The R package `simFrame`: An object-oriented approach towards simulation studies in statistics

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Content

Motivation

Research projects in statistcs are often based on extensive simulation studies (e.g., project AMELI, see Alfons et al. 2009).

- If many scientists or institutions are involved, a precise outline for the simulation studies is required.
- Otherwise results obtained by different researchers may be incomparable, which in turn makes it impossible to draw meaningful conclusions.

A common framework for simulation may assist statisticians in defining and following such common guidelines. Requirements include:

- running simulations with only a few commands,
- adding contamination to investigate robust methods,
- inserting missing values to evaluate methods for incomplete data,
- visualization of simulation results and
- easy extensibility for special needs.

The R package `simFrame` (Alfons 2010) ...

- is an object-oriented framework for statistical simulation based on S4 classes and methods (Chambers 1998, 2008) focused on applications in robust statistics.
- offers a wide range of simulation designs with a minimal amount of programming.
- gives maximum control over input and output due to the object-oriented implementation, while at the same time providing clear interfaces for extensions by user-defined classes and methods.
- allows certain proportions of the data to be contaminated or set to `NA`.
- selects an appropriate plot method for the simulation results automatically depending on their structure.

Categorization of statistical simulation

- Statistical simulation is frequently divided into the following categories:

  Model-based simulation: data sets are generated repeatedly from a distributional model or a mixture of distributions.

  - Application: Evaluation of methods that make theoretical assuptions about the underlying data.
  - Example: Comparison of outlier detection methods, which typically assume a multivariate normal distribution.

  Design-based simulation: samples are drawn repeatedly from a finite population.

  - Application: Evaluation of methods in survey statistics.
  - Example: Comparison of different estimation methods for point and variance estimates of poverty measures.

- Both types of simulations are supported by `simFrame`.

Design of the framework

- Statistical simulation in R is often done using bespoke use-once-and-throw-away scripts.

  $\longrightarrow$ This approach has its limitations if a research project is based on extensive simulation studies.
- Design of `simFrame`: Simulations are performed using the generic function `runSimulation()`, whose behavior is determined by control objects.
  - The user supplies a function that is applied in every iteration.
  - Switching from one simulation design to another can easily be done by just plugging in different control objects.
  - Only a few lines of code are necessary, the user does not have to worry about loops or collecting the results in a suitable data structure.
  - Comparability of the results from different researchers in a project is ensured if the same control objects are used.

General implementation

- Most of `simFrame` is implemented as S4 classes and methods, except some utility functions and some C code.
- Control classes ...
  - contain all necessary information to perform the corresponding tasks (data generation, sampling, contamination, insertion of missing values).
  - are the basis for method selection for generic functions, which in most cases provides the interfaces for extensions by developers.
- Available package vignettes:
  - `vignette("simFrame-intro")`: detailed discussion of the implementation (Alfons et al. 2010b, submitted to JSS).
  - `vignette("simFrame-eusilc")`: further code examples that show the strengths of the framework.

Simplified UML class diagram

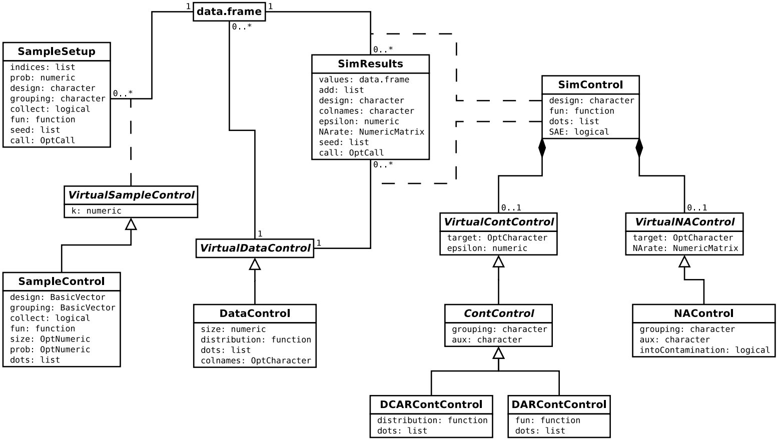


Figure: Simplified UML class diagram of `simFrame`

Running simulations

The generic function `runSimulation()` is the interface for running simulation studies.

- Methods for model-based and design-based simulation are implemented.
- In addition, the control class `SimControl` determines how the simulation runs are performed.
  - A function to be applied in every simulation run needs to be specified.
  - Control objects for contamination and the insertion of missing values may be supplied.

Notes on the function to be applied in each simulation run:

- There are some requirements, which are listed in Alfons et al. (2010b).
- It is evaluated using `try` to prevent loss of results if computations fail in one of the simulation runs.

Visualization

Visualization methods for the simulation results are based on `lattice` graphics (Sarkar 2008, 2010).

`simBwplot()`: boxplots of the simulation results.

`simDensityplot()`: densityplot of the simulation results.

`simXyplot()`: for different contamination levels or missing value rates, the (average) results are plotted against the contamination levels or missing value rates.

The `plot()` method for the simulation results selects a suitable graphical representation automatically.

Parallel computing

Statistical simulation is embarrassingly parallel, hence computational performance can be increased by parallel computing. In `simFrame`, parallel computing is implemented using the R package `snow` (Rossini et al. 2007, Tierney et al. 2008, 2009).

`clusterSetup()`: setting up multiple samples on a cluster.

`clusterRunSimulation()`: running simulations on a cluster.

- All objects and packages required for the computations (including `simFrame`) need to be made available on every worker process.
- In order to ensure reproducibility of the simulation results, random number streams (L'Ecuyer et al. 2002, Sevcikova and Rossini 2009) should be used. These are supported by `snow` via the function `clusterSetupRNG()`.

Example: Gini coefficient I

- EU-SILC is a complex household survey used as basis for measuring risk-of-poverty and social cohesion in Europe.
- The Gini coefficient is a well-known measure of inequality.
- In this simple example, different estimation methods for the Gini coefficient are compared in a design-based simulation study.
- The standard estimation method (Eurostat definition; EU-SILC 2004) is compared to two semiparametric approaches, which fit a Pareto distribution to the upper tail of the data.
  - Hill (1975) introduced the maximum-likelihood estimator, which is therefore referred to as Hill estimator.
  - The partial density component estimator (PDC; Vandewalle et al. 2007) follows a robust approach.
- All these methods are implemented in the R package `laeken` (Alfons et al. 2010a).

Example: Gini coefficient II

First, the required packages and the data set are loaded, and the seed of the random number generator is set.

```
> library(simFrame)
> library(laeken)
> data(eusilcP)
> set.seed(12345)
```

Next, a control object for drawing 100 samples from the population is defined (stratified by regions, sampling of whole households).

```
> sc <- SampleControl(design = "region", grouping = "hid",
+     size = c(75, 250, 250, 125, 200, 225, 125, 150, 100),
+     k = 100)
```

Then, a control object for contamination is defined. The contamination level is set to 0.5% because EU-SILC data typically contain a very low amount of outliers.

```
> cc <- DCARContControl(target = "eqIncome", epsilon = 0.005,
+     grouping = "hid", dots = list(mean = 5e+05, sd = 10000))
```

Example: Gini coefficient III

The function for the simulation runs is quite simple as well.

```
> sim <- function(x, k) {
+     g <- gini(x$eqIncome, x$.weight)$value
+     eqIncHill <- fitPareto(x$eqIncome, k = k, method = "thetaHill",
+         groups = x$hid)
+     gHill <- gini(eqIncHill, x$.weight)$value
+     eqIncPDC <- fitPareto(x$eqIncome, k = k, method = "thetaPDC",
+         groups = x$hid)
+     gPDC <- gini(eqIncPDC, x$.weight)$value
+     c(standard = g, Hill = gHill, PDC = gPDC)
+ }
```

With all necessary objects available, running the simulation experiment is only one more command. Note that simulations are performed separately for each gender.

```
> results <- runSimulation(eusilcP, sc, contControl = cc,
+     design = "gender", fun = sim, k = 125)
```

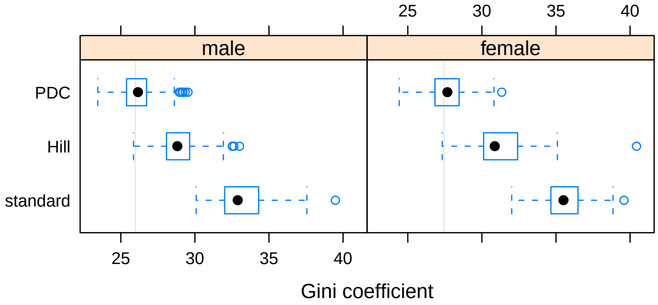
Example: Gini coefficient IV

In order to add a reference line to the plot of the results, the true values are computed from the population.

```
> tv <- simSapply(eusilcP, "gender", function(x) gini(x$eqIncome)$value)
```

An appropriate visualization method is selected automatically by the `plot()` method.

```
> plot(results, true = tv, xlab = "Gini coefficient")
```



Conclusions and outlook

- The flexible, object-oriented implementation of `simFrame` allows researchers to make use of a wide range of simulation designs with a minimal amount of programming.
- Control classes are used to handle data generation, sampling, contamination and the insertion of missing values.
- Developers can easily extend the existing framework with user-defined classes and methods.
- An appropriate plot method for the simulation results is selected automatically.
- Parallel computing using `snow` is supported to increase computational performance.
- Future plans include to extend the framework with different sampling methods and more specialized contamination and missing data models.

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