mlr3proba: Machine Learning Survival Analysis in R

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Abstract

As machine learning has become increasingly popular over the last few decades, so too has the number of machine learning interfaces for implementing these models. However, no consistent interface for evaluation and modelling of survival analysis has emerged despite its vital importance in many fields, including medicine, economics, and engineering. mlr3proba is part of the mlr3 ecosystem of machine learning packages for R and facilitates mlr3’s general model tuning and benchmarking by providing a multitude of performance measures and learners for survival analysis with a clean and systematic infrastructure for their evaluation. mlr3proba provides a comprehensive machine learning interface for survival analysis, which allows survival modelling to finally be up to the state-of-art.

Keywords: machine learning, survival analysis, R, benchmarking, AutoML

1. Introduction

mlr3proba introduces survival modelling to the mlr3 (Lang et al., 2019a) ecosystem of machine learning packages. Survival modelling is the field of Statistics concerned with making predictions about the time until an event (often death) takes place. By utilising a probabilistic supervised learning (Gressmann et al., 2018) framework mlr3proba allows for multiple survival analysis predictions: predicting the time to an event, the probability of an event over time, and the relative risk of an event. mlr3proba includes an extensive collection of classical and machine learning models, and many specialised survival measures.

R (R Core Team, 2020) is a favoured programming language for both survival analysis and machine learning as it has an extensive library of statistical functions and models implemented in both its core functionality, and in open source packages from CRAN and Bioconductor. mlr3proba leverages these packages by connecting a multitude of machine learning models and measures for survival analysis. By interfacing these packages, mlr3proba currently supports simulation of survival data, classical survival models, prediction of survival distributions by machine learning, and support for high-dimensional data (for example genomics and imaging). Interfacing other packages in the mlr3 family allows optimisation and benchmarking for all of these.
2. Implemented Functionality

A standard pipeline for survival analysis consists of: i) Defining a survival task as a set of features and survival outcome (time until the event and a censoring indicator); ii) Training a model on survival data, with the possibility of optimisation via tuning of hyper-parameters; iii) Making predictions from the trained model on new data; iv) Evaluating the quality of predictions with survival-specific measures, possibly including visualisation.

mlr3proba streamlines this process by: i) Standardising survival tasks, with the Surv object from the survival (Therneau, 2015) package, into a single object capable of handling left-, interval-, and right-censoring (TaskSurv); ii) Unifying all survival learners (LearnSurv*) with iii) prediction objects that clearly distinguish model prediction types (PredictionSurv); iv) Unifying survival measures for different survival prediction types (MeasureSurv*).

More than 20 survival learners are currently implemented, ranging from classical statistical models like Cox regression (Cox, 1972) to machine learning methods including Random Survival Forests (Ishwaran et al., 2008), gradient boosting machines, and many others. When models return a survival probability prediction, these are cast into standardized distribution objects using the distr6 package (Sonabend and Kiraly, 2019), which allows clean post-processing, such as predicting survival and hazard functions, among other uses.

For comparison of different models, 19 survival measures are implemented in mlr3proba, including discrimination measures (variants of concordance indices) and scoring rules, for example the (time-dependent) Graf score (Graf et al., 1999). Several of these are implemented directly in mlr3proba with an Rcpp (Eddelbuettel and Francois, 2011) implementation for fast and reliable performance.

Careful design and documentation of models and measures clearly demonstrates the precise return type provided by models and evaluated by measures, which has historically been problematic in survival analysis (see section 3). Model tuning and optimisation is available via mlr3tuning (Lang et al., 2019b) and preprocessing, feature selection, and more general pipelines from mlr3pipelines (Binder et al., 2020).

3. Return Types

A key advantage of mlr3proba, is a clear distinction between model prediction types. Survival models can be used to produce a variety of different prediction types but implementation has historically not reflected this. In other supervised learning fields this is not a problem as regression always predicts a continuous value for the outcome, and classification either predicts a category or a probability (the two can immediately be seen to be different). However in survival analysis there are several different possible predictions that could be made and without clear documentation, these can look very similar. For example, if a user wanted to compare predictions from Cox PH and survival tree models without mlr3proba, this would require the following steps: i) Train and predict from the models using two separate packages; ii) identify that the model predictions are not directly comparable; iii) use a third package to transform the predictions into a compatible form (for example combining a relative risk prediction with a baseline hazard estimation); iv) identify which measures can be used to evaluate this form; and v) find the package that includes these measures and potentially write functions to interface with the package.
In `mlr3proba`, this distinction is made clear by defining four distinct prediction types: i) `response`, which returns the predicted survival time (expected time until the event occurs); ii) `lp`, which returns a prediction for the linear predictor of a linear model; iii) `crank`, a continuous ranking for comparing the relative risk between observations in the test sample; iv) `distr`, a survival distribution implemented via `distr6`, which includes functionality for evaluating the survival and hazard function.

This problem of return types is important as different types are not comparable and historically this has not been successfully managed, leading to impractical benchmark experiments. By defining these prediction types as different objects in `mlr3proba`, incompatible benchmark experiments are avoided by internal validation checks. Finally, by making use of `mlr3pipelines` (Binder et al., 2020), transformations between prediction types can be made, with clear documentation and parameter setting that ensure a simple interface for the user. The example in Listing 1 demonstrates a GBM learner using the `distrcompositor` to transform a linear predictor prediction to a distribution by assuming a PH form and estimating the baseline survival function with the Kaplan-Meier estimator (Kaplan and Meier, 1958). Mathematically, this transformation is \( S_{PH}(\tau) = \hat{S}_0(\tau)^{\exp(\hat{\eta})} \) where \( \hat{S}_0 \) is the baseline hazard estimated by the Kaplan-Meier estimator and \( \hat{\eta} \) is the predicted linear predictor.

4. Related Work

There are an increasing number of machine learning packages across programming languages, including `caret` (Kuhn, 2008), `mlr` (Bischl et al., 2016), `tidymodels` (Kuhn and Wickham, 2020), and `scikit-learn` (Pedregosa et al., 2011). However, functionality for survival analysis has been mostly limited to ‘classical’ statistical models with relatively few packages supporting a machine learning framework.

R ships with the package `survival` (Therneau, 2015), which supports left-, interval-, and right-censoring, competing risks, time-dependent models, stratification, and model evaluation. However the package is limited to classical statistical models, with no support for machine learning and limited support for formal comparison or non-linear models.

`pec` (Mogensen et al., 2014) implements no models itself but instead interfaces with many different survival packages to create survival probability predictions. The package’s main focus is on model evaluation via prediction error curves (‘pec’s) with little support for model building/training and predicting.

`skpro` (Gressmann et al., 2018) is a probabilistic supervised learning interface in Python. `skpro` extends the `scikit-learn` (Pedregosa et al., 2011) interface to probabilistic models and appears to be the only package (in any language) dedicated to domain-agnostic probabilistic supervised learning. The interface provides an infrastructure for machine learning based survival analysis with design choices influencing `mlr3proba`, but `skpro` does not currently support survival models.

`pysurvival` (Fotso et al., 2019) is another Python package, which implements classical and machine learning survival analysis models. The package has the advantage of being able to natively leverage neural network survival models, which are almost exclusively implemented in Python. Whilst not directly interfacing the `scikit-learn` interface, the package introduces unified functions for model fitting, predicting, and evaluation.
scikit-survival (Pühlsterl, 2019) builds directly on scikit-learn to implement a few survival models and measures in a machine learning framework. Unlike pysurvival, no neural networks are included, thus the two packages complement each other well.

5. Example

Listing 1 gives an example of how to benchmark three survival models, set hyper-parameter values, and make use of the distribution compositor.

Line 1: Required packages are loaded, mlr3proba always requires mlr3. Lines 2-3: Kaplan-Meier and Cox PH learners are constructed with default parameters. Line 4: A decision tree is initialized with user-specified choices for the hyper-parameters maxdepth and minsplit. Lines 5-6: The GBM learner is wrapped in the distrcompositor to transform its ranking prediction to a probabilistic prediction. Line 7: Learners are combined into a list for use in the benchmark function. Line 8: Benchmarking is performed on a pre-specified task using the rats dataset from survival. Line 9: Three-fold cross-validation is specified. Line 10: The infrastructure for the experiment is automatically determined by supplying the task(s), learners, and resampling method. Line 11: Learners are resampled according to the chosen scheme and benchmarked. Line 12: Predictions are aggregated over all folds and scored with Uno’s concordance index (Uno et al., 2011) to provide a final comparison.

Listing 1: Example code for constructing, benchmarking, and evaluating survival models.

6. Availability, Documentation, and Code Quality Control

Packages in the mlr3 ecosystem are released under the GNU Lesser General Public License version 3 (LGPL-3) on GitHub (https://github.com/mlr-org) and CRAN. Documentation is available at https://mlr3proba.mlr-org.com/. Survival learners are available from the mlr3learners GitHub organisation (https://github.com/mlr3learners). Further use-case centric information is available in the (work-in-progress) mlr3 book (https://mlr3book.mlr-org.com) and examples in the mlr3 gallery (https://mlr3gallery.mlr-org.com). An extensive suite of unit tests is run on different continuous integration systems. Contributor guidelines detail expectations and requirements for external contributions.
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