Machine Learning with R

mlr

Introduction

***mlr* offers a unified interface for the basic building blocks of machine learning: tasks, learners, hyperparameters, etc.**

Tasks contain a description of a task (classification, regression, clustering, etc.) and a data set.

Learners specify a machine learning algorithm (GLM, SVM, xgboost, etc.) and its parameters.

Hyperparameters are learner settings that can be specified directly or tuned. A **parameter set** lists the possible hyperparameters for a given learner.

Wrapped Models are learners that have been trained on a task and can be used to make predictions.

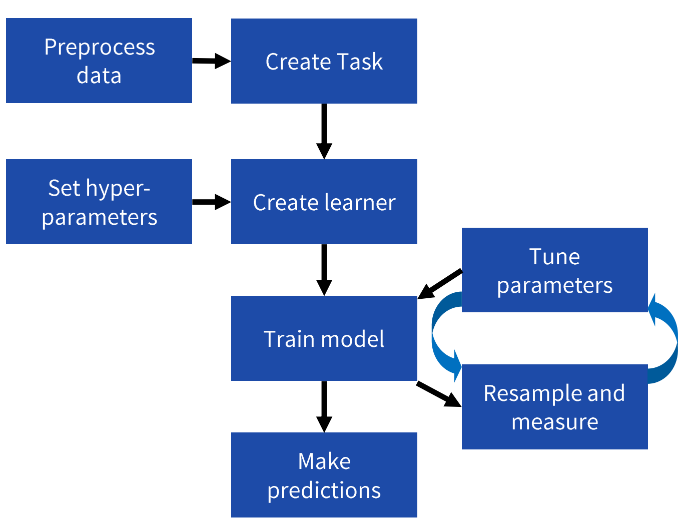
Predictions are the results of applying a model to either new data or the original training data.

Measures control how learner performance is evaluated, e.g. RMSE, LogLoss, AUC, etc.

Resampling estimates generalization performance by separating training data from test data. Common strategies include holdout and cross-validation.

Links: Tutorial | CRAN | Github

mlr workflow



Setup

Preprocessing data

`createDummyFeatures(obj=,target=,method=,cols=)`
Creates (0,1) flags for each non-numeric variable excluding `target`. Can be applied to entire dataset or only specific `cols`

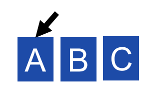
`normalizeFeatures(obj=,target=,method=,cols=,range=,on.constant=)`
Normalizes numerical features according to specified `method`:
- `"center"` (subtract mean)
- `"scale"` (divide by std. deviation)
- `"standardize"` (center and scale)
- `"range"` (linear scale to given range, default `range=c(0,1)`)

`mergeSmallFactorLevels(task=,cols=,min.perc=)`
Combine infrequent factor levels into a single merged level

`summarizeColumns(obj=)` where `obj` is a data.frame or task. Provides type, NA, and distributional data about each column

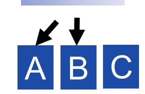
See also `capLargeValues` `dropFeatures` `removeConstantFeatures` `summarizeLevels`

Creating a task

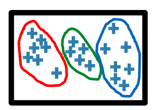


`makeClassifTask(data=,target=)`
Classification of a target variable, with optional positive class `positive`

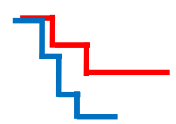
`makeRegrTask(data=,target=)`
Regression on a target variable



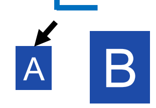
`makeMultilabelTask(data=,target=)`
Classification where the target can belong to more than one class per observation



`makeClusterTask(data=)`
Unsupervised clustering on a data set



`makeSurvTask(data=,target=c("time","event"))`
Survival analysis with a survival time column and an event column



`makeCostSensTask(data=,costs=)`
Cost-sensitive classification where each observation-cost pair has a specified cost

Other arguments that can be passed to a `task`:
- `weights=` Weighting vector to apply to observations
- `blocking=` Factor vector where each level indicates a block of observations that will not be split up in resampling

Making a learner

`makeLearner(cl=,predict.type=,...,par.vals=)`
Choose an algorithm class to perform the task and determine what that algorithm will predict
- `cl=`name of algorithm, e.g. `"classif.xgboost"` `"regr.randomForest"` `"cluster.kmeans"`
- `predict.type="response"` returns a prediction type that matches the source data; `"prob"` returns a predicted probability for classification problems only; `"se"` returns the a standard error of the prediction for regression problems only. Only certain learners can return `"prob"` and `"se"`
- `par.vals=` takes a list of hyperparameters and passes them to the learner; parameters can also be passed directly (`...`)

You can make multiple learners at once with `makeLearners()`

mlr has integrated over 170 different learning algorithms
- Full list: `View(listLearners())` shows all learners
- Available learners for a task: `View(listLearners(task))`
- Filtered list: `View(listLearners("classif", properties=c("prob", "factors")))` shows all classification learners `"classif"` which can predict probabilities `"prob"` and handle factor inputs `"factors"`
- See also `getLearnerProperties()`

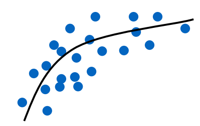
Training & Testing

Setting hyperparameters

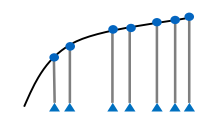
`setHyperPars(learner=,...)`
Set the hyperparameters (settings) for each learner, if you don't want to use the defaults. You can also specify hyperparameters in the `makeLearner()` call

`getParamSet(learner=)`
Show the possible universe of parameters for your learner; can take a learner directly, or a text string such as `"classif.qda"`

Train a model and predict



`train(learner=,task=)`
Train a model (`WrappedModel`) by applying a learner to a task. By default, the model will train on all observations. The underlying model can be extracted with `getLearnerModel()`



`predict(object=,task=,newdata=)`
Use a trained model to make predictions on a task or data set. The resulting `pred` object can be viewed with `View(pred)` or accessed by `as.data.frame(pred)`

Measuring performance

`performance(pred=,measures=)`
Calculate performance of predictions according to one or more of several measures (use `listMeasures()` for full list):
- classif `acc auc bac ber brier[.scaled] f1 fdr fn fnr fp fpr gmean multiclass[.au1u .aunp .aunu .brier] npv ppv qsr ssr tn tnr tp tpr wkappa`
- regr `arsq expvar kendalltau mae mape medae medse mse msle rae rmse rmsle rrse rsq sae spearmanrho sse`
- cluster `db dunn G1 G2 silhouette`
- multilabel `multilabel[.f1 .subset01 .tpr .ppv .acc .hamloss]`
- costsens `mcp meancosts`
- surv `cindex`
- other `featperc timeboth timepredict timetrain`

For detailed performance data on classification tasks, use:
- `calculateConfusionMatrix(pred=)`
- `calculateROCMeasures(pred=)`

Resampling a learner

`makeResampleDesc(method=,...,stratify=)`
`method` must be one of the following:
- `"CV"` (cross-validation, for number of folds use `iters=`)
- `"LOO"` (leave-one-out cross-validation, for folds use `iters=`)
- `"RepCV"` (repeated cross-validation, for number of repetitions use `reps=`, for folds use `folds=`)
- `"Subsample"` (aka Monte-Carlo cross-validation, for iterations use `iters=`, for train % use `split=`)
- `"Bootstrap"` (out-of-bag bootstrap, uses `iters=`)
- `"Holdout"` (for train % use `split=`)

`stratify` keeps target proportions consistent across samples.

`makeResampleInstance(desc=,task=)` can reduce noise by ensuring the resampling is done identically every time.

`resample(learner=,task=,resampling=,measures=)`
Train and test model according to specified resampling strategy.

mlr includes several pre-specified resample descriptions: `cv2` (2-fold cross-validation), `cv3`, `cv5`, `cv10`, `hout` (holdout with split 2/3 for training, 1/3 for testing).
Convenience functions also exist to `resample()` with a specific strategy: `crossval()`, `repcv()`, `holdout()`, `subsample()`, `bootstrapOOB()`, `bootstrapB632()`, `bootstrapB632plus()`

Refining Performance

Tuning hyperparameters

Set search space using `makeParamSet(make<type>Param())`
- `makeNumericParam(id=,lower=,upper=,trafo=)`
- `makeIntegerParam(id=,lower=,upper=,trafo=)`
- `makeIntegerVectorParam(id=,len=,lower=,upper=,trafo=)`
- `makeDiscreteParam(id=,values=c(...))` (can also be used to test discrete values of numeric or integer parameters)

`trafo` transforms the parameter output using a specified function, e.g. `lower=-2,upper=2,trafo=function(x) 10^x` would test values between 0.01 and 100, scaled exponentially
Other acceptable parameter types include `Logical LogicalVector CharacterVector DiscreteVector`

Set a search algorithm with `makeTuneControl<type>()`
- `Grid(resolution=10L)` Grid of all possible points
- `Random(maxit=100)` Randomly sample search space
- `MBO(budget=)` Use Bayesian model-based optimization
- `Irace(n.instances=)` Iterated racing process
- Other types: `CMAES`, `Design`, `GenSA`

Tune using `tuneParams(learner=,task=,resampling=,measures=,par.set=,control=)`

Quickstart

Prepare data for training and testing

```
library(mlbench)
data(Soybean)
soy = createDummyFeatures(Soybean,target="Class")
tsk = makeClassifTask(data=soy,target="Class")
ho = makeResampleInstance("Holdout",tsk)
tsk.train = subsetTask(tsk,ho$train.inds[[1]])
tsk.test = subsetTask(tsk,ho$test.inds[[1]])
```

Convert the factor inputs in the Soybean dataset into (0,1) dummy features which can be used by the XGboost algorithm. Create a task to precict the "Class" column. Create a train set with 2/3 of data and a test set with the remaining 1/3 (default).

Create learner and evaluate performance

```
lrn = makeLearner("classif.xgboost",nrounds=10)
cv = makeResampleDesc("CV",iters=5)
res = resample(lrn,tsk.train,cv,acc)
```

Create an XGboost learner which will build 10 trees. Then test performance using 5-fold cross-validation. Accuracy should be between 0.90-0.92.

Tune hyperparameters and retrain model

```
ps = makeParamSet(makeNumericParam("eta",0,1),
  makeNumericParam("lambda",0,200),
  makeIntegerParam("max_depth",1,20))
tc = makeTuneControlMBO(budget=100)
tr = tuneParams(lrn,tsk.train,cv5,acc,ps,tc)
lrn = setHyperPars(lrn,par.vals=tr$x)
```

Tune hyperparameters `eta`, `lambda`, and `max_depth` by defining a search space and tuning using Model Based Optimization (MBO) to control the search. Then perform 100 rounds of 5-fold cross-validation, improving accuracy to ~0.93. Update the XGboost learner with the tuned hyperparameters.

```
mdl = train(lrn,tsk.train)
prd = predict(mdl,tsk.test)
calculateConfusionMatrix(prd)
mdl = train(lrn,tsk)
```

Train the model on the train set and make predictions on the test set. Show performance as a confusion matrix. Finally, re-train model on the full set to use on new data. You are now ready to go out into the real world and make 93% accurate predictions!

Legend for functions (not all parameters shown):
`function(required_parameters=,optional_parameters=)`

Configuration

mlr's default settings can be changed using `configureMlr()`:

- `show.info` Whether to show verbose output by default when training, tuning, resampling, etc. (`TRUE`)
- `on.learner.error` How to handle a learner error. `"stop"` halts execution, `"warn"` returns NAs and displays a warning, `"quiet"` returns NAs with no warning (`"stop"`)
- `on.learner.warning` How to handle a learner warning. `"warn"` displays a warning, `"quiet"` supresses it (`"warn"`)
- `on.par.without.desc` How to handle a parameter with no description. `"stop"`, `"warn"`, `"quiet"` (`"stop"`)
- `on.par.out.of.bounds` How to handle a parameter with an out-of-bounds value. `"stop"`, `"warn"`, `"quiet"` (`"stop"`)
- `on.measure.not.applicable` How to handle a measure not applicable to a learner. `"stop"`, `"warn"`, `"quiet"` (`"stop"`)
- `show.learner.output` Whether to show learner output to the console during training (`TRUE`)
- `on.error.dump` Whether to create an error dump for crashed learners if `on.learner.error` is not set to `"stop"` (`TRUE`)

Use `getMlrOptions()` to see current settings

Parallelization

mlr works with the `parallelMap` package to take advantage of multicore and cluster computing for faster operations. mlr automatically detects which operations are able to run in parallel.

To begin parallel operation use:
`parallelStart(mode=,cpus=,level=)`

- `mode` determines how the parallelization is performed:
  - `"local"` no parallelization applied, simply uses `mapply`
  - `"multicore"` multicore execution on a single machine, uses `parallel::mclapply`. Not available in Windows.
  - `"socket"` multicore execution in socket mode
  - `"mpi"` Snow MPI cluster on one or multiple machines using `parallel::makeCluster` and `parallel::clusterMap`
  - `"BatchJobs"` Batch queuing HPC clusters using `BatchJobs::batchMap`
- `cpus` determines how many logical cores will be used
- `level` controls parallelization: `"mlr.benchmark"` `"mlr.resample"` `"mlr.selectFeatures"` `"mlr.tuneParams"` `"mlr.ensemble"`

To end parallelization, use `parallelStop()`

Imputation

`impute(obj=,target=,cols=,dummy.cols=,dummy.type=)` Applies specified logic to data frame or task containing NAs and returns an imputation description which can be used on new data

- `obj=`data frame or task on which to perform imputation
- `target=`specify target variable which will not be imputed
- `cols=`column names and logic for imputation*
- `dummy.cols=`column names to create a NA (T/F) column*
- `dummy.type=`set to `"numeric"` to use (0,1) instead of (T/F)

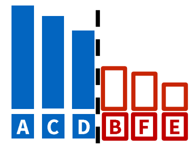
*Can also use `classes` and `dummy.classes` in place of `cols`

Imputation logic is passed to `cols` or `classes` via a list, e.g.: `cols=list(V1=imputeMean())` where `V1` is the column to which to apply the imputation, and `imputeMean()` is the imputation method. Available imputation methods include:
`imputeConst(const=)` `imputeMedian()` `imputeMode()`
`imputeMin(multiplier=)` `imputeMax(multiplier=)`
`imputeNormal(mean=,sd=)`
`imputeHist(breaks=,use.mids=)`
`imputeLearner(learner=,features=)`
`impute` returns a list containing the imputed dataset or task as well as an imputation description that can be used to reapply the same imputation to new data using `reimpute`

`reimpute(obj=,desc=)` Imputes missing values on a task or dataset (`obj`) using a description (`desc`) created by `impute`

Feature Extraction

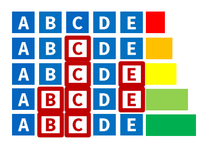
Feature filtering



`filterFeatures(task=,method=, perc=,abs=,threshold=)` Uses a learner-agnostic feature evaluation method to rank feature importance, then includes only features in the top n percent (`perc=`), top n (`abs=`), or which meet a set performance threshold (`threshold=`).

Outputs a task with features that failed the test omitted. `method` defaults to `"randomForestSRC.rfsrc"`, but can be set to:
`"anova.test"` `"carscore"` `"cforest.importance"` `"chi.squared"` `"gain.ratio"` `"information.gain"` `"kruskal.test"` `"linear.correlation"` `"mrmr"` `"oneR"` `"permutation.importance"` `"randomForest.importance"` `"randomForestSRC.rfsrc"` `"randomForestSRC.var.select"` `"rank.correlation"` `"relief"` `"symmetrical.uncertainty"` `"univariate.model.score"` `"variance"`

Feature selection



`selectFeatures(learner=,task=, resampling=,measures=,control=)` Uses a feature selection algorithm (`control`) to resample and build a model repeatedly using different feature sets each time in order to find the best set.

Available controls include:

- `makeFeatSelControlExhaustive(max.features=)` Try every combination of features up to optional `max.features`
- `makeFeatSelControlRandom(maxit=,prob=, max.features=)` Randomly sample features with probability `prob` (default 0.5) until `maxit` (default 100) iterations; return the best one found
- `makeFeatSelControlSequential(method=,maxit=, max.features=,alpha=,beta=)` Perform an iterative search using a `method` from the following: `"sfs"` forward search, `"sbs"` backward search, `"sffs"` floating forward search, `"sfbs"` floating backward search. `alpha` indicates minimum improvement required to add a feature; `beta` indicates minimum required to remove a feature
- `makeFeatSelControlGA(maxit=,max.features=,mu=, lambda=,crossover.rate=,mutation.rate=)` Genetic algorithm trains on random feature vectors, then uses crossover on the best performers to produce 'offspring', repeated over generations. `mu` is size of parent population, `lambda` is size of children population, `crossover.rate` is probability of choosing a bit from first parent, `mutation.rate` is probability of flipping a bit (on or off)

`selectFeatures` returns a `FeatSelResult` object which contains optimal features and an optimization path. To apply feature selection result (`fsr`) to your task (`tsk`), use:
`tsk = subsetTask(tsk,features=fsr$x)`

Benchmarking

`benchmark(learners=,tasks=,resamplings=,measures=)` Allows easy comparison of multiple learners on a single task, a single learner on multiple tasks, or multiple learners on multiple tasks. Returns a benchmark result object.

Benchmark results can be accessed with a variety of functions beginning with `getBMR<object>:` `AggrPerformance` `FeatSelResults` `FilteredFeatures` `LearnerIds` `LeanerShortNames` `Learners` `MeasureIds` `Measures` `Models` `Performances` `Predictions` `TaskDescs` `TaskIds` `TuneResults`

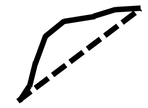
mlr contains several toy tasks which are useful for benchmarking:
`agri.task` `bc.task` `bh.task` `costiris.task` `iris.task` `lung.task` `mtcars.task` `pid.task` `sonar.task` `wpbc.task` `yeast.task`

Visualization

Performance

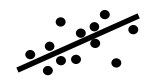
`generateThreshVsPerfData(obj=,measures=)` Measure performance at different probability cutoffs to determine optimal decision threshold for binary classification problems

- `plotThreshVsPerf(obj)` Plot visual representation of threshold curve(s) from `ThreshVsPerfData`



- `plotROCCurves(obj)` Plot receiver operating characteristic (ROC) curve from `ThreshVsPerfData`. Must set `measures=list(fpr,tpr)`

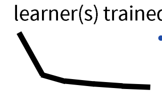
Residuals



- `plotResiduals(obj=)` Plots residuals for `Prediction` or `BenchmarkResult`

Learning curve

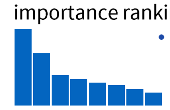
`generateLearningCurveData(learners=,task=, resampling=,percs=,measures=)` Measure performance of learner(s) trained on different percentages of task data



- `plotLearningCurve(obj=)` Plot curve showing learner performance vs. proportion of data used, uses `LearningCurveData`

Feature importance

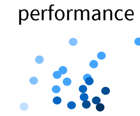
`generateFilterValuesData(task=,method=)` Get feature importance rankings using specified filter method



- `plotFilterValues(obj=)` Plot bar chart of feature importance based on filter method using `FilterValuesData`

Hyperparameter tuning

`generateHyperParsEffectData(tune.result=)` Get the impact of different hyperparameter settings on model performance



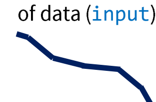
- `plotHyperParsEffect(hyperpars.effect.data=,x=,y=,z=)` Create a plot showing hyperparameter impact on performance using `HyperParsEffectData`

See also:

- `plotOptPath(op=)` Display details of optimization process. Takes `<obj>$opt.path`, where `<obj>` is an object of class `tuneResult` or `featSelResult`
- `plotTuneMultiCritResult(res=)` Show pareto front for results of tuning to multiple performance measures

Partial dependence

`generatePartialDependenceData(obj=,input=)` Get partial dependence of model (`obj`) prediction over each feature of data (`input`)

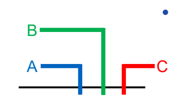


- `plotPartialDependence(obj=)` Plots partial dependence of model using `PartialDependenceData`

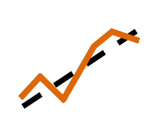
Benchmarking

- `plotBMRBoxplots(bmr=)` Distribution of performances
- `plotBMRSummary(bmr=)` Scatterplot of avg. performances
- `plotBMRRanksAsBarChart(bmr=)` Rank learners in bar plot

Other

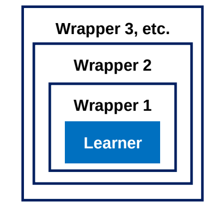


- `generateCritDifferencesData(bmr=, measure=,p.value=,test=)` Perform critical-differences test using either the Bonferroni-Dunn (`"bd"`) or `"Nemenyi"` test
- `plotCritDifferences(obj=)`



- `generateCalibrationData(obj=)` Evaluate calibration of probability predictions vs. true incidence
- `plotCalibration(obj=)`

Wrappers



Wrappers fuse a learner with additional functionality. mlr treats a learner with wrappers as a single learner, and hyperparameters of wrappers can be tuned jointly with underlying model parameters. Models trained with wrappers will apply them to new data.

Preprocessing and imputation

`makeDummyFeaturesWrapper(learner=)`
`makeImputeWrapper(learner=,classes=,cols=)`
`makePreprocWrapper(learner=,train=,predict=)`
`makePreprocWrapperCaret(learner=,...)`
`makeRemoveConstantFeaturesWrapper(learner=)`

Class imbalance

`makeOverBaggingWrapper(learner=)`
`makeSMOTEWrapper(learner=)`
`makeUndersampleWrapper(learner=)`
`makeWeightedClassesWrapper(learner=)`

Cost-sensitive learning

`makeCostSensClassifWrapper(learner=)`
`makeCostSensRegrWrapper(learner=)`
`makeCostSensWeightedPairsWrapper(learner=)`

Multilabel classification

`makeMultilabelBinaryRelevanceWrapper(learner=)`
`makeMultilabelClassifierChainsWrapper(learner=)`
`makeMultilabelDBRWrapper(learner=)`
`makeMultilabelNestedStackingWrapper(learner=)`
`makeMultilabelStackingWrapper(learner=)`

Other

`makeBaggingWrapper(learner=)`
`makeConstantClassWrapper(learner=)`
`makeDownsampleWrapper(learner=,dw.perc=)`
`makeFeatSelWrapper(learner=,resampling=,control=)`
`makeFilterWrapper(learner=,fw.perc=,fw.abs=, fw.threshold=)`
`makeMultiClassWrapper(learner=)`
`makeTuneWrapper(learner=,resampling=,par.set=, control=)`

Nested Resampling

mlr supports **nested resampling** for complex operations such as tuning and feature selection through wrappers. In order to get a good estimate of generalization performance and avoid data leakage, both an outer (for tuning/feature selection) and an inner (for the base model) resampling process are advised.

- Outer resampling can be specified in `resample` or `benchmark`
- Inner resampling can be specified in `makeTuneWrapper`, `makeFeatSelWrapper`, etc.

Ensembles

`makeStackedLearner(base.learners=,super.learner=, method=)` Combines multiple learners to create an ensemble

- `base.learners=`learners to use for initial predictions
- `super.learner=`learner to use for final prediction
- `method=`how to combine base learner predictions:
  - `"average"` simple average of all base learners
  - `"stack.nocv"`,`"stack.cv"` train super learner on results of base learners, with or without cross-validation
  - `"hill.climb"` search for optimal weighted average
  - `"compress"` with a neural network for faster performance