Software Manual
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RoCoCo

An R Package Implementing a Robust Rank Correlation Coefficient and a Corresponding Test

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Scope and Purpose of this Document

This document is a user manual for the R package `rococo`. It is only meant as a gentle introduction into how to use the basic functions implemented in this package. Not all features of the R package are described in full detail. Such details can be obtained from the documentation enclosed in the R package. Further note the following: (1) this is not an introduction to robust rank correlation; (2) this is not an introduction to R. If you lack the background for understanding this manual, you first have to read literature on these subjects.

Contents

1 Introduction

Correlation measures are among the most basic tools in statistical data analysis and machine learning. They are applied to pairs of observations to measure to which extent the two observations comply with a certain model. The most prominent representative is surely *Pearson's product moment coefficient* [1, 13], often nonchalantly called *correlation coefficient* for short. Pearson's product moment coefficient can be applied to numerical data and assumes a linear relationship as the underlying model; therefore, it can be used to detect linear relationships, but no non-linear ones.

Rank correlation measures [7, 10, 12] are intended to measure to which extent a monotonic function is able to model the inherent relationship between the two observables. They neither assume a specific parametric model nor specific distributions of the observables. They can be applied to ordinal data and, if some ordering relation is given, to numerical data too. Therefore, rank correlation measures are ideally suited for detecting monotonic relationships, in particular, if more specific information about the data is not available. The two most common approaches are *Spearman's rank correlation coefficient* (short *Spearman's rho*) [15, 16] and *Kendall's tau (rank correlation coefficient)* [2, 9, 10]. Another simple rank correlation measure is the *gamma rank correlation measure* according to Goodman and Kruskal [7].

The rank correlation measures cited above are designed for ordinal data. However, as argued in [5], they are not ideally suited for measuring rank correlation for numerical data that are perturbed by noise. Consequently, [5] introduces a family of robust rank correlation measures. The idea is to replace the classical ordering of real numbers used in Goodman's and Kruskal's gamma [7] by some fuzzy ordering [8, 3, 4] with smooth transitions — thereby ensuring that the correlation measure is continuous with respect to the data.

2 Installation

2.1 Installation via CRAN

The R package `rococo` (current version: 1.0.1) is part of the *Comprehensive R Archive Network (CRAN)*[1]. The simplest way to install the package, therefore, is to enter the following command into your R session:

```
> install.packages("rococo")
```

2.2 Manual installation

If, for what reason ever, you prefer to install the package manually, download the package file suitable for your computer system and copy it to your harddisk. Open the package's page at CRAN[2] and then proceed as follows.

[1] `http://cran.r-project.org/`

[2] `http://cran.r-project.org/web/packages/rococo/index.html`

Manual installation under Windows

1. Download `rococo_1.0.1.zip` and save it to your harddisk
2. Open the R GUI and select the menu entry

   ```
   Packages | Install package(s) from local zip files...
   ```

   (if you use R in a different language, search for the analogous menu entry). In the file dialog that opens, go to the folder where you placed `rococo_1.0.1.zip` and select this file. The package should be installed now.

Manual installation under Linux/UNIX/MacOS

1. Download `rococo_1.0.1.tar.gz` and save it to your harddisk.
2. Open a shell window and change to the directory where you put `rococo_1.0.1.tar.gz`. Enter

   ```
   R CMD INSTALL rococo_1.0.1.tar.gz
   ```

   to install the package.

2.3 Compatibility issues

Both the Windows and the Linux/UNIX/MacOS version available from CRAN have been built using the latest version, R 2.13.0. However, the package should work without severe problems on R versions $\geq$2.12.0.

3 Getting Started

To load the package, enter the following in your R session:

```
> library(rococo)
```

You will probably see a message that package `Rcpp` has been loaded (in case it has not been loaded previously in the current R session). Apart from this, you can be sure that the package has been installed successfully if this command terminates without any further error message or warning. If so, the package is ready for use now.

The package includes both a user manual (this document) and a reference manual (help pages for each function). To view the user manual, enter

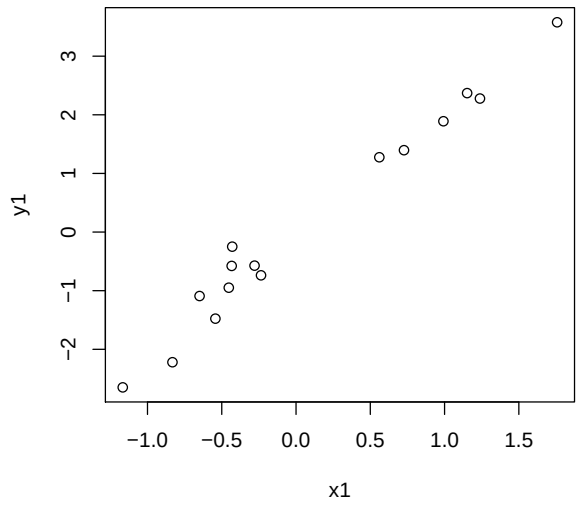
```
> vignette("rococo")
```

Help pages can be viewed using the `help` command. It is recommended to start with

```
> help(rococo)
```

For demonstration purposes, let us first create an artificial toy data set:

```
> x1 <- rnorm(15)
> y1 <- 2 * x1 + rnorm(length(x1), sd = 0.25)
> plot(x1, y1)
```



Obviously, these are linearly correlated Gaussian data, so Pearson's product moment correlation coefficient [1, 13] would be the optimal choice. We use these data anyway, only for illustration purposes. The function `rococo()` can be used to compute the robust rank correlation coefficient as follows:

```
> rococo(x1, y1)

[1] 0.9167946
```

To perform a robust rank correlation test, use the function `rococo.test`:

```
> rococo.test(x1, y1, alternative = "two.sided")

        Robust Gamma Rank Correlation:

data: x1 and y1 (length = 15)
similarity: linear
rx = 0.1357292 / ry = 0.2663235
t-norm: min
alternative hypothesis: true gamma is not equal to 0
sample gamma = 0.9167946
estimated p-value = 8.245524e-06 (0 of 1000 values)
```

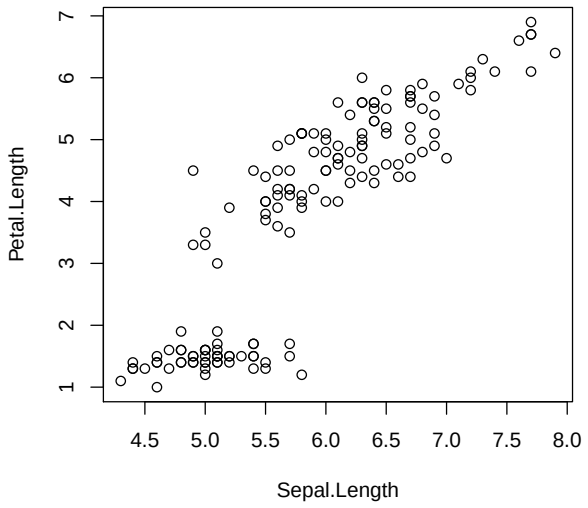
The argument `alternative` works in the same way as for the standard function `cor.test()`.

The function `rococo.test()` is a generic method that can be called on two numeric vectors (as above) or, alternatively, using a formula to conveniently extract two columns from a data frame:

```
> data(iris)
> plot(~Sepal.Length + Petal.Length, iris)
> rococo.test(~Sepal.Length + Petal.Length, iris, alternative = "two.sided")
```

```
        Robust Gamma Rank Correlation:

data: Sepal.Length and Petal.Length (length = 150)
similarity: linear
rx = 0.13 / ry = 0.35
t-norm: min
alternative hypothesis: true gamma is not equal to 0
sample gamma = 0.7940949
estimated p-value = < 2.2e-16 (0 of 1000 values)
```



All examples above use default settings for the fuzzy orderings that are used to define the rank correlation coefficient. In the following section, we introduce the concept behind the robust gamma rank correlation coefficient in greater depth and describe how to adjust the corresponding settings properly.

4 Adjusting Similarities and t-Norms

4.1 Background

The robust gamma rank correlation coefficient requires the definition of two *strict fuzzy orderings* [4], R_X and R_Y. A strict fuzzy ordering is a two-place function that measures to which degree its second argument is strictly larger than its first argument. Given a data set consisting of n pairs of observations (where $n \geq 2$)

$$(x_i, y_i)_{i=1}^n, \tag{1}$$

R_X is used for comparing x observations and R_Y is used for comparing y observations.

Given a data set as in Eq. (1), the strict fuzzy orderings R_X and R_Y are used to compute two important numbers, the *number of concordant pairs* $\tilde{C}$ and the number of *discordant pairs* $\tilde{D}$:

$$\tilde{C} = \sum_{i=1}^{n} \sum_{j \neq i} \bar{T}(R_X(x_i, x_j), R_Y(y_i, y_j))$$
$$\tilde{D} = \sum_{i=1}^{n} \sum_{j \neq i} \bar{T}(R_X(x_i, x_j), R_Y(y_j, y_i))$$

The function $\bar{T}$ is a triangular (t-norm) [11] that is used to aggregate degrees of relationships between pairs of x observations and the corresponding degrees for y observations (see below). The final *robust gamma rank correlation coefficient* is then computed as

$$\tilde{\gamma} = \frac{\tilde{C} - \tilde{D}}{\tilde{C} + \tilde{D}}$$

in perfect analogy to Goodman's and Kruskal's gamma [7].

4.2 Choosing the Family of Similarities

It should be clear from the description above that the robust gamma rank correlation coefficient requires the following ingredients:

1. A fuzzy ordering R_X for the x observations
2. A fuzzy ordering R_Y for the y observations
3. A t-norm $\bar{T}$ for aggregation.

For R_X and R_Y, the `rococo` package provides five possible choices which are identified by the *similarity* that is used to define the strict fuzzy ordering (for more details see [4, 5]). Table 1 provides an overview.

Obviously, in all five cases, the strict fuzzy ordering R is computed from the similarity E in the following way:

$$R(x, x') = \begin{cases} 1 - E(x, x') & \text{if } x' > x \\ 0 & \text{otherwise} \end{cases}$$

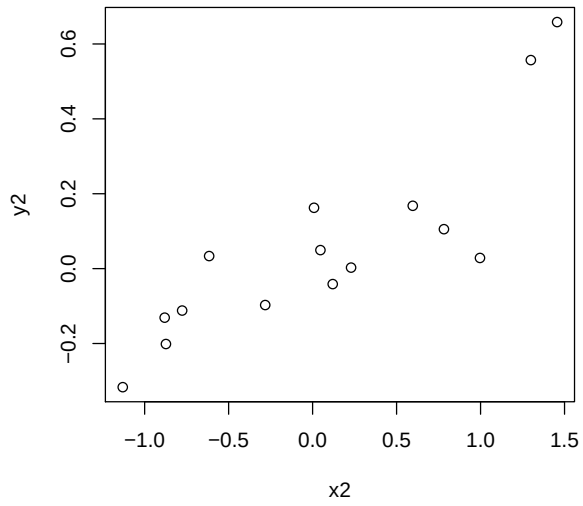
Table 1: Overview of strict fuzzy orderings implemented in the `rococo` package:

Setting	Similarity	Strict fuzzy ordering
`"linear"`	$E(x,x') = \max(0, 1 - \frac{1}{r}\lvert x - x'\rvert)$	$R(x,x') = \max(0, \min(1, \frac{1}{r}(x' - x)))$
`"exp"`	$E(x,x') = \exp(-\frac{1}{r}\lvert x - x'\rvert)$	$R(x,x') = \max(0, 1 - \exp(-\frac{1}{r}(x' - x)))$
`"gauss"`	$E(x,x') = \exp(-\frac{1}{2r^2}(x - x')^2)$	$R(x,x') = \begin{cases} 1 - \exp(-\frac{1}{2r^2}(x - x')^2) & \text{if } x \leq x' \\ 0 & \text{otherwise} \end{cases}$
`"epstol"`	$E(x,x') = \begin{cases} 1 & \text{if } \lvert x - x'\rvert \leq r \\ 0 & \text{otherwise} \end{cases}$	$R(x,x') = \begin{cases} 1 & \text{if } x' > x + r \\ 0 & \text{otherwise} \end{cases}$
`"classical"`	$E(x,x') = \begin{cases} 1 & \text{if } x = x' \\ 0 & \text{otherwise} \end{cases}$	$R(x,x') = \begin{cases} 1 & \text{if } x' > x \\ 0 & \text{otherwise} \end{cases}$

Further note that the choices `"epstol"` and `"classical"` are not continuous. The former is the well-known ε-intolerant similarity that has been discussed widely in the context of the Poincaré paradox (note that this similarity is not a transitive relation). The latter setting `"classical"` corresponds to the classical Goodman and Kruskal gamma.

The functions `rococo()` and `rococo.test()` choose the first variant `"linear"` by default, both for x and y observations. If one wants to choose a different setting or two different strict fuzzy orderings for x and y observations, the `similarity` argument can be used. For demonstrating this, we create a noisy data set from a function f that has a large flat area:

```
> x2 <- rnorm(15)
> f2 <- function(x) {
+     if (x > 0.8)
+         x - 0.8
+     else if (x < -0.8)
+         x + 0.8
+     else 0
+ }
> y2 <- sapply(x2, f2) + rnorm(length(x2), sd = 0.1)
> plot(x2, y2)
```



As said before, `"linear"` is the default choice:

```
> rococo.test(x2, y2, alternative = "greater")

        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity: linear
rx = 0.1385442 / ry = 0.02385542
t-norm: min
alternative hypothesis: true gamma is greater than 0
sample gamma = 0.7436693
estimated p-value = 0.0001191489 (0 of 1000 values)
```

This default setting makes sense in particular if no information about the data, their distribution, or not even the noise distribution is known. Now let us try some different settings:

```
> rococo.test(x2, y2, similarity = "gauss", alternative = "greater")

        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity: gauss
rx = 0.1385442 / ry = 0.02385542
t-norm: min
alternative hypothesis: true gamma is greater than 0
sample gamma = 0.8037081
estimated p-value = 0.0001128236 (0 of 1000 values)
```

```
> rococo.test(x2, y2, similarity = c("classical", "gauss"),
+     alternative = "greater")

        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity for x: classical
similarity for y: gauss (ry = 0.02385542)
t-norm: min
alternative hypothesis: true gamma is greater than 0
sample gamma = 0.7216286
estimated p-value = 0.0001855216 (0 of 1000 values)
```

Particularly note the latter of the two examples: different settings for x and y observations can be done by supplying a vector to the `similarity` argument, where the first element determines the choice for x observations and the second element determines the choice for y observations.

4.3 Parametrizing Similarities

So far, we have neglected that four of the five similarities/fuzzy orderings listed in Table 1 require an additional parameter r. In all four cases, r controls the importance of observations that are close to each other. The smaller r, the more similar observations are taken into account when computing the numbers of concordant and discordant pairs. This entails that, the smaller r, the easier noise can corrupt the result. The larger r, the less similar observations are considered, i.e. the more noise-tolerant the result will be. However, that does not mean that the largest possible r is the best choice. An overly large r can result in unspecific and unsignificant results. The `rococo` package allows for setting one r for both x and y observations:

```
> rococo.test(x2, y2, similarity = "gauss", r = 0.1, alternative = "greater")

        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity: gauss
rx = 0.1 / ry = 0.1
t-norm: min
alternative hypothesis: true gamma is greater than 0
sample gamma = 0.8799177
estimated p-value = 0.0002530797 (0 of 1000 values)
```

It is also possible to specify different values of r for x and y observations. Analogously to the parameter `similarity`, this can be done by supplying a two-element vector to the parameter `r`:

```
> rococo.test(x2, y2, similarity = c("linear", "gauss"), r = c(0.05,
+     0.1), alternative = "greater")
```

```
        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity for x: linear (rx = 0.05)
similarity for y: gauss (ry = 0.1)
t-norm: min
alternative hypothesis: true gamma is greater than 0
sample gamma = 0.852226
estimated p-value = 0.0001945368 (0 of 1000 values)
```

It should be clear from the formulas in Table 1 that $r = 0$ is either invalid or does not make sense. The `rococo` package still admits choosing a zero value. In this case, `rococo` makes an *automatic adjustment* of r to 10% of the interquartile range (the difference between the 75% and the 25% quantile) of the observation under consideration:

```
> rococo.test(x2, y2, similarity = c("linear", "gauss"), r = 0,
+     alternative = "greater")

        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity for x: linear (rx = 0.1385442)
similarity for y: gauss (ry = 0.02385542)
t-norm: min
alternative hypothesis: true gamma is greater than 0
sample gamma = 0.7626111
estimated p-value = 0.0001024683 (0 of 1000 values)

> IQR(x2) * 0.1

[1] 0.1385442

> IQR(y2) * 0.1

[1] 0.02385542
```

In the results above, note the values `rx` and `ry` in the output of `rococo.test()`. These are the values that have been specified or that have been determined automatically. The computations of 10% of the interquartile range should demonstrate that this is what takes place when r is set to 0. Note that this is also done by default if the argument `r` is not specified.

Table 2: Overview of strict fuzzy orderings implemented in the `rococo` package:

Setting	t-Norm
`"min"` (default)	$T_{\mathbf{M}}(x, y) = \min(x, y)$
`"prod"`	$T_{\mathbf{P}}(x, y) = x \cdot y$
`"lukasiewicz"`	$T_{\mathbf{L}}(x, y) = \max(0, x + y - 1)$

4.4 Choosing the t-Norm for Aggregation

As mentioned above, the robust gamma rank correlation coefficient further requires to specify a t-norm $\bar{T}$ that is used for aggregation of the ordering measures from x and y observations. The `rococo` package offers three built-in t-norms that can be selected by specifying the `tnorm` argument when calling the functions `rococo()` and `rococo.test()`. Table 2 provides an overview. Here is an example that uses the product t-norm for aggregation:

```
> rococo.test(x2, y2, similarity = c("linear", "gauss"), tnorm = "prod",
+     alternative = "greater")

        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity for x: linear (rx = 0.1385442)
similarity for y: gauss (ry = 0.02385542)
t-norm: prod
alternative hypothesis: true gamma is greater than 0
sample gamma = 0.7621023
estimated p-value = 0.0002170714 (1 of 1000 values)
```

The choice of the t-norm $\bar{T}$ is not particularly critical and should not have a strong influence on the significance of results. Most users will suffice with the default setting `"min"`. The choice `"prod"` produces similar, but slightly smoother results which may be suitable in combination with the only differentiable fuzzy ordering (`similarity="gauss"`).

Even though the choice is not critical, the `rococo` package also offers the choice of user-defined t-norms by supplying a two-place function as `tnorm` argument. Here is an example with some Yager t-norm [11, 17]:

```
> DrastictNorm <- function(x, y) {
+     if (x == 1)
+         y
+     else if (y == 1)
+         x
```

```
+     else 0
+ }
> YagertNorm <- function(lambda) {
+     fun <- function(x, y) {
+         if (lambda == 0)
+             DrastictNorm(x, y)
+         else if (is.infinite(lambda))
+             min(x, y)
+         else max(0, 1 - ((1 - x)^lambda + (1 - y)^lambda)^(1/lambda))
+     }
+     attr(fun, "name") <- paste("Yager t-norm with lambda =",
+         lambda)
+     fun
+ }
> rococo(x2, y2, tnorm = YagertNorm(0.5))

[1] 0.7419704

> rococo.test(x2, y2, tnorm = YagertNorm(0.2))

        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity: linear
rx = 0.1385442 / ry = 0.02385542
t-norm: Yager t-norm with lambda = 0.2
alternative hypothesis: true gamma is not equal to 0
sample gamma = 0.7417189
estimated p-value = 0.0002896577 (0 of 1000 values)
```

Note that the `rococo` package performs only a few basic checks on a user-defined t-norm. It remains the duty of the user to ensure that the function is actually a valid t-norm.

The three built-in t-norms (see Table 2) are efficiently implemented in C++ and called with the help of the `Rcpp` package [6] while user-defined t-norms have to be evaluated in R loops. Even though we use the `compiler` package (if available) to pre-compile the user-defined t-norm, this may still result in a drastic slowdown of computations, particularly for larger data sets or when using `rococo.test()` with `exact=TRUE` (see end of next section).

5 A Note on Permutation Testing

Classical rank correlation measures only depend on the sorting of x and y observations. Thus, for a given number of samples n, one can deduce the distribution of the test statistic under the $\mathcal{H}_0$ hypothesis as a simple function of the number of samples n. We neither want to make any prior assumption about the distribution of data nor does the complex inner structure of the robust

gamma rank correlation coefficient and the variety of possible parameter settings allow for an analytic deduction of the test statitistic's distribution. However, as extensive experiments have shown, we can assume that the test statistic is approximately normally distributed around 0, where only the standard deviation depends on the data distribution and the parameter settings of the rank correlation measures. Therefore, we use *permutation testing* for estimating the standard deviation of the test statistic under the assumption of independence. This is done in the following way: For a given data set $(x_i, y_i)_{i=1}^n$, we first compute the robust rank correlation coefficient according to the specified parameters. Then we create K random shuffles of $(y_i')_{i=1}^n$ and compute the robust rank correlation coefficient for $(x_i, y_i')_{i=1}^n$ according to the specified parameters. Due to the shuffling, $(x_i)_{i=1}^n$ and $(y_i')_{i=1}^n$ are independent, where $(y_i')_{i=1}^n$ has the same marginal distribution as $(y_i)_{i=1}^n$. Thus, the robust rank correlation coefficients obtained for a sufficiently large number of shuffles allows for estimating the distribution of the test statistics under the $\mathcal{H}_0$ hypothesis with given marginal distributions and we can estimate the test's p-value by the resulting normal distribution. Assume that $\tilde{\gamma}$ is the observed gamma rank and that $\tilde{\sigma}$ is the estimated standard deviation from 0 computed from the observed test statistics on the random shuffles. Then the p-values can be computed as ($P_{\mu,\sigma}$ denotes the cummulative distribution function of the normal distribution with mean μ and variance σ^2)

- $2 \cdot (1 - P_{0,\tilde{\sigma}}(|\tilde{\gamma}|))$ in case we perform a two-sided test,
- $1 - P_{0,\tilde{\sigma}}(\tilde{\gamma})$ in case we perform a one-sided test with alternative hypothesis that there is a positive correlation, and
- $P_{0,\tilde{\sigma}}(\tilde{\gamma})$ in case we perform a one-sided test with alternative hypothesis that there is a negative correlation.

This p-value is stored in the slot `p.value` of the resulting output object of `rococo.test()`. As usual in R, $< 2.2e-16$ is displayed if the p-value is lower than machine precision. Moreover, the output object also contains a slot `count` which corresponds to the number of times

- the test statistics' absolute value exceeded the absolute value of the test statistic for the unshuffled data in case we perform a two-sided test,
- the test statistic was greater than the test statistic for the unshuffled data in case we perform a one-sided test with alternative hypothesis that there is a positive correlation, and
- the test statistic was less than the test statistic for the unshuffled data in case we perform a one-sided test with alternative hypothesis that there is a negative correlation.

This count allows for an alternative method of determining a p-value as a relative frequency. Users who want to use this method can compute the p-value as the quotient of the above count (slot `count`) over the number of trials (slot `numtests`).

The number of shuffles performed by `rococo.test()` is controlled by the parameter `numtests` (the default is 1000). It is clear that, the smaller the number of shuffles, the less exact the estimation is. We concur that 1000 samples are sufficient (at least with high probability) if one wants to test whether the association is significant with a significance threshold of 95% or 99%. If the user, however, is interested in much more exact estimates of the p-value or if he/she wants to test against much more stringest significance thresholds, it may be necessary to perform much higher

numbers of shuffles. Needless to mention, this will also result in an increase of computation times, where the computation time grows linearly with the number of shuffles.

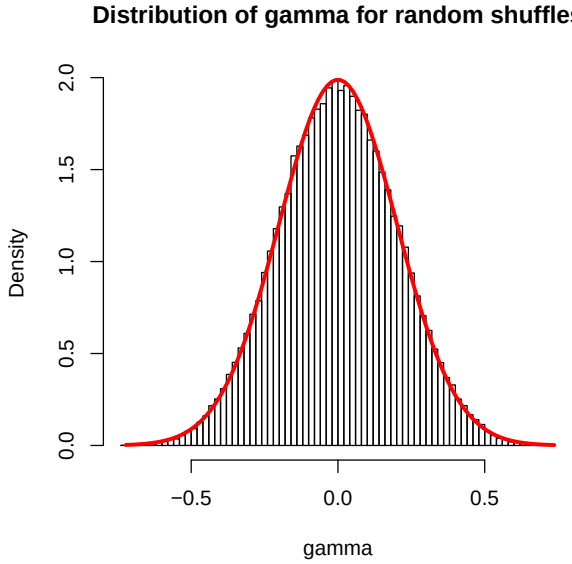
Here is an example with 100,000 shuffles, where we use the option `storeValue=TRUE` to get access to the rank correlation values for all random shuffles:

```
> res <- rococo.test(x2, y2, numtests = 1e+05, storeValues = TRUE)
> res

        Robust Gamma Rank Correlation:

data: x2 and y2 (length = 15)
similarity: linear
rx = 0.1385442 / ry = 0.02385542
t-norm: min
alternative hypothesis: true gamma is not equal to 0
sample gamma = 0.7436693
estimated p-value = 0.0002180539 (9 of 100000 values)
```

```
> hist(res@perm.gamma, breaks = 100, probability = TRUE, xlab = "gamma",
+     main = "Distribution of gamma for random shuffles")
> plot(function(x) dnorm(x, mean = 0, sd = res@H0gamma.sd),
+     min(res@perm.gamma), max(res@perm.gamma), col = "red",
+     lwd = 3, add = TRUE)
```



The histogram and the density of the corresponding normal distribution (red curve) match almost perfectly.

For small data sets (not more than 10 samples), the package further provides computations of *exact p-values*. This can be enforced by passing the argument `exact=TRUE` to `rococo.test()`. In this case, *all possible permutations* are considered (using the Steinhaus-Johnson-Trotter algorithm; see, e.g., [14]) and the exact p-value is computed as the quotient of the above count (slot `count`) over the number of trials (the factorial of the length of `x` and `y`):

```
> rococo.test(x2[1:8], y2[1:8], exact = TRUE)


        Robust Gamma Rank Correlation:

data: x2[1:8] and y2[1:8] (length = 8)
similarity: linear
rx = 0.1201968 / ry = 0.03707752
t-norm: min
alternative hypothesis: true gamma is not equal to 0
sample gamma = 0.9239921
exact p-value = 0.0003968254 (16 of 40320 values)
```

Using the exact test for 10 samples results in $10! = 3628800$ permutations that have to be considered. For the built-in t-norms, such a computation should finish within a few seconds. However, in conjunction with a user-defined t-norm, computations may be significantly longer, in the range of several minutes.

6 How to Cite This Package

If you use this package for research that is published later, you are kindly asked to cite it as follows:

> U. Bodenhofer and F. Klawonn (2008). Robust rank correlation coefficients on the basis of fuzzy orderings: initial steps. *Mathware Soft Comput.* **15**(1):5–20.

To obtain a BibTEX entry of the reference, you can enter the following into your R session:

```
> toBibtex(citation("rococo"))
```

Acknowledgment

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References

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