

Simulation Tools for Small Area Estimation: Introducing the R-package **saeSim**

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Abstract

The abstract of the article in English

Keywords: package, small area estimation, reproducible research, simulation, R.

1. Introduction

The objective of small area estimation is to produce reliable statistics (means, quantiles, proportions, etc.) for domains where little or no sampled units are available. Groups may be areas or other entities, for example defined by socio-economic characteristics. New statistical methods are applied in model-based and design-based simulation studies. Considering the demands for reproducible research we propose a framework for simulation studies inside the field of small area estimation.

Reproducible Research has become a widely discussed topic in general and also in the field of statistics. Thanks to the many mostly open-source tools like the R-language (R Core Team 2014) and L^AT_EX, and also packages like knitr (Yihui 2013) and Sweave (Leisch 2002) and more recently rmarkdown (Allaire, McPherson, Xie, Wickham, Cheng, and Allen 2014), the integration of text and source code for statistical analysis is possible. Not only are tools available to make research reproducible, also the demand of making the analysis of articles reproducible is rising which is supported by the rising number of Open Access Journals. Publishing source-code and data alongside an article draws special attention to authoring an analysis. However, the requirements for source code are different from the written words in the article itself.

Instead of imagining that our main task is to instruct a computer what to do, let us concentrate rather on explaining to human beings what we want a computer to do. (Knuth 1992, p.99)

In this article we want to introduce a new package for the R-language to support the process of making simulation studies reproducible as well as supporting a *human-readable* interface. With this package we have three objectives in specific: First, making tools for data generation available and reusable. Second, unify the process behind simulation studies inside the field of

Small Area Estimation. And third, making source-code of simulation studies available, such that it supports the conducted research in a transparent manner.

In section 2 we will give a short introduction to small area estimation and the role of simulation studies within that field. Section 3 will then introduce a framework for simulation studies and how it is supported by `saeSim`. To illustrate some of the package’s features we present a case study in section 4.

2. Small area estimation

The objective of small area estimation is to produce reliable statistics (means, quantiles, proportions, etc.) for domains where little or no sampled units are available. Groups may be areas or other entities, for example defined by socio-economic characteristics. The demand for such estimators is rising as they are used for fund allocation, educational and health programs (Pfeffermann 2013). As direct estimation of such statistics are considered to be unreliable, methods in small area estimation try to improve the domain predictions by borrowing strength from neighboured or *similar* domains. This can be achieved by using additional information from census data to assist the prediction for non-sampled domains or domains with little information. For the purpose of this article we will introduce two basic models frequently used in small area estimation, the unit-level model introduced by Battese, Harter, and Fuller (1988) and the area-level model introduced by Fay and Herriot (1979).

The unit level model (Battese *et al.* 1988) can be expressed as:

$$\begin{aligned} y_{ij} &= x_{ij}^\top \beta + v_i + e_{ij} \\ v_i &\stackrel{iid}{\sim} N(0, \sigma_v^2) \\ e_{ij} &\stackrel{iid}{\sim} N(0, \sigma_e^2) \end{aligned}$$

where $i = 1, \dots, D$ and $j = 1, \dots, n_i$. y_{ij} is the the dependent variable for domain i and unit j , and x_{ij} the corresponding auxiliary information for that unit. Furthermore v and e are independent. This model can be seen as a linear mixed model from which the best linear unbiased predictor (BLUP) can be derived and is used for the domain prediction (Rao 2003).

Due to reasons of confidentiality unit-level information is not always available. Instead only aggregates, or rather the direct estimators may be supplied. However, these direct estimations are known to be unreliable, hence in such situations area-level models can be valuable. The area-level model introduced by Fay and Herriot (1979) is build on a sampling model:

$$y_i = \mu_i + e_i,$$

where y_i is a direct estimator of a statistic of interest μ_i for an area i with $i = 1, \dots, D$ and D being the total number of areas. The sampling error e_i is assumed to be independent and normally distributed with known variances $\sigma_{e,i}^2$, i.e. $e_i | \mu_i \sim N(0, \sigma_{e,i}^2)$. The model is modified with the linking model by assuming a linear relationship between the true area statistic μ_i and some auxiliary variables x_i :

$$\mu_i = x_i^\top \beta + v_i,$$

with $i = 1, \dots, D$. Note that x_i is a vector containing area-level (aggregated) information for P variables and β is a vector ($1 \times P$) of regression coefficients describing the (linear) relationship. The model errors v_i are assumed to be independent and normally distributed, i.e. $v_i \sim N(0, \sigma_v^2)$. Furthermore e_i and v_i are assumed to be independent. Combining the sampling and linking model leads to:

$$y_i = x_i^\top \beta + v_i + e_i. \tag{1}$$

Model 1 is effectively a random-intercept model where the distribution of the error term e_i is heterogeneous and known.

3. A simulation framework

In our opinion simulation studies can best be summarised when understood as a process of data manipulation. Thus the main focus of **saeSim** is to define the steps in that process which can then be *cleanly* defined and repeated. Before we go into any detail of the functionality of the package we will discuss the process behind simulation studies and later how **saeSim** maps this process into R.

Simulation studies in small area estimation address three different levels, the population, the sample and data on aggregated level, as illustrated in figure 1. The **population-level** defines the data on which a study is conducted and may be a true population, synthetic population data or randomly generated variates from a model. We see three different point of views to define a population. First *design-based*, which means that a simulation study is based on true or synthetic data of *one* population. Second a *semi-model-based* point of view, where only one population is drawn from a model and is fixed in the whole simulation study. And third, *model-based* studies which have changing random populations drawn from a model.

The scope of this article is not to promote any of those viewpoints, but simply to identify the similarity in them. The *base* (first component in figure 1) of any simulation study is a data table, the question is, if this data is *fixed* or *random* over the course of the simulation. Or from a more technical point of view, is the data generation (the second step in figure 1) repeated in each simulation run or omitted? Depending on the choice of a fixed or random population it is necessary to recompute the population domain-statistics like domain means and variances, or other statistics of interest (third component in figure 1).

The **sample-level** is when domain predictions are conducted for unit-level models. Independently of how the population is treated, fixed or random, this phase consists of two steps, first drawing a sample, and second conducting computations on the samples (fourth and fifth component in figure 1). Given a sample, design or model based small area methods are applied. Of interest are estimated parameters, which can be estimated model parameters or domain predictions as well as measures of uncertainty for the estimates.

As the sample-level is when unit-level models are applied, the **aggregate-level** is when area-level models are applied (the seventh and last component in figure 1). Area-level models in small area estimation typically only use information available for domains (in contrast to units). Thus, the question for simulation studies for area-level methods is, if the data is generated on unit-level and used after the aggregation (sixth component in figure 1) or if the data is generated directly on area-level, i.e. drawn from an area-level model. Depending on whether unit-level data and sampling are part of the simulation the aggregate-level follows the generation of the population or is based on the aggregated sample. Again, we do not promote a specific viewpoint but simply allow steps in the process of simulation to be omitted.

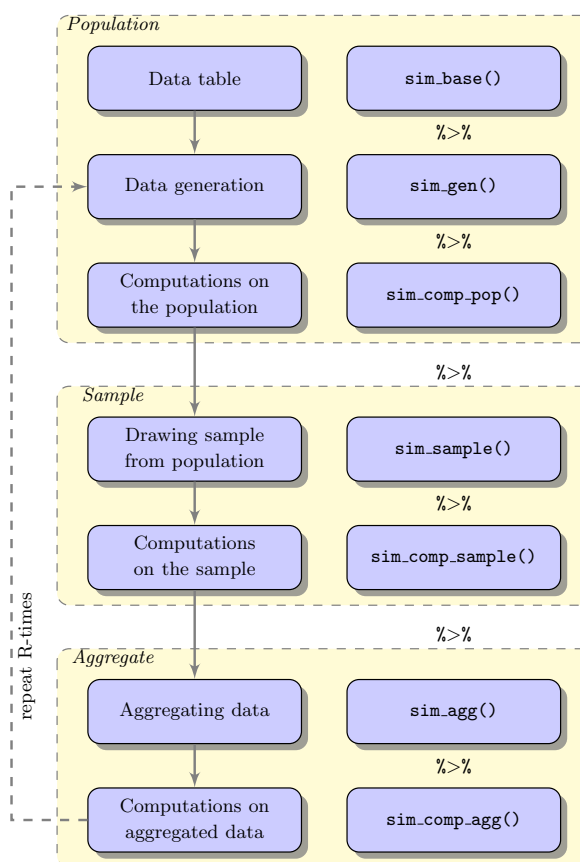


Figure 1: Process of simulation.

Depending on the topic of research steps in this simulation framework can be more relevant than others or completely irrelevant. We see these steps more as a complete list of phases one can encounter, thus single components can be omitted if not relevant in specific applications. For example *data generation* is not relevant if you have population data, or the *sample-level* is not used, when the sample is directly drawn from the model.

From this considerations, *saeSim* maps the different steps into R. Two layers with separate responsibilities need to be discussed. The first is *how* different simulation components can be combined, and the second *when* or in which order they are applied. Regarding the first, in *saeSim* we put a special emphasis on the interface of each component, which is to use functions which take a `data.frame` as argument and have a `data.frame` as return value. This is a widely used approach for data manipulation and promoted recently in the package *dplyr* (Wickham and Francois 2014). This definition of interfaces, the return value of one component is the input of the next, is also used in *saeSim*.

Understanding a simulation as a process of manipulating one data object, see the second column in figure 1 how the different steps in a simulation can be accessed. It is important to note that the functions in figure 1 control the process, the second layer, i.e. *when* components are applied. Each of these functions take a simulation setup object to be modified and a function with the discussed interface as arguments. Hence a simulation setup is a collection of functions to be applied in a certain sequence. Also the second-layer functions have a defined interface: a `sim_setup` as input to be modified and a `sim_setup` as output. Thus, components can be chained together using the *pipe operator* (`%>%`) from the package *magrittr* (Bache and Wickham 2014).

With *saeSim* we want to contribute tools for simulation studies in the field of small area estimation. We see the need for sharing tools for data generation and simulation amongst the scientific community and thus defined an interface for these tools as well as a platform to make them accessible. By defining the steps behind a simulation we hope to promote a reasonable way to communicate them alongside publications and during research. In the next section we will present a case study and focus more on the concrete functionality provided by the package.

4. Case study

Braking the responsibility into what is applied and when it is applied addresses several aspects of reproducibility. First, by defining the interface between all components, it is easy to combine them in any combination and thus easy to share and reuse. Second, by controlling when components are applied we avoid the necessity of control structures in syntax and emphasise on the definition of components. The following example shows these aspects of the package using a predefined simulation setup:

```
> setup1 <- sim_base_lm() %>% sim_sample(sample_number(5))
> setup2 <- sim_base_lm() %>% sim_sample(sample_fraction(0.05))
```

Without knowing anything about the setup defined in `sim_base_lm` we can see that `setup1` and `setup2` only differ in the applied sampling scheme. `sim_sample` is responsible to control when a function is applied (after the population-level) and `sample_number(5)` and `sample_fraction(0.05)` define the explicit way of drawing samples. The pipe operator `%>%` is used to add new components to the setup. As said before the composition of a simulation in that manner will focus on the definition of components and hide control structures. The next example will repeat the simulation stored in `setup1` two times. The results are returned in a list of `data.frames` which have five rows as we sample 5 observations:

```
> setup1 %>% sim(R = 2) %>% sapply(nrow)
```

```
[1] 5 5
```

As a side remark: The pipe operator, `%>%`, is designed to make otherwise nested expressions more readable as a line can be read from left to right, instead of inside out (Bache and Wickham 2014). As a minimal example see the following lines which are equivalent:

```
> sum(1:10)
```

```
[1] 55
```

```
> 1:10 %>% sum
```

```
[1] 55
```

4.1. Model-based simulation

The first task for the model-based simulation is to generate the data under the model:

$$y_i = 100 + 2 \cdot x_i + v_i + e_i$$

where $x_i \stackrel{iid}{\sim} N(0, 4^2)$, $v_i \stackrel{iid}{\sim} N(0, 1)$ and $e_i \stackrel{indep}{\sim} N(0, \sigma_i^2)$ with $\sigma_i^2 = 0.1, 0.2, \dots, 4$ and $i = 1, \dots, 40$ as index for the domains. Also are x_i , v_i and e_i independent from each other. The starting point is always a data table as *base-component*, in this case just with an id variable named `idD` and constructed with the function `base_id`. Any random number generator in R can be used, however we have a strictly *normal* model, for which some predefined functions can be used.

```
> library(saeSim)

> setup <- base_id(nDomains = 40, nUnits = 1) %>%
+   sim_gen_x(mean = 0, sd = 4) %>%
+   sim_gen_v(mean = 0, sd = 1)
> setup
```

	idD	x	v
1	1	-2.5058152	-0.1645236
2	2	0.7345733	-0.2533617
3	3	-3.3425144	0.6969634
4	4	6.3811232	0.5566632
5	5	1.3180311	-0.6887557
6	6	-3.2818735	-0.7074952

Note that if you print a simulation setup to the console, as in the above example, one simulation run is performed and only the first rows of the resulting data table are printed. This enables interactivity with the object itself, however it hides that the setup object is a collection of functions to be called. The error component e_i in the model has different variances which is not covered by a predefined function. Thus, as a *generator* function we will define a function which takes a `data.frame` as input and returns it after adding a variable named `vardir` with the variances and the variable `e` with the generated random numbers:

```
> gen_e <- function(dat) {
+   dat$vvaridir <- seq(0.1, 4, length.out = nrow(dat))
+   dat$e <- rnorm(nrow(dat), sd = sqrt(dat$vvaridir))
+   dat
+ }
> setup <- setup %>% sim_gen(gen_e)
> setup
```

	idD	x	v	vvaridir	e
1	1	-2.2746749	-0.5059575	0.1	0.1344285
2	2	-0.5407145	1.3430388	0.2	-0.1067262
3	3	4.7123480	-0.2145794	0.3	0.5797550
4	4	-6.0942672	-0.1795565	0.4	0.5606229
5	5	2.3757848	-0.1001907	0.5	-0.4378710
6	6	1.3318015	0.7126663	0.6	1.7088396

The last step in data generation is to construct the response variable which will be named `y` and added to the data. Also we will add the *true* area statistic under the model to the data:

```
> setup <- setup %>%
+   sim_resp_eq(y = 100 + 2 * x + v + e) %>%
+   sim_comp_pop(comp_var(trueStat = y - e))
```

Not all necessary functions can be provided by the package. As said before, one of the main objectives was to define the interface between components. To add the area-level predictions from a Fay-Herriot model we need to define a function for that. The function takes a `data.frame` as input and returns the modified version. Here we use the function `eblupFH` from the package `sae` (Molina and Marhuenda 2013) to estimate the EBLUP under the FH model. Finally we add `comp_FH` to the process:

```
> library(sae)

> comp_FH <- function(dat) {
+   modelFH <- eblupFH(y ~ x, vvaridir, data = dat)
+   dat$FH <- modelFH$eblup
+   dat
+ }
> setup <- setup %>% sim_comp_agg(comp_FH)
> setup
```

	idD	x	v	vvaridir	e	y	trueStat	FH
1	1	1.637607	0.7073107	0.1	0.1258998	104.10843	103.98253	104.06121
2	2	6.755493	1.0341077	0.2	-0.1822523	114.36284	114.54509	114.23876
3	3	6.346354	0.2234804	0.3	0.7253263	113.64151	112.91619	113.45213
4	4	-1.323631	-0.8787076	0.4	-0.4434978	96.03053	96.47403	96.45416
5	5	-9.140942	1.1629646	0.5	-0.4105563	82.47052	82.88108	82.46045
6	6	9.990646	-2.0001649	0.6	-0.7754272	117.20570	117.98113	118.08379

The object `setup` stores all necessary information to run one iteration of the simulation. To start more repetitions, `sim` is called, which will return $R = 100$ (as the number of repetitions) `data.frames` containing the simulated data from each iteration as a list. We use `rbind_all` from the package `dplyr` to append the resulting list:

```
> library(dplyr)
```

```
> simResults <- sim(setup, R = 100) %>% rbind_all
> simResults %>% select(idD, idR, simName, trueStat, y, FH)
```

Source: local data frame [4,000 x 6]

	idD	idR	simName	trueStat	y	FH
1	1	1		107.87088	108.21065	108.30528
2	2	1		113.29033	114.13809	113.80733
3	3	1		105.88208	105.55180	105.63108
4	4	1		84.61171	84.36450	84.63272
5	5	1		103.68692	103.39260	103.42371
6	6	1		104.26130	103.97032	103.79131
7	7	1		97.85114	97.54439	97.43298
8	8	1		101.93187	101.66741	101.49500
9	9	1		92.51517	93.88300	93.67397
10	10	1		104.07055	103.37302	104.01407
...

An additional variable `idR` is automatically added as an ID-variable for the iteration as well as a variable `simName` which purpose is to distinguish between scenarios, should there be more than one. At this time we do not provide further tools to process the resulting data. As it is a `data.frame` many packages for processing that data are available in R, in this case `dplyr` (Wickham and Francois 2014) and `reshape2` (Wickham 2007) have been used. The Rmd-file for this article can be checked for further detail, thus we do not see need to provide further tools from here on.

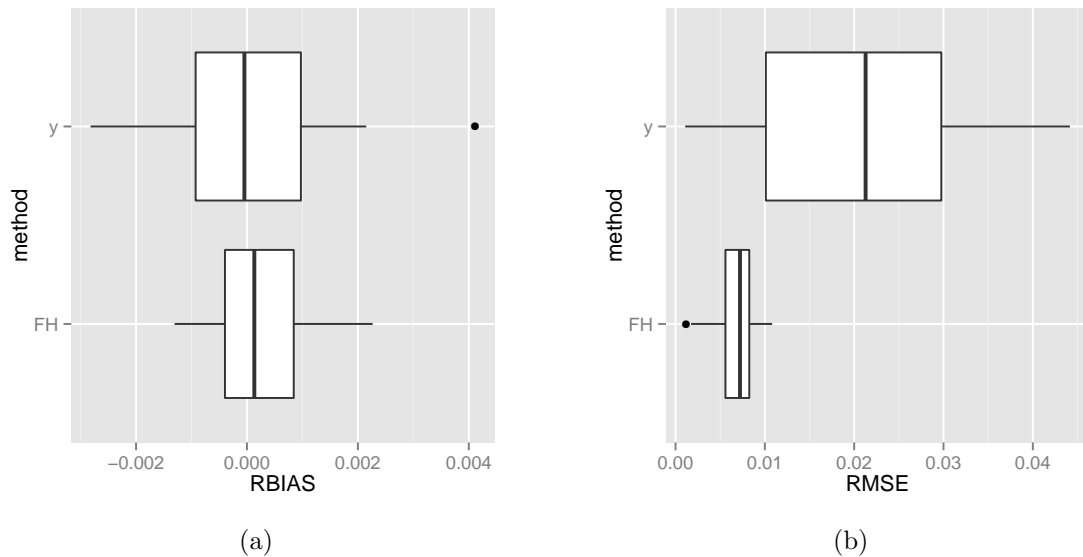


Figure 2: RBIAS and RMSE for the conducted model-based simulation

4.2. Design-based simulation

In the design-based simulation we want to illustrate the use of `saeSim` when starting from data of a population. For this purpose we use a synthetic population generated from Austrian EU-SILC (European Union Statistics on Income and Living Conditions) data. We use this data to illustrate the functionality of the package, the data consists of 25 thousand households and does not represent the true population size of Austria. It is published alongside the R-package `simFrame` (Alfons, Templ, and Filzmoser 2010) where it is used as example data. To

keep this study as simple as possible, we further restrict the data for the main income holder and will only use some of the provided auxiliary information.

```
> data(eusilcP, package = "simFrame")
> simDat <- eusilcP %>%
+   mutate(agesq = age^2, eqIncome = as.numeric(eqIncome)) %>%
+   filter(main) %>%
+   select(region, eqIncome, age, agesq, gender)
> head(simDat)
```

	region	eqIncome	age	agesq	gender
1	Upper Austria	11128.45	25	625	male
2	Styria	19694.85	53	2809	male
3	Styria	5066.24	30	900	female
4	Upper Austria	31480.01	32	1024	male
5	Vienna	17813.40	77	5929	female
6	Lower Austria	13501.53	35	1225	male

For the purpose of the design-based case study we want to apply the earlier introduced BHF estimator which is implemented in the R-package *sae* (Molina and Marhuenda 2013). The function we use, *ebupBHF*, expects three data objects to produce the predictions. The sampled data, the population means of the auxiliary variables and the population sizes in each domain. To store these informations and make them available during the simulation we attach them as attributes to the population data. There are other options but setting attributes to the processed data is supported in the package and presents a very flexible form of processing data on different aggregation levels.

```
> attr(simDat, "popMeans") <- group_by(simDat, region) %>%
+   summarise(age = mean(age),
+             agesq = mean(agesq),
+             genderFemale = mean(as.integer(gender) - 1),
+             trueStat = mean(eqIncome))
> attr(simDat, "popMeans")
```

Source: local data frame [9 x 5]

	region	age	agesq	genderFemale	trueStat
1	Burgenland	54.50063	3269.677	0.3366708	22005.42
2	Lower Austria	51.95259	3009.934	0.3777874	19813.37
3	Vienna	46.98310	2486.448	0.4662797	20395.84
4	Carinthia	51.81428	2995.735	0.3540337	19486.18
5	Styria	50.64087	2886.845	0.3573538	19335.39
6	Upper Austria	50.18644	2795.804	0.3443871	20517.29
7	Salzburg	51.44943	2965.268	0.4189108	19890.33
8	Tyrol	51.76707	2995.451	0.3975648	19350.89
9	Vorarlberg	49.06904	2697.382	0.3583756	22156.12

```
> attr(simDat, "popN") <- group_by(simDat, region) %>% summarise(N = n())
> attr(simDat, "popN")
```

Source: local data frame [9 x 2]

region	N
--------	---


```

1   Burgenland  799
2 Lower Austria 4619
3       Vienna  5857
4   Carinthia  1723
5       Styria  3386
6 Upper Austria 4071
7       Salzburg 1671
8       Tyrol   1889
9   Vorarlberg  985

```

Before we come to the estimation configuration, the first step is to add a sampling scheme. As stated earlier, the starting point of a simulation setup is to provide a `data.frame` as *base-component* which, in this case, is the population data. Then the sampling component is added, in which we define to draw 10 per cent of the observations from each domain with simple random sampling.

```

> setup <- simDat %>%
+   sim_sample(sample_fraction(0.1, groupVars = "region"))
> setup

```

```

      region eqIncome age agesq gender
1 Burgenland 23572.28  67  4489  male
2 Burgenland 24056.37  26   676  male
3 Burgenland 21613.73  46  2116  male
4 Burgenland 11750.30  40  1600  male
5 Burgenland  9664.08  80  6400 female
6 Burgenland 19369.91  63  3969 female

```

What now needs to be done, is to define the components which add the desired estimates to the data. Here we will compute the mean of income in each domain as the direct estimator and the EBLUP under the BHF model. Although this could be done in one step, we will separate the two computations to illustrate how to combine several estimations and define each component independent of one another. This focus on the definition of each component and meeting the convention of the defined interface is the intended approach. It will automatically organise the simulation and each component is arranged using the simulation framework. Hence, we will define two functions, one for adding the direct estimates and one for adding the EBLUP.

```

> comp_direct <- function(dat) {
+   attr(dat, "sampleMean") <-
+     dat %>% group_by(region) %>% summarise(direct = mean(eqIncome))
+   dat
+ }
> comp_BHF <- function(dat) {
+   popMeans <- select(attr(dat, "popMeans"), -trueStat)
+   modelBHF <-
+     eblupBHF(eqIncome ~ age + agesq + gender, region, meanxpop = popMeans,
+               popnsize = attr(dat, "popN"), data = dat)
+   attr(dat, "BHF") <- modelBHF$eblup
+   dat
+ }

```

Another positive aspect of the above definitions is, that each step is relatively small and the purpose clearly defined, which will make them easy to understand, modify and reproduce. Finally we will combine the simulation results in an *aggregation-component*, possibly

followed by the application of area-level models but skipped in this example. The result of this aggregation step will be a `data.frame` with one row for each region.

```
> agg_results <- function(dat) {
+   cbind(attr(dat, "sampleMean"),
+         BHF = attr(dat, "BHF")$eblup,
+         trueStat = attr(dat, "popMeans")$trueStat)
+ }
```

To combine the simulation setup and the defined components we arrange them using the function `sim_comp_sample` to ensure that the direct estimator and the EBLUP is computed on the sampled data, and `sim_agg` to add the above aggregation step.

```
> setup <- setup %>%
+   sim_comp_sample(comp_BHF) %>%
+   sim_comp_sample(comp_direct) %>%
+   sim_agg(agg_results)
> setup
```

	region	direct	BHF	trueStat
1	Burgenland	21933.95	21255.53	22005.42
2	Lower Austria	18885.08	19036.29	19813.37
3	Vienna	20734.08	20720.48	20395.84
4	Carinthia	19211.55	19377.21	19486.18
5	Styria	18704.75	18955.96	19335.39
6	Upper Austria	20636.94	20504.37	20517.29

To repeat the simulation R times the simulation setup can be passed to the function `sim`, the resulting list is directly combined using `rbind_all`.

```
> simResults <- setup %>% sim(R = 50) %>% rbind_all
> simResults
```

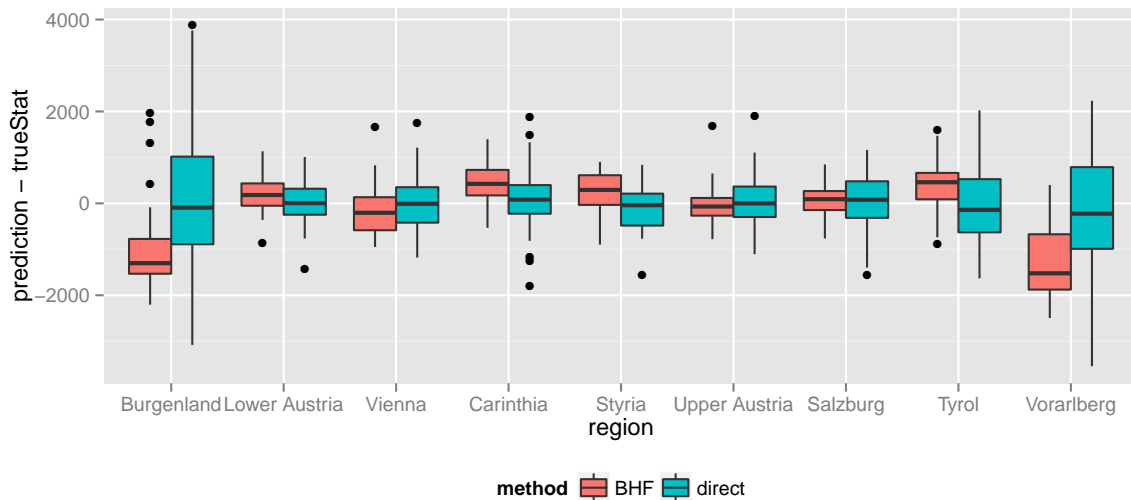
Source: local data frame [450 x 6]

	region	direct	BHF	trueStat	idR	simName
1	Burgenland	23083.61	20800.16	22005.42	1	
2	Lower Austria	20414.91	20264.56	19813.37	1	
3	Vienna	20756.78	20422.85	20395.84	1	
4	Carinthia	19581.64	19912.42	19486.18	1	
5	Styria	19443.11	19757.42	19335.39	1	
6	Upper Austria	20417.38	20356.38	20517.29	1	
7	Salzburg	19900.44	20009.83	19890.33	1	
8	Tyrol	18493.29	19540.25	19350.89	1	
9	Vorarlberg	21166.20	20444.35	22156.12	1	
10	Burgenland	21340.42	20510.92	22005.42	2	
..

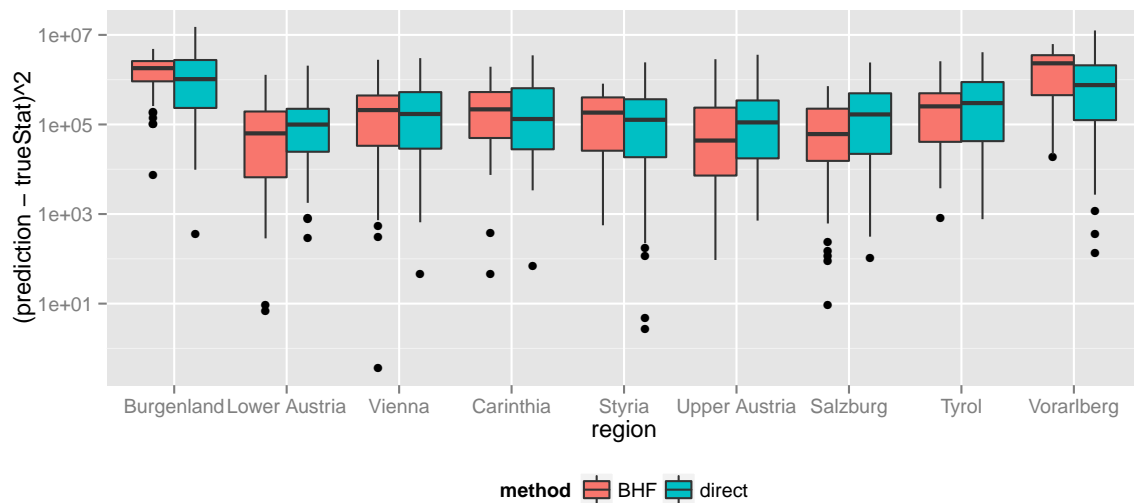
To further process simulation results we present two graphics, using the package `ggplot2` (Wickham 2009) and `reshape2` (Wickham 2007) for

```
> ggDat <- melt(simResults,
+               id.vars = c("region", "trueStat"),
+               measure.vars = c("BHF", "direct"),
+               variable.name = "method",
+               value.name = "prediction")
```

```
> ggplot(ggDat, aes(x = region, y = prediction - trueStat, fill = method)) +
+   geom_boxplot() + theme(legend.position = "bottom")
```



```
> ggplot(ggDat, aes(x = region, y = (prediction - trueStat)^2, fill = method)) +
+   geom_boxplot() + scale_y_log10() + theme(legend.position = "bottom")
```



5. Outlook

Use this package to share and publish simulation studies alongside papers. Contribute to the package to make your ideas available. Contribute to the package and make your whole simulation study available.

- Link to simFrame
- Package Features
 - outliers
 - sampling
 - non-linear models

- How to contribute?
- parallel computations

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