University of Duisburg-Essen Faculty of Business Administration and Economics Chair of Econometrics



# tidyMC

## Monte Carlo Simulations made easy and tidy

### Report

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### Introduction

Monte Carlo Simulations (henceforth MCS) are used to study the properties of econometrics inference techniques by simulation. They are almost always part of theoretical econometric research to study the performance of some inference technique. They supplement theoretical research most often in one of four ways. Firstly, they are used to assess the performance of asymptotically valid techniques in smaller samples. Secondly, they are used to assess how robust a technique is to violations of its theoretical assumptions. Thirdly, they allow to compare the performance of different techniques for a given data generating process (DGP). Fourthly, MCS allows to investigate the properties of inference techniques for which no analytic solution exists. Moreover, MCS itself can be used as a statistical inference technique. For example, Bootstrap Inference can be conceptualized as a special case of MCS. Beyond these examples, there are many more areas where MCS is used. However, independent of its use-case, easy and efficient implementation of MCS is currently only sparsely available.

With our tidyMC package, we want to enable researchers to easily and efficiently include MCS in their research using the programming language R (R Core Team, 2022). For one, tidyMC allows to easily speed up MCS by providing efficient parallelization options over a pre-specified parameter grid. Because MCS involves repeated computation, using parallel workers allows for significant computation time reductions. For another, tidyMC returns an easy to work with output. The output allows to access the result of all simulations for every parameter combination in the parameter grid. Moreover, tidyMC provides functions to effectively communicate the results of the MCS. Using the output, the simulation results can then be easily visualized using the package's plot function. Because the function returns a ggplot object, researchers can customize the object to their liking. Additionally, the package provides a function that converts the results into publication-ready LaTex tables. The table is heavily customizable and thereby allows researchers to effectively communicate their results.

This report is structured as follows. Section @ref(Monte Carlo Simulation) gives an introduction to why and how Monte Carlo Simulations work and provides a simple OLS example. Section @ref(Vignette) presents tidyMC's vignette. The vignette gives an easy-to-follow guide on how to implement MCS using the tidyMC package. Section @ref(Package Principles) explains the coding practices we followed and gives a conceptual overview of how we implemented MCS in R. Section @ref(Comparison to other Monte Carlo Approaches in R) compares the performance of tidyMC to the performance of the MonteCarlo package and other potential MCS implementations. Section @ref(Conclusion) concludes.

### Monte Carlo Simulation

MCS allows analyzing the properties of classic econometric inference techniques. As a simulation-based technique, MCS applies a statistical procedure to many synthetically created samples. The repeated application of the procedure to a fully known DGP helps to investigate the properties of statistical techniques in a wide set of settings. It is possible to use MCS as a simulation-based inference technique itself. In this section, we want to give a brief overview of how and in which circumstances MCS work, mainly following Kiviet et al. (2012).

#### Pseudo Random Number Generation and the Data Generating Process

Using MCS on computers has the great advantage that, with the necessary information, the simulation results can be replicated on most machines. This is possible because, given seed and algorithm, the

numbers created by a random number generator are completely reproducible. MCS generally start with a synthetically created i.i.d. sample. Computers are, however, not able to generate truly random draws from different distributions. Instead, the computer draws from different distributions that are generated through pseudo-random draws from a uniform distribution. Draws from a uniform distribution are created by using so-called random number generators (RNG). These algorithms are applied to a natural number, called the seed. The resulting values are pseudo-random because they are indistinguishable from truly random numbers but are fully determined by the combination of the algorithm and the seed. The combined knowledge of the algorithm and the seed allows exact replication of a series of pseudo-random numbers generated. The purpose of the tidyMC package is to additionally allow easy parallelization of the MCS. With parallel computing, special attention has to be paid to creating disjoint and sufficiently long sets of draws from a uniform distribution. Our package builds on the L'Ecuyer-CMRG RNG streams implemented in furrr::furrr\_options. The algorithm creates reproducible sets of numbers for each parallel worker, using an integer seed of at most length 7. Alternatively, a seed of length 1 is accepted, which internally is mapped to a valid seed of length 7. Because the algorithm creates a subset of random numbers for each worker, the stream and hence the MCS results are only reproducible if the same number of parallel workers is used. Moreover, our function allows the users to supply a user-generated list of random numbers. Draws from other distributions are then simulated using their CDF and the draws from the uniform distribution. Complex multivariate distributions can then be simulated as functions of different standard distributions. This allows us to generate and work with distributions that are analytically not manageable @[kiviet2012monte].

### Monte Carlo Distribution Approximation

MCS is most commonly used to infer properties of the distribution of statistics in a fixed setting, i.e. for a prespecified DGP, hence the simulation results hold only for this. Since it additionally only approximates the distribution numerically, we need to control for the resulting approximation inaccuracies. In MCS we generally simulate the distribution of a statistic  $q_n$ . The statistic can often be expressed as a function of a parameter vector  $\beta$ , some deterministic variables D, some random variables v, and a given number of observations, s.t.  $q_n = q_n(\beta, D, v, n)$ . What a Monte Carlo Simulation ultimately achieves is a numerical approximation of the true distribution of  $q_n$  for the specified DGP. Let  $q_n^R$  be the statistic generated by the  $R^th$  Monte Carlo Simulation. Then the histogram of all  $q_n^R$  is an unbiased and consistent estimator of  $q_n$ . Thus, the precision of the approximation is controlled by setting the number of Monte Carlo estimates. We can then use different statistics such as mean and variance on  $q_n^R$  to summarize the distribution of the statistic for the prespecified DGP. The approach can of course be easily extended to a vector of statistics  $q_n$  (Kiviet et al., 2012).

### Monte Carlo Best Practices

Kiviet et al. (2012) gives a few things that need to be considered when doing and presenting MCS. The results must allow the audience to get a precise picture of the Monte Carlo experiment. MCS generally involves testing the attributes of  $q_n$  not only for one DGP but for a wide set of DGPs that may include nuisance parameters that may significantly alter the distribution.

Instead of going through every use case, we next describe one specific MCS use case. The insights from that use case should however be easily transferable to other MCS applications. One way to perform MCS is mimic analytic derivations. For example, if properties of an asymptotically consistent technique are studied, the MCS should include different nuisance parameters over increasing sample sizes. The

report of the results should then include the technique's key performance indicators, such as bias and efficiency, over different combinations of nuisance parameters and sample sizes. As the parameters are the explanatory variables of the MCS (Kiviet et al., 2012), their values have to be chosen with care to appropriately represent the results from the experiment. The reported representative selection of sample size and nuisance parameters should then show the - potentially nonlinear - behavior of the key indicators of the performance of the technique. As the later sections will show, tidyMC provides easy options to define an arbitrarily large parameter grid to use for the MCS as well as user-defined performance indicators. The packages' summary functions allow the researcher to get a quick overview of the results of the combinations defined in the parameter grid. The plot and table functions allow afterwards to easily communicate the desired results. Due to the flexible design of the tidyMC, the parameter grid can easily be extended to include different estimators for comparisons. It also allows using the distribution of the data itself to generate a new sample, from which we can then infer the properties of an estimator (Kiviet et al., 2012)}.

### **OLS** consistency

To demonstrate how a MCS works, we provide an example using the estimation of a linear model using the ordinary least squares (OLS) estimator (Hayashi, 2011). Given a dependent variable y and a set of i.i.d. regressors  $X = \{x_1, x_2\}$  we consider the linear DGP

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \varepsilon, \tag{1}$$

where  $\beta = \{\beta_0, \beta_1, \beta_2\}$  are the coefficients and  $\varepsilon$  is a normally distributed error term with variance  $\sigma^2$ , i.e.  $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$ . The corresponding OLS estimators  $\hat{\beta}$  and  $s^2$  for  $\beta$  and  $\sigma^2$  are

$$\hat{\beta} = (X'X)^{-1}X'y,\tag{2}$$

$$s^2 = \frac{1}{n - k - 1} \hat{\epsilon}' \hat{\epsilon},\tag{3}$$

where k=2 is the number of regressors and  $\hat{\varepsilon}$  is the vector of residuals. Both estimators are consistent and unbiased (Hayashi, 2011). Accordingly OLS should be able to correctly estimate the coefficients for every sample size, while the precision of the estimates should increase in the sample size.

Using a MCS we can demonstrate the properties of the OLS estimator. Fixing the coefficients  $\beta = \{1, 4, 5\}$  and  $\sigma^2 = 3$ , we generate different DGPs using different normal distributions to generate the dependent variables  $x_1$  and  $x_2$ . Additionally, we generate  $\varepsilon$  from its respective distribution, and we estimate OLS on this sample. The number of observations we use is set to  $n = \{100, 200, 300\}$ , which will be used to assess the convergence of the OLS estimators. We repeat the estimation 1000 times for each n.

The results demonstrate the performance of OLS estimation with increasing sample sizes. As expected figures 1, ??fig:ols\_b1\_se) and table 1 confirm that a bigger sample size leads to a more precise estimation of the underlying population values. Comparing both panels, we see that this behavior is just confirmed, as the estimated values do not differ and they become more precise. Moreover, the densities present show the unbiasedness of the estimator and the decrease of its standard deviation with more observations.

Table 1: Ommited variable bias MC results

N. Observations	$x_2$ Included or not	$\hat{eta}_0$	S.d. $\hat{\beta}_0$	$\hat{eta}_1$	S.d. $\hat{\beta}_1$	$\hat{eta}_2$	$s^2$
N = 10							
100	1	0.956	0.226	4.034	0.087	4.999	2.872
200	1	1.031	0.167	3.987	0.060	5.004	3.022
300	1	1.014	0.138	3.990	0.052	4.994	3.086
N = 1000							
100	1	0.994	0.236	4.000	0.088	5.003	2.938
200	1	0.996	0.166	4.001	0.062	5.002	2.974
300	1	1.002	0.135	4.000	0.050	5.000	2.976
- TD - 1	1000 1		1	-			

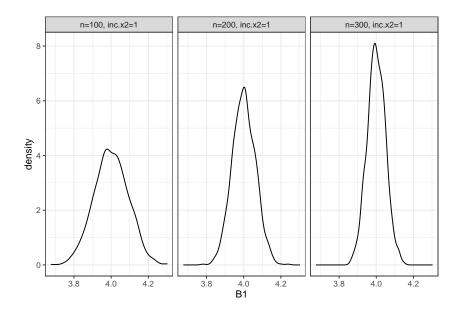


Figure 1: MC  $\beta_1$  results

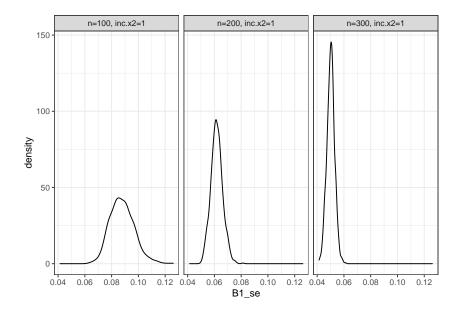


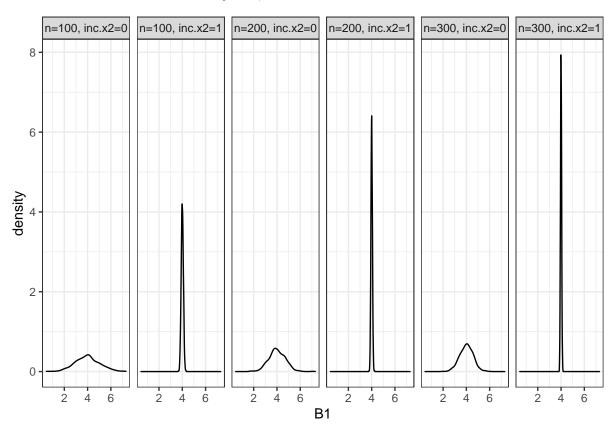
Figure 2: MC S.d.  $\beta_1$  results

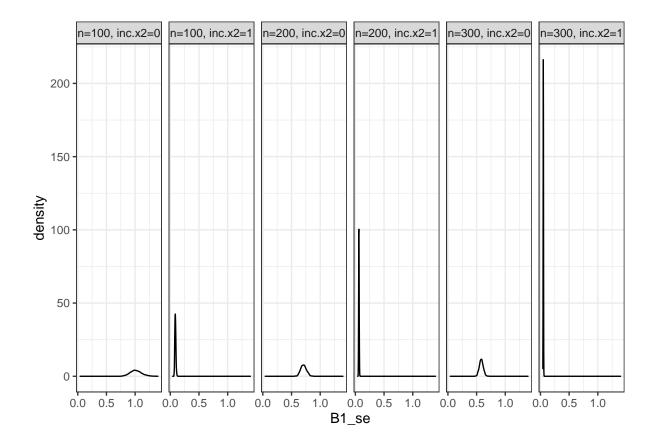
### Omitted variable problem

Moreover, a common problem for estimation is the inclusion of suitable regressors into the model. One of these is the absence of relevant variables in the model, also called omitted variable problem. In this subsection we test the impact of this problem in OLS estimation (Hayashi, 2011).

We test the effects of estimating a model using only  $x_1$  when the underlying DGP follows the structure of (1). If  $x_1$  and  $x_2$  are correlated, the absence of one of them in the regression model will cause the available variable to be correlated with the error term, thus violating one of the main assumptions OLS. This correlation will lead to a biased estimation of  $\beta_1$  (assuming  $x_1$  is contained in the model and  $x_2$  is omitted). If there is no correlation between  $x_1$  and  $x_2$  and  $x_2$  is omitted,  $x_1$  and the error term will still be uncorrelated. Thus, in that case, we expect  $\hat{\beta}_1$  to still be an unbiased estimator for  $\beta_1$ . In any case, the exclusion of the relevant variable  $x_2$  will result in a less efficient estimation of  $\beta_1$ , as the estimated model tries to explain the effect of  $x_2$  by  $x_1$ .

We set the structure of the estimated DGP identical to the base case, only that  $\mathbf{x_2}$  is excluded from the estimation model. To show the loss in efficiency we present the density plots for the Monte Carlo results for  $\hat{\beta}_1$  and its standard error in figures @ref(fig:ommit\_b1) and @ref(fig:ommit\_b1\_se). There is a clear difference in term of the variance of the estimated MC coefficients between the case where  $\mathbf{x_2}$  is included into the model and not. In other words, the variance of  $\hat{\beta}_1$  decreases much slower for increasing n if  $\mathbf{x_2}$  is not included in the model. This can also be seen for the standard deviation of  $\hat{\beta}_1$ : if  $\mathbf{x_2}$  is included in the model, the standard deviation of  $\hat{\beta}_1$  converges to 0 for already small sample sizes n. However, if  $\mathbf{x_2}$  is not included in the model, the standard deviation of  $\hat{\beta}_1$  converges much slower to 0, and thus bigger sample sizes would be needed to obtain the same degree of efficiency for  $\hat{\beta}_1$ . Nonetheless, we observe that the OLS estimate remains unbiased in any case, since  $\mathbf{x_1}$  and  $\mathbf{x_2}$  are uncorrelated.





# Vignette

In the following vignette we are going to present how to obtain the results of the @ref(OLS consistency) and @ref(Omitted variable problem) chapters by using the tidyMC package.

# Package overview

Monte Carlo Simulations aim to study the properties of statistical inference techniques. At its core, a Monte Carlo Simulation works through the application of the techniques to repeatedly drawn samples from a pre-specified data generating process. The tidyMC package aims to cover and simplify the whole workflow of running a Monte Carlo simulation in either an academic or professional setting. Thus, tidyMC aims to provide functions for the following tasks:

- Running a Monte Carlo Simulation for a user defined function over a parameter grid using future\_mc()
- Summarizing the results by (optionally) user defined summary functions using summary.mc()
- Creating plots of the Monte Carlo Simulation results, which can be modified by the user using plot.mc() and plot.summary.mc()
- Creating a LaTeX table summarizing the results of the Monte Carlo Simulation using tidy\_mc\_latex()

In the following subsections we will show how you can implement those tasks using the tidyMC package.

### Installing tidyMC

Until now, the tidyMC package is not on CRAN, thus you need to download the development version from GitHub as follows:

```
# install.packages("devtools")
devtools::install_github("stefanlinner/tidyMC")
```

Afterwards you can load the package:

```
library(tidyMC)
```

Moreover, the following packages will be used in this vignette:

```
# install.packages("magrittr")
library(magrittr)
# install.packages("ggplot2")
library(ggplot2)
# install.packages("kableExtra")
library(kableExtra)
```

### Run your first Monte Carlo Simulation with future\_mc()

future\_mc() allows you to run a Monte Carlo Simulation for a user defined function and given parameters. The first argument of future\_mc() is fun which has to be a function that handles the generation of data, the application of the method of interest and the evaluation of the result for a single repetition and parameter combination. future\_mc() handles the generation of loops over the desired parameter grids and the repetition of the Monte Carlo experiment for each of the parameter constellations. Consider the following example for fun and note that it performs the required tasks of generating data, applying the method and evaluating the results:

```
# fun
ols_test <-
function(b0, b1, b2, n, sigma2, param_x1, param_x2, inc.x2){

# generation of data
x1 <- rnorm(n = n, mean = param_x1[1], sd = param_x1[2])
x2 <- rnorm(n = n, mean = param_x2[1], sd = param_x2[2])
e <- rnorm(n, sd = sqrt(sigma2))
y <- b0 + b1*x1 + b2*x2 + e

if (inc.x2 == 0){
    x2 <- x2 * inc.x2
}

# application of method
estim <- lm(y ~ x1 + x2)</pre>
```

The second argument of future\_mc() is repetitions which should be an integer specifying the number of Monte Carlo iterations. While the third argument param\_list has to be a list whose components are named after the parameters of fun which should vary for the different Monte Carlo Simulation and each component is a vector containing the desired grid values for the parameter. Consider the following example for param\_list and note that its components are named accordingly to the parameters of ols\_test: n and inc.x2, respectively:

```
# param_list
param_list_ols <-
list(n = c(100, 200, 300), inc.x2 = c(0,1))</pre>
```

future\_mc() takes care of creating all possible parameter combinations of param\_list and runs the Monte Carlo Simulation over all of these for all possible combinations. If you don't want to run a Monte Carlo Simulation for every possible parameter combination you can alternatively define param\_table with a data.frame or data.table containing the parameter combinations you are interested in. The ... argument can be used to specify further arguments of fun which are not contained in param\_list. Those arguments will be held fixed for all parameter combinations. In our OLS example those arguments are b0, b1, b2, sigma2, param\_x1, and param\_x2.

Moreover, there are four formal requirements that fun and thus ols\_test have to fulfill:

- The arguments of fun which are present in param\_list have to be scalar values. Note that the arguments of ols\_test which are contained in param\_list\_ols: n and inc.x2 are scalar values. The remaining arguments of ols\_test are allowed to take non-scalar values.
- Every variable used inside fun has either to be defined inside fun or given as an argument through the ... argument.
- The value returned by fun has to be a named list. In our example the names of the returned list are b0, b1, b2, and sigma2.
- The names of the returned values and those of the arguments contained in param\_list need to be different. Moreover, they cannot be params, repetitions or setup as these names are already occupied. Note that b0, b1, b2, and sigma2 are the names of the returned values as well as names of arguments of ols\_test. However, none of those arguments is contained in param\_list\_ols. If we would add either of those variables to param\_list\_ols we would need to change the name of the returned value for the respective variable.

We recommend to even further restrict the return value of fun to be a named list of scalars. This allows you to use all comfort functions of the tidyMC package. As you can see, we did that for ols\_test.

The argument parallelisation\_plan allows the user to set a parallelisation plan. While the argument parallelisation\_options allows the user to fine tune functions, such as furrr::future\_map() by furrr::furrr\_options(). The argument seed for furrr::furrr\_options() can be specified in parallelisation\_options following the formal requirements of its respective documentation. Moreover, the user can also decide not to run the Monte Carlo in parallel by setting parallel = FALSE. To construct parallelisation\_plan the user needs to provide a list named after the arguments of future::plan. The main argument strategy needs to provide the specific type of parallelisation the user would like to use and the number of cores which are used in the function. Some of the options for strategy are: multisession, multicore and cluster. We strongly recommend the user to read the documentation of the future package for a more detailed instruction of how to set up the different strategies.

As a default (check = TRUE) future\_mc() runs a quick check by running a single test-iteration for each parameter combination in order to check for possible errors in fun. If a error occurs the user not only receives the error message but also the parameter combinations for which the error occurred:

```
set.seed(101)
first_mc_ols <- future_mc(
    fun = ols_test,
    repetitions = 1000,
    param_list = param_list_ols,
    b0 = 1,
    b1 = 4,
    b2 = 5,
    sigma2 = -2,
    param_x1 = c(0,5),
    param_x2 = c(0,6),
    check = TRUE
)</pre>
```

```
## Running single test-iteration for each parameter combination...
## Warning in sqrt(sigma2): NaNs produced

## Warning in rnorm(n, sd = sqrt(sigma2)): NAs produced

## Warning in sqrt(sigma2): NaNs produced

## Warning in rnorm(n, sd = sqrt(sigma2)): NAs produced

## Warning in sqrt(sigma2): NaNs produced

## Warning in rnorm(n, sd = sqrt(sigma2)): NAs produced

## Warning in sqrt(sigma2): NaNs produced

## Warning in rnorm(n, sd = sqrt(sigma2)): NAs produced

## Warning in rnorm(n, sd = sqrt(sigma2)): NAs produced

## Warning in sqrt(sigma2): NaNs produced
```

```
## Warning in rnorm(n, sd = sqrt(sigma2)): NAs produced
## Warning in sqrt(sigma2): NaNs produced
## Warning in rnorm(n, sd = sqrt(sigma2)): NAs produced
## Error in future_mc(fun = ols_test, repetitions = 1000, param_list = param_list_ols, :
   Function error: NaNs produced
   At the parameters: n = 100, inc.x2 = 0
##
##
   Function error: NaNs produced
##
   At the parameters: n = 200, inc.x2 = 0
##
##
  Function error: NaNs produced
## At the parameters: n = 300, inc.x2 = 0
##
  Function error: NaNs produced
## At the parameters: n = 100, inc.x2 = 1
##
##
  Function error: NaNs produced
   At the parameters: n = 200, inc.x2 = 1
##
##
## Function error: NaNs produced
## At the parameters: n = 300, inc.x2 = 1
```

The attentive reader might already have noticed that we specified sigma2 = -2 which doesn't make sense, as the variance of the error term cannot be negative. This results in a failed check for all parameter combinations, as this parameter is held fixed for any combination. Once we correct that mistake, we can run our first Monte Carlo Simulation:

```
set.seed(101)
first_mc_ols <- future_mc(
   fun = ols_test,
   repetitions = 1000,
   param_list = param_list_ols,
   b0 = 1,
   b1 = 4,
   b2 = 5,
   sigma2 = 2, # correctly specify sigma2
   param_x1 = c(0,5),
   param_x2 = c(0,6),
   check = TRUE
)</pre>
```

## Running single test-iteration for each parameter combination...
##
##
Test-run successfull: No errors occurred!

```
## Running whole simulation: Overall 6 parameter combinations are simulated \dots
```

##
## Simulation was successfull!
## Running time: 00:00:04.686848

future\_mc returns a list of type mc and length 11 consisting of a tibble (first\_mc\_ols\$output) containing the return value of fun for each iteration and parameter combination. In our case first\_mc\_ols\$output contains a column for each output b0, b1, b2, and sigma2, as well as a column for each parameter in param\_list\_ols and a column containing the nice\_names of the parameter combinations. Overall the first\_mc\_ols\$output consists of 6000 rows, i.e., for each parameter combination 1.000 rows:

#### first\_mc\_ols\$output

```
## # A tibble: 6,000 x 7
##
                            n inc.x2
                                                        b2 sigma2
      params
                                          b0
                                                 b1
##
      <chr>
                        <dbl>
                               <dbl>
                                       <dbl> <dbl> <dbl>
                                                            <dbl>
##
    1 n=100, inc.x2=0
                          100
                                       1.28
                                               3.38
                                                             776.
    2 n=100, inc.x2=0
                          100
                                    0 -4.27
                                               3.89
                                                        NA
                                                             773.
##
##
    3 n=100, inc.x2=0
                          100
                                    0 5.85
                                               4.36
                                                        NA
                                                            1130.
    4 n=100, inc.x2=0
                          100
                                    0 1.57
                                               4.69
                                                        NA
                                                            1067.
## 5 n=100, inc.x2=0
                          100
                                    0 -0.802 3.93
                                                        NA
                                                             873.
                                    0 1.26
##
   6 \text{ n=} 100, \text{ inc.} x2=0
                          100
                                               4.44
                                                       NA
                                                             880.
   7 n=100, inc.x2=0
                          100
                                    0 5.01
                                               4.22
                                                       NA
                                                             852.
## 8 n=100, inc.x2=0
                          100
                                    0 - 1.49
                                               3.99
                                                       NΑ
                                                             938.
## 9 n=100, inc.x2=0
                          100
                                       3.07
                                               3.80
                                                       NA
                                                             779.
## 10 n=100, inc.x2=0
                          100
                                       2.06
                                               3.73
                                                       NA
                                                             999.
## # ... with 5,990 more rows
```

If ols\_test would not return a named list of scalars, but a named list of non-scalars, then first\_mc\_ols\$output would not contain a column for each output, but a single column containing the named list of non-scalars for each iteration and parameter combination.

Moreover, first\_mc\_ols returns much other information about the Monte Carlo Simulation that can be printed in a dense representation:

#### first\_mc\_ols

```
##
           x2 <- x2 * inc.x2
##
       estim \leftarrow lm(y \sim x1 + x2)
##
##
       out <- list(b0 = estim$coefficients[1], b1 = estim$coefficients[2],</pre>
           b2 = estim$coefficients[3], sigma2 = var(estim$residuals))
##
       return(out)
##
## }
##
##
    The following 6 parameter combinations:
##
       n inc.x2
## 1 100
## 2 200
              0
## 3 300
              0
## 4 100
## 5 200
               1
## 6 300
               1
## are each simulated 1000 times.
##
##
    The Running time was: 00:00:04.686848
##
##
    Parallel: TRUE
##
   The following parallelisation plan was used:
## $strategy
## multisession:
## - args: function (..., workers = availableCores(), lazy = FALSE, rscript_libs = .libPaths(), envi
## - tweaked: FALSE
## - call: NULL
##
##
   Seed: TRUE
##
```

#### Summarize your results with summary.mc()

If fun returns a named list of scalars the user can use summary.mc() to summarize all Monte Carlo results. The first argument of the function is an object of class mc returned by future\_mc(). The next argument sum\_funs determines which summarizing functions will be used on the simulation results. The functions can be provided for any combination of: parameter combinations resulting from param\_list, and the outputs of fun. Every specified function can only take one argument, which is the vector (with length repetitions) for every output. We will present all customization options of sum\_funs in a step wise manner.

The first option of summarizing the results is given by just providing the mc object to summary.mc. In this case, mean() will be applied to all numeric values and summary() to all non-numeric data types. When the summarizing functions return one numeric value (like mean()) the results are twofold:

• First, a single scalar result of the function evaluated using the complete output vector is returned in the first element.

• Second, a vector with length repetitions of numeric results from the step wise calculation of the function's result across the output's vector. We call this resulting vector as the "path" of the summarizing function.

Additionally, to save computation time the parameter which\_path is available to the user who wants to specify for which outputs the "path" should be calculated. The user needs to provide a character vector with the output names'. Moreover, the options "all" (the default) and "none" are also available.

For the OLS example since all outputs of ols\_test are numeric, the returned object will be a named nested list composed of four elements named after the nice\_names returned by future\_mc(). Each of this elements are itself lists containing the summarized outputs, i.e. b0, b1, b2, and sigma2. Lastly each of these are composed by the "path" and scalar result of mean().

```
# Default
summary_default <- summary(first_mc_ols)
summary_default</pre>
```

```
## Results for the output b0:
##
      n=100, inc.x2=0: 0.9185223
##
      n=100, inc.x2=1: 1.003477
##
      n=200, inc.x2=0: 1.02396
##
      n=200, inc.x2=1: 1.002091
      n=300, inc.x2=0: 1.000223
##
      n=300, inc.x2=1: 1.002196
##
##
##
## Results for the output b1:
##
      n=100, inc.x2=0: 3.985091
      n=100, inc.x2=1: 4.000044
##
      n=200, inc.x2=0: 4.005565
##
      n=200, inc.x2=1: 4.000216
##
      n=300, inc.x2=0: 4.001195
##
      n=300, inc.x2=1: 4.000031
##
##
##
## Results for the output b2:
      n=100, inc.x2=0:
##
## [1] NA
##
      n=100, inc.x2=1: 5.001864
##
##
      n=200, inc.x2=0:
##
  [1] NA
##
##
      n=200, inc.x2=1: 5.001091
      n=300, inc.x2=0:
##
##
  [1] NA
##
##
      n=300, inc.x2=1: 5.000132
```

```
##
##
## Results for the output sigma2:
##
      n=100, inc.x2=0: 892.7561
##
      n=100, inc.x2=1: 1.958776
##
      n=200, inc.x2=0: 895.652
##
      n=200, inc.x2=1: 1.982949
      n=300, inc.x2=0: 900.6887
##
      n=300, inc.x2=1: 1.983788
##
##
##
```

#### str(summary\_default[[1]])

```
## List of 4
    $ b0
            :List of 2
##
                        : num 0.919
     ..$ mean
##
     ..$ mean_over_reps: num [1:1000] 1.278 -1.497 0.954 1.108 0.726 ...
##
    $ b1
            :List of 2
##
     ..$ mean
                        : num 3.99
     ..$ mean_over_reps: num [1:1000] 3.38 3.63 3.88 4.08 4.05 ...
##
##
            :List of 1
     ..$ mean: num NA
##
    $ sigma2:List of 2
##
##
     ..$ mean
                        : num 893
     ..$ mean_over_reps: num [1:1000] 776 774 893 936 923 ...
##
```

This nested list structure should give an idea of the reach and flexibility the sum\_funs argument is allowed to have, since the user can specify a function for each element in this list.

For an intermediate level of customization, the user can provide a combination of summarizing functions for every output, which will be used for all parameter combination. In the case of the OLS example, if we want to apply mean() on all estimated coefficients, but we want to use var() on the MC results of sigma2, the sum\_funs should have the following structure:

```
# summarizing output the same way for each parameter combination with one function combination sum_sols <-list(b0 = mean, b1 = mean, b2 = mean, sigma2 = var)
```

Moreover, the user can specify any function provided it takes the output vector as only available argument.

Lastly for the last level of customization, a nested list named after the nice\_names where every element follows the structure of the last example (components named after the outputs and each component is a function) can be specified. We present an example for this:

```
quantile_sum <- function(x) quantile(x, probs = 0.75)

# summarizing output differently for different parameter combinations
sum_funs2 <-</pre>
```

```
list(
    list(b0 = quantile_sum, b1 = min, b2 = min, sigma2 = mean),
    list(b0 = mean, b1 = quantile_sum, b2 = mean, sigma2 = mean),
    list(b0 = median, b1 = median, b2 = median, sigma2 = mean),
    list(b0 = max, b1 = max, b2 = max, sigma2 = mean),
    list(b0 = min, b1 = min, b2 = min, sigma2 = quantile_sum),
    list(b0 = mean, b1 = mean, b2 = quantile_sum, sigma2 = quantile_sum)
)
names(sum_funs2) <- first_mc_ols$nice_names
summary_out_param_spec <- summary(first_mc_ols, sum_funs = sum_funs2)</pre>
```

We would like to reiterate that the provided summary functions are not restricted regarding the complexity of their return value. However, the path of the summarized output over all simulation repetitions is only returned if the provided summary functions return a single numeric value. Thus, the following comfort functions plot.summary.mc() and tidy\_mc\_latex() will only work in this specific case.

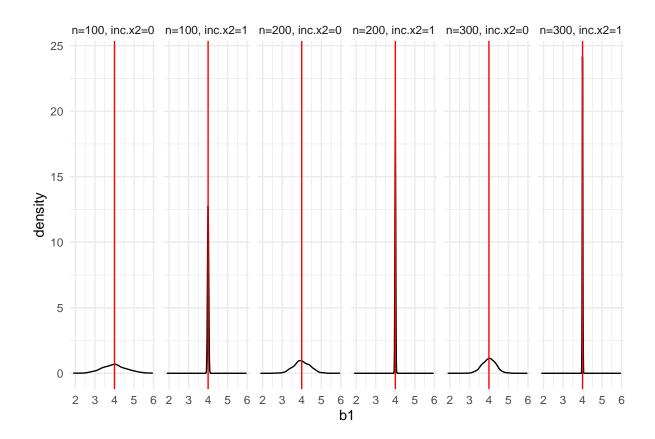
#### Plot your Monte Carlo Simulation with plot.mc() and plot.summary.mc()

If fun returns a named list of scalars the user can use plot.mc() to generate a list of objects of class gg and ggplot2 for all Monte Carlo results. The first argument of the function is an object of class mc returned by future\_mc(). Using the argument plot the user can indicate whether the generated plots should be printed immediately or only returned as a list. The list will contain one plot for each output of fun comparing the results of the different simulation setups. In general, plot.mc() generates density plots for numeric outputs and bar plots for non-numeric outputs. In our example a plot for b0, b1, b2, and sigma2 will be returned in a list of length four and as b0, b1, b2, and sigma2 are all numeric outputs plot.mc() will return density plots for each of those:

```
mc_ols_plot <- plot(first_mc_ols, plot = FALSE)
names(mc_ols_plot)
## [1] "b0" "b1" "b2" "sigma2"</pre>
```

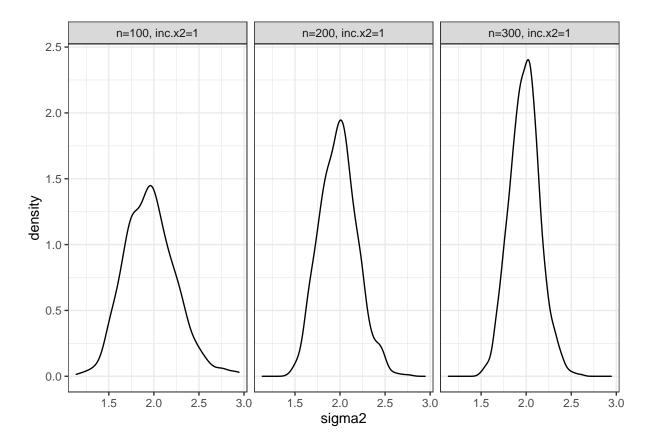
As the single list elements are of class gg and ggplot2, we can easily customize and extend the single plots using familiar ggplot2 commands:

```
mc_ols_plot$b1 +
ggplot2::geom_vline(xintercept = 4, col = "red") +
ggplot2::theme_minimal()
```



When creating the plots the user can also subset the setups which he/she would like to see in the plots using the first\_mc\_ols\$nice\_names in the function argument which\_setup, or a named list in parameter\_comb. The single components of the list have to be named after the parameters specified in param\_list and contain vectors specifying the values of the parameters to filter by. In the ols example we can filter by the parameters n and inc.x2:

```
# subsetting by nice_names
mc_ols_plot_subset1 <-
   plot(first_mc_ols, plot = FALSE, which_setup = first_mc_ols$nice_names[4:6])
#subsetting by parameter values
mc_ols_plot_subset2 <-
   plot(first_mc_ols, plot = FALSE, parameter_comb = list(inc.x2 = 1))
mc_ols_plot_subset1$sigma2</pre>
```

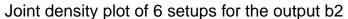


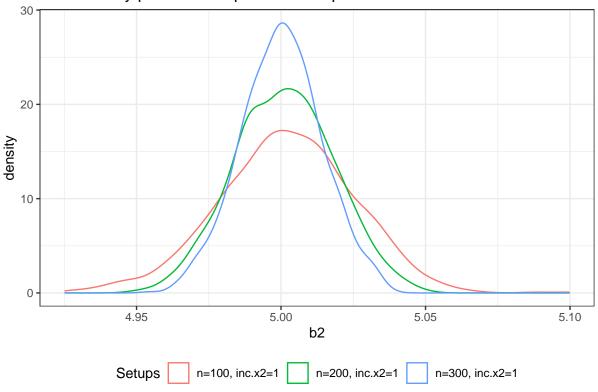
Thus, if the user wants distinct plots for every parameter combination, one needs to subset the plot for any single setup in first\_mc\_ols\$nice\_names.

Finally, you can also plot the simulation results for several parameter combination in one single plot by specifying the argument join with the respective first\_mc\_ols\$nice\_names:

```
mc_ols_plot_joint <- plot(first_mc_ols, plot = FALSE, join = first_mc_ols$nice_names)
mc_ols_plot_joint$b2</pre>
```

## Warning: Removed 3000 rows containing non-finite values (stat\_density).

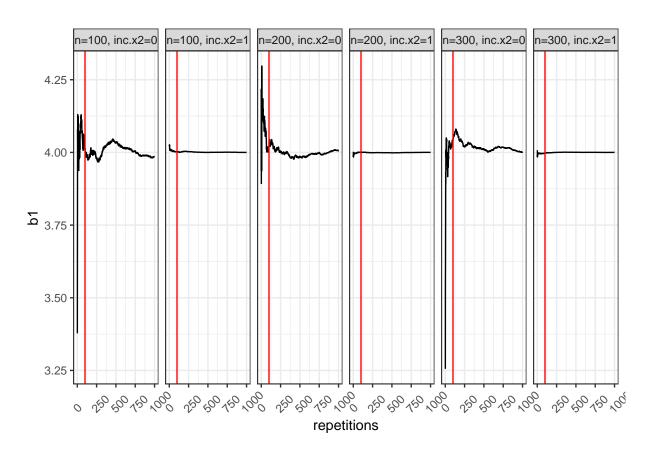




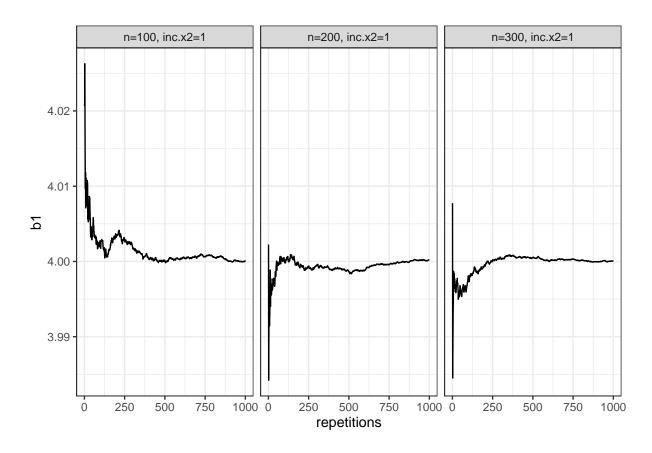
Please be aware that the only one of the three arguments which\_setup, parameter\_comb, and join can be specified at the same time.

If the provided summary functions in summary.mc() return a single numeric value and thus a path of the summarized output over all simulation repetitions is returned, the user can use plot.summary.mc() to plot those paths. The first argument of the function is an object of class summary.mc returned by summary.mc(). Just as plot.mc(), plot.summary.mc() returns a list of objects of class gg and ggplot2. The list will contain one line plot for each output of fun displaying the paths of the results of the different simulation setups. The arguments plot, which\_setup, parameter\_comb, and join can be specified the same way as for plot.mc:

```
sum_mc_plot <- plot(summary_default, plot = FALSE)
sum_mc_plot$b1 +
   ggplot2::geom_vline(xintercept = 100, col = "red") +
   ggplot2::theme(axis.text.x = element_text(angle = 45, hjust = 0.1, vjust = 0.2))</pre>
```

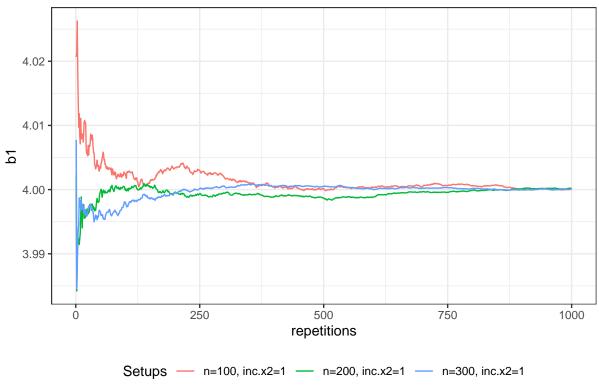


```
sum_mc_plot_subset1 <-
   plot(summary_default, plot = FALSE, which_setup = first_mc_ols$nice_names[4:6])
sum_mc_plot_subset2 <-
   plot(summary_default, plot = FALSE, parameter_comb = list(inc.x2 = 1))
sum_mc_plot_subset2$b1</pre>
```



```
sum_mc_plot_joint <-
plot(summary_default, plot = FALSE, join = first_mc_ols$nice_names[4:6])
sum_mc_plot_joint$b1</pre>
```

### Joint time series of 3 setups for the output b1



### Create a LaTeX table of your results with tidy\_mc\_latex()

Using tidy\_mc\_latex the user can present the results from future\_mc directly into a LaTeX document using all the benefits from the kableExtra package. The first and main argument x needed by tidy\_mc\_latex is a summary.mc object obtained from summary.mc(). To present the results in a comprehensive manner the function requires that all summarized outputs in summary.mc be scalar numeric results for all parameter combinations. In case, the summarizing function returns more than one argument then this will be presented in the table as an NA value. The second argument of the function is repetitions\_set which allows the user to see the certain values of the "path" of the summarized results of fun. To illustrate this we use the MC results for the OLS example:

```
tidy_mc_latex(
    x = summary(first_mc_ols),
    repetitions_set = c(10, 1000)
) %>%
    kableExtra::kable_styling(latex_options = "HOLD_position")
```

Table 2: Monte Carlo simulations results

	inc.x2	b0	b1	b2	sigma2			
n	IIIC.X2	DU	DI	02	Siginaz			
N = 1	N = 10							
100	0	1.354	4.043	NA	906.484			
100	1	0.989	4.011	4.999	1.915			
200	0	2.326	4.156	NA	871.074			
200	1	1.025	3.996	5.002	2.015			
300	0	0.083	4.006	NA	950.222			
300	1	0.989	3.997	4.997	2.058			
N = 1	N = 1000							
100	0	0.919	3.985	NA	892.756			
100	1	1.003	4.000	5.002	1.959			
200	0	1.024	4.006	NA	895.652			
200	1	1.002	4.000	5.001	1.983			
300	0	1.000	4.001	NA	900.689			
300	1	1.002	4.000	5.000	1.984			

The resulting table is composed of two panels, which corresponds to the length of repetitions\_set. In them the columns correspond to the results of the summarizing functions for b0, b1, b2, and sigma2, and the rows correspond to specific combinations of the parameters provided in parameter\_list. The footnote in the table shows the number of repetitions and the total parameter combinations provided to future\_mc.

Moreover, the next three arguments in tidy\_mc\_latex are comfort options to select which results of summary.mc depending on the parameter combinations will be presented in the table. On one hand, The argument which\_setup allows the user to make use of the nice\_names of the parameter combinations in the returned object by future\_mc() to subset the rows in the table. On the other hand, the argument parameter\_comb is used to directly filter the parameters by their values. This argument requires a named list, containing vector or scalar values of all parameters to be filtered from. The user must only provide one of this arguments at a time. We show how to make use of both parameters to subset the rows of table for n = 100 and  $inc_{x2} = 1$ :

```
tidy_mc_latex(
    x = summary(first_mc_ols),
    repetitions_set = c(10, 1000),
    which_setup = first_mc_ols$nice_names[1]) %>%
    kableExtra::kable_styling(latex_options = "HOLD_position")
```

Table 3: Monte Carlo simulations results

n	inc.x2	b0	b1	sigma2			
N = 10							
100	0	1.354	4.043	906.484			
N = 1000							
100	0	0.919	3.985	892.756			

Total repetitions = 1000, total parameter combinations = 6

```
tidy_mc_latex(
    x = summary(first_mc_ols),
    repetitions_set = c(10, 1000),
    parameter_comb = list(n = 100, inc.x2 = 1)) %>%
    kableExtra::kable_styling(latex_options = "HOLD_position")
```

Table 4: Monte Carlo simulations results

n	inc.x2	b0	b1	b2	sigma2		
N = 10							
100	1	0.989	4.011	4.999	1.915		
N = 1000							
100	1	1.003	4.000	5.002	1.959		

The user can also subset the outputs of the original function (columns in the table) using the parameter which\_out. This is done using a character vector with the names of the outputs, e.g. to only show the columns for b0 and sigma2 the user needs to set which\_out = c("b0", "sigma2").

Lastly, by providing a named list to the argument kable\_options, the user can change all arguments of the underlying function kable::kbl(). The names of the list have to be equal to the names of the arguments of the function and the contents of every element also has to fulfill its requirements. We provide an example of how this list should be constructed, but for optimal usage we strongly recommend the user to see the documentation of the kable::kbl() function.

To allow for further customization the returned object by tidy\_mc\_latex is of class knitr\_kable, therefore the user can utilize most functions from the kableExtra package in the standard tidyverse manner. For example:

Table 5: Ommited variable problem MC results

Number of observations	$x_2$ included or not	$\beta_0$	$\beta_1$	$\beta_2$	$s^2$
N = 10					
100	0	1.354	4.043	NA	906.484
100	1	0.989	4.011	4.999	1.915
200	0	2.326	4.156	NA	871.074
200	1	1.025	3.996	5.002	2.015
300	0	0.083	4.006	NA	950.222
300	1	0.989	3.997	4.997	2.058
N = 1000					
100	0	0.919	3.985	NA	892.756
100	1	1.003	4.000	5.002	1.959
200	0	1.024	4.006	NA	895.652
200	1	1.002	4.000	5.001	1.983
300	0	1.000	4.001	NA	900.689
300	1	1.002	4.000	5.000	1.984

### Comparison to other Monte Carlo Approaches in R

### Design of the functions

As already stated our conceptualization of an MCS implementation is based upon the basic requirements of this technique and framing the functions into the tidyverse structure (Wickham, 2017). Previously, the MonteCarlo package (Leschinski, 2019) already developed a convenient framework for the study and paralellised implementation of MCS, to which we compare the structure of our package. The main function for running a MCS in the MonteCarlo is the function of the eponymous name.

Both our future\_mc and the MonteCarlo functions have two main divisions on their structure. First, we have the set-up of the arguments, data containers and error checking, parts of the function. Which can be called as the preamble of the simulation. Lastly, the actual simulation of the MC study over a parameter grid specified by the user. The main differences between our implementation and the MonteCarlo packages lay in these two steps of the functions.

On one hand, the whole development of our package draws from the benefits of the tidyverse functions. For example: the creation of parameter grids, the structure of the data and repeated calculations, rely heavily in functions provided by the stringr (Wickham, 2022), tibble and purrr (Henry & Wickham, 2020) packages. Most importantly, for all repeated calculations that normally are handled by for loops we implement them with their purrr counterparts. These are all implemented keeping in mind the type of the object to be handled in order to reduce computation time, i.e. the mapping functions are tailored for dealing with specific data types. In contrast, the MonteCarlo function is built within a base R framework. Moreover, to offer flexibility to the user, the function uses a high number of strings for the creation of for loops, containers and parameter grids which are then parsed and evaluated inside the function.

On the other hand, when it comes to the implementation of the parallelised simulation both functions differ totally from each other. The MonteCarlo function is built around the implementation of the snow (Tierney et al., 2021) and snowfall packages. These packages let the user perform calculations by a master/worker scheme, this means that the main function call distributes tasks to the "workers" (CPUs). Thus, all workers resolve the tasks they are given and convey their results to the main R session

giving the instructions. In contrast, future\_mc draws its computing power from the future package [futurepackage through the furrr package API (Vaughan & Dancho, 2022). The future package conceptualizes parallel computation based on task processing constructs called futures which are tasks that are resolved in background process while the main session continues to run. The benefit of this is twofold, for one all tasks are centralized in a queue and are supplied to the workers as soon as they are available which keeps calculation times consistent across workers. For the other, the main session can still delegate tasks and perform operations, provided that no results are required from the unresolved futures. In the design of future\_mc we reap these benefits through the use of the furrr::pmap() function, to which we provide the user's function and his/her desired parameter grid replicated as many times as the number of Monte Carlo repetitions.

### Package Principles in tidyMC

In developing the tidyMC package, we followed the principle of "fail early and often", i.e. if a function is misspecified, we want our function to fail as early as possible and also return readable and informative error messages. To achieve this goal, the first part of each function in our package consists of assertions to the input parameters, as these are specified by the user and are therefore error-prone. After making sure that the input parameters are correctly specified, the following core of the function should work without problems and can thus be executed. In our package, we ensure the class and general structure of the input parameters by using the checkmate package, as the checkmate (Lang, 2017) commands can almost always be written in a readable line of code, produce readable error messages and are written in C, so we don't have to worry about execution time overhead.

Since one of our main focuses is to embed our functions in tidyMC into the tidyverse structure, we have used functions from packages of the tidyverse whenever possible. This is particularly evident in the following three cases: First, we use stringr::str\_c() instead of paste() as this is generally faster and more stable. Second, we mostly work with tibbles instead of data.frames, as they provide more consistent subsetting behaviour and we take advantage of tibbles' higher flexibility by storing lists in columns. Thirdly, for all repeated calculations that are normally handled by for loops, we implement their purre counterparts. These are all implemented taking into account the type of the object being handled to reduce computation time.

To work collaboratively on our package code, we use the version control system Git and manage our Git project with GitHub. This ensures that our pieces of code are merged correctly and nothing gets lost along the way. It also allows us to track our development over time and easily revert to older versions of our package. We also relied heavily on Hadley Wickham's book, which is a great summary of best practices in package programming. As recommended by Wickham, when we wanted to use functions from another package, we added the appropriate package to the NAMESPACE file by usethis::use\_package("pkg\_name") and then used the form package::function() when calling a function from another package in our code. This way, all dependencies are clear to the reader. To reduce package dependencies outside the tidyverse, we tried to avoid using packages that are not part of the tidyverse whenever possible.

Our typical development workflow (inspired by Hadley Wickham) looks as follows:

- We implement the desired feature in our code relying on tidyverse functions
- We run an example to check whether the functionality is implemented correctly
- We use devtools::load\_all to make our (updated) function available for experimentation

- We try to take care of the function documentation using roxygen2 (Wickham et al., 2022) right away, as at this point all requirements for the function and the functionality are best in our mind
- We run devtools::check and fix all occurring notes, warnings, and errors
- A group member who was not involved in the coding runs several examples using the function to test its functionality
  - Whenever a bug occurs, it is reported to the developer of the function, who takes care of fixing the bug
  - The bug is converted into a failing test (using testthat (Wickham, 2011) and the developer's task is to make this test pass. This test ensures that the same bug will not occur a second time.

### Speed comparison

To test the performance of tidyMC we evaluated the function:

```
# test_func <- function(param = 0.1, n = 100, x1 = 1, x2 = 2){
#
# data <- rnorm(n, mean = param) + x1 + x2
# stat <- mean(data)
# stat_2 <- var(data)</pre>
```

to benchmark the performance of the tidyMcpackage against competing implementations. To compare the performances we tested all Monte Carlo implementations using different setups. We compute the Monte Carlos simulations using either one, two, or four cores and either one, ten, or 100 parameter combinations. For each of these setups, we compare the speed and required memory for 100, 1000, and 10000 Monte Carlo repetitions. All comparisons were run on a 2021 Macbook Pro with the M1 processor and 8 Gb of Ram.

Our first comparison is between the MonteCarlopackage and the tidyMCpackage. Figure xyz(a) shows the median simulation speed over the different setups, while Figure xyz(b) shows the median memory use. In both figures, we see that when using multiple cores, tidyMC outperforms Monte Carlo in terms of speed and memory. The figure also shows that MonteCarlois quicker, when only one core is used. However tidyMC is much more memory efficient, especially with large studies that either use many repetitions or that use many parameters. (ADD COLORS AND PLOT DECRIPTION)

Our second comparison is between the parallelization over parameters, the parallelization over repetitions, and the tidyMC parallelization over everything. For the comparison, we have only used the very core function of our package, without any pretests and other utility functions. Figure xyz(a) shows the median simulation speed over the different setups, while Figure xyz(b) shows the median memory use. The blue line shows the results from tidyMC, the red line the results from the parallelization over the parameters, and the green line the results from parallelizing over the repetitions. The plots show that in terms of speed our approach of parallelizing over all combinations is superior in all settings to the two other settings. However, in terms of memory usage, tidy MC generally performs worse than the other two. In contrast, parallelizing over repetitions is generally the most memory efficient.

#### Unresolved Issues

With the help of various online resources, especially Stackoverflow, we were able to fix all errors, warnings and notes returned by devtools::check() in a satisfactory way (for us), except for one:

```
> checking R code for possible problems ... NOTE
  tidy_mc_latex: no visible binding for global variable '.'
  Undefined global functions or variables:
    .
```

Figure 3: Unresolved Note.

If this note occurs in the context of a dplyr function, the problem can easily be solved by using the rlang::.data pronoun after adding rlang .data to the @importFrom tag in your roxygen2 header, as explained e.g. in this post. However, if this note does not occur in the context of a dplyr function, but as in our case with purrr::map(), there is (at least to our knowledge) no such nice solution, as also this stackoverflow post is not answered. Thus, we decided to use the second option presented in the R-blogger post and set

```
. <- NULL
```

at the respective part in the code. This solution is often used when working with the data.table package and deals with the note in the RCMD-check as the variable . then has a visible binding (to NULL). However, it feels a bit "hacky" to us and we would like to know if there is another more natural solution to that problem.

### Conclusion

With the tidyMC package we provide researchers with an easy and comfortable way to perform their own Monte Carlo Studies. We provide a general setup, that easily allows for Monte Carlo Studies in all possible flavors. In this report, we used OLS to demonstrate how tidyMC may be used to efficiently set up Monte Carlo Simulations over a parameter grid with parallelization. Building on the tidyverse, the tidyMC package uses the powerful furrr package to efficiently parallelize the Monte Carlo study over an arbitrarily complex parameter grid. We compared the tidyMC approach to R's currently most popular package for Monte Carlos Simulations, the MonteCarlopackage, as well as two alternative approaches. We find that tidyMC generally outperforms the alternatives in terms of speed and memory required. Especially with larger Monte Carlo Studies using more parallel workers, our implementation is much quicker and much less memory intensive. To ease getting a quick overview of the simulation results we provide a comprehensive summary function. Lastly, to allow easy communication of the Monte Carlo results, we provide a build in plot function and a function to generate LaTeX tables. Both functions are highly customizable, allowing the user to tailor the output to his needs. Because our package is built largely on top of other tidyverse packages, it integrates very nicely into the package collection. However, its easy usage should benefit all types of R users.

While we have implemented many different options for the user, there is still room for extensions. Right now the plot function only allows for plotting densities. In a future version, we may add further plotting options. Furthermore, it may be beneficial to add predesigned options for different kinds of flavors of Monte Carlo Simulations. Our current implementation is as general as possible. Specifying the plot and

table functions for specific use cases would likely lead to a more comfortable user experience. For example, if different estimators are compared, it might make sense to add preset plot functions that more effectively allows visualizing the differences in performance. However, given the level of generality for which we designed that package, we believe that its current implementation may nonetheless lead to good results for all potential users.

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