R `mlr3` w/ ChatGPT

feat. `mlr3`

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- Syntax
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- Resampling
- Benchmarking

Introduction

Who am I?

- Graduate School of Public Health, SNU (2019.03 ~ 2021.02)
- Seoul National University Bundang Hospital (2021.06 ~)
- Data (NHIS, MIMIC-IV, Registry data, KNHNAES …)
- Comento mentor (R for healthcare) (2022.07 ~)

ML framework in R

What is `mlr3`?

`mlr3`: **M**achine **L**earning in **R** **3**

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I want to learn `mlr3` in R. I would like you to introduce the package in detail.

`mlr3` is a versatile machine learning framework in R. It provides a coherent interface to a large number of classification, regression, multilabel, and survival analysis methods. The `mlr3` package, along with its associated ecosystem of packages, is intended to be a successor to the `mlr` package, offering improved design, more efficient operations, and greater flexibility.

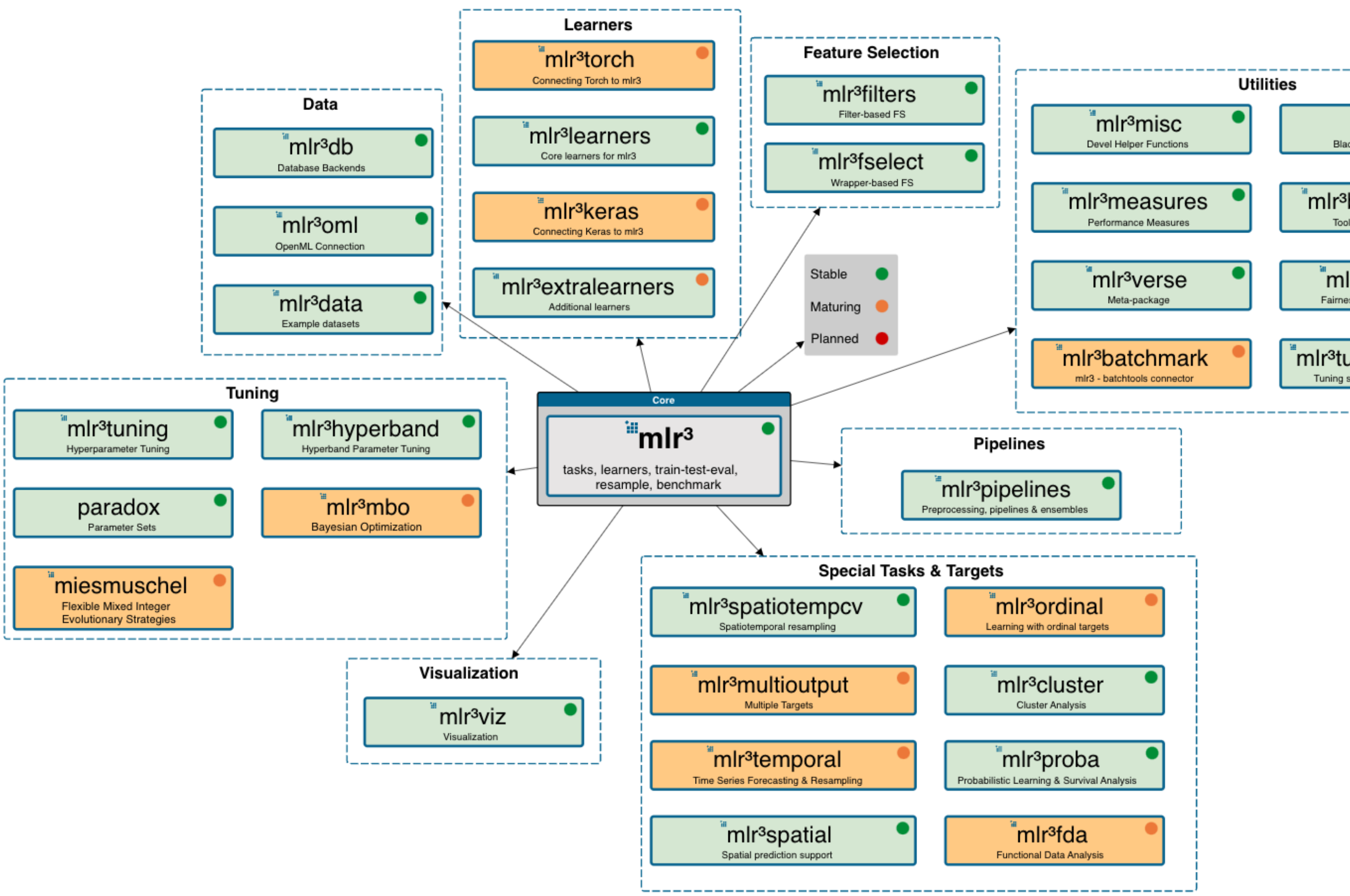


Figure 1: source: https://mlr3.mlr-org.com

`mlr3` & `mlr3verse`

Why `mlr3`?

- National Health Insurance System Data (NHIS-HEALS, NHIS-NSC)
- `dplyr` → `data.table`
- `Python` : `scikit-learn` = `R` : ??
- `mlr3`: `data.table` based package

Syntax

`mlr3` vs `tidymodels`

> 2. Syntax and Usage:
>   - `` `mlr3` ``: mlr3 uses a more traditional R object-oriented programming approach. Its syntax and structure are quite different from the tidyverse style and could be more difficult to grasp for beginners or those used to tidyverse-style workflows.
>   - `` `tidymodels` ``: tidymodels is designed to work seamlessly with the rest of the tidyverse, using consistent, "tidy" syntax. If you are already familiar with tidyverse packages like `` `dplyr` `` or `` `ggplot2` ``, you will likely find `` `tidymodels` `` more intuitive and easier to use.

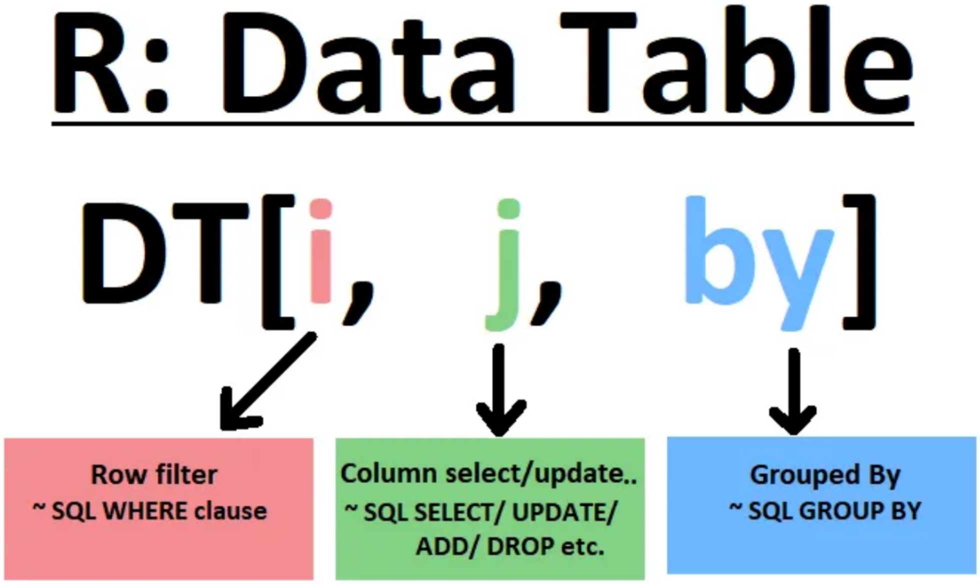
Core 1. `R6`

Object Oriented Programming (OOP)

- Objects: `foo = bar$new()`
- Methods: `$new()`
- Fields: `$baz`

```
task = TaskClassif$new("xxx") # Objects
task$new()  # Methods
task$feature_names # Fields
```

Core 2. `data.table`




```
DT[i >= 10] # filter rows
DT[, .(X,Y)] # select columns
DT[, mean(X), by=Y] # aggregate by group
```

Utils 1. Dictionary

```
# Getting a specific object with `$get(key)`
mlr_learners$get("regr.rpart")
```

```
<LearnerRegrRpart:regr.rpart>: Regression Tree
* Model: -
* Parameters: xval=0
* Packages: mlr3, rpart
* Predict Types:  [response]
* Feature Types: logical, integer, numeric, factor, ordered
* Properties: importance, missings, selected_features, weights
```

Utils 1. Dictionary

```r
# Searching objects with $keys()
mlr_measures$keys() |> head()
```

```
[1] "aic"            "bic"            "classif.acc"    "classif.auc"
[5] "classif.bacc"   "classif.bbrier"
```

Utils 1. Dictionary

```r
# OR with `as.data.table()`
as.data.table(mlr_learners) |> head()
```

key	label	task_type	feature_types	packages	properties	predict_types
classif.cv_glmnet	NA	classif	logical, integer, numeric	mlr3 , mlr3learners, glmnet	multiclass , selected_features, twoclass , weights	response, prob
classif.debug	Debug Learner for Classification	classif	logical , integer , numeric , character, factor , ordered	mlr3	hotstart_forward, missings , multiclass , twoclass	response, prob
classif.featureless	Featureless Classification Learner	classif	logical , integer , numeric , character, factor , ordered , POSIXct	mlr3	featureless , importance , missings , multiclass , selected_features, twoclass	response, prob
classif.glmnet	NA	classif	logical, integer, numeric	mlr3 , mlr3learners, glmnet	multiclass, twoclass , weights	response, prob
classif.kknn	NA	classif	logical, integer, numeric, factor , ordered	mlr3 , mlr3learners, kknn	multiclass, twoclass	response, prob
classif.lda	NA	classif	logical, integer, numeric, factor , ordered	mlr3 , mlr3learners, MASS	multiclass, twoclass , weights	response, prob

Utils 2. Sugar functions

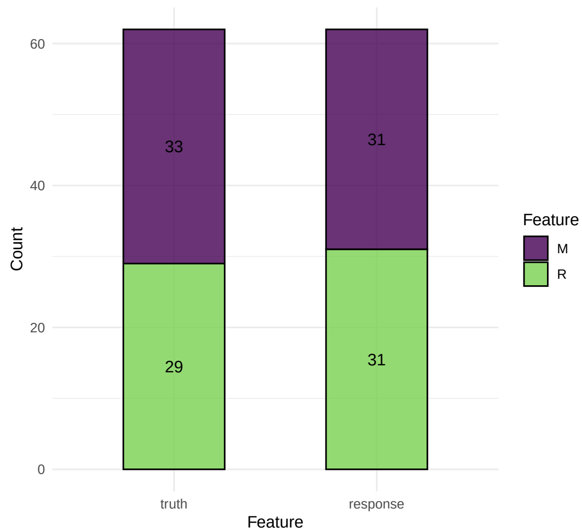
- `R6` class → `S3` type functions

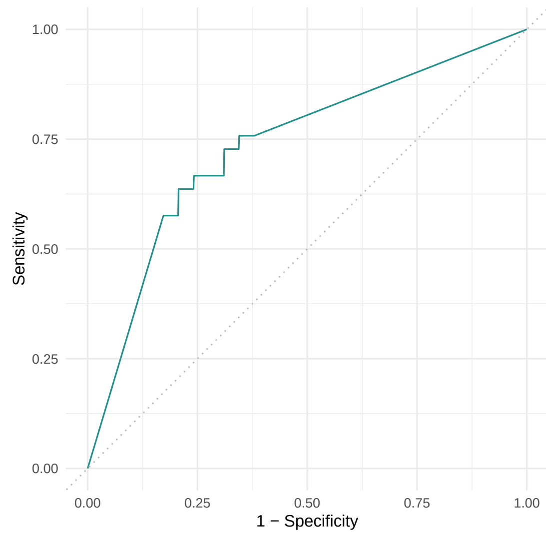
```r
# No sugar
LearnerClassifLogReg$new()

# Sugar
lrn("classif.log_reg")
```

Utils 3. `mlr3viz`

- `autoplot()` visualization

```r
autoplot(pred)
autoplot(pred, type="roc")
```





Basic modeling

Ask ChatGPT!

1. Tasks

- Objects with data and metadata
- Default datasets
- Dictionary: `mlr_tasks`
- Sugar function: `tsk()`

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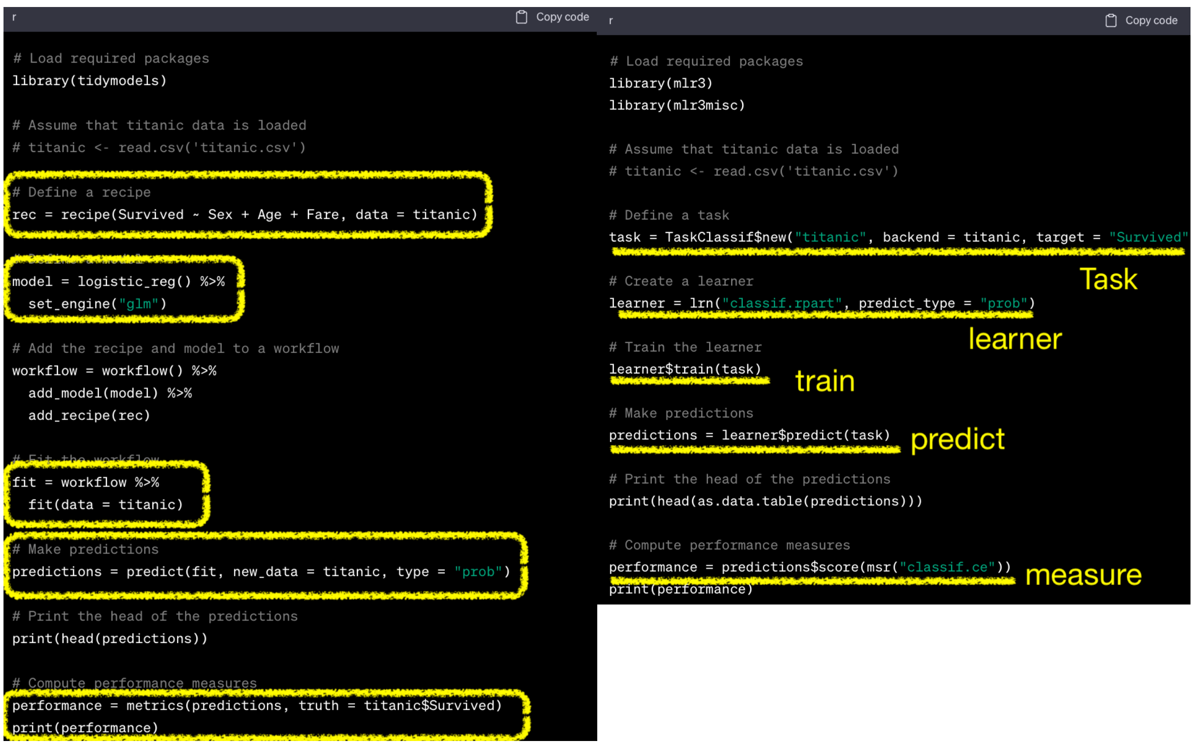
Okay, I would like to make a classification model of random forest with the `titanic` dataset, which predicts survival of passenger. I need you to write the R codes of the `mlr3` way and `tidymodels` way.



```r
# Load required packages
library(tidymodels)

# Assume that titanic data is loaded
# titanic <- read.csv('titanic.csv')

# Define a recipe
rec = recipe(Survived ~ Sex + Age + Fare, data = titanic)

# Define a model
model = logistic_reg() %>%
  set_engine("glm")

# Add the recipe and model to a workflow
workflow = workflow() %>%
  add_model(model) %>%
  add_recipe(rec)

# Fit the workflow
fit = workflow %>%
  fit(data = titanic)

# Make predictions
predictions = predict(fit, new_data = titanic, type = "prob")

# Print the head of the predictions
print(head(predictions))

# Compute performance measures
performance = metrics(predictions, truth = titanic$Survived)
print(performance)
```

```r
# Load required packages
library(mlr3)
library(mlr3misc)

# Assume that titanic data is loaded
# titanic <- read.csv('titanic.csv')

# Define a task
task = TaskClassif$new("titanic", backend = titanic, target = "Survived"

# Create a learner
learner = lrn("classif.rpart", predict_type = "prob")

# Train the learner
learner$train(task)

# Make predictions
predictions = learner$predict(task)

# Print the head of the predictions
print(head(as.data.table(predictions)))

# Compute performance measures
performance = predictions$score(msr("classif.ce"))
print(performance)
```

```r
# R6 methods
# mlr_tasks$get("titanic")

# Sugar function
tsk("titanic")
```

```
<TaskClassif:titanic> (1309 x 11): Titanic
* Target: survived
* Properties: twoclass
* Features (10):
  - chr (3): cabin, name, ticket
  - dbl (2): age, fare
  - fct (2): embarked, sex
  - int (2): parch, sib_sp
  - ord (1): pclass
```

1. Tasks

Or External data as `task`

- `as_task_regr()` : regression
- `as_task_classif()`: classification
- `as_task_clust()`: clustering

```r
task_mtcars = as_task_regr(mtcars,
                           target = "mpg")
task_mtcars
```

```
<TaskRegr:mtcars> (32 x 11)
* Target: mpg
* Properties: -
* Features (10):
  - dbl (10): am, carb, cyl, disp, drat, gear, hp, qsec, vs, wt
```

2. Learners

- ML algorithms
- Dictionary: `mlr_learners`
- Sugar function: `lrn()`
- regression (`regr.~`), classification(`classif.~`), and clustering (`clust.~`)

- `library(mlr3learners)`

> **Extra learners**
>
> - only for `github` not CRAN
> - e.g., `lightGBM`
>
> ```
> # remotes::install_github("mlr-org/mlr3extralearners@*release")
> library(mlr3extralearners)
> ```

2. Learners

- `$train()`, `$predict()`

```
task = tsk("german_credit")
learner_dt = lrn("classif.rpart", predict_type="prob")
split = partition(task, ratio=.7)
learner_dt$train(task, row_ids = split$train)
prediction = learner_dt$predict(task, row_ids = split$test)
```

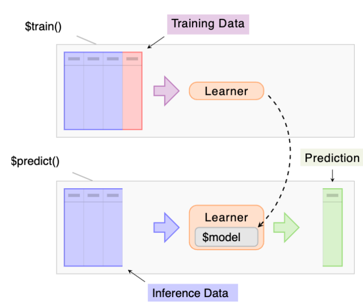


Figure 2: source: mlr3books

2. Learners

confusion matrix

```
prediction$confusion
```

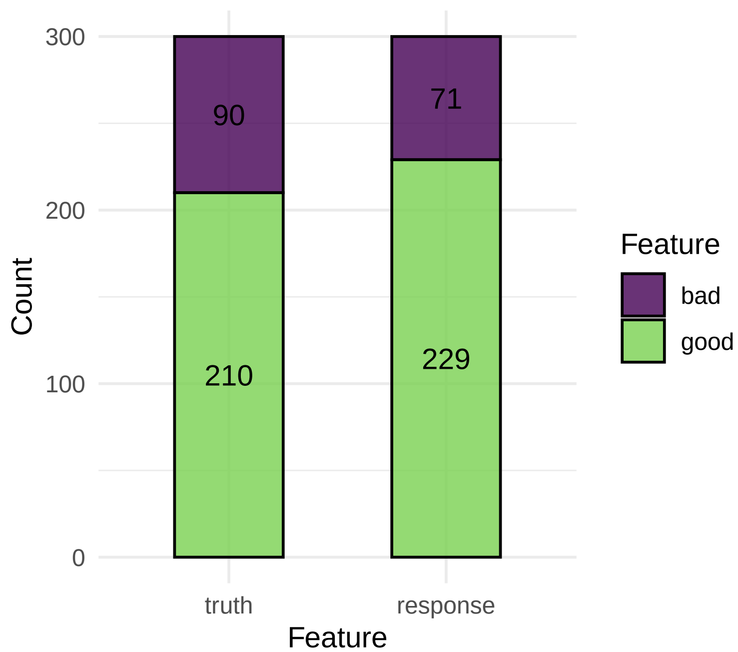
```
        truth
response good bad
```

```
good   184   45
bad     26   45
```

2. Learners

Or with `mlr3viz`

```
autoplot(prediction)
```



Hyperparameter

```
# with learner
learner = lrn("classif.rpart", maxdepth = 1)

# Or
learner$param_set$set_values(xval = 2, maxdepth=3, cp=.5)

learner$param_set$values
```

```
$xval
```

```
[1] 2

$maxdepth
[1] 3

$cp
[1] 0.5
```

Hyperparameter

Setting hyperparameters

- `$param_set` of learners
- setting class, lower, upper

```
as.data.table(learner$param_set) |> head()
```

id	class	lower	upper	levels	nlevels	is_bounded	special_vals	default	storage_type	tags
cp	ParamDbl	0	1	NULL	Inf	TRUE	NULL	0.01	numeric	train
keep_model	ParamLgl	NA	NA	TRUE, FALSE	2	TRUE	NULL	FALSE	logical	train
maxcompete	ParamInt	0	Inf	NULL	Inf	FALSE	NULL	4	integer	train
maxdepth	ParamInt	1	30	NULL	30	TRUE	NULL	30	integer	train
maxsurrogate	ParamInt	0	Inf	NULL	Inf	FALSE	NULL	5	integer	train
minbucket	ParamInt	1	Inf	NULL	Inf	FALSE	NULL	<environment: 0x134ede100>	integer	train

3. Measures

- Evaluation of performances
- Dictionary: `mlr_measures`
- Sugar function: `msr()`, `msrs()`
- `classif.~`, `regr.~`
- `$score()`

```
as.data.table(mlr_measures) |> head()
```

key	label	task_type	packages	predict_type	task_properties
aic	Akaike Information Criterion	NA	mlr3	NA	
bic	Bayesian Information Criterion	NA	mlr3	NA	
classif.acc	Classification Accuracy	classif	mlr3 , mlr3measures	response	
classif.auc	Area Under the ROC Curve	classif	mlr3 , mlr3measures	prob	twoclass
classif.bacc	Balanced Accuracy	classif	mlr3 , mlr3measures	response	
classif.bbrier	Binary Brier Score	classif	mlr3 , mlr3measures	prob	twoclass

3. Measures

`msr()`: a single performance

```
measure = msr("classif.acc")
prediction$score(measure)
```

```
classif.acc
  0.7633333
```

3. Measures

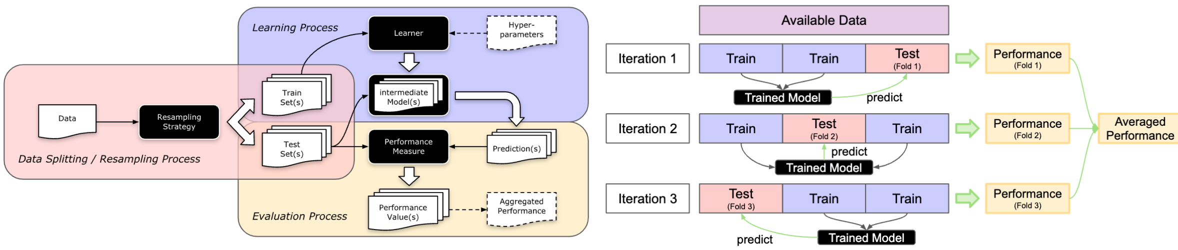
`msrs()`: multiple performances

```
# Multiple measurements
measures = msrs(c("classif.acc","classif.ppv","classif.npv","classif.auc"))
prediction$score(measures)
```

```
classif.acc classif.ppv classif.npv classif.auc
  0.7633333   0.8034934   0.6338028   0.7558730
```

Resampling

Resampling



- Split available data into multiple training and test sets
- **Reliable** performance
- Prevent **Overfitting**

`tidymodels` vs `mlr3`

Resampling

- Dictionary: `mlr_resamplings`
- Sugar function: `rsmp()`

```
as.data.table(mlr_resamplings)
```

key	label	params	iters
bootstrap	Bootstrap	ratio , repeats	30
custom	Custom Splits		NA
custom_cv	Custom Split Cross-Validation		NA
cv	Cross-Validation	folds	10
holdout	Holdout	ratio	1
insample	Insample Resampling		1
loo	Leave-One-Out		NA
repeated_cv	Repeated Cross-Validation	folds , repeats	100
subsampling	Subsampling	ratio , repeats	30

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Okay, then I would like to resample the models by 10-fold cross validation. I need you to write the R codes of the `mlr3` way and `tidymodels` way.

```r
# Load required packages
library(tidymodels)
library(ranger)

# Load the data
data("Titanic", package = "datasets")
titanic <- as.data.frame(Titanic)
titanic$Survived <- as.factor(ifelse(titanic$Survived == "No", 0, 1))

# Define the model
model <- rand_forest(trees = 500) %>%
  set_engine("ranger") %>%
  set_mode("classification")

# Define the recipe
rec <- recipe(Survived ~ ., data = titanic)

# Create the workflow
workflow <- workflow() %>%
  add_model(model) %>%
  add_recipe(rec)

# Define resampling strategy (10-fold cross-validation)
folds <- vfold_cv(titanic, v = 10, strata = "Survived")

# Resample and evaluate model
results <- workflow %>%
  fit_resamples(resamples = folds)

# Print out performance measures
collect_metrics(results)
```

```r
# Load required packages
library(mlr3)
library(mlr3learners)

# Load the data
data("Titanic", package = "datasets")
titanic <- as.data.frame(Titanic)
titanic$Survived <- as.factor(ifelse(titanic$Survived == "No", 0, 1))

# Define task
task <- TaskClassif$new(id = "titanic", backend = titanic, target = "Survive

# Define learner (random forest)
learner <- lrn("classif.ranger", num.trees = 500)

# Define resampling strategy (10-fold cross-validation)
resampling <- rsmp("cv", folds = 10) 1
rr <- resample(task, learner, resampling) 2

# Print out performance measures
rr$aggregate(measures = msr("classif.ce")) 3
```

Resampling

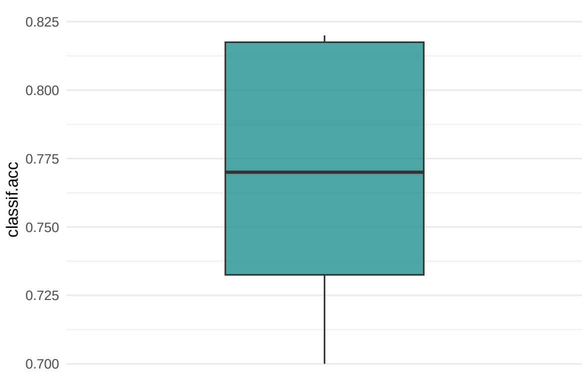
- `resample()`: initiate resampling
- `$aggregate()`: aggregate resampling performance

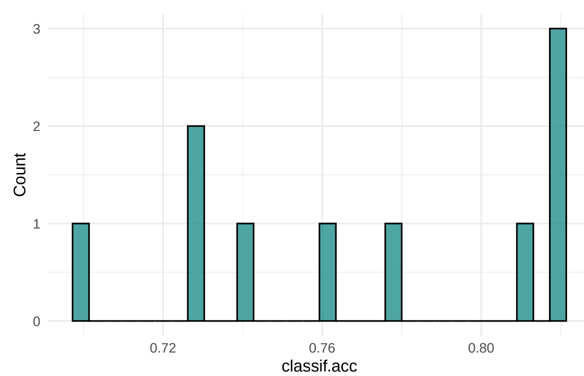
```
task = tsk("german_credit")
learner = lrn("classif.ranger", predict_type="prob")
resample = rsmp("cv", folds=10)
rr  = resample(task, learner, resample, store_model=T)
measures = msrs(c("classif.acc","classif.ppv","classif.npv","classif.auc"))
rr$aggregate(measures)
```

```
classif.acc classif.ppv classif.npv classif.auc
  0.7710000   0.7890524   0.6956910   0.7979774
```

Resampling

```
autoplot(rr, type="boxplot", measure = msr("classif.acc"))
autoplot(rr, type="histogram", measure = msr("classif.acc"))
```





Benchmarking

`tidymodels` vs `mlr3`

Benchmarking

- Comparison of multiple learners on a single task (or multiple tasks).

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Okay, lastly I would like to benchmark model performances. Here's the conditions
- algorithms: logistic regression, random forest, and XGBoost.
- resample: 10-fold cross validations.
- performance measurements: sensitivity, specificity, precision, f1-socre, and auroc.

```r
# Load required packages
library(tidymodels)
library(parsnip)
library(dials)
library(workflows)
library(xgboost)

# Load the data
data("Titanic", package = "datasets")
titanic <- as.data.frame(Titanic)
titanic$Survived <- as.factor(ifelse(titanic$Survived == "No", 0, 1

# Define the models
log_reg_model <- logistic_reg() %>%
  set_engine("glm") %>%
  set_mode("classification")

rand_forest_model <- rand_forest(trees = 500) %>%
  set_engine("ranger") %>%
  set_mode("classification")

xgboost_model <- boost_tree() %>%
  set_engine("xgboost") %>%
  set_mode("classification")

models <- list(log_reg = log_reg_model, rand_forest = rand_forest

# Define the recipe
rec <- recipe(Survived ~ ., data = titanic)

# Define resampling strategy (10-fold cross-validation)
folds <- vfold_cv(titanic, v = 10, strata = "Survived")

# Define the workflow and resampling for each model, then combine t
results <- map_dfr(models, ~ {
  workflow <- workflows::workflow() %>%
    add_recipe(rec) %>%
    add_model(.x)

  resamples <- fit_resamples(workflow, resamples = folds, metrics =

  resamples %>%
    collect_metrics() %>%
    mutate(model = .y)
})

print(results)
```

```r
# Load required packages
library(mlr3)
library(mlr3learners)
library(mlr3extras)
library(mlr3measures)
library(mlr3tuning)

# Load the data
data("Titanic", package = "datasets")
titanic <- as.data.frame(Titanic)
titanic$Survived <- as.factor(ifelse(titanic$Survived == "No", 0, 1))

# Define task
task <- TaskClassif$new(id = "titanic", backend = titanic, target = "Sur

# Define learners (logistic regression, random forest, XGBoost)
learners <- lapply(
  c("classif.log_reg", "classif.ranger", "classif.xgboost"),
  lrn, predict_type = "prob"
)

# Define resampling strategy (10-fold cross-validation)
resampling <- rsmp("cv", folds = 10)

# Define benchmark design
design <- benchmark_grid(
  tasks = task,
  learners = learners,
  resamplings = resampling
)

# Run benchmark
bmr <- benchmark(design)

# Print performance measures
bmr$aggregate(msrs(c("classif.sensitivity", "classif.specificity", "cla
```

- `benchmark_grid()`: design a benchmarking

```
tasks = tsks(c("german_credit", "sonar", "breast_cancer"))

learners = list(
  lrn("classif.log_reg", predict_type="prob", id="LR"),
  lrn("classif.rpart", predict_type="prob", id="DT"),
  lrn("classif.ranger", predict_type="prob", id="RF")
)

rsmp = rsmp("cv", folds=5)

design = benchmark_grid(
  tasks = tasks,
  learners = learners,
  resamplings = rsmp)
```

Benchmarking

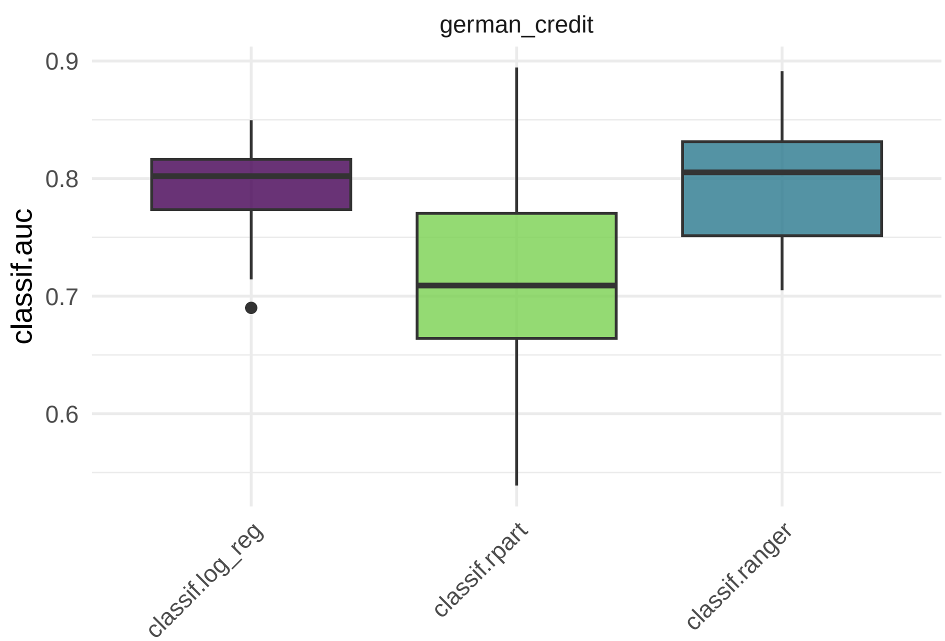
- `benchmark()`: execute benchmarking

```
bmr = benchmark(design)
measures = msrs(c("classif.acc","classif.ppv", "classif.npv", "classif.auc"))
as.data.table(bmr$aggregate(measures))[,-c("nr","resample_result","resampling_id","iters")
```

task_id	learner_id	classif.acc	classif.ppv	classif.npv	classif.auc
german_credit	LR	0.7540000	0.7959935	0.6128794	0.7682786
german_credit	DT	0.7220000	0.7720000	0.5715187	0.7009023
german_credit	RF	0.7670000	0.7866093	0.6820459	0.7916496
sonar	LR	0.7027875	0.7229497	0.6805154	0.7122449
sonar	DT	0.7262485	0.7250771	0.7382659	0.7524838
sonar	RF	0.8174216	0.8101012	0.8425397	0.9232502
breast_cancer	LR	0.9252791	0.9361270	0.9195608	0.9418515
breast_cancer	DT	0.9502362	0.9167371	0.9675106	0.9543396
breast_cancer	RF	0.9751181	0.9549859	0.9860113	0.9938067

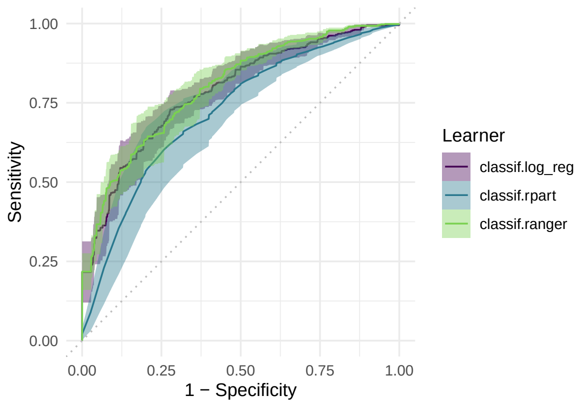
Benchmarking result

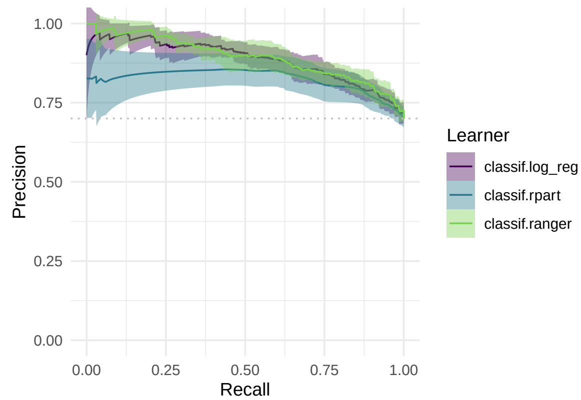
```
task = tsk("german_credit")
learners = list(
  lrn("classif.log_reg", predict_type="prob"),
  lrn("classif.rpart", predict_type="prob"),
  lrn("classif.ranger", predict_type="prob")
)
cv10 = rsmp("cv", folds=10)
design = benchmark_grid(
  task = task,
  learners = learners,
  resamplings = cv10)
bmr = benchmark(design)
autoplot(bmr, measure = msr("classif.auc"))
```



Benchmarking result

```r
autoplot(bmr, type = "roc")
autoplot(bmr, type = "prc")
```





More about `mlr3`

- Hyperparameter optimization
- Feature selection
- ML pipelines

Summary

`mlr3`

- `R6`, `data.table` based ML framework
- Sugar function + Dictionary
- Task, Learner, Measure
- Resampling
- Benchmarking
- Still in development (ver 0.16.0)
- A great textbook: **mlr3book**

Thank you for listening!