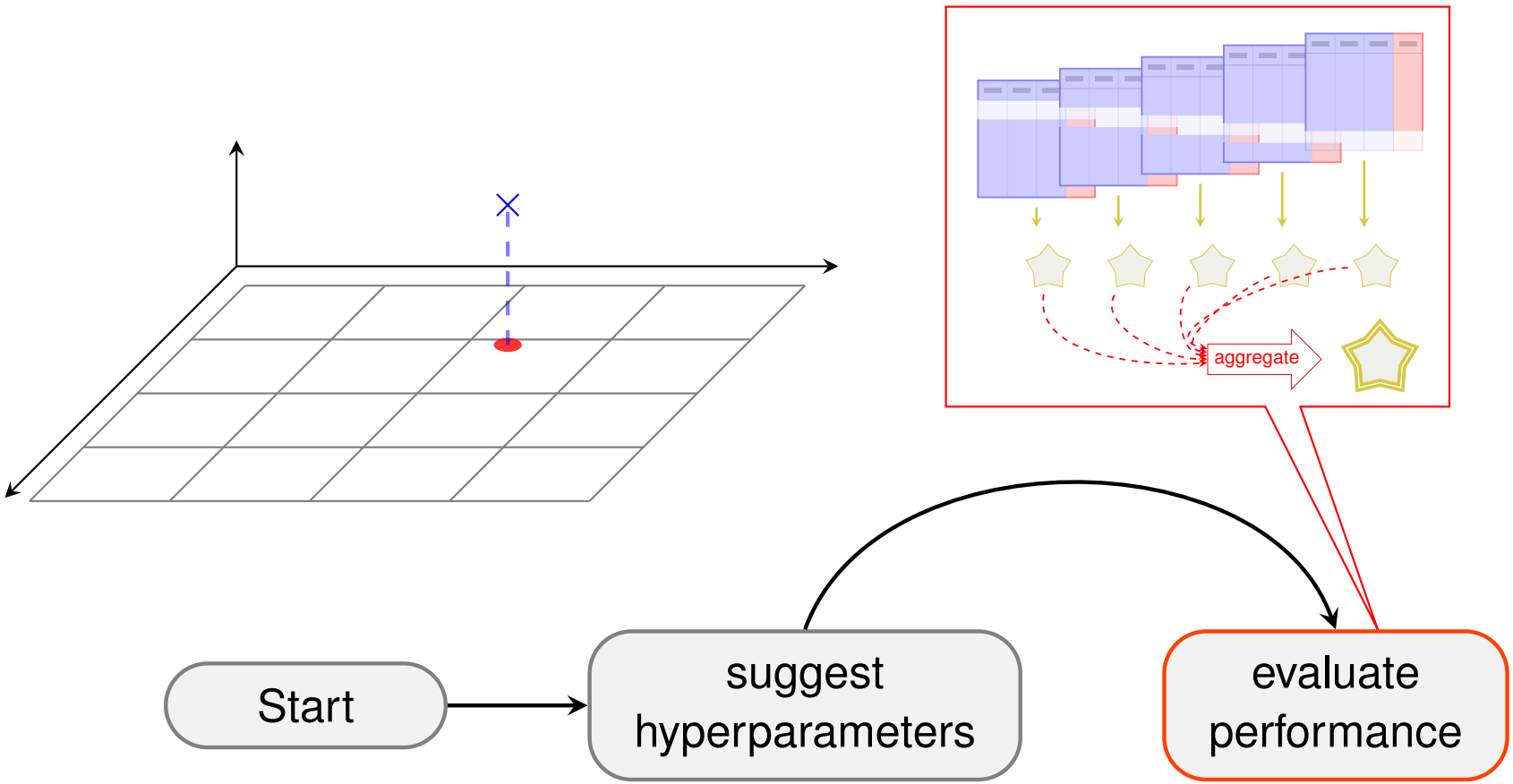

aggregate
Start
suggest hyperparameters
evaluate performance

TUNING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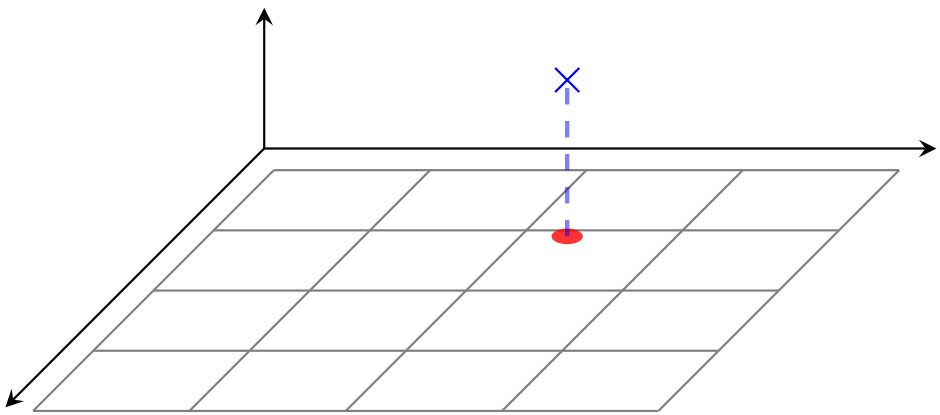

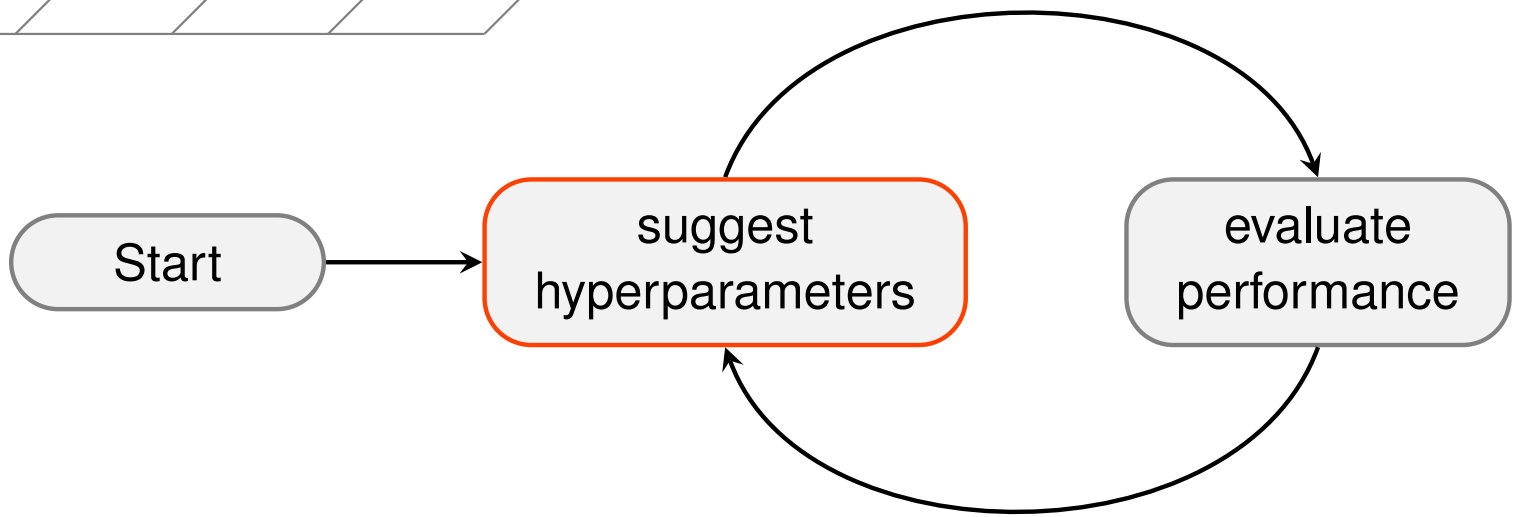

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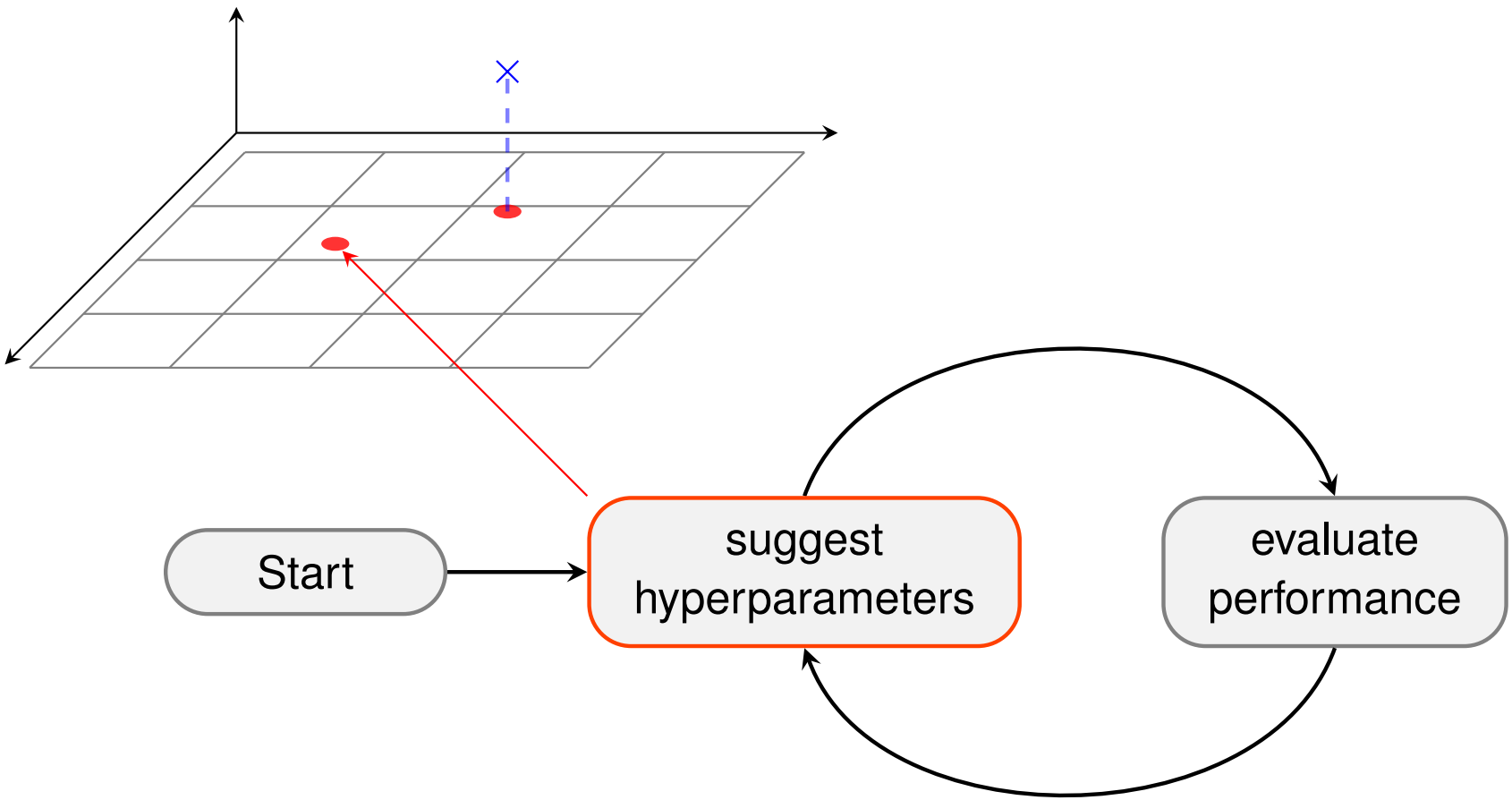

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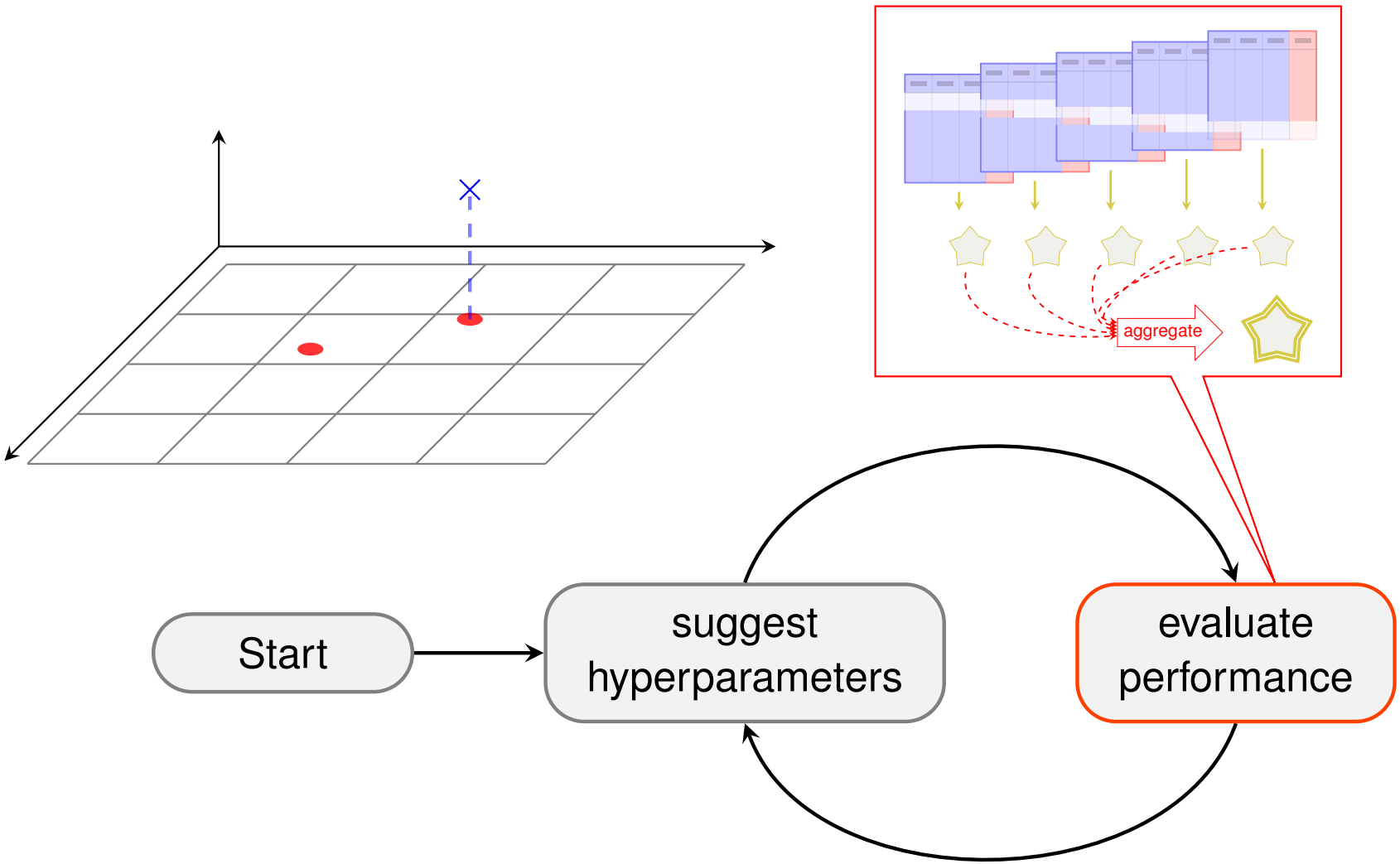
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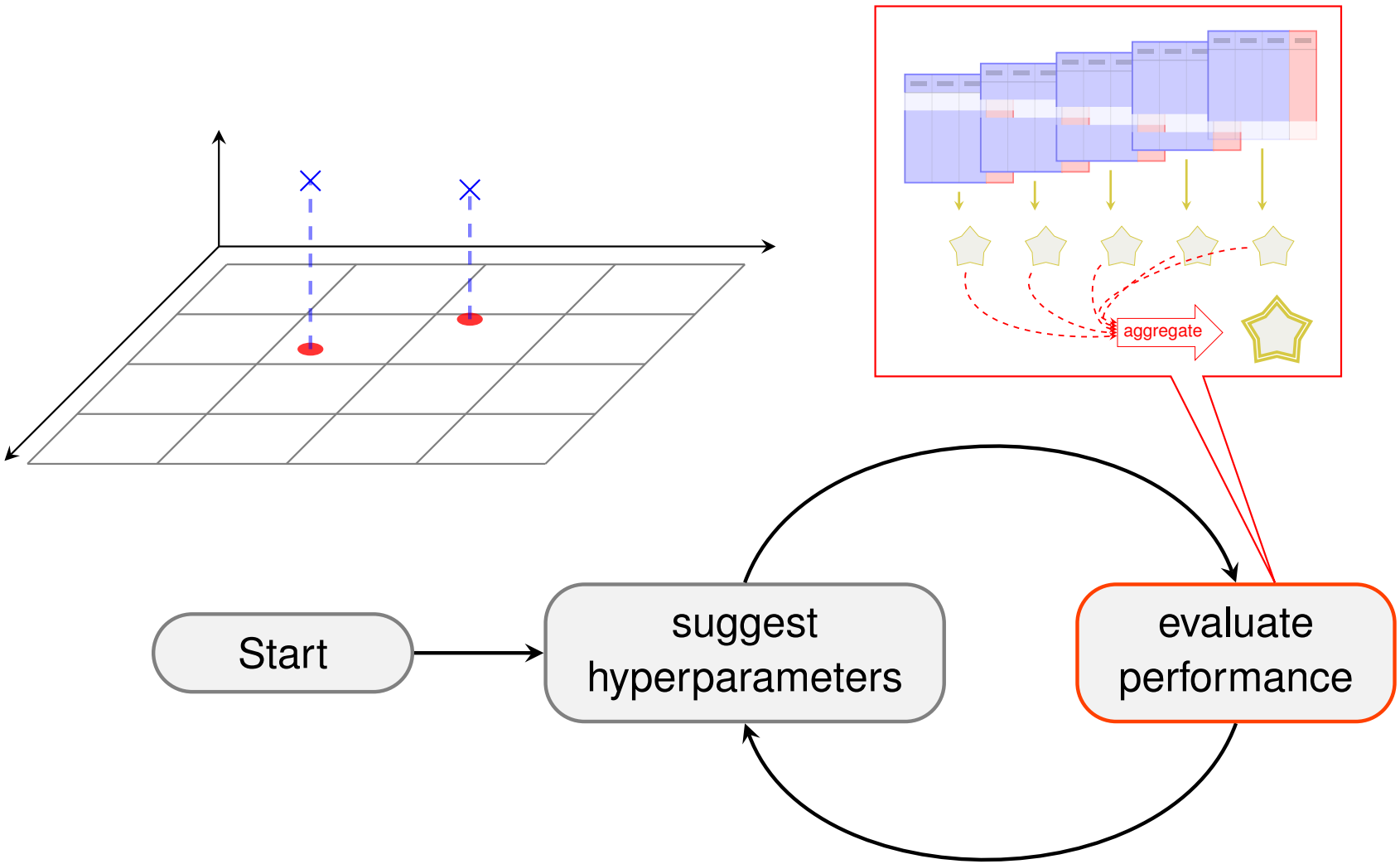
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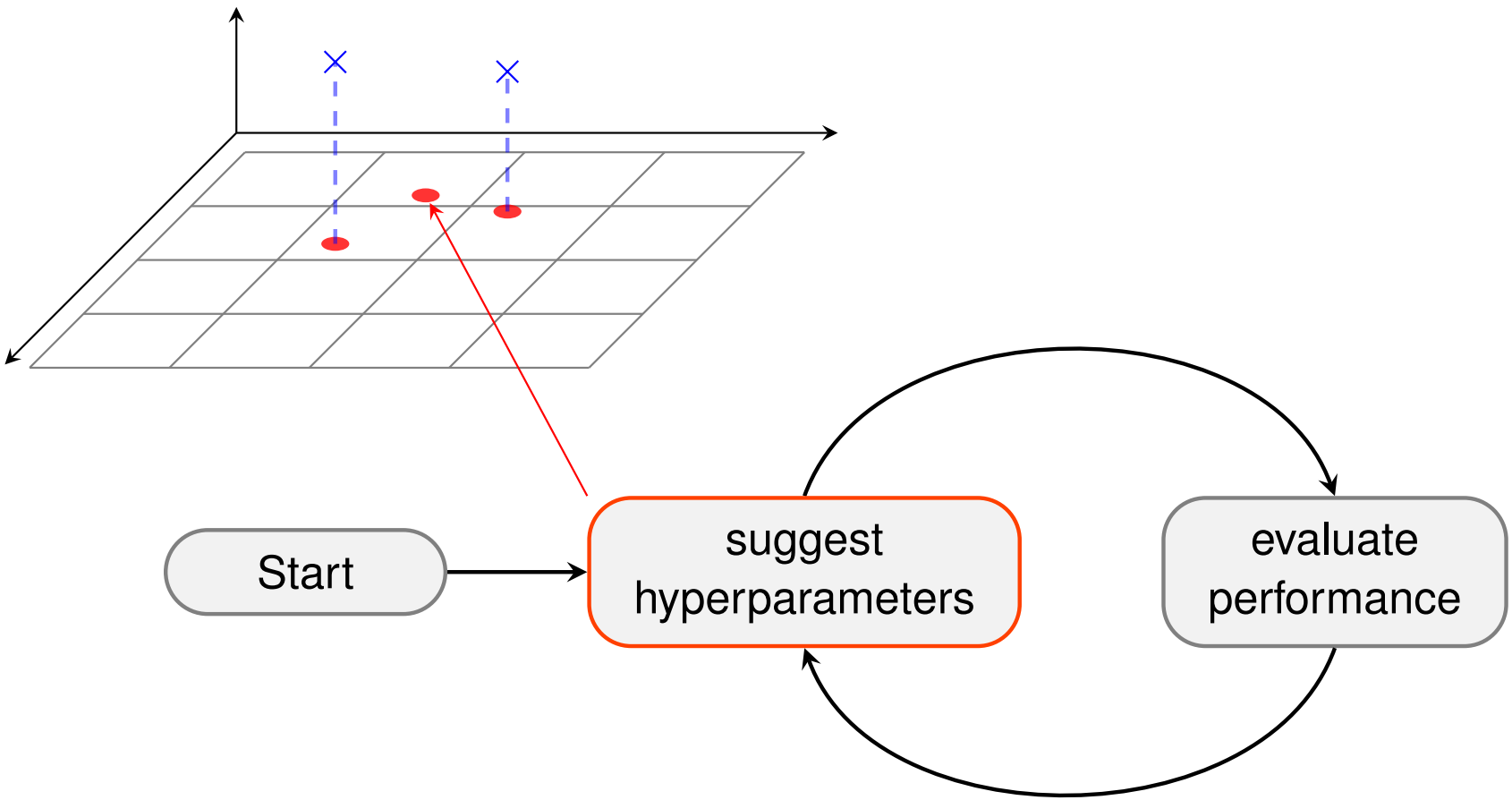

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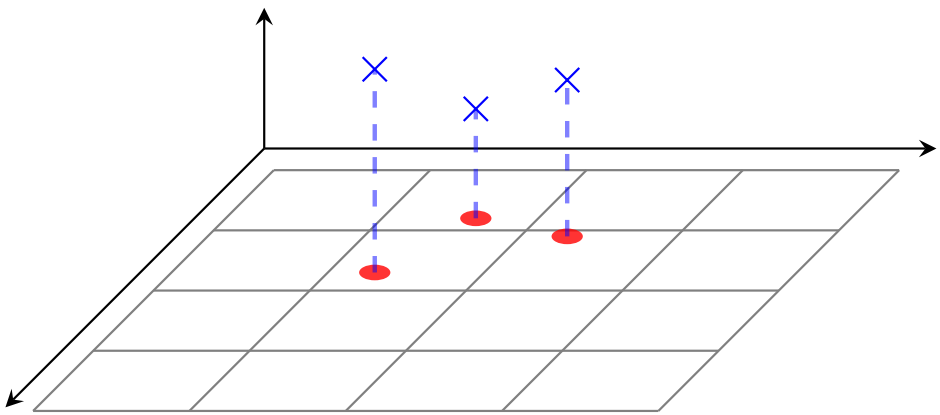

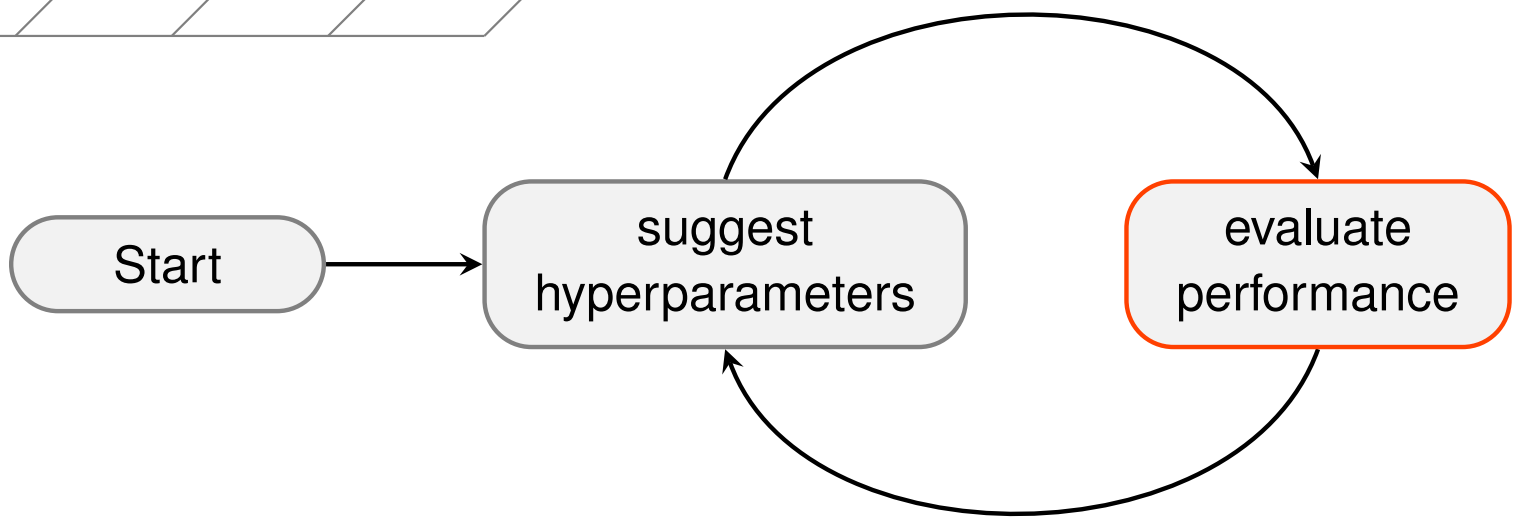

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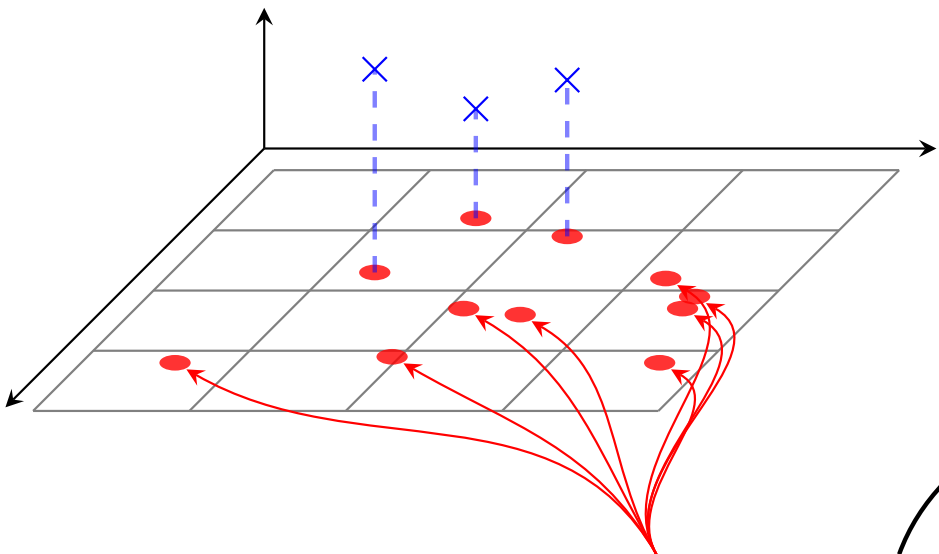
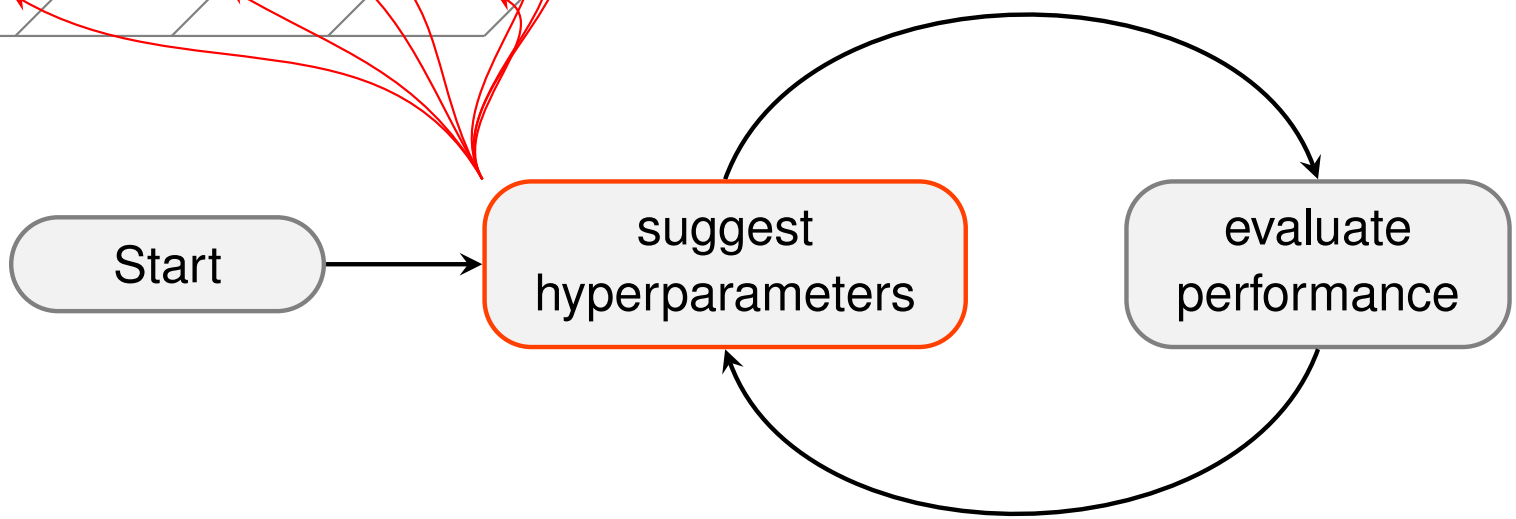


Batch evaluation



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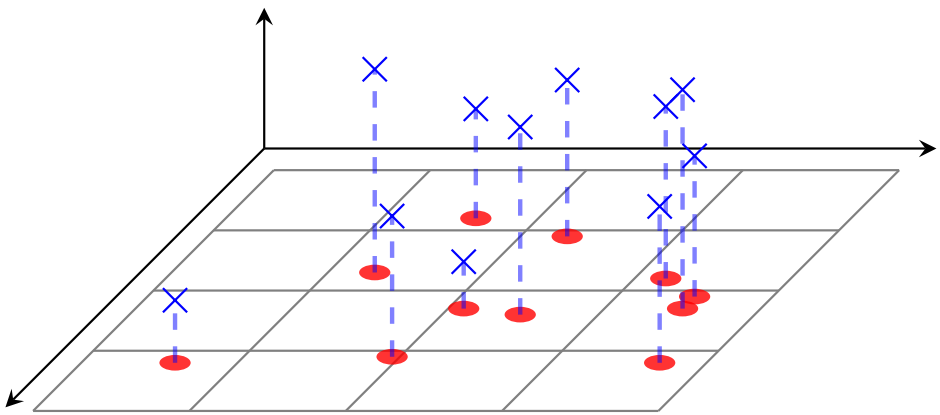

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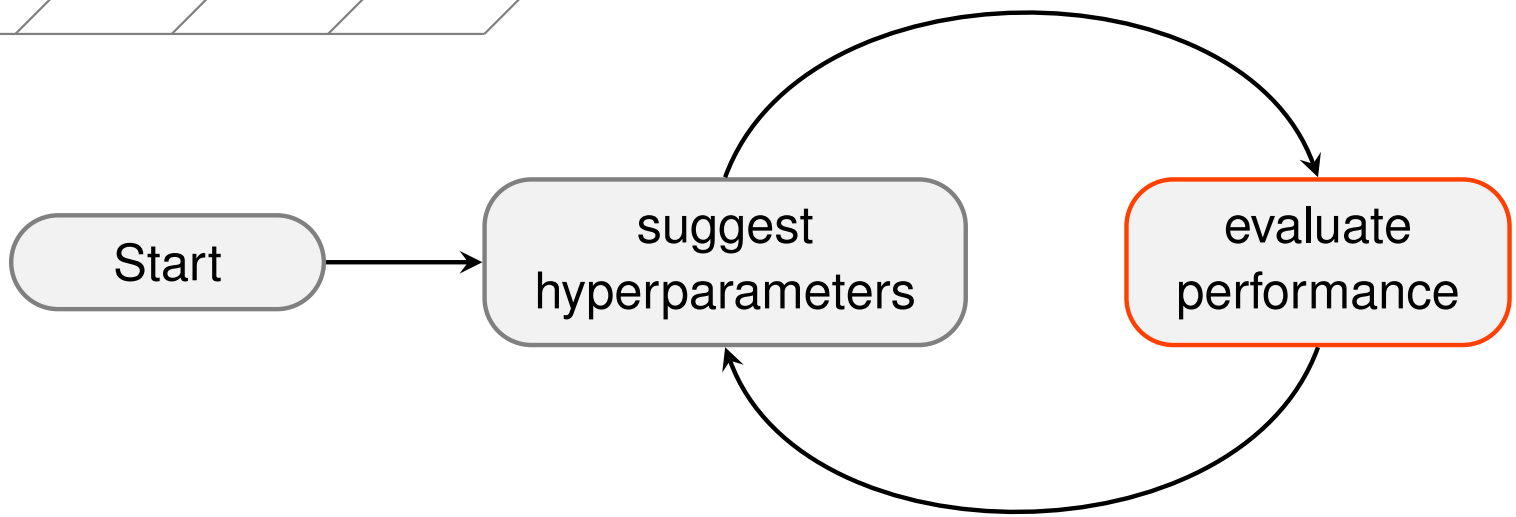

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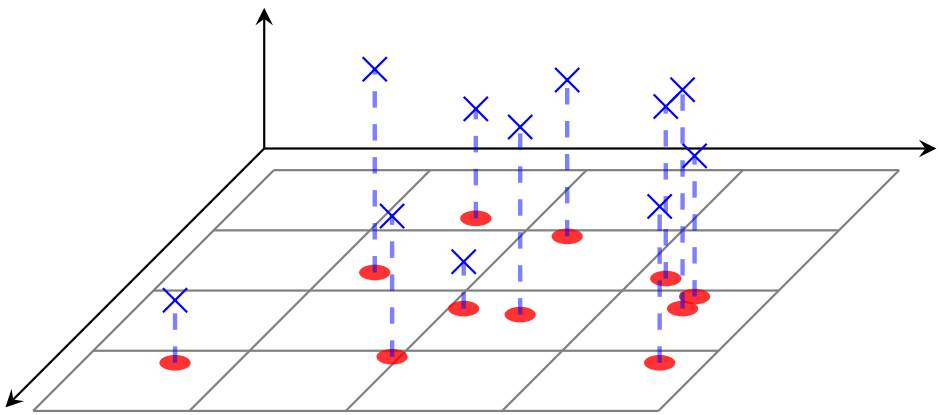

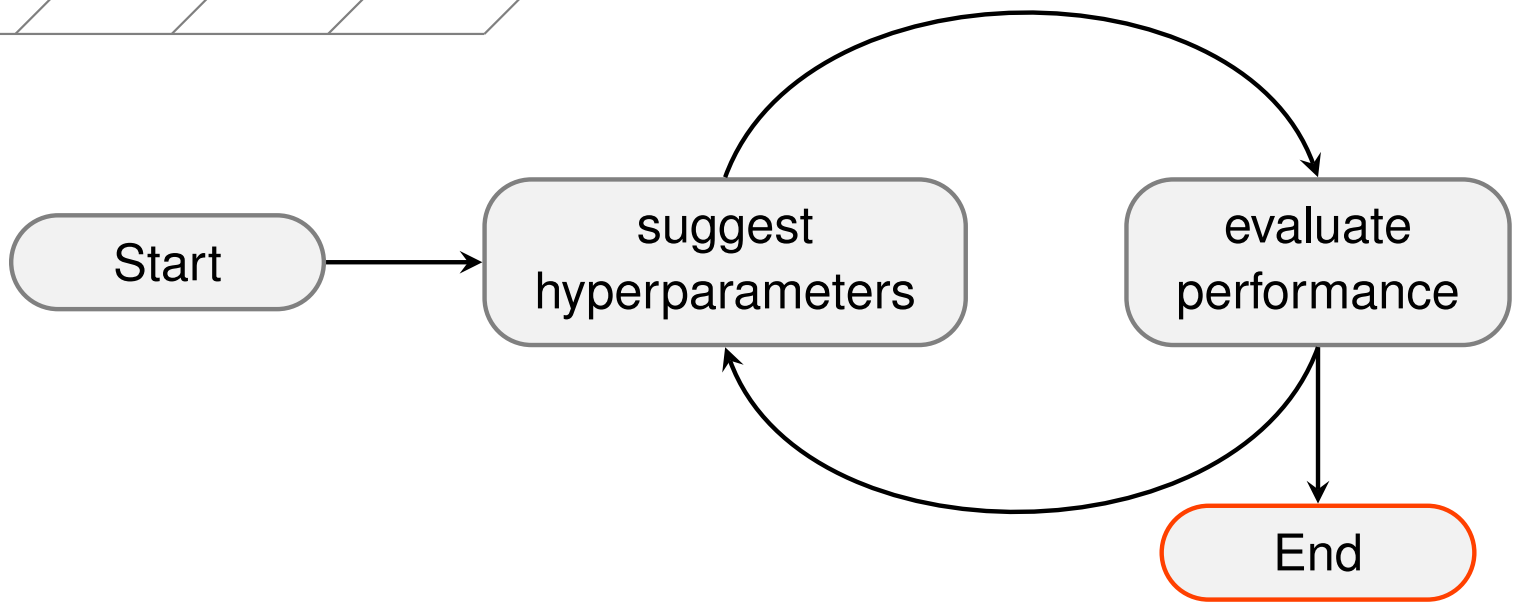

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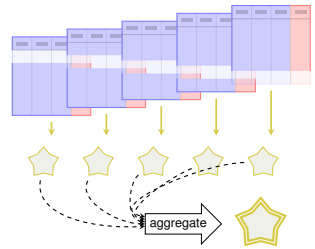
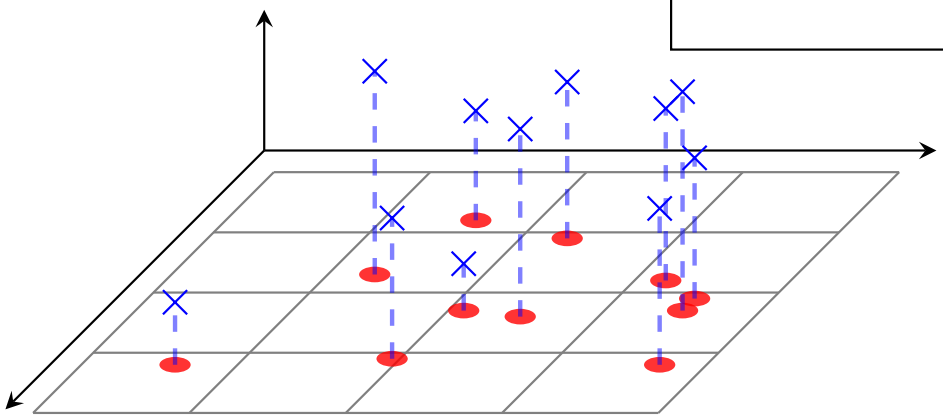
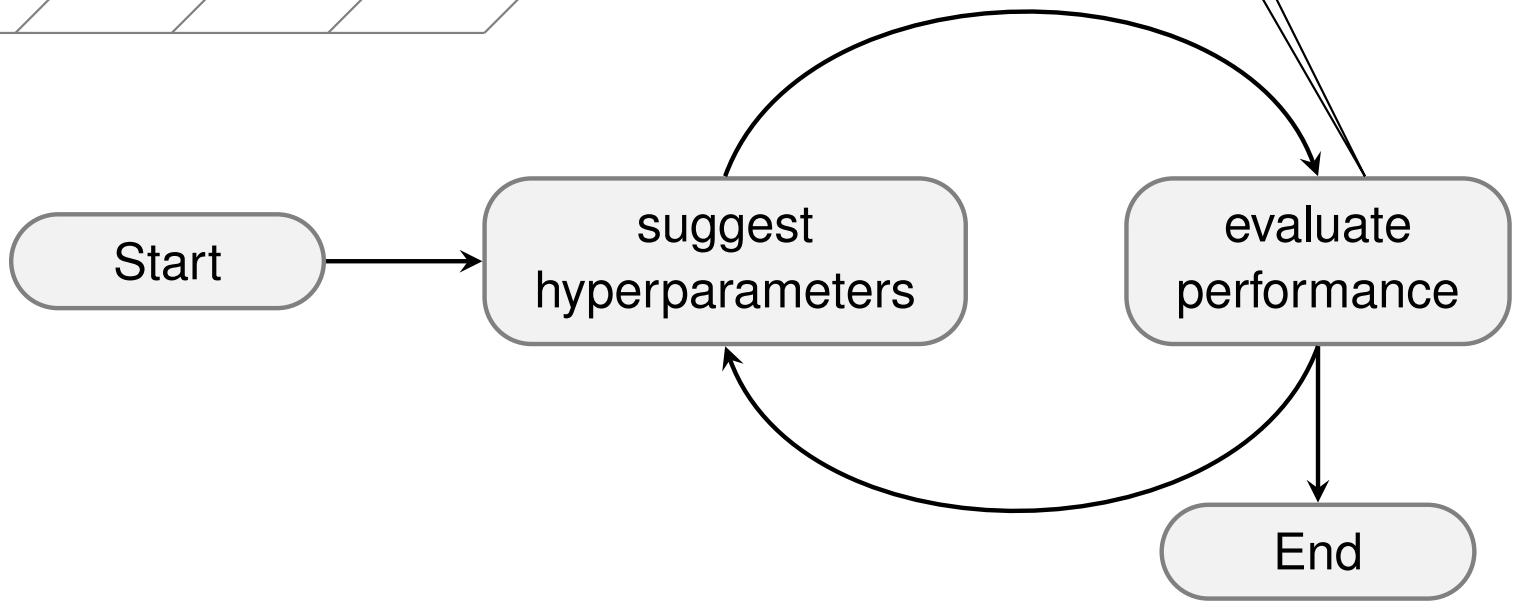


`Learner (lrn())`
`Task`
`Resampling (rsmp())`
`Measure (msr())`





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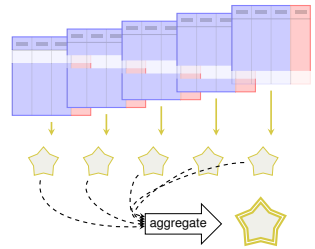

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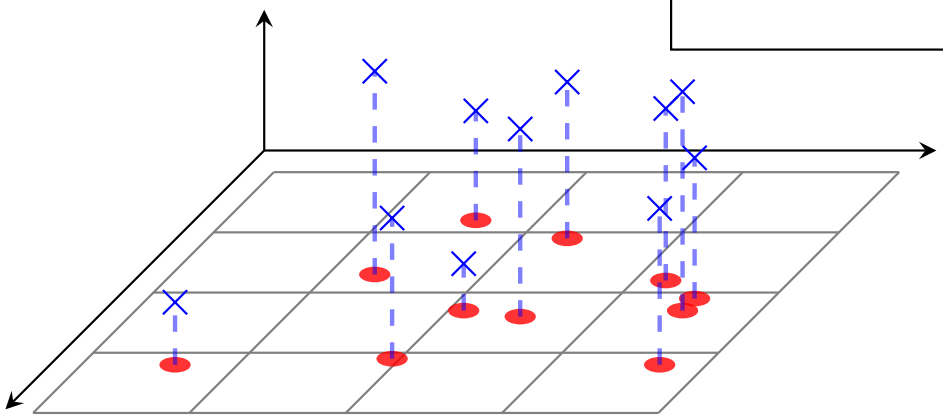


Start

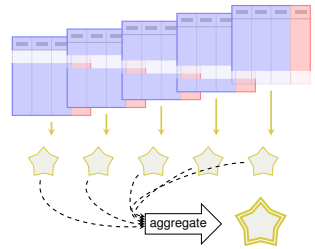
suggest hyperparameters

evaluate performance

End

search space
`Tuner`

TUNING



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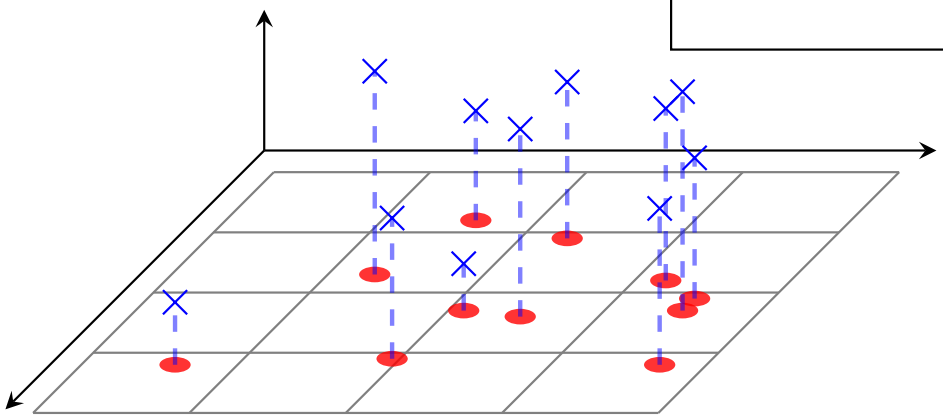


Start

suggest hyperparameters

evaluate performance

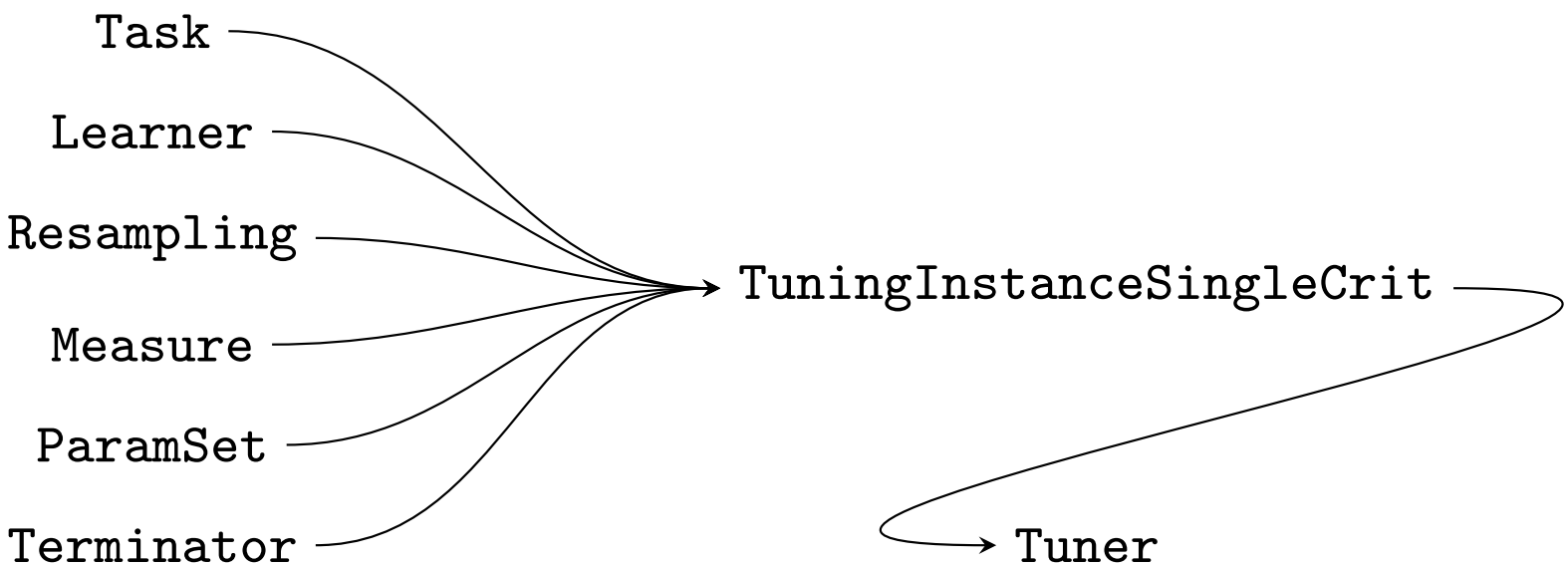
search space
`Tuner`

`Terminator` (when to finish)

End

Tuning in mlr3

OBJECTS IN TUNING



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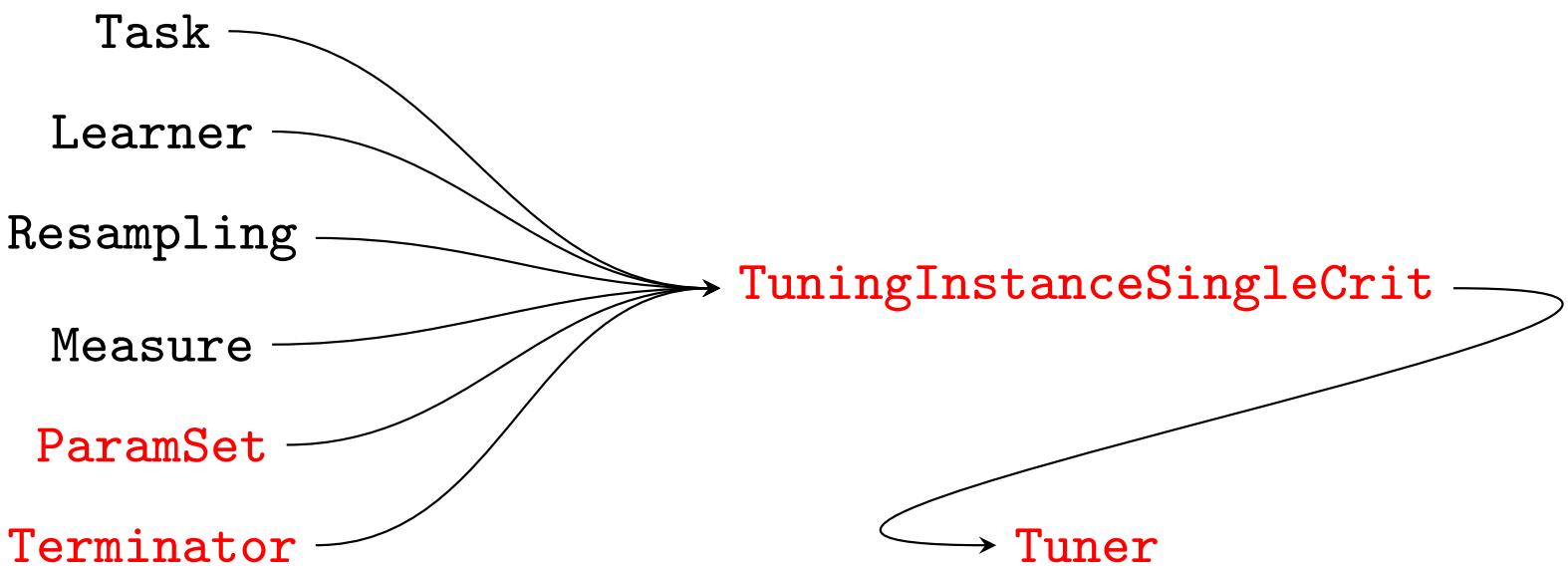
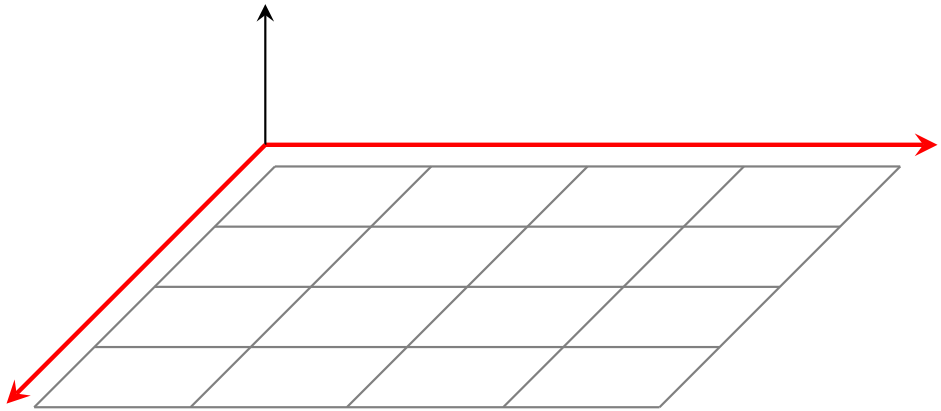


SEARCH SPACE



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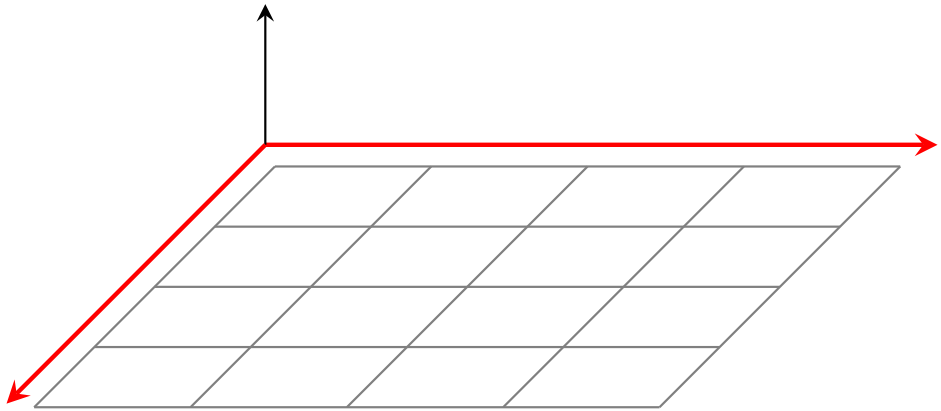
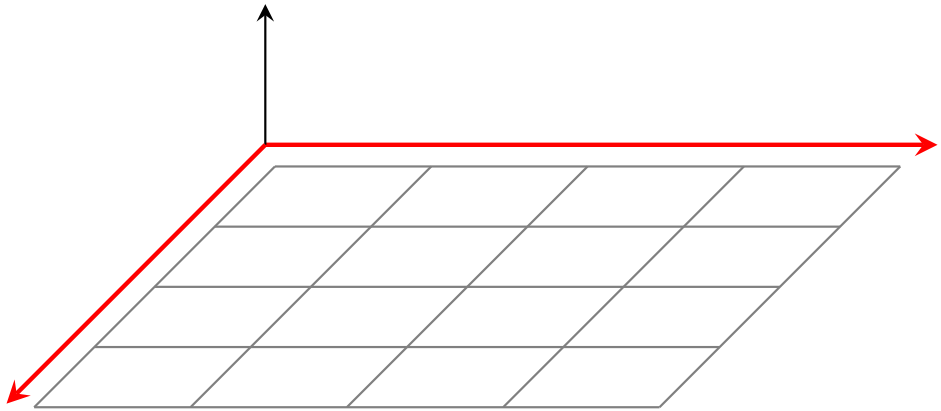


```
ParamSet$new(list(param1, param2, ...))
```

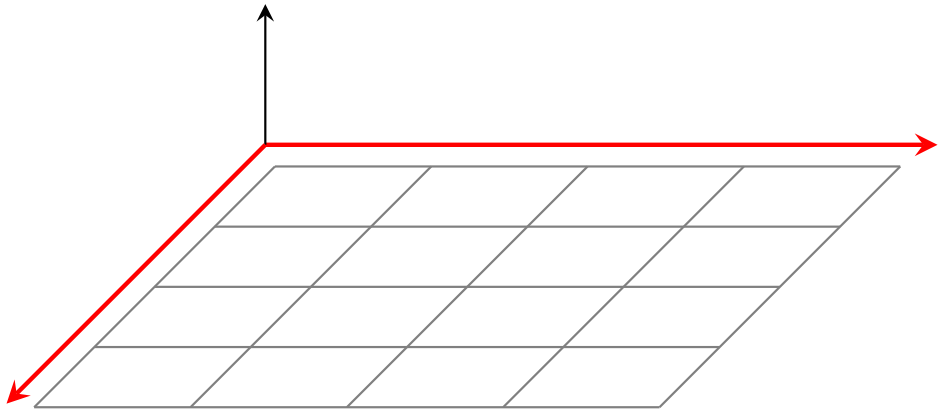
SEARCH SPACE



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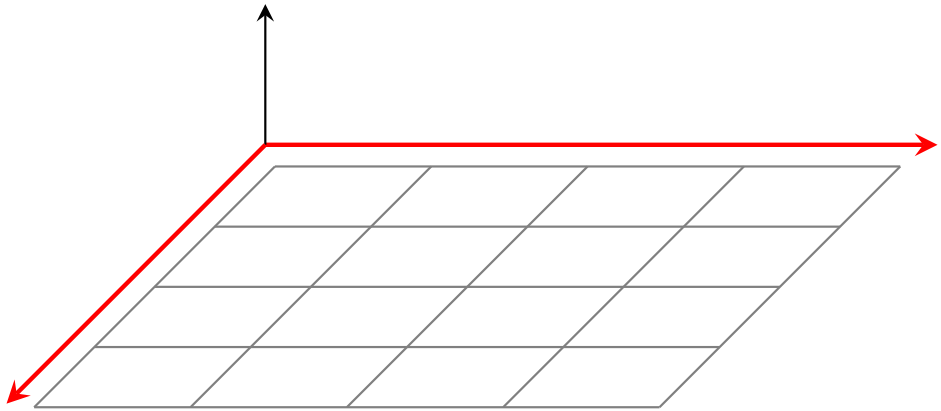
```
library("paradox")
searchspace_knn = ParamSet$new(list(
  ParamInt$new("k", lower = 1, upper = 20)
))
```

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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- `Terminator` class

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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
  ```
  ```

TERMINATION

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- `Terminator` class
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#> 5:     perf_reached
#> 6:         run_time
#> 7:       stagnation
#> 8: stagnation_batch
```

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

TUNING METHOD

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- `Tuner` class

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- `Tuner` class
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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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-
```
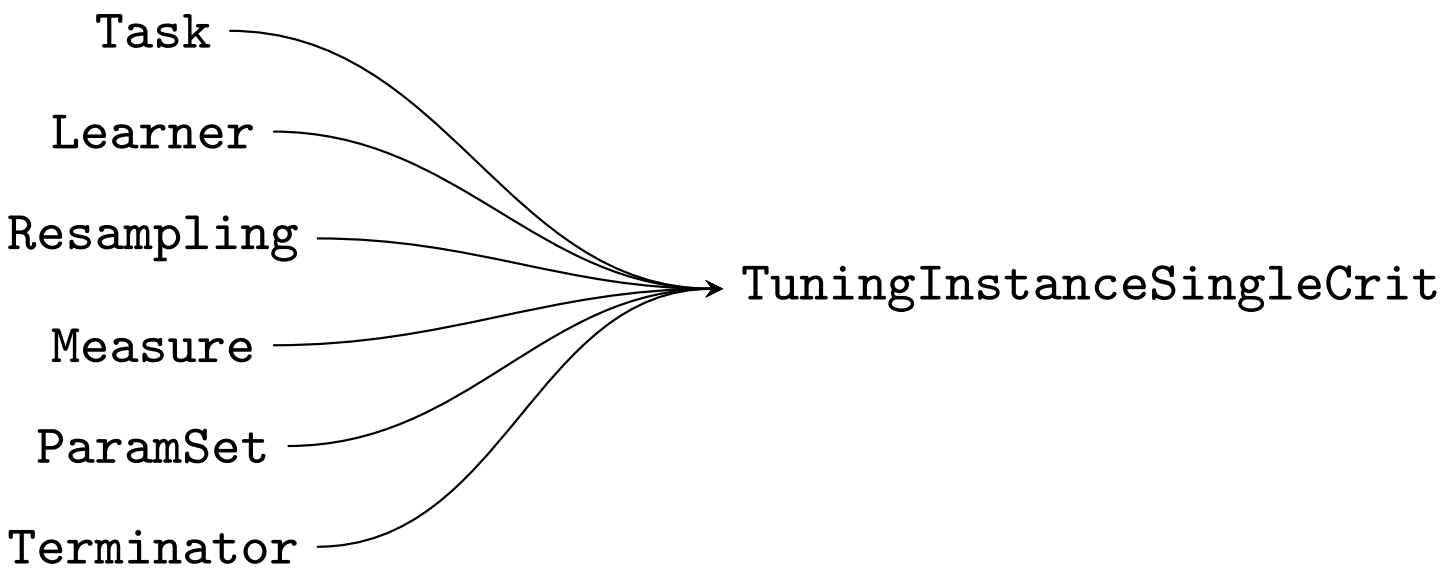
gsearch = tnr("grid_search", resolution = 3)

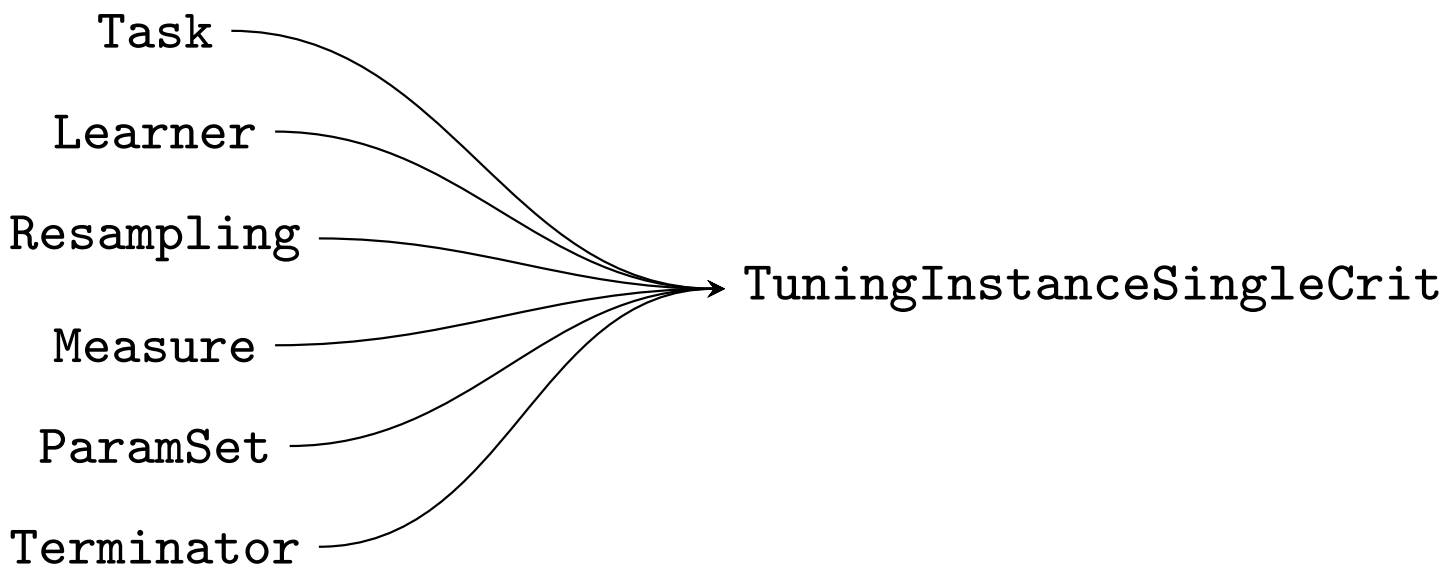
print(gsearch)
#> <TunerGridSearch>
#> * Parameters: resolution=3, batch_size=1
#> * Parameter classes: ParamLgl, ParamInt, ParamDbl, ParamFct
#> * Properties: dependencies, single-crit, multi-crit
#> * Packages: -
```

TUNING METHOD

- 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: -
  ```
- common parameter `batch_size` for parallelization
  ```

CALLING THE TUNER



CALLING THE TUNER



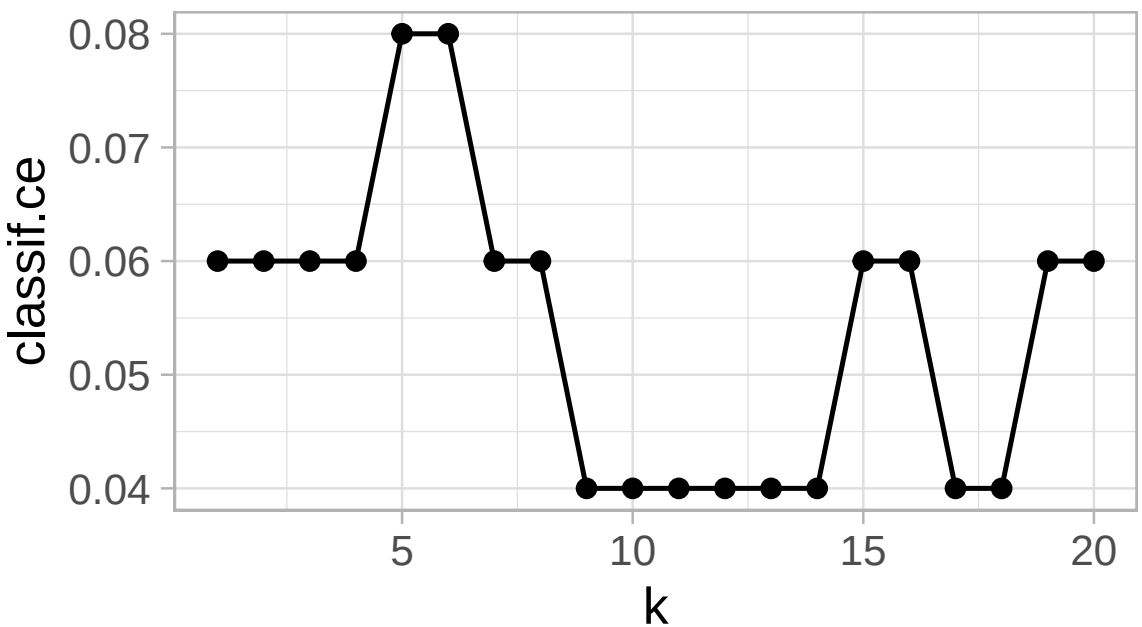

```
inst = TuningInstanceSingleCrit$new(task = tsk("iris"),
  learner = lrn("classif.kknn", kernel = "rectangular"),
  resampling = rsmp("holdout"), measure = msr("classif.ce"),
  terminator = trm("none"), search_space = searchspace_knn
)
```

CALLING THE TUNER

```
gsearch$optimize(inst)

#> INFO  [10:07:50.176] [bbotk] Starting to optimize 1 parameter(s) with '<Optim
#> INFO  [10:07:50.247] [bbotk] Evaluating 1 configuration(s)
#> INFO  [10:07:51.452] [bbotk] Result of batch 1:
#> INFO  [10:07:51.455] [bbotk]   k classif.ce                                  u
#> INFO  [10:07:51.455] [bbotk]  10       0.04 f40e0ddd-c858-4e54-8cf7-3b31bdce
#> INFO  [10:07:51.456] [bbotk] Evaluating 1 configuration(s)
#> INFO  [10:07:51.552] [bbotk] Result of batch 2:
#> INFO  [10:07:51.554] [bbotk]  k classif.ce                                 uh
#> INFO  [10:07:51.554] [bbotk]  1       0.06 be9d13a6-b039-4c6a-b1e7-7b759bfc1
#> INFO  [10:07:51.555] [bbotk] Evaluating 1 configuration(s)
#> INFO  [10:07:51.694] [bbotk] Result of batch 3:
#> INFO  [10:07:51.695] [bbotk]   k classif.ce                                  u
#> INFO  [10:07:51.695] [bbotk]  20       0.08 891af82b-6c9c-4b37-9d33-477d12e3
#> INFO  [10:07:51.703] [bbotk] Finished optimizing after 3 evaluation(s)
#> INFO  [10:07:51.704] [bbotk] Result:
#> INFO  [10:07:51.706] [bbotk]   k learner_param_vals  x_domain classif.ce
#> INFO  [10:07:51.706] [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

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

```
gsearch = tnr("grid_search", resolution = 3)

inst = TuningInstanceSingleCrit$new(task = tsk("iris"),
  learner = lrn("classif.kknn", kernel = "rectangular"),
  resampling = rsmp("holdout"), measure = msr("classif.ce"),
  terminator = trm("evals", n_evals = 2), search_space = searchspace_knn)

gsearch$optimize(inst)

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

Parameter Transformation

PARAMETER TRANSFORMATION

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Example:

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Example:

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

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Example:

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2. transform by $\exp()$ in `trafo` function

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Example:

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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)

```
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?

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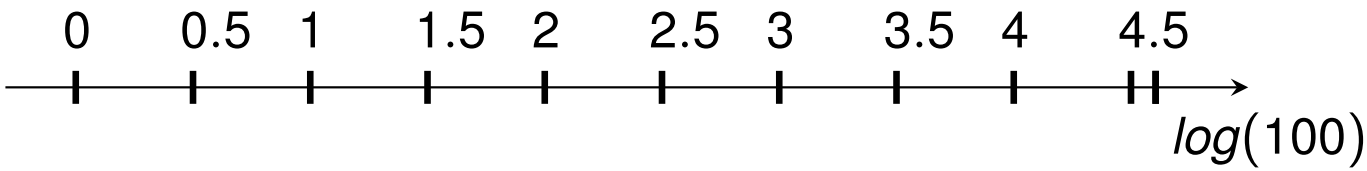
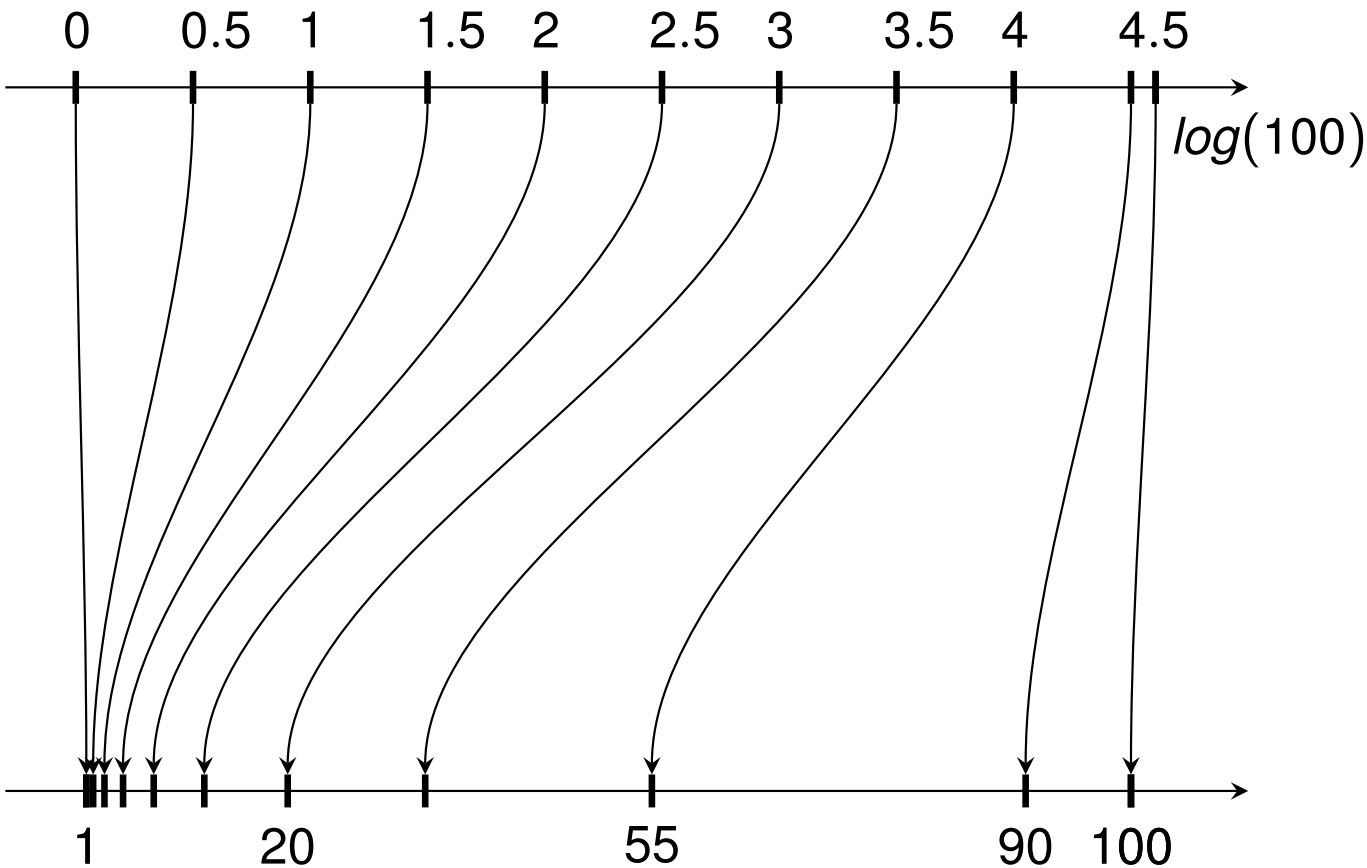
What is our transformation doing?



PARAMETER TRANSFORMATION

What is our transformation doing?



PARAMETER TRANSFORMATION

Tuning again. . .

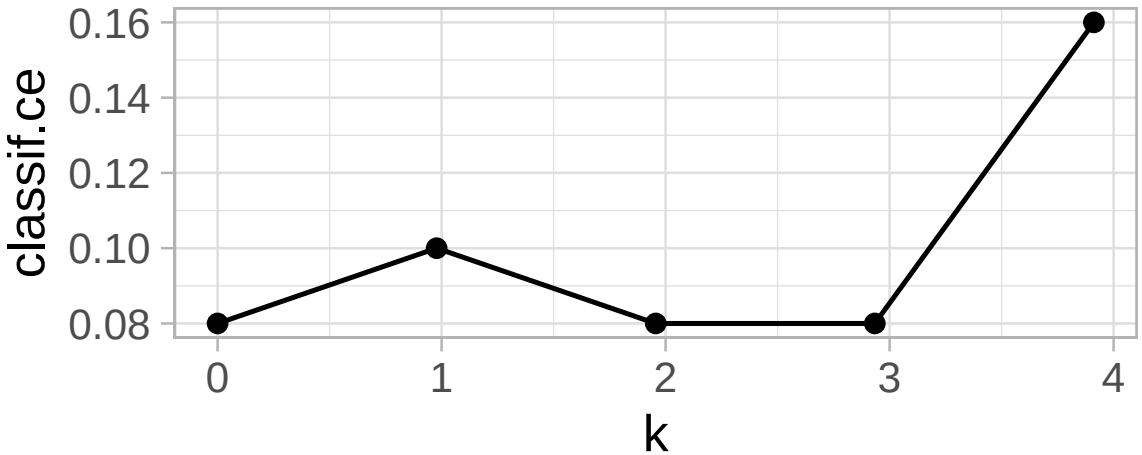
PARAMETER TRANSFORMATION

Tuning again. . .

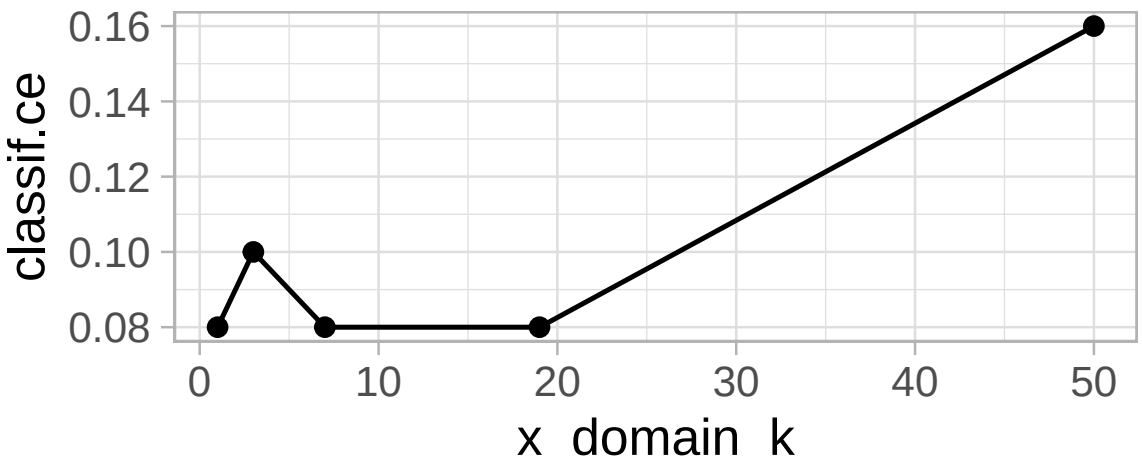
```
inst$result

#>      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

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




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



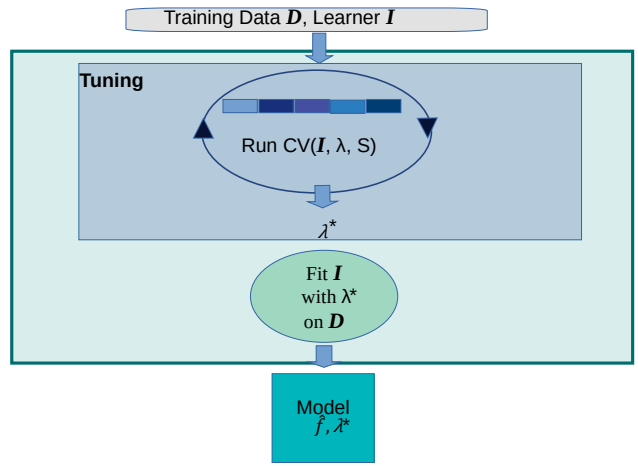
Nested Resampling

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

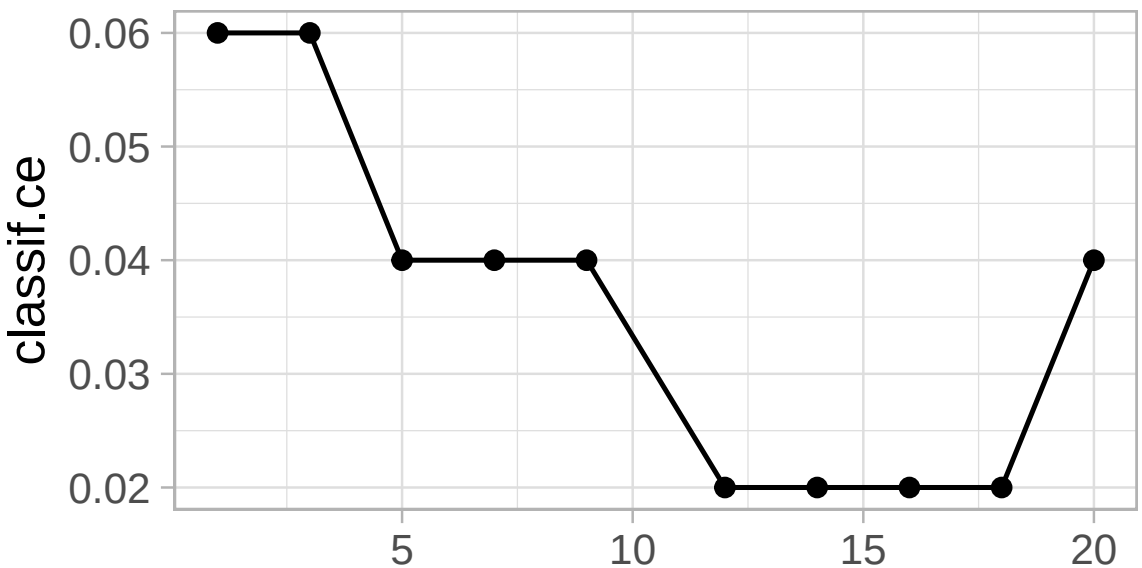
```
optlrn = AutoTuner$new(
  learner = lrn("classif.kknn", kernel = "rectangular"),
  resampling = rsmp("holdout"), measure = msr("classif.ce"),
  terminator = trm("none"),
  tuner = tnr("grid_search", resolution = 10),
  search_space = searchspace_knn)
```

```
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

```
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("")
```