LMU LUDWIG-MAXIMILIANS-UNIVERSITÄT MÜNCHEN

Tuning Machine Learning Algorithms with mlr3

mlr3tuning

Department of Statistics – LMU Munich

Intro

TUNING

- Behavior of most methods depends on *hyperparameters*

TUNING

- Behavior of most methods depends on *hyperparameters*
- We want to choose them so our algorithm performs well

TUNING

- Behavior of most methods depends on *hyperparameters*
- We want to choose them so our algorithm performs well
- Good hyperparameters are data-dependent

TUNING

- Behavior of most methods depends on *hyperparameters*
- We want to choose them so our algorithm performs well
- Good hyperparameters are data-dependent

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

TUNING

- Behavior of most methods depends on *hyperparameters*
- We want to choose them so our algorithm performs well
- Good hyperparameters are data-dependent

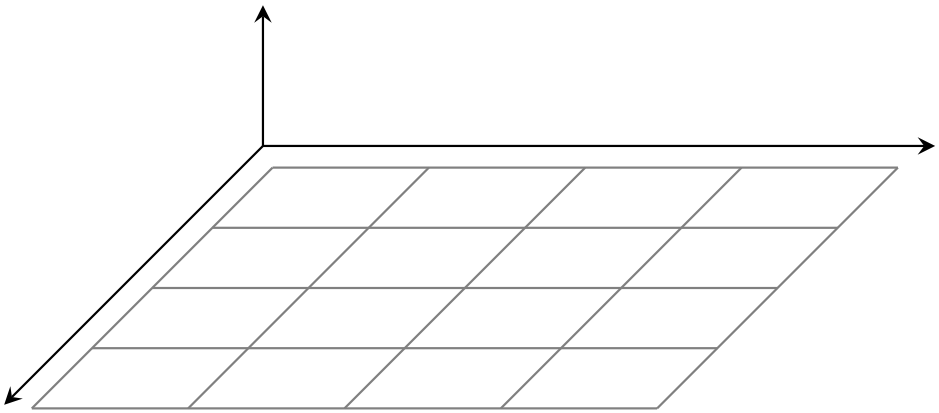
$\Rightarrow$ We do *black box optimization* (“Try stuff and see what works”)

Tuning toolbox for `mlr3`:

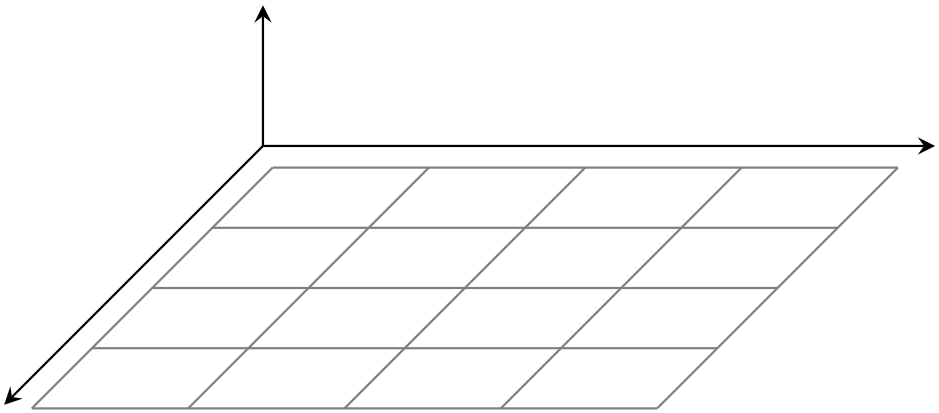
```
library("mlr3tuning")
```

Tuning

TUNING

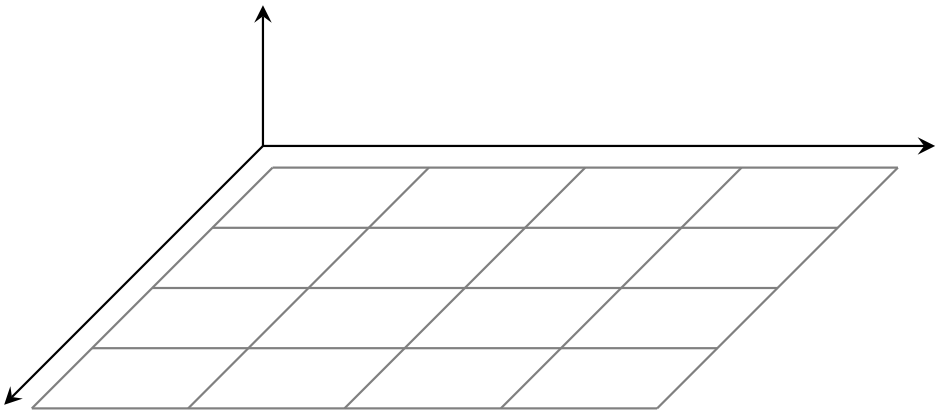


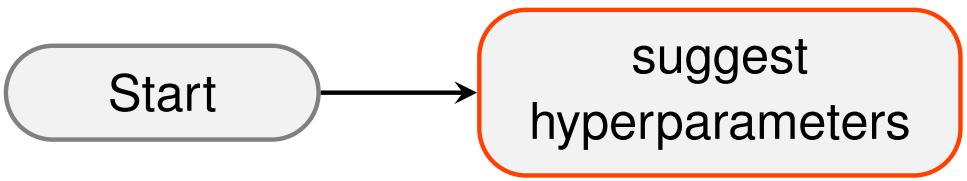
TUNING



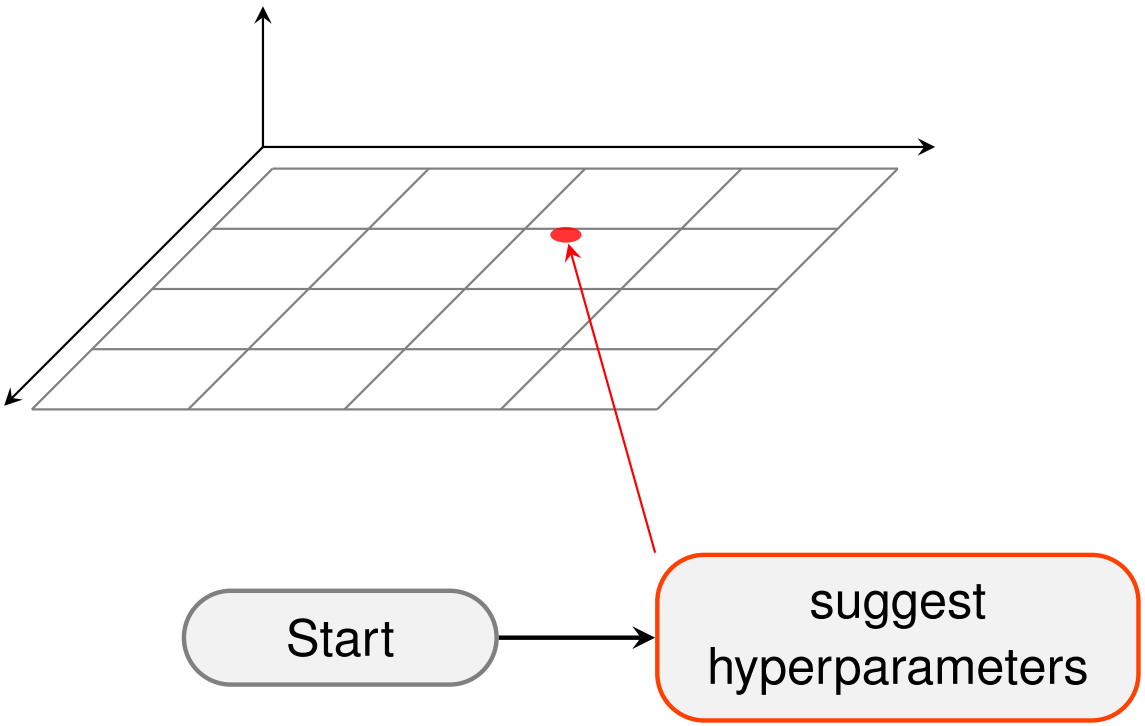
Start

TUNING

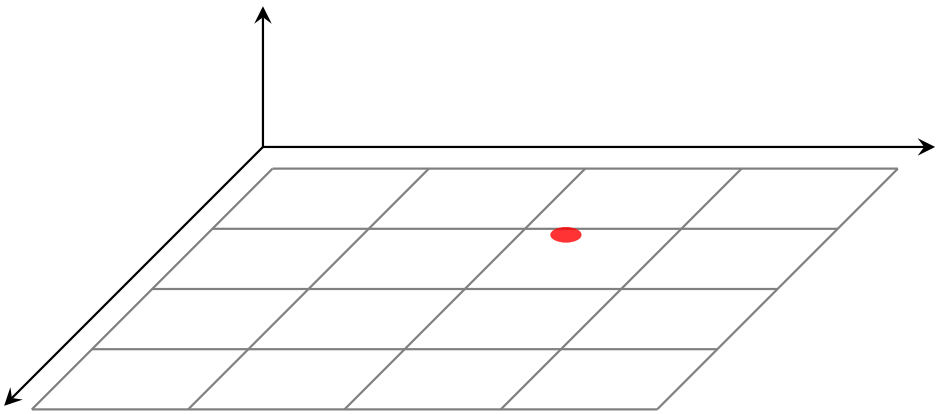


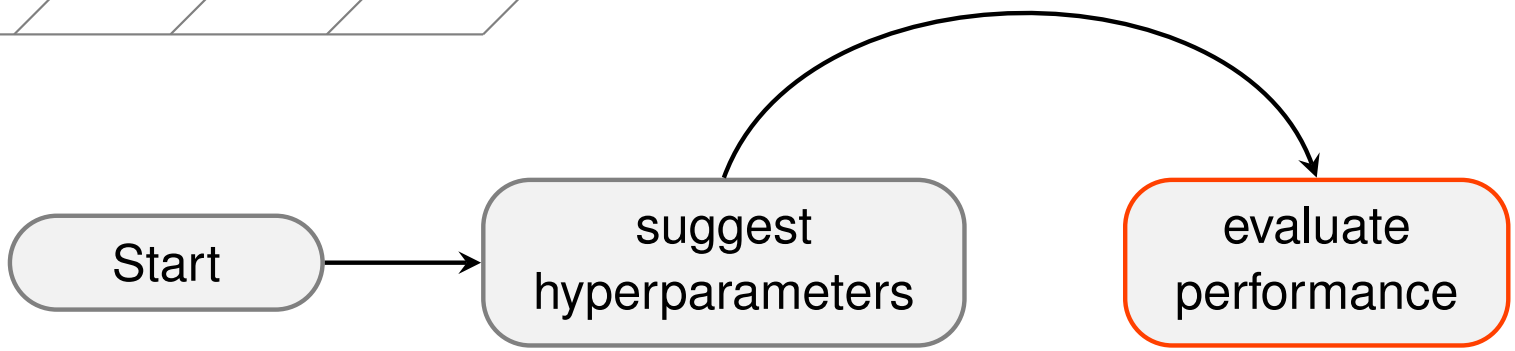


TUNING

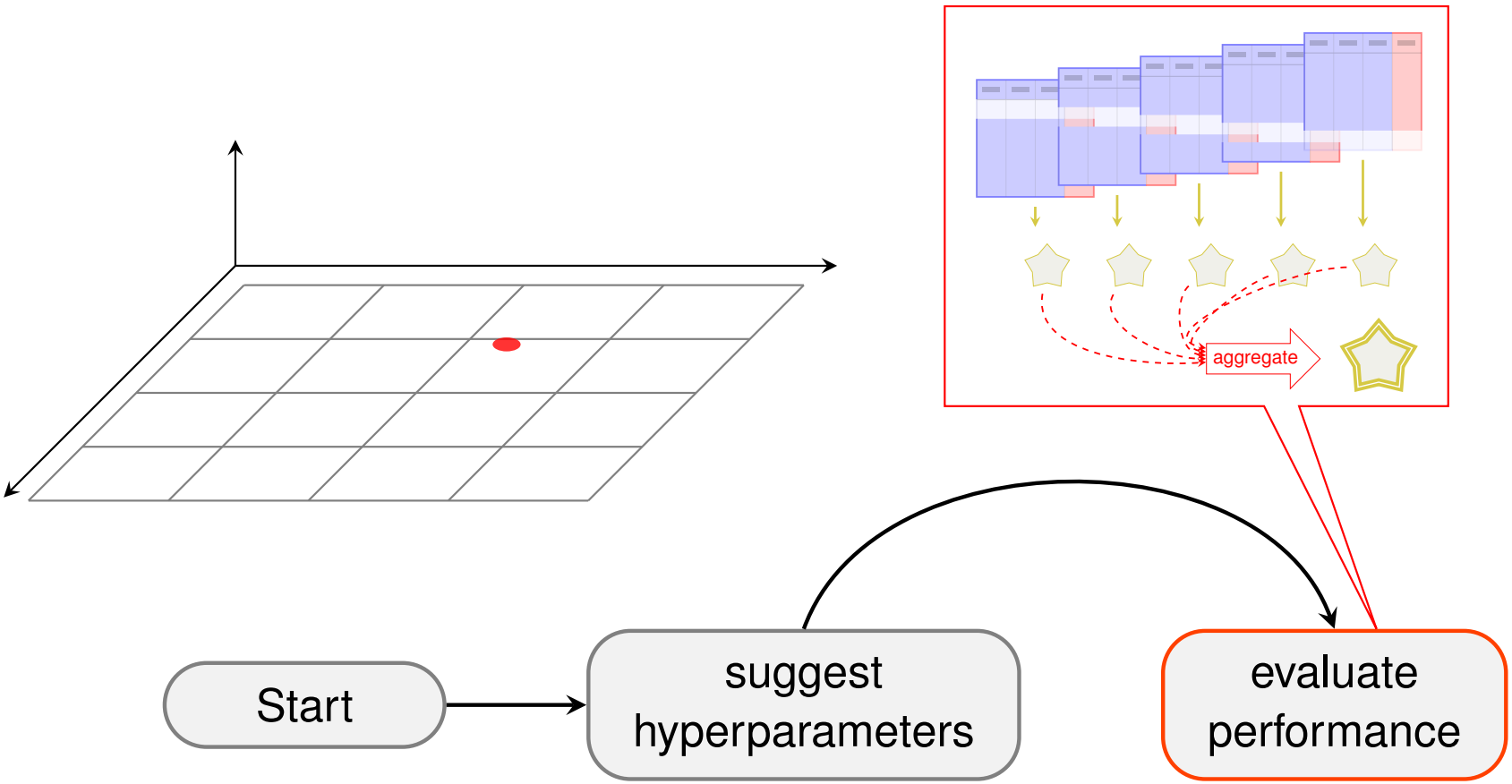


TUNING

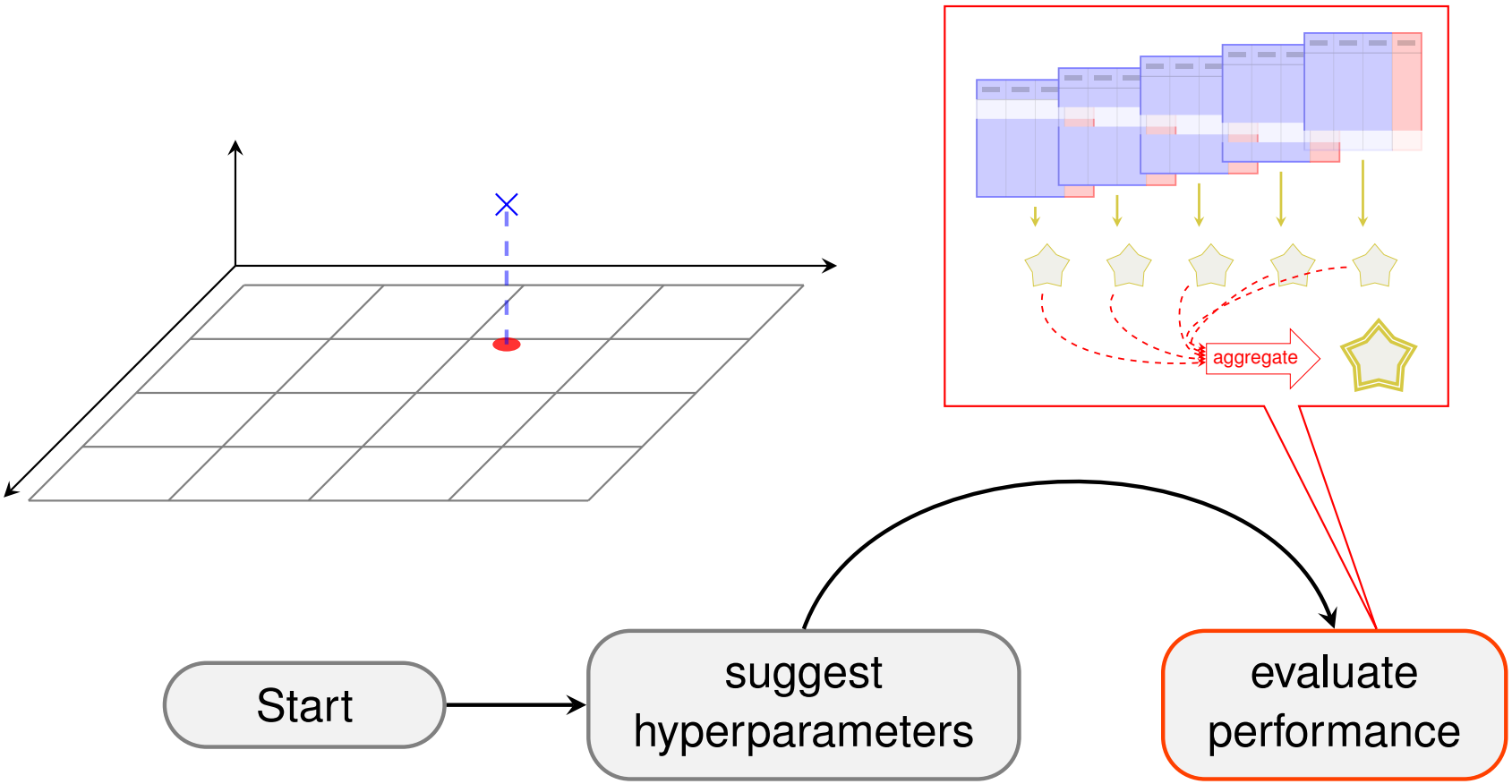




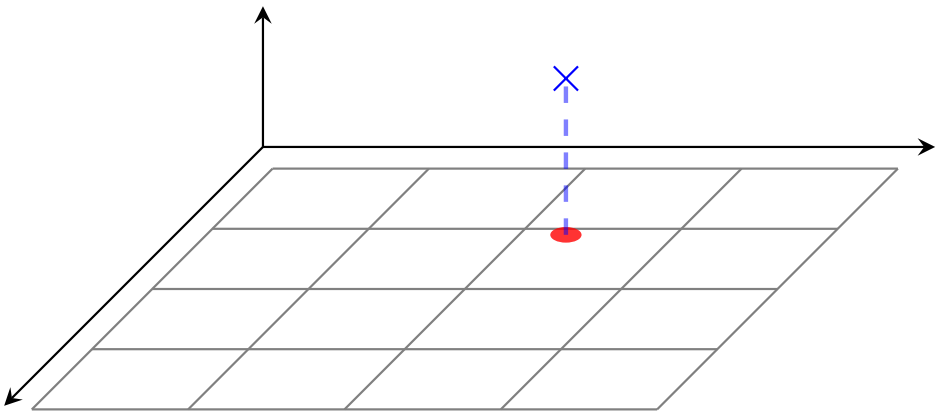
TUNING

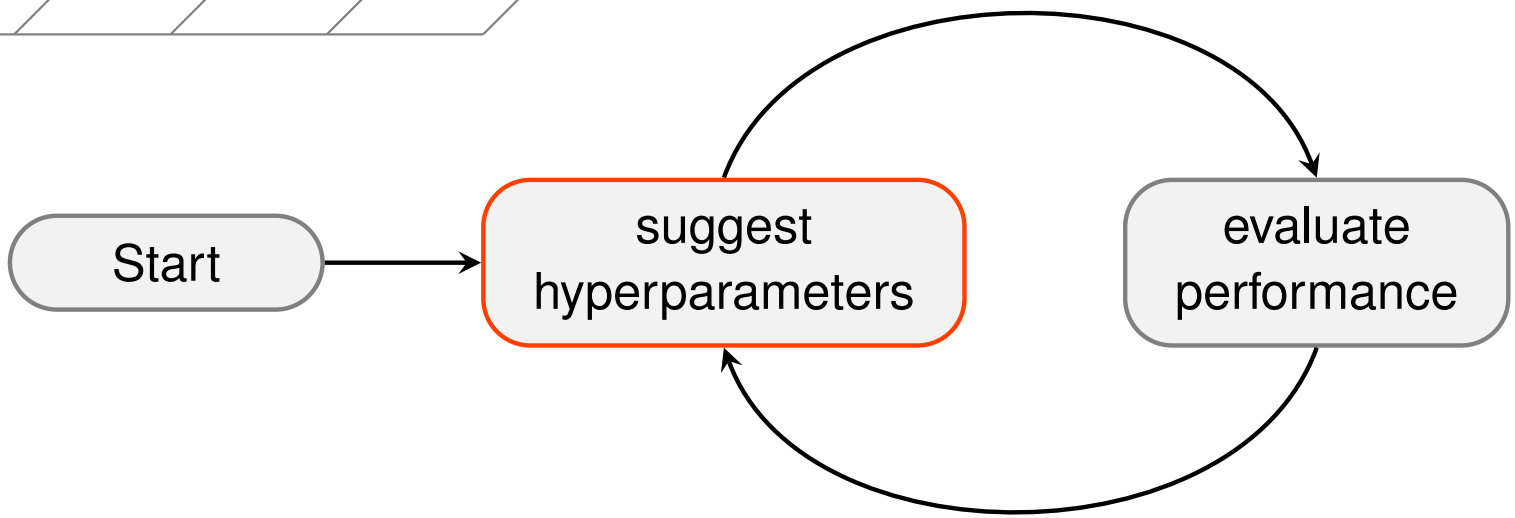

aggregate
Start
suggest hyperparameters
evaluate performance

TUNING

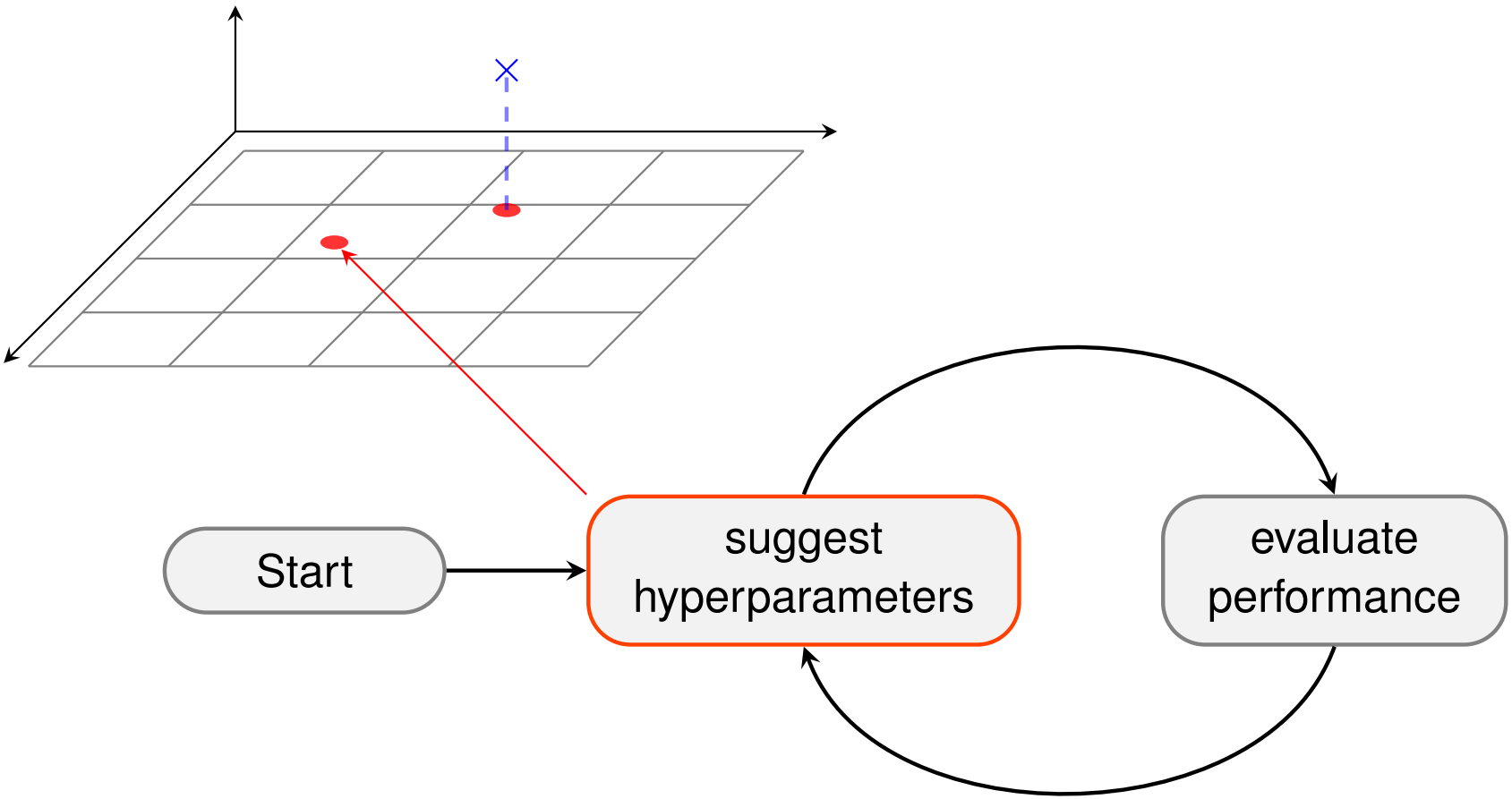

aggregate
Start
suggest hyperparameters
evaluate performance

TUNING

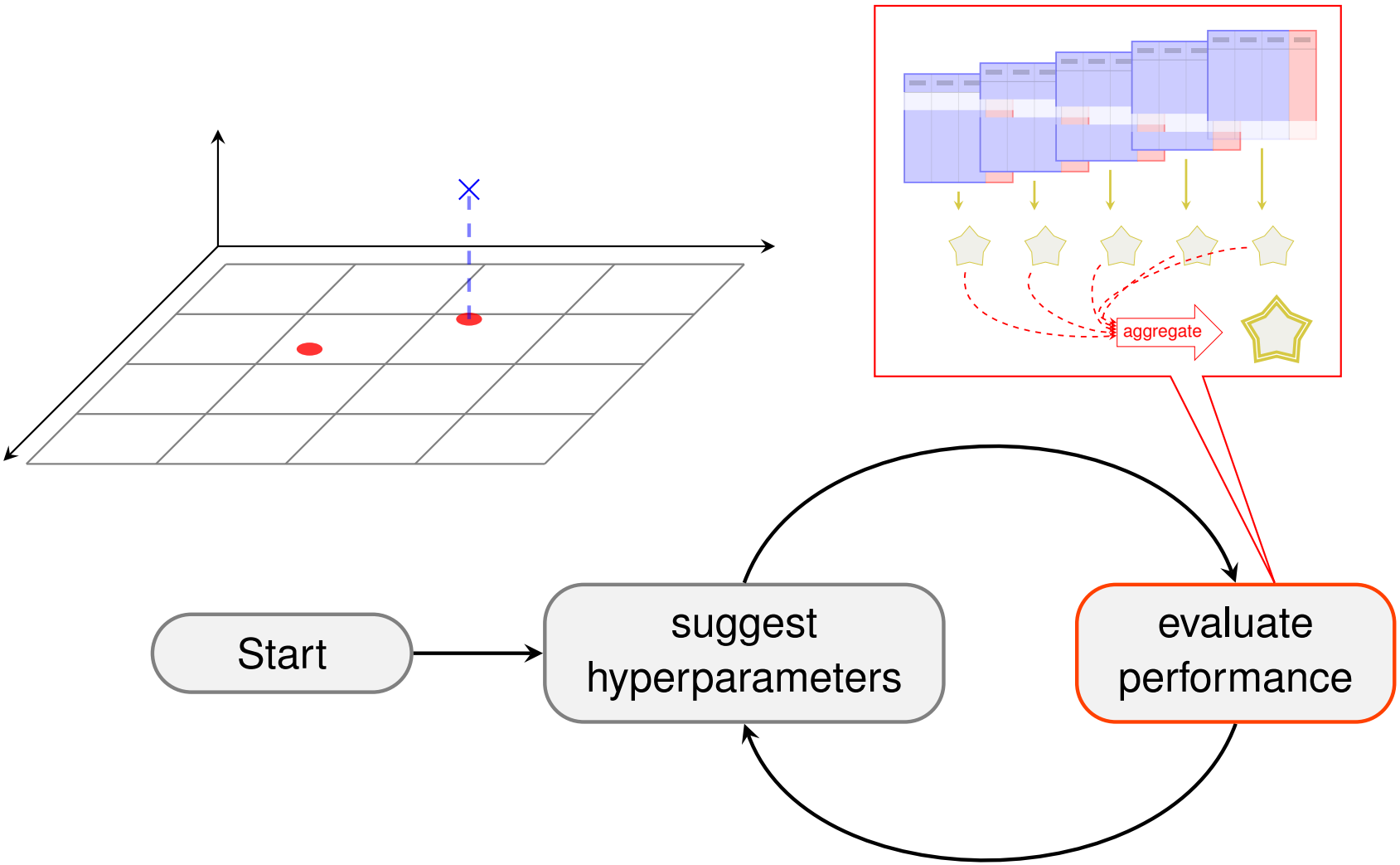




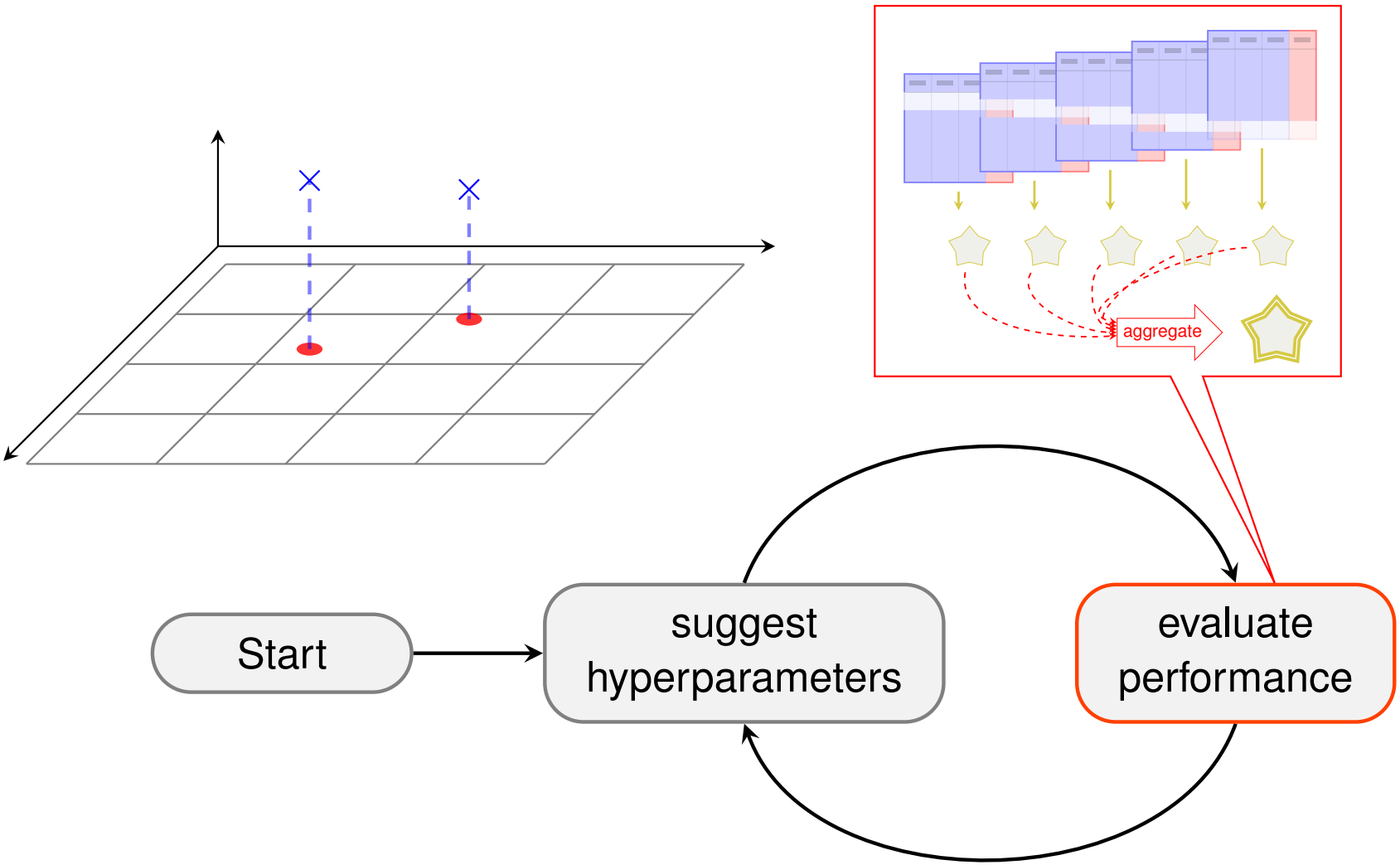
TUNING



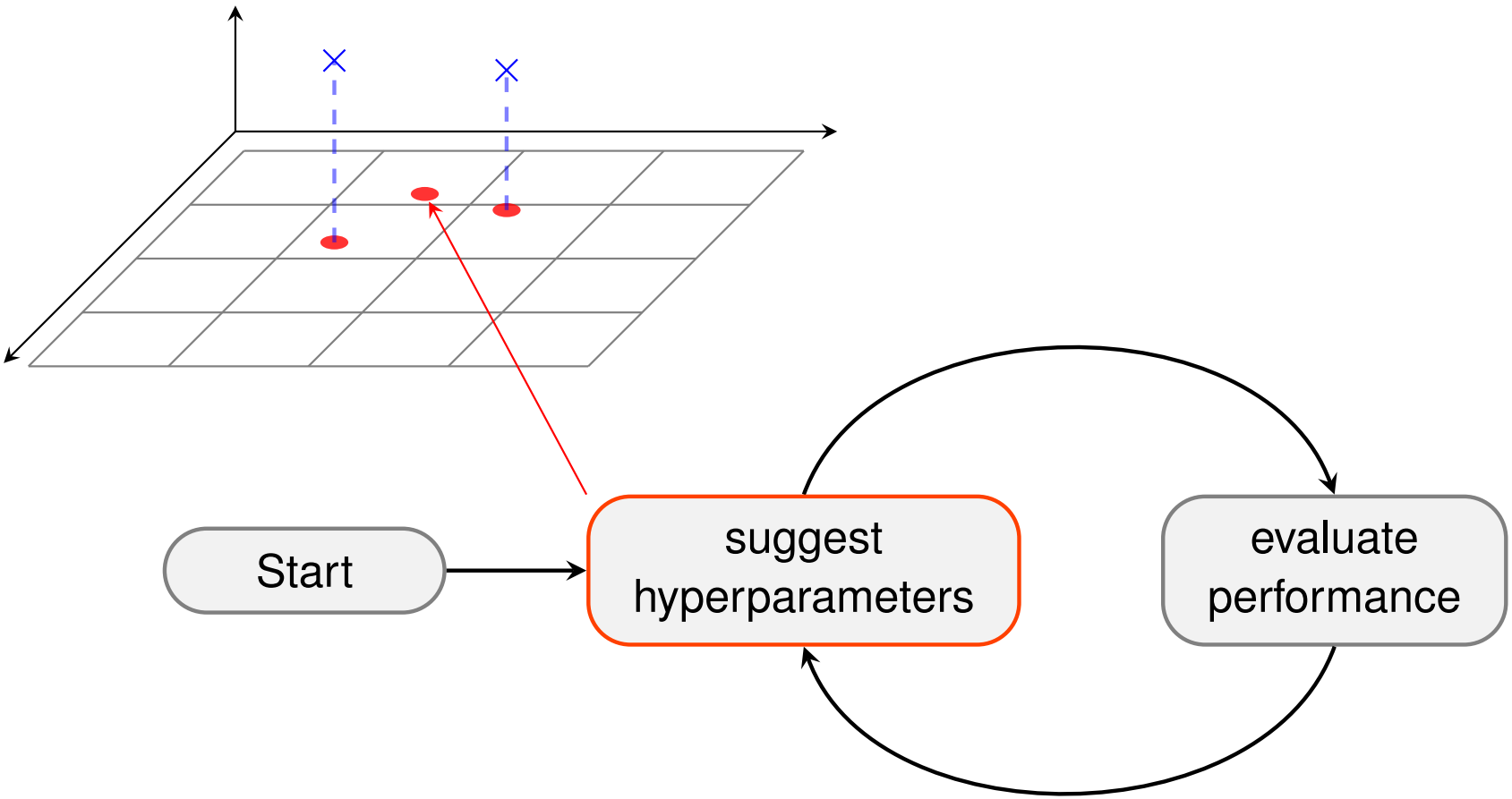
TUNING


aggregate
Start
suggest
hyperparameters
evaluate
performance

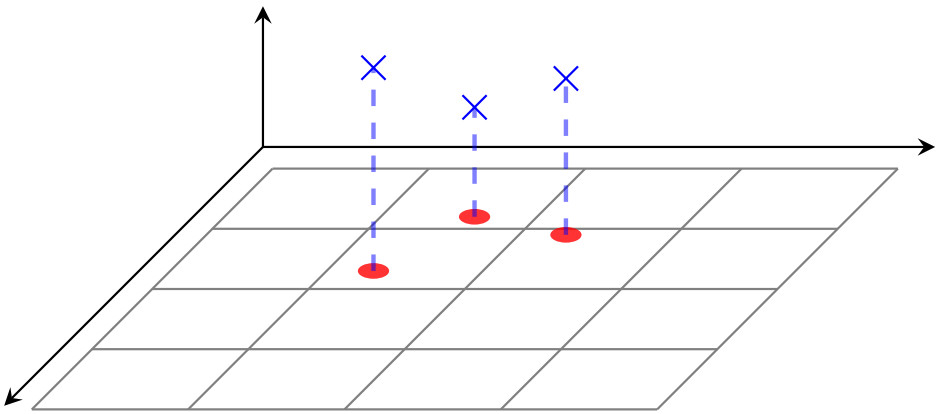
TUNING

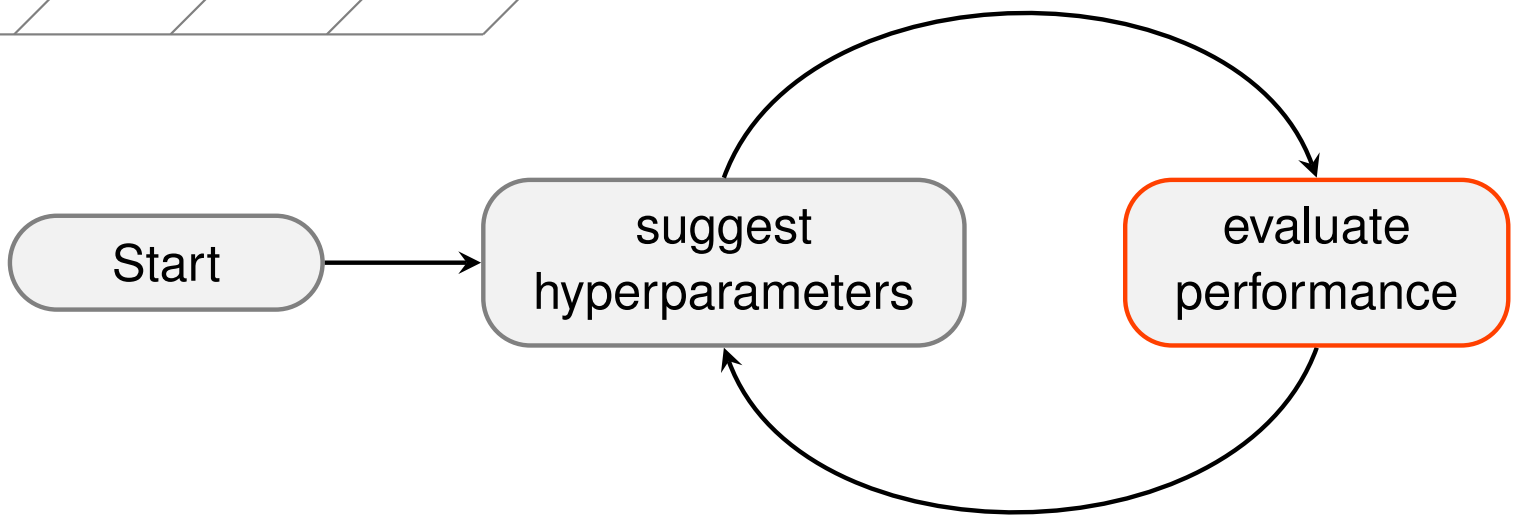

aggregate
Start
suggest
hyperparameters
evaluate
performance

TUNING

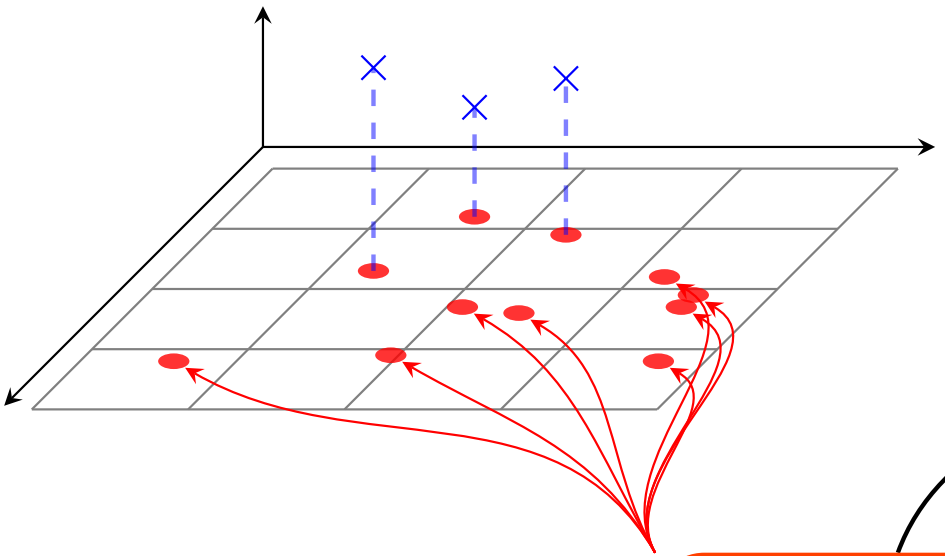


TUNING

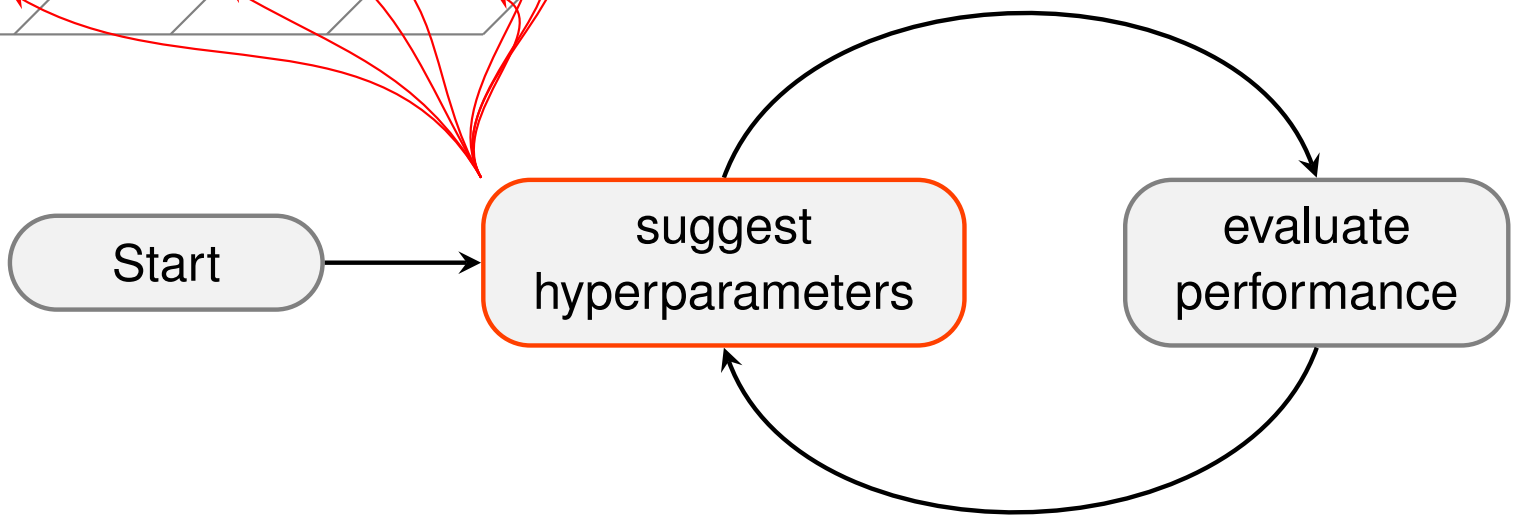




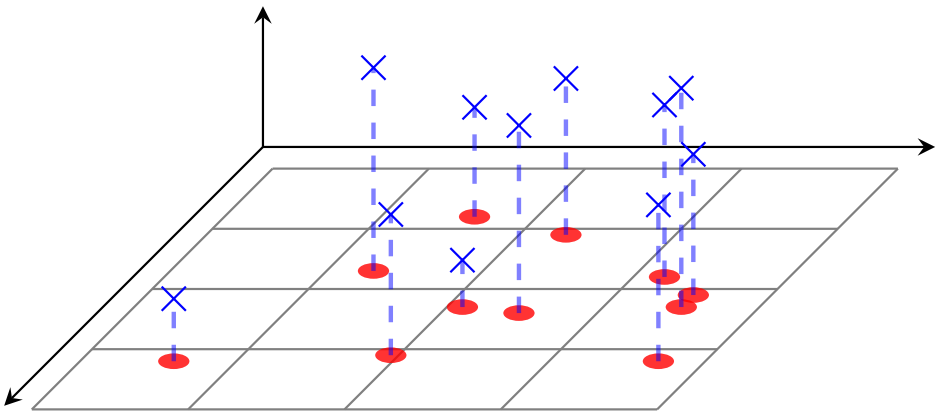
TUNING



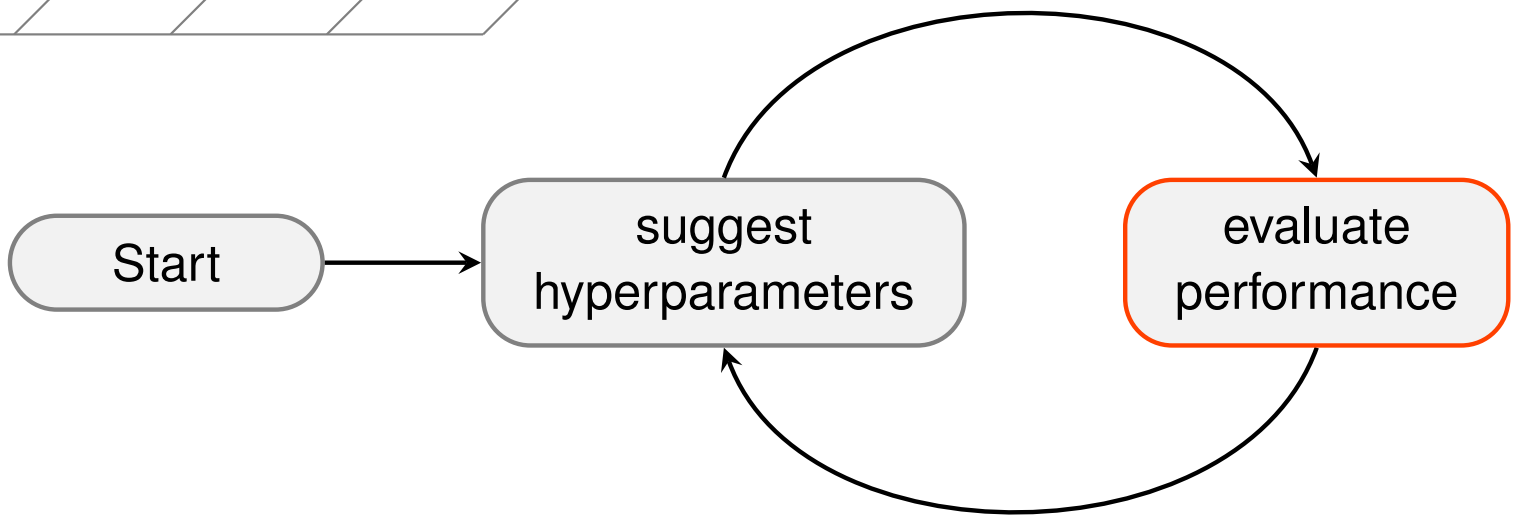
Batch evaluation



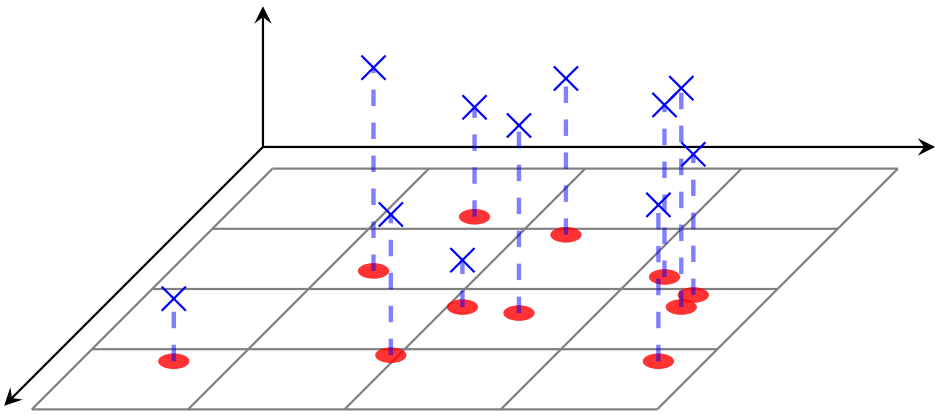
TUNING

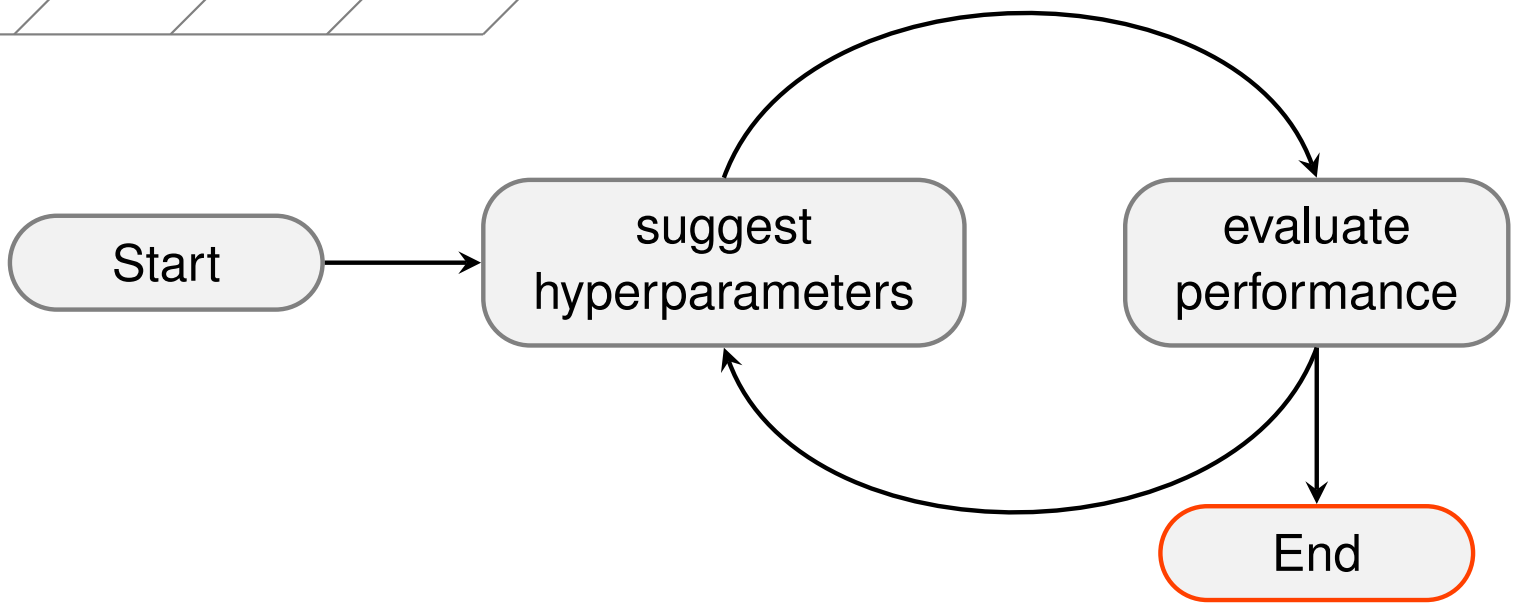


Batch evaluation

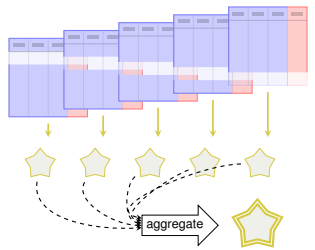


TUNING

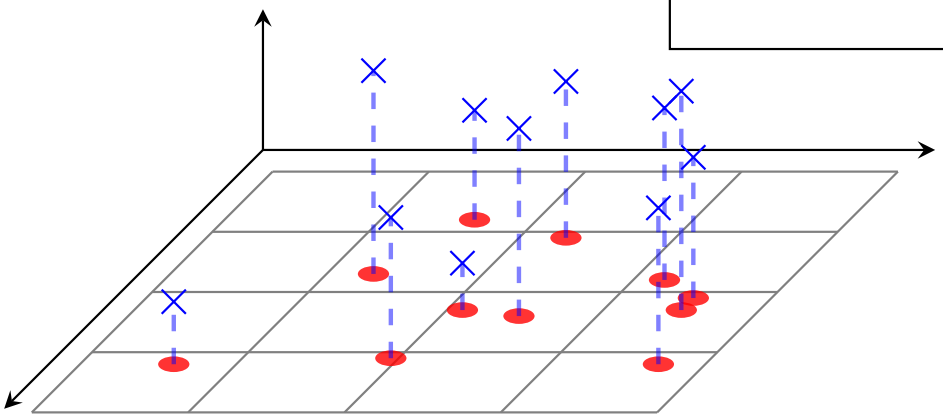


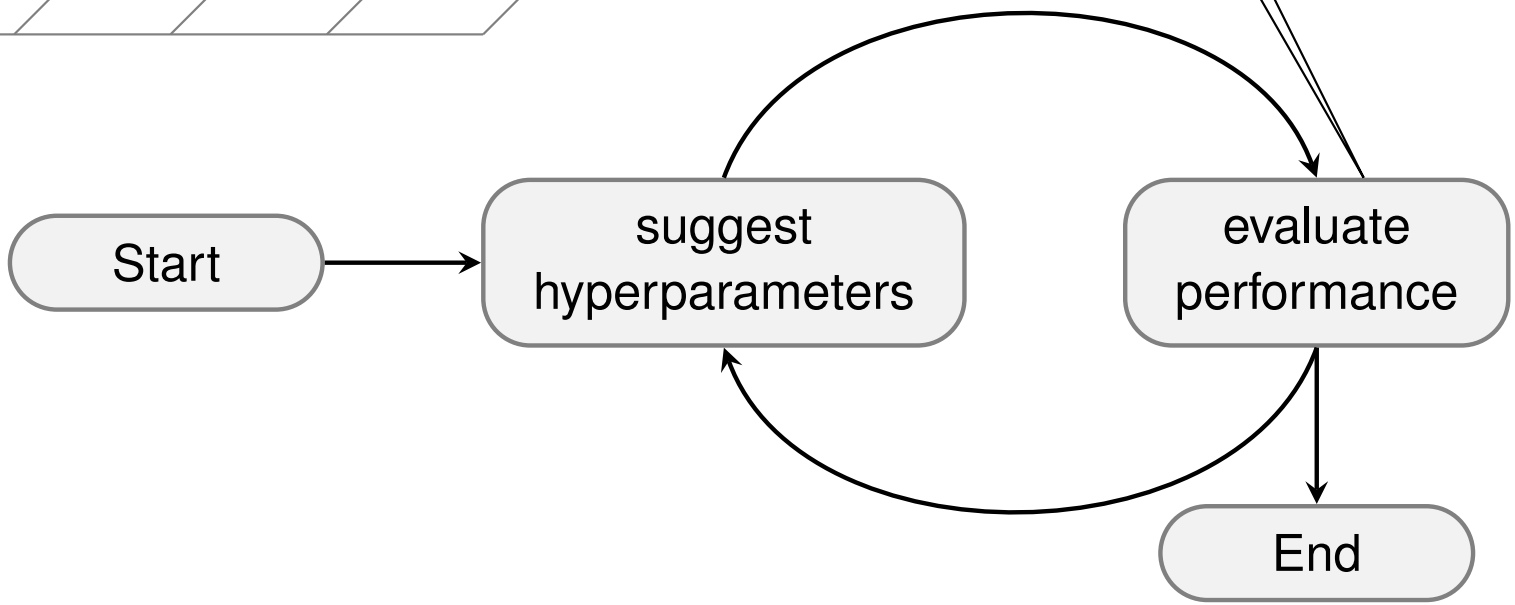


TUNING

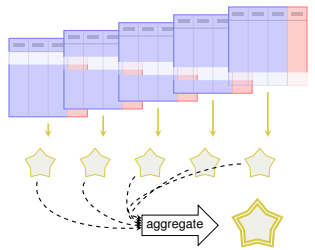


`Learner (lrn())`
`Task`
`Resampling (rsmp())`
`Measure (msr())`

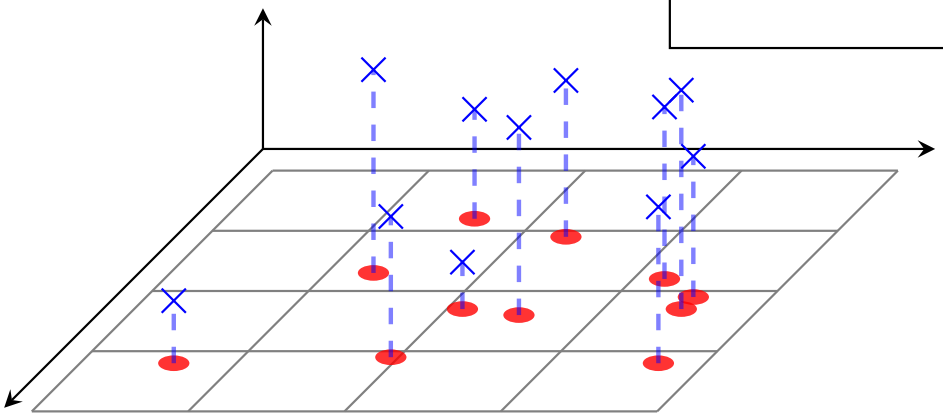




TUNING



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



Start

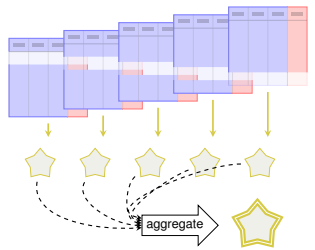
suggest hyperparameters

evaluate performance

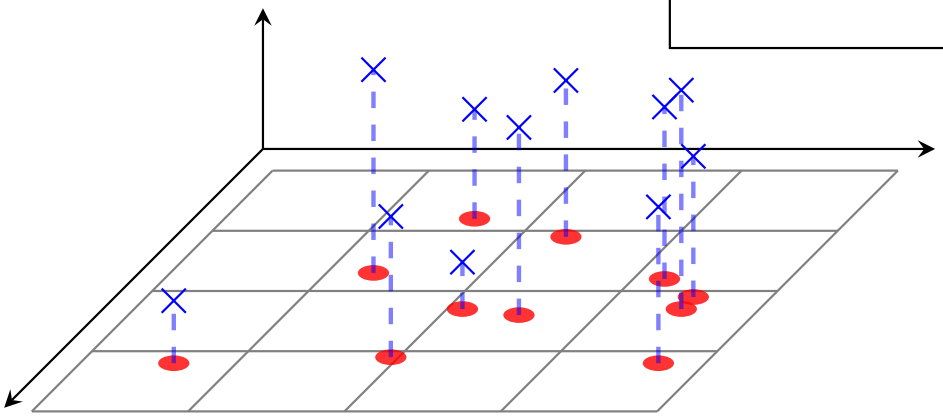
End

search space
`Tuner`

TUNING



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



Start

suggest hyperparameters

evaluate performance

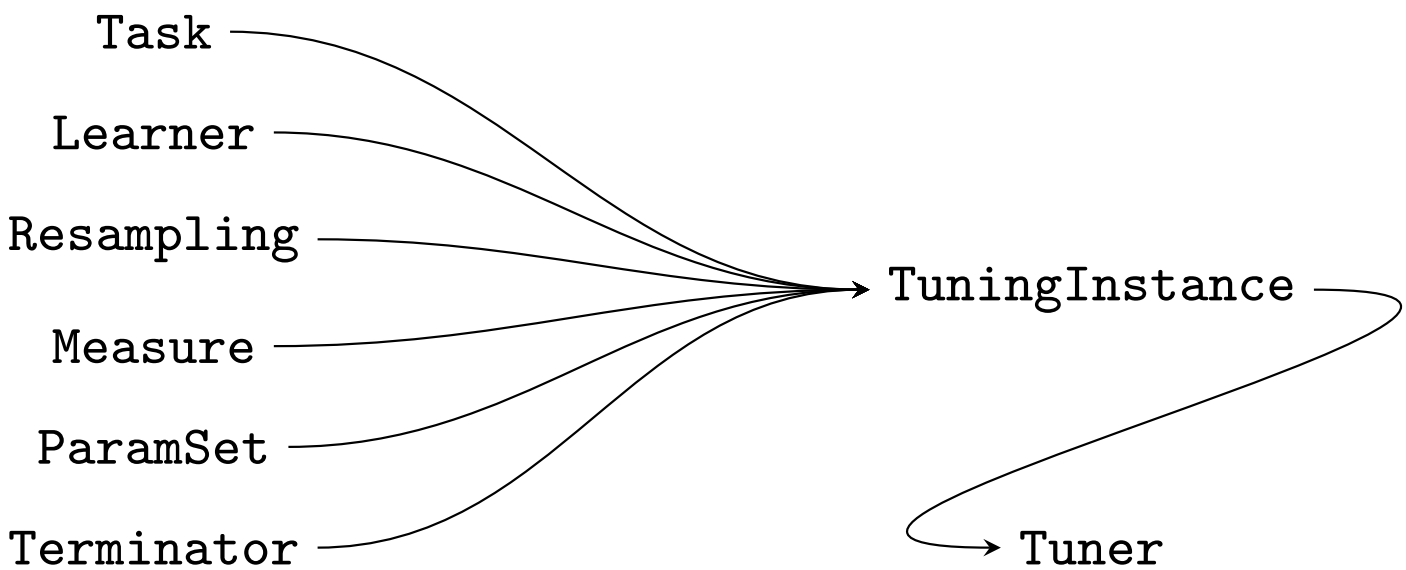
search space
`Tuner`

`Terminator` (when to finish)

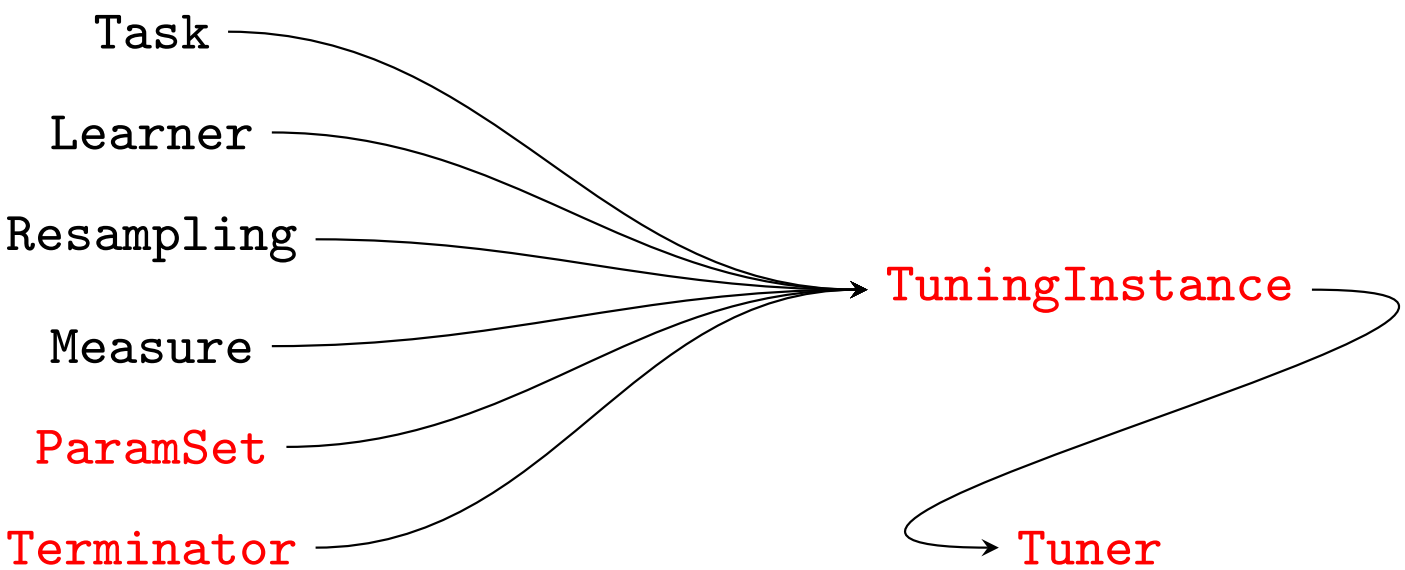
End

Tuning in mlr3

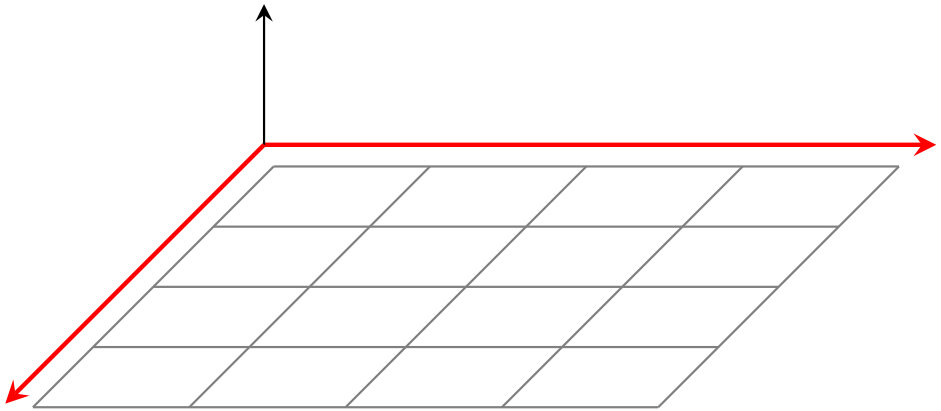
OBJECTS IN TUNING



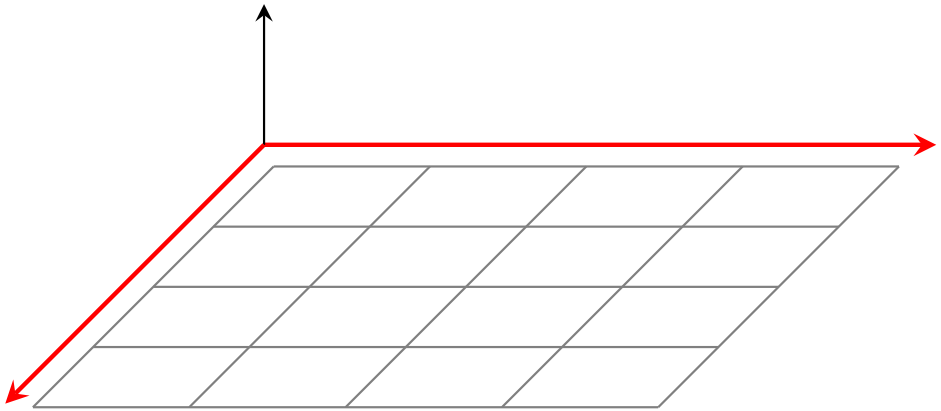
OBJECTS IN TUNING



SEARCH SPACE

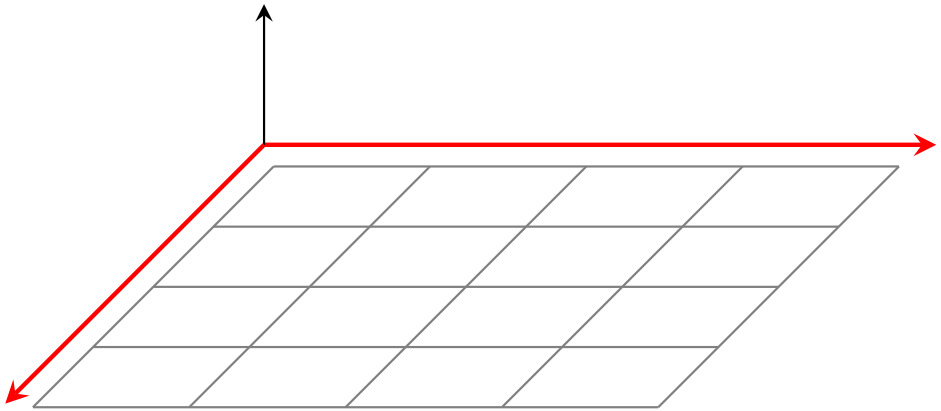


SEARCH SPACE



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

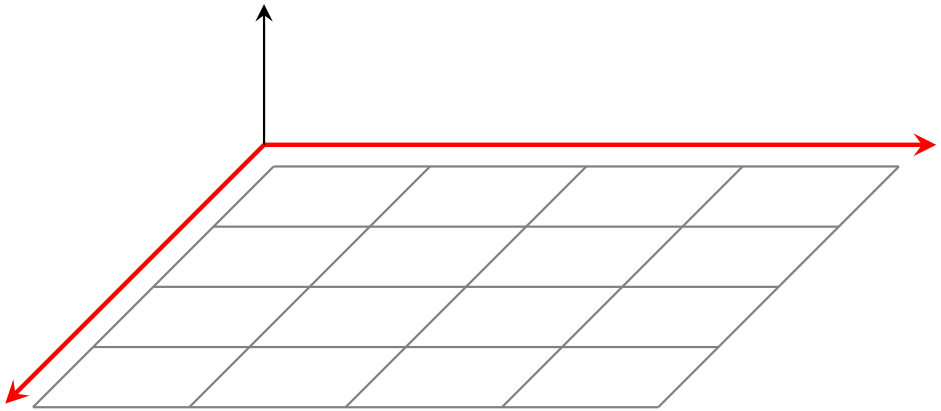
SEARCH SPACE



```
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



```
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)`

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

TERMINATION

- Tuning needs a *termination condition*: when to finish

TERMINATION

- Tuning needs a *termination condition*: when to finish
- `Terminator` class

TERMINATION

- Tuning needs a *termination condition*: when to finish
- `Terminator` class
- `mlr_terminators` dictionary, `term()` short form

TERMINATION

- Tuning needs a *termination condition*: when to finish
- `Terminator` class
- `mlr_terminators` dictionary, `term()` short form
- ```
  as.data.table(mlr_terminators)
  ```

  ```
  #>              key
  #> 1:   clock_time
  #> 2:         combo
  #> 3:         evals
  #> 4:   model_time
  #> 5:          none
  #> 6: perf_reached
  #> 7:   stagnation
  ```
  ```

TERMINATION

- Tuning needs a *termination condition*: when to finish
- `Terminator` class
- `mlr_terminators` dictionary, `term()` short form

```
as.data.table(mlr_terminators)
```

```
#>              key
#> 1:   clock_time
#> 2:         combo
#> 3:         evals
#> 4:   model_time
#> 5:          none
#> 6: perf_reached
#> 7:   stagnation
```

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

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

TUNING METHOD

- need to choose a *tuning method*

TUNING METHOD

- need to choose a *tuning method*
- `Tuner` class

TUNING METHOD

- need to choose a *tuning method*
- `Tuner` class
- `mlr_tuners` dictionary, `tnr()` short form

TUNING METHOD

- need to choose a *tuning method*
- `Tuner` class
- `mlr_tuners` dictionary, `tnr()` short form
- ```
  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

TUNING METHOD

- load `Tuner` with `tnr()`, set parameters
-
```
gsearch = tnr("grid_search", resolution = 20)

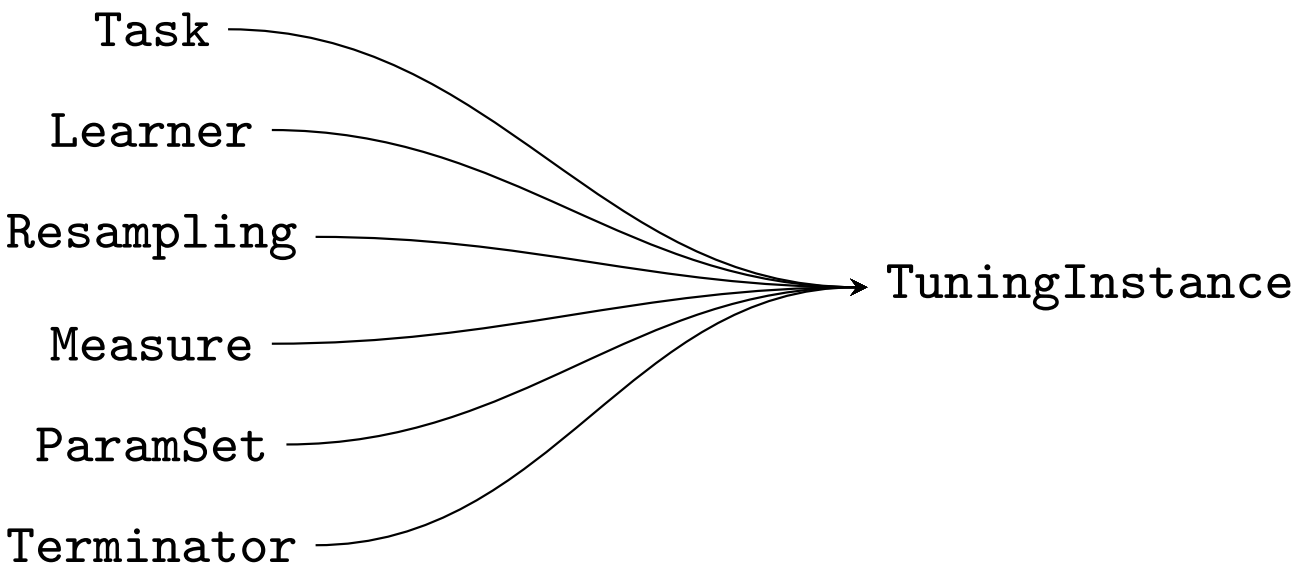
print(gsearch)
#> <TunerGridSearch>
#> * Parameters: resolution=20, batch_size=1
#> * Packages: -
#> * Properties: dependencies
```

TUNING METHOD

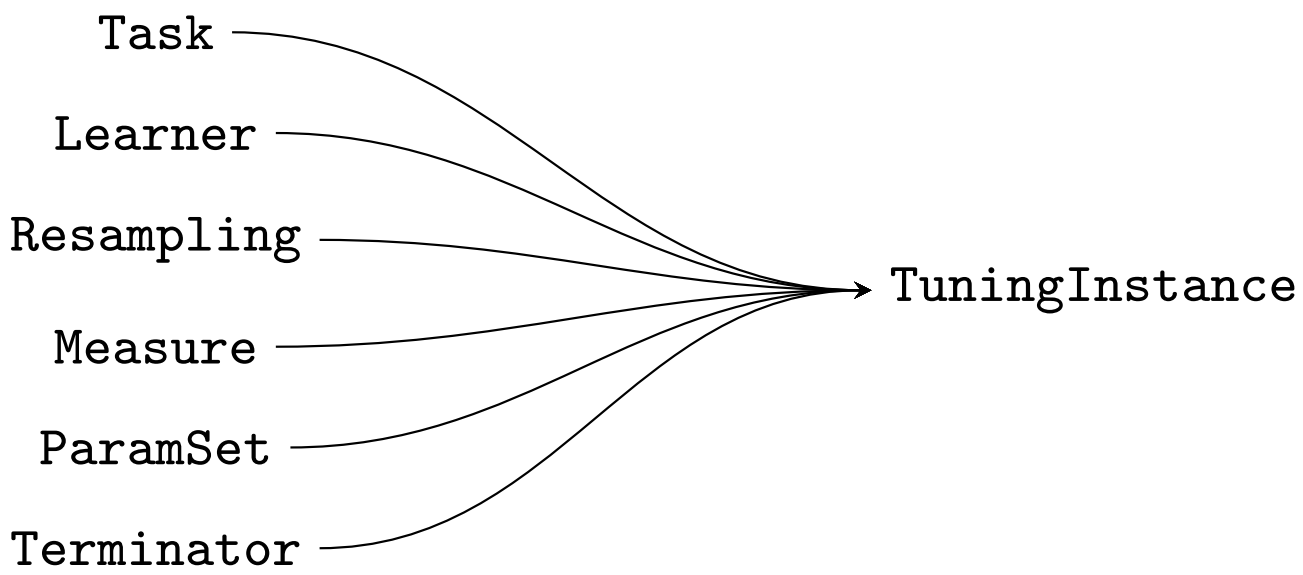
- load `Tuner` with `tnr()`, set parameters
- ```
  gsearch = tnr("grid_search", resolution = 20)

  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

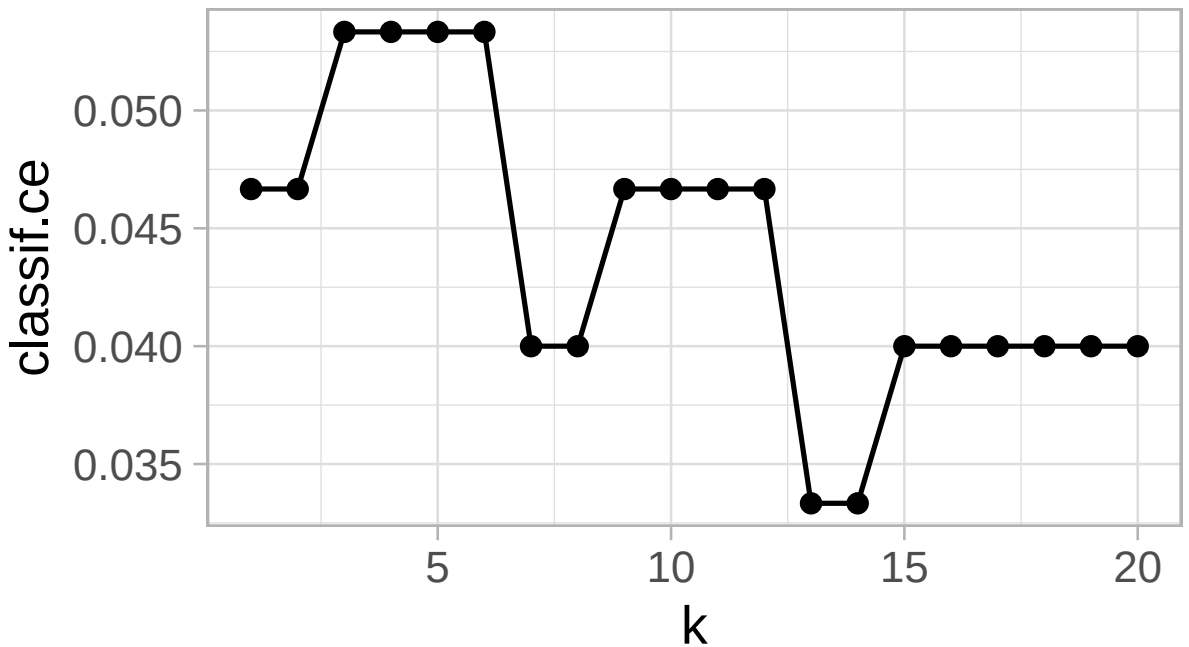
```
gsearch$tune(inst)
```

```
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

PARAMETER TRANSFORMATION

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

PARAMETER TRANSFORMATION

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

$\Rightarrow$ Transformations

PARAMETER TRANSFORMATION

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

$\Rightarrow$ Transformations

- Part of `ParamSet`

PARAMETER TRANSFORMATION

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

$\Rightarrow$ Transformations

- Part of `ParamSet`

Example:

PARAMETER TRANSFORMATION

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

$\Rightarrow$ Transformations

- Part of `ParamSet`

Example:

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

PARAMETER TRANSFORMATION

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

$\Rightarrow$ Transformations

- Part of `ParamSet`

Example:

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

PARAMETER TRANSFORMATION

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

$\Rightarrow$ Transformations

- Part of `ParamSet`

Example:

1. sample from $\log(1) \ldots \log(100)$ (`k_before_trafo`)
2. transform by $\exp()$ in `trafo` function
3. don't forget to `round` (k must be integer)

PARAMETER TRANSFORMATION

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

$\Rightarrow$ Transformations

- Part of `ParamSet`

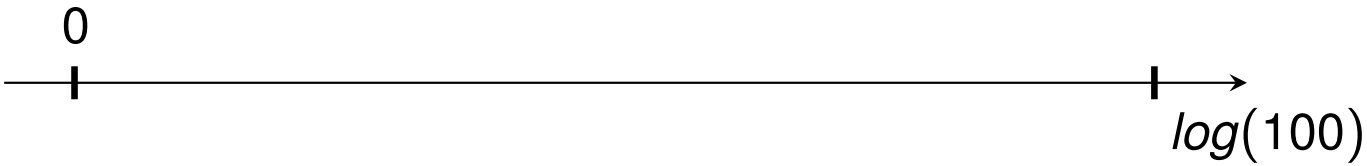
Example:

1. sample from $\log(1) \ldots \log(100)$ (`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))))
}
```

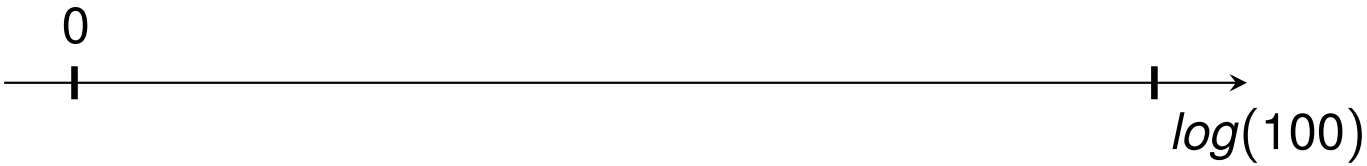
PARAMETER TRANSFORMATION

What is our transformation doing?



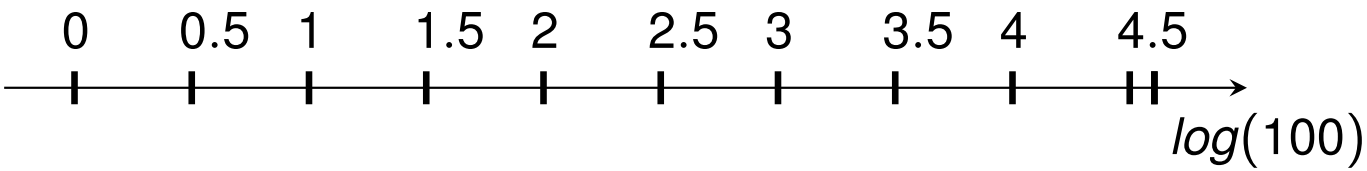
PARAMETER TRANSFORMATION

What is our transformation doing?



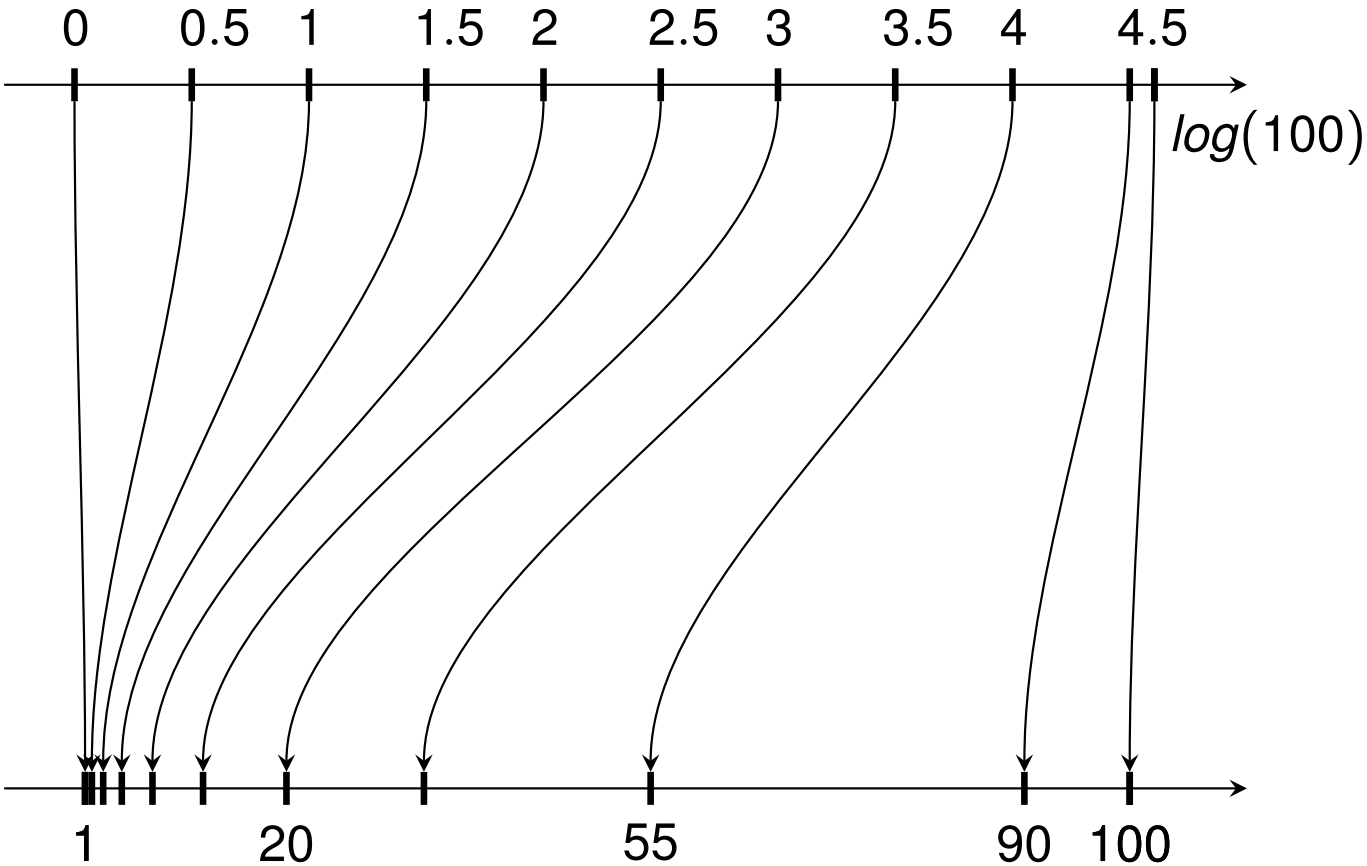
PARAMETER TRANSFORMATION

What is our transformation doing?



PARAMETER TRANSFORMATION

What is our transformation doing?



PARAMETER TRANSFORMATION

Tuning again. . .

PARAMETER TRANSFORMATION

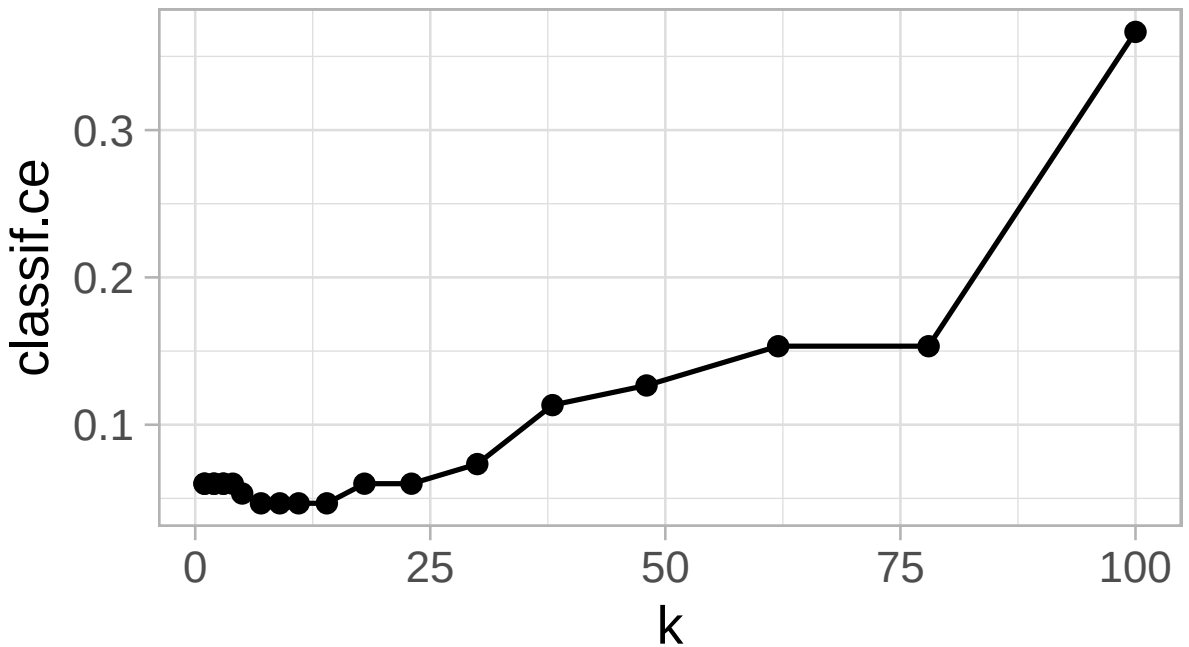
Tuning again...

```
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

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
- Predicing: Just use final model

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
  - Predicing: Just use final model

- **AutoTuner**

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
  - Predicing: 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:classif.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
```

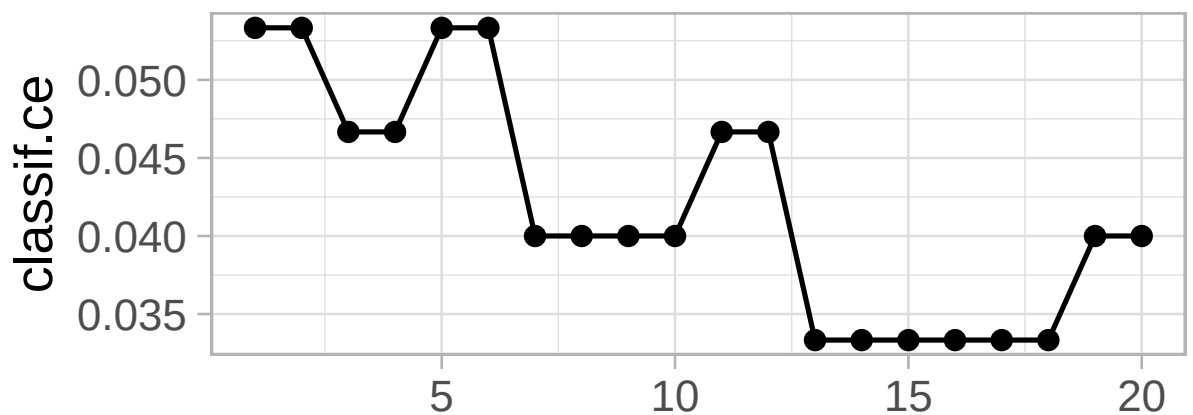
NESTED RESAMPLING

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

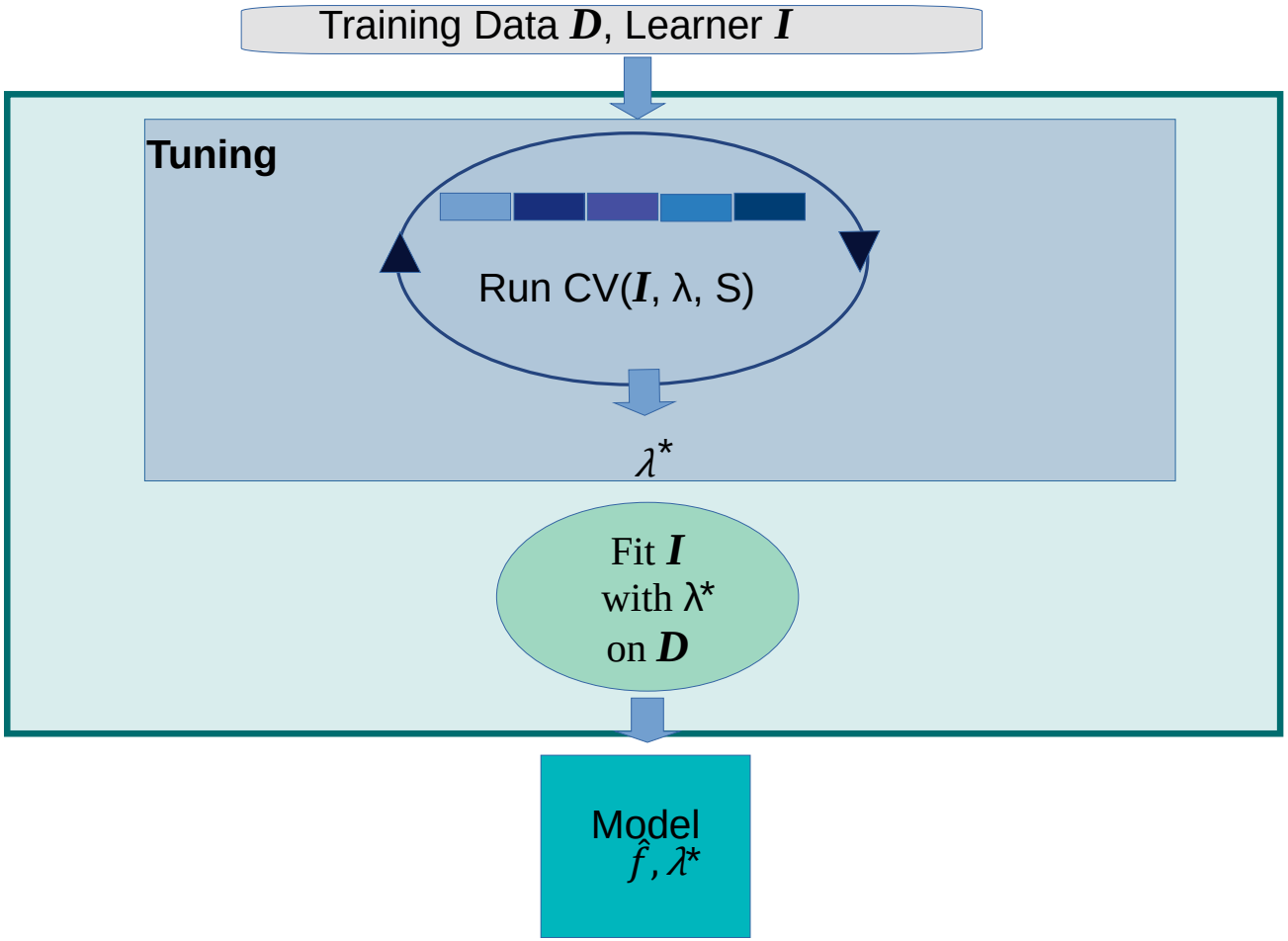
```
optlrn$model$learner

#> <LearnerClassifKKNN:classif.kknn>
#> * Model: data.table
#> * Parameters: kernel=rectangular, k=18
#> * Packages: withr, kknn
#> * Predict Type: response
#> * 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
```

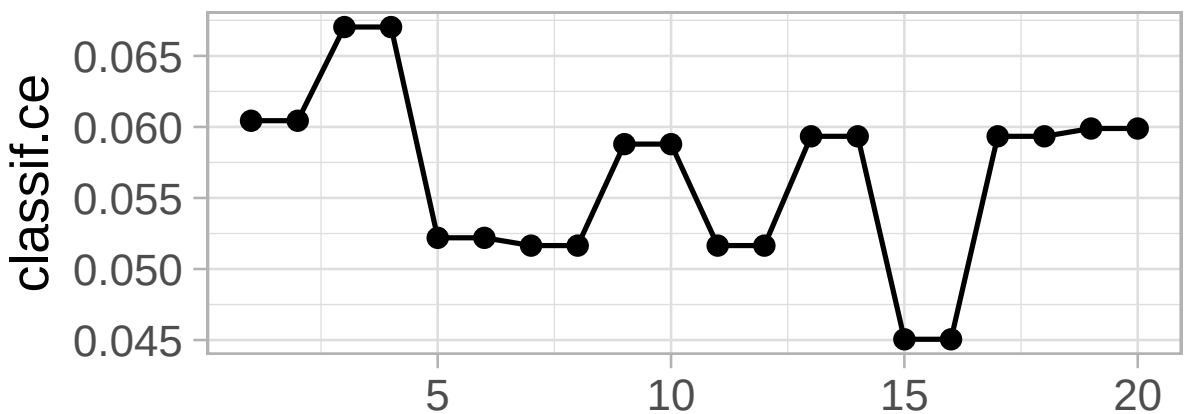
NESTED RESAMPLING

```
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()`