

ScottKnott: A Package for Performing the Scott-Knott Clustering Algorithm in R

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ABSTRACT. Scott-Knott is an hierarchical clustering algorithm used in the application of ANOVA, when the researcher is comparing treatment means, with a very important characteristic: it does not present any overlapping in its grouping results. We wrote a code, in R, that performs this algorithm starting from vectors, matrix, data.frame, aov or aov.list objects. The results are presented with letters representing groups, as well as through graphics using different colors to differentiate distinct groups. This R package, named *ScottKnott* is the main topic of this article.

Keywords: Scott-Knott, multiple comparisons, R core team.

1 INTRODUCTION

Scott-Knott (SK) is a hierarchical clustering algorithm used as an exploratory data analysis tool. It was designed to help researchers working with an ANOVA experiment, wherein the comparison of treatment means is an important step in order, to find distinct homogeneous groups of those means whenever the situation leads to a significant *F-test*.

The multiple comparison procedures commonly used to solve this problem usually divide the set of treatment means into groups that are not completely distinct. Therefore, many treatments end up belonging to different groups simultaneously, this is called overlapping [6].

In fact, as the number of treatments increases, so do the number of overlappings making it difficult for the experimental users to distinguish the real groups to which the treatments should belong. In this case, the division of treatments in completely distinct groups is the most important solution. Even though the goal of multiple comparison methods is an all-pair comparison, not a division of the treatment means into groups, biologists, plant breeders and many others expect those tests to make that division in groups.

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The possibility of using cluster analysis in place of multiple comparison procedures was suggested by [15] since the results of cluster type analysis, represent a type of solution for dividing treatments into distinct groups.

The SK algorithm is a hierarchical cluster analysis approach used to partition treatments into distinct groups. Many other hierarchical cluster analysis approaches have been proposed since Scott, A.J. and Knott, M. [18] published their results, such as, for example [13], [9], and [6]. However, the SK has been the most widely used approach due to its simple intuitive appeal, and also the good results it always provides [12, 4, 11, 14].

The SK procedure uses a clever algorithm of cluster analysis, where, starting from the whole group of observed mean effects, it divides, and keeps dividing the subgroups in such a way that the intersection of any of the two formed groups remains empty. In the words of A.J. Scott and M. Knott: “We study the consequences of using a well-known method of cluster analysis to partition the sample treatment means in a **balanced design** and show how a corresponding likelihood ratio test gives a method of judging the significance of the difference among groups obtained” [18]. Besides, simulation studies reveal that in comparison with the most used multiple comparison procedures, the SK procedure has a very good performance [10, 5]. We also try to motivate the reader into the practice of the SK algorithm by bringing a real data example and compare the SK with other procedures, namely the clustering (`hclust`, package `stats`) and Tukey test (package `agricolae`).

The main objective of this paper is the **ScottKnott** R package, which implements the SK procedure [18]. The package is available on the Comprehensive R Archive Network (CRAN) website and can be accessed at: <http://CRAN.R-project.org/package=ScottKnott>.

The R Package **ScottKnott** consists of two methods, `SK` and `SK.nest`. The `SK` method performs the algorithm on treatments of main factors whereas `SK.nest` does the same on nested designs of factorial, split-plot and split-split-plot experiments. They return objects of classes `SK`, and `SK.nest` containing the groups of means plus other variables necessary for `summary` and `plot`. The generic functions `summary` and `plot` are used to obtain and print a summary and a plot.

Nowadays, the R environment for computational statistics has become the working language of computational statistics worldwide. Moreover, the huge processing power and memory space of modern computers has made it possible to write computer codes for almost every statistical methodology, indeed, this has eventually become, one of the main working tasks for statisticians and, as a result, statistical journals have been giving more space to the publication of software guides. Among them, the most important are the R packages.

2 REAL DATA STUDY

As a motivation we will use an experiment conducted at EMBRAPA Milho e Sorgo (The Brazilian Agricultural Research Corporation, Corn and Sorghum Section). It was published in [16] page 167. The experiment consists of 16 treatments (cultivars) of sorghum conducted in a balanced squared lattice design and the yield by plot (*kg/plot*). For our purposes, the experiment can be considered an incomplete randomized block design with 4 blocks, 16 treatments,

and 5 repetitions, that is, the yield of each treatment is measured 5 times. These data are available in the **ScottKnott** package as `sorghum`.

The objective of this study is to compare the 16 treatment means, as a first step of the whole analysis, and the question is: are there groups of treatments which could be considered homogeneous? In other words, would it be possible to find groups for which the treatment means belonging to those groups that represent cultivars yielding the same weight of sorghum and the differences in the observed results being due to random variability?

We understand that this way of questioning is very important for the agricultural researcher and might be even more important than testing for the difference between treatment means for every pair of those means. There is a total of 120 of those pairs.

Even though this first study is just exploratory, it will give the researcher the insight he/she needs to continue the analysis.

This exploratory analysis was carried out using the SK algorithm, whose results were compared to two other methods.

```
> library(ScottKnott)
> data(sorghum)
> av <- aov(y ~ r/bl + x,
+         data=sorghum$dfm)
> sk <- SK(av,
+         which='x',
+         sig.level=0.05)
> plot(sk,
+       title=NULL,
+       col=c('black',
+            'gray'))
```

The first is the function `hclust` found in the package **stats**, which performs hierarchical cluster analysis on a set of dissimilarities. The used agglomeration method was “ward”. We calculated the mean value of the 5 repetitions for each treatment and used it in the `hclust` function.

```
> dat.cl <- sorghum$dfm[order(sorghum$dfm$x), ][, 4]
> dim(dat.cl) <- c(5, 16)
> dimnames(dat.cl) <- list(paste('r',
+                               1:5,
+                               sep=''),
+                          1:16)
> dat.cl.m <- apply(dat.cl,
+                  2,
+                  mean)
> cl <- hclust(dist(dat.cl.m),
+             'ward')
> plot(cl,
+       main='')
```

The second, was the Tukey's HSD test which is a multiple comparison procedure that is also used by researchers to divide the treatment means into groups. We used the Rpackage **agricolae** to build the graph.

```
> library(agricolae)
> tk <- HSD.test(av,
+               'x',
+               group=TRUE,
+               alpha=0.05)
> bar.group(tk$groups,
+           ylim=c(0, 12),
+           density=4,
+           border="black")
```

Figure 1 shows the result of the SK algorithm. It divided the means into two groups. The two main groups found using the function `hclust` (Fig. 2) are not exactly the same as those found using the SK algorithm, but they are as similar as it was expected. The treatment means 14, 8, 5, 7, 9, 3 belong to the same group in both figures, and the treatments 1, 2, 4, which belong to the same group of the above treatments in Figure 1; in Figure 2, on the other hand, they belong to the second main group. Nevertheless, they are grouped together at the lowest level. The `hclust` function cuts at the big gap between treatments 9 and 3 and the function `SK` at the big gap between treatments 2 and 12.

Figure 3 shows the result using the Tukey's HSD test. It finds 3 groups, marked by the letters *a*, *b* and *c*. Almost all of the treatments are classified to the 3 groups and this overlapping makes very difficult for the researcher to decide in which groups those means should be sorted.

What makes the SK algorithm more convenient in such cases is that, in addition to dividing the treatments in groups without overlapping, its result also uses a probabilistic approach aimed at finding the groups: the SK algorithm takes the maximum between group sum of squares, which is used in a likelihood ratio test with an asymptotic χ^2 distribution. This approach is very useful when the number of treatments is large.

It is also possible to change the value of the parameter **sig.level** of the SK function by getting different groupings, and the researcher can check what makes sense in practice.

3 COMPARATIVE PERFORMANCE OF SK METHOD

In performance studies involving statistical tests, it is often very difficult to obtain the rates of type I error and power in an analytical manner. The most usual way to get that information is through simulation using Monte Carlo methods. [3] show that the difference between analytical values and Monte Carlo's is very small thus making its use an optimal way to get the necessary information. Their results are similar to those found by [2].

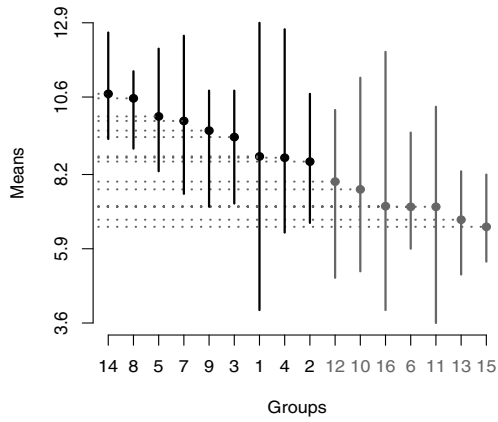


Figure 1: Yield of sorghum using Skott-Knott algorithm, $\alpha = 5\%$.

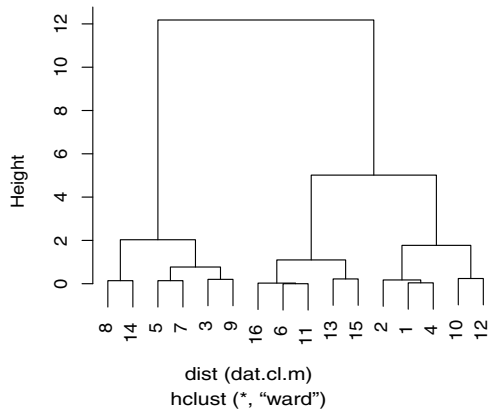


Figure 2: Yield of sorghum using hclust, distance = euclidean and agglomeration method = ward.

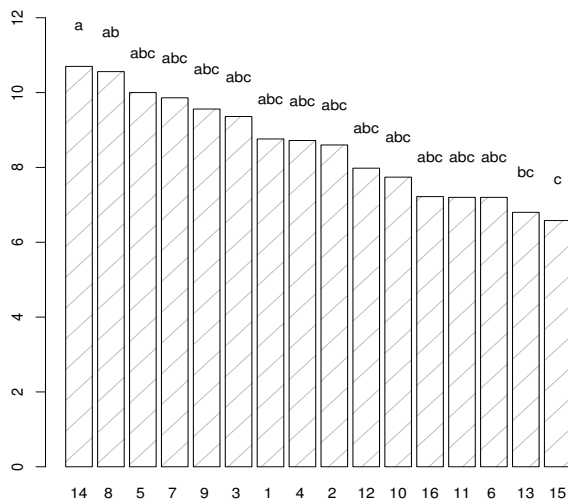


Figure 3: Yield of sorghum using Tukey, $\alpha = 5\%$.

Despite the fact that SK is a clustering procedure, we can use simulation results to compare its performance to Tukey test and others, as if it were a multiple comparison procedure.

Two of the most common measures to compare “Multiple Comparison Procedures” found in the literature are:

- The ratio between the number of type I errors (reaching the result that $\mu_i \neq \mu_j$ when truly $\mu_i = \mu_j$) and the number of comparisons, is defined as *comparisonwise error rate*.
- The ratio between the number of experiments with one or more type I errors and the total number of experiments is defined as *experimentwise error rate* [7, 19].

Two simulation studies conducted at the Federal University of Lavras, Brazil, used Monte Carlo methods to evaluate the performance of the SK method [3, 2]. One [10] showed that it possesses high power and an error rate that is almost always in accordance with the nominal levels using both comparisonwise and experimentwise error rates (Table 1). That is, the rates are not far from α value or **sig.level** as defined in the last paragraph of section 4.1.

The other, [5] evaluated the power and the type I error rates of the SK, Tukey and SNK test, in a wide variety of experimental situations, in conditions of normality and non-normality error distribution (Table 2). They concluded that the SK is more powerful than the other two and is also robust against violations of normality assumptions. Both performed 2000 simulations for each experiment with 5, 10, 20 and 80 treatments with 4, 10 and 20 replications α value of 1% and 5% plus coefficients of variation of 1%, 10%, 20% and 30%.

4 METHOD

4.1 Methodology

Suppose we have a set of independent sample treatment means in the analysis of variance context, each treatment with the same number of replications, all normal variates, that is a **balanced design**. Furthermore, suppose that ANOVA leads to a significant *F-test* for the difference among the treatment means. Moreover, by rejecting the homogeneity of the treatment means there is still the problem of finding out the number of homogeneous groups and which are the treatment means contained in each group.

It should be noted that we follow [6] in what we mean by homogeneity of treatments: “Once more it should be borne in mind that non rejection of equality is by no means equivalent to proving equality. We carefully defined homogeneity as non rejection of equality. Nor should it be inferred that treatments belonging to different “homogeneous groups” are (significantly) different; treatments belonging to the same group, however, are not.” The SK procedure is a hierarchical clustering algorithm that attempts to find out those groups without overlapping.

Let us consider k as the number of treatments. As it starts, the SK procedure will either find two distinct groups dividing the treatment means or it will determine those k treatment means

Table 1: Error rates by comparisons (ERC) and experiment (ERE), for the Scott-Knott test, depending on the number of repetitions (REP), number of treatments (TRAT), coefficient of variation (CV) and nominal levels of significance at $\alpha = 1\%$ and $\alpha = 5\%$.

REP	TRAT	CV	1%		5%	
			%ERC	%ERE	%ERC	%ERE
4	5	1	0.13**	0.25**	3.47**	6.60*
4	5	30	0.22**	0.45**	2.85**	5.40
10	5	1	0.67	1.25	3.11**	5.90
10	5	30	0.54	1.00	3.31**	6.35
20	5	1	0.54	1.05	3.41**	6.25
20	5	30	0.69	1.25	3.41**	6.40*
4	10	1	0.30**	0.65	2.12**	4.20
4	10	30	0.25**	0.55	2.48**	4.90
10	10	1	0.55	1.10	2.61**	5.25
10	10	30	0.41**	0.80	2.68**	5.45
20	10	1	0.66	1.35	2.45**	5.05
20	10	30	0.77	1.55	2.42**	5.15
4	20	1	0.17**	0.35**	2.16**	4.40
4	20	30	0.33**	0.65	1.91**	4.00
10	20	1	0.31**	0.65	2.28**	4.80
10	20	30	0.44**	0.90	2.49**	5.05
20	20	1	0.42**	0.85	2.98**	6.10
20	20	30	0.50**	1.05	2.56**	5.35
4	80	1	0.27**	0.55	1.74**	3.55**
4	80	30	0.33**	0.65	1.81**	3.70**
10	80	1	0.47**	0.95	2.27**	4.60
10	80	30	0.47**	0.95	1.75**	3.55**
20	80	1	0.50**	1.00	2.31**	4.70
20	80	30	0.55	1.10	2.70**	5.50

Source: Adapted of [10]. *Exceeded the upper limit of the confidence interval accurate, with 99% confidence to nominal levels of significance of 1% (1.727044) and 5% (6.391386). **Exceeded the upper limit of the confidence interval accurate, with 99% confidence to nominal levels of significance of 1% (0,518787) and 5% (3,828164).

homogeneous belonging to just one group. To do so, it should divide the $2^{k-1} - 1$ possible partitions of the k means in two nonempty groups, but it is enough to look at the $k - 1$ partitions formed by ordering the treatment means and divide them between two successive ones [18]. Let T_1 and T_2 be the totals of two of those groups with k_1 and k_2 treatments in each one, so that $k_1 + k_2 = k$, that is:

$$T_1 = \sum_{i=1}^{k_1} y(i) \quad T_2 = \sum_{i=k_1+1}^{k_1+k_2} y(i)$$

where $y(i)$, $i = 1 : m$ are the ordered treatment means and y the grand mean [16].

Table 2: Type I error rates by experiment (%), to the Tukey, SNK and Scott Knott tests, for different CV and distributions, considering the number of treatments (p) equal to 10 and 20 replications for nominal levels of significance 1% to 5%.

Distributions	CV	Tests					
		Tukey		SNK		Scott-Knott	
		$\alpha = 1\%$	$\alpha = 5\%$	$\alpha = 1\%$	$\alpha = 5\%$	$\alpha = 1\%$	$\alpha = 5\%$
Normal	1	1.20	5.70	1.20	5.70	0.90	6.35
	10	1.15	5.05	1.15	5.10	1.25	6.90
	20	1.30	4.60	1.30	4.60	1.20	6.20
	30	1.00	4.75	1.00	4.80	1.45	6.00
Lognormal	1	1.15	4.80	1.20	5.05	1.45	5.30
	10	0.60	3.80	1.20	6.50	2.00	7.10
	20	0.85	4.15	1.55	8.70	2.35	8.15
	30	0.35	3.55	0.90	9.25	1.65	7.15
Exponential	1	0.95	5.00	0.95	5.05	1.45	7.25
	10	1.00	5.35	1.10	5.40	1.30	6.35
	20	0.85	4.35	0.85	4.40	1.45	6.10
	30	1.30	5.20	1.35	5.45	1.95	6.00
Weibull 3.6	1	1.25	5.50	1.25	5.55	1.70	6.25
	10	0.70	4.35	0.70	4.35	1.10	5.75
	20	0.60	4.05	0.60	4.85	1.30	5.80
	30	1.00	4.80	1.00	4.90	1.60	6.60

Source: [5].

Also, let B be the between groups sum of squares. That is:

$$B = \frac{T_1^2}{k_1} + \frac{T_2^2}{k_2} - \frac{(T_1 + T_2)^2}{k_1 + k_2}$$

Let B_o be the maximum value, taken over the $k - 1$ partitions of the k treatments into two groups, of the between groups sum of squares B . After finding out those groups, we use the likelihood ratio test for the null hypothesis of equality of all means against the alternative that they belong to the two groups found above. If we reject this hypothesis then the two groups are kept, otherwise the group of k treatment means is considered homogeneous. We then repeat this procedure for each group separately and stop until all of the formed groups become homogeneous.

The statistics used for the likelihood ratio test is:

$$\lambda = \frac{\pi}{2(\pi - 2)} \times \frac{B_o}{\sigma_o^2}$$

where σ_o^2 is the maximum likelihood estimator of $\frac{\sigma^2}{r}$.

Let $s^2 = \frac{MSE}{r}$ be the unbiased estimator of $\frac{\sigma^2}{r}$, ν be degrees of freedom associated with that estimator, then

$$\sigma_o^2 = \frac{\sum_{i=1}^k (y(i) - y)^2 + \nu s^2}{k + \nu}$$

λ is asymptotically a χ^2 distributed random variable with $\nu_o = \frac{k}{\pi-2}$ degrees of freedom. Therefore we can use that to set the cutoff point for a given α value each time we perform the test.

We can think the p-value of likelihood ratio test as a distance to be measured between the two selected groups and the type I error (α value) chosen to be the cut off. If the p-value is smaller than α , the groups are too far away from each other and should be separated (they are heterogeneous), otherwise, they become just one group (homogeneous).

“Choosing an appropriate value for α is difficult. If α is too small, the splitting process will terminate too soon, on the other hand, if α is too large, the process will go too far and split homogeneous sets of means” [18].

As we start dividing the first groups into other smaller groups, we repeat the same algorithm for each group. We keep doing that until every formed group is either homogeneous or just contains one observed mean.

It is important to emphasize the fact that the above defined α value is not the nominal error rate of the type I error of the algorithm as a whole. If we set the α value as 5% then every test the SK procedure performs to divide (or not) a sub-group has a type I error rate of 5%. Nevertheless, we cannot say that the former type I error rate is 5%. This α value is the parameter called **sig.level** in the SK function.

4.2 ScottKnott package

The **ScottKnott** package was written in R language [17]. The results are objects of the class `list`, `SK` and `SK.nest`, which are used as an input to the generic functions `summary` and `plot`. It performs the clustering algorithm on three designs and three experiments. Once again, it must be emphasized again that the two functions `SK` and `SK.nest` **only work on balanced designs**. The designs are: Completely Randomized Design (CRD), Randomized Complete Block Design (RCBD) and Latin Squares Design (LSD). The experiments are: Factorial Experiment (FE), Split-Plot Experiment (SPE) and Split-Split-Plot Experiment (SSPE).

The **ScottKnott** package has two main functions: `SK` and `SK.nest`. The `SK` function is used for clustering the treatment means of a main factor. The `SK.nest` function, in turn, is used for clustering treatment means relative to interactions among factors, that is whenever the treatment means belong to a factor nested in others. For example, the treatment means of factor A, for level 1 of factor B, and level 1 of factor C. As shown above, the `SK.nest` function supports no more than two nestings.

The `summary` function generates an output where the different groups are displayed as letters of the alphabet. The `plot` function generates distinct groups that are differentiated by colors.

The main algorithm is the `MaxValue` function which builds groups of means according to the method of SK. It is basically an algorithm for a pre-order path in a binary decision tree. Every node of this tree, represents a different group of means and, when the algorithm reaches this node it takes the decision to either split the group in two, or to form a group of means. At the end all the leaves of the tree are the groups of homogeneous means.

The `SK` and `SK.nest` functions are methods for objects of class `vector`, `matrix` or `data.frame` joined as default, whereas `aov` and `aovlist` are methods for single experiments.

The main parameters used by those methods are:

- `x`: A design matrix, `data.frame` or an `aov` object.
- `y`: A vector of response variable. It is only necessary to inform this parameter if `x` represents the design matrix.
- `which`: The name of the factor to be used in the clustering. The name must be inside quoting marks.
- `model`: If `x` is a `data.frame` object, the model to be used in the `aov` must be specified.
- `error`: The error to be considered. Only used in cases of *split-plot* or *split-split-plot* experiments.
- `sig.level`: Level of Significance, α value, used in the SK and `SK.nest` algorithms to create the groups of means. The default value is 0.05.
- `f1`: A vector of length 1 providing the level of the first factor in the tested nesting order.
- `f2`: A vector of length 1 providing the level of the second factor in the tested nesting order.
- `id.trim`: The number of characters to trim the label of the factor levels.
- `...`: Further arguments (required by generic).

4.2.1 Split-Split-Plot Experiment (SSPE)

We show an example on how to use the **ScottKnott** package. An object of `aovlist` class will be used in the `SK.nest` function.

SSPE is the object containing the data set for a Split-Split-Plot Experiment (SSPE). It is a simulated data aimed at modelling a SSPE with 3 plots, each one split 3 times, each split, split again 5 times and 4 repetitions per split-split.

It can be called using the command below:

```
> data(SSPE)
> nav <- with(SSPE,
+           aov(y ~ blk + P*SP*SSP + Error(blk/P/SP),
+           data=dfm))
```

SSP factor is nested in *SP* factor, which is nested in *P* factor. The value 1 of the parameter fl_1 and 1 of parameter fl_2 mean that the first level of factors *P* and *SP*, respectively, are chosen. The comparison is made only among levels (treatments) of factor *SSP* belonging to that particular combination of levels of factor *P* and factor *SP*. Look at the `aov(model)` and `SK.nest` (which) functions for the order at which the factors appear.

```
> nsk <- SK.nest(nav,
+               which='P:SP:SSP',
+               error='Within',
+               fl1=1,
+               fl2=1)
> summary(nsk)
```

```
Nested: P/SP/SSP
      Levels  Means SK(5%)
p1/sp1/ssp5 456.3500    a
p1/sp1/ssp4 438.9850    a
p1/sp1/ssp3 392.0725    a
p1/sp1/ssp2 349.3500    b
p1/sp1/ssp1 294.6800    b
```

```
> plot(nsk,
+       rl.col=c(rep('black', 3),
+                 rep('gray', 2)),
+       title='')
```

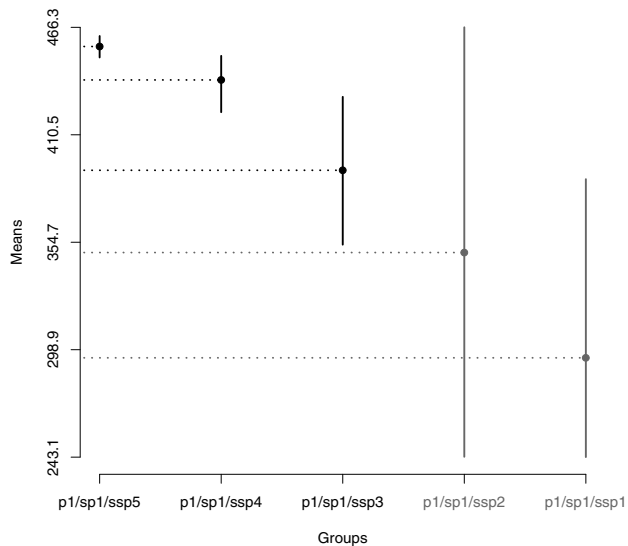


Figure 4: Split-Split-Plot Experiment (SSPE). Nested analysis ($ssp/sp=1/p=1$), $\alpha = 5\%$.

Further examples are documented in the folder *demo* of the R-package **ScottKnott**.

5 THE PACKAGE USAGE

The best measurement of how much the ScottKnott package is used around the world is to count the number of times it has been downloaded since it became available at the CRAN (The Comprehensive R Archive Network). Unfortunately, only one (<http://cran-logs.rstudio.com>), out of 88 mirrors, has control of downloads. Therefore, the numbers shown below are very underestimated. Two other factors contribute with that underestimation: the download control effected by that mirror began on October 1, 2012 and the ScottKnott package has been available since January 2009, and second, this mirror is not Brazilian, whereas Brazilian statisticians are those who mostly use the ScottKnott method. In any case, a little information is better than none at all.

Figure 5 lists the countries that have downloaded the ScottKnott package between periods from October 1, 2012 to August 30, 2013. The country with the highest number of downloads is the United States. The “other” category comprises 55 countries with the number of downloads below 10.

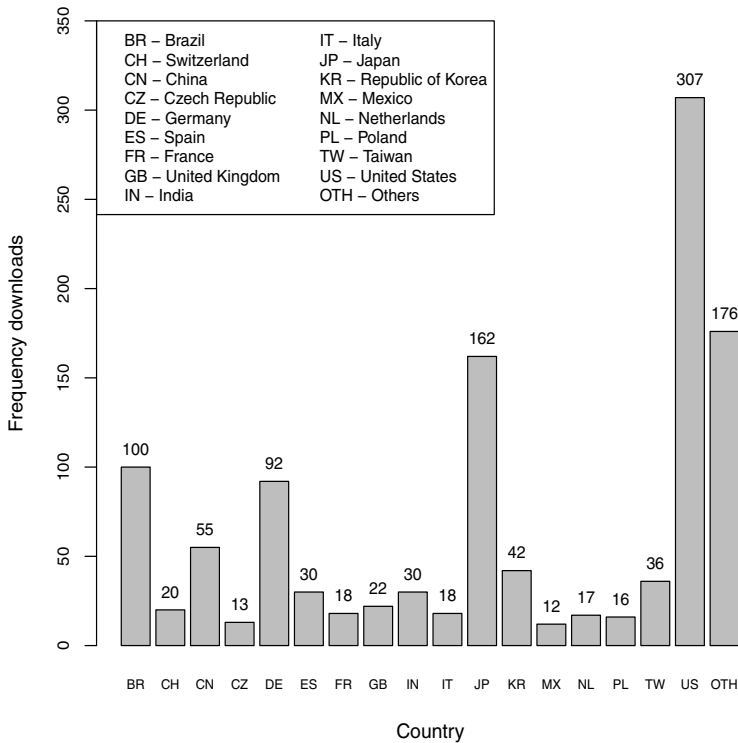


Figure 5: Number of downloads of the ScottKnott package by countries between October 1, 2012 and August 30, 2013.

The number of downloads performed per month since the implementation of the download control can be seen in Figure 6.

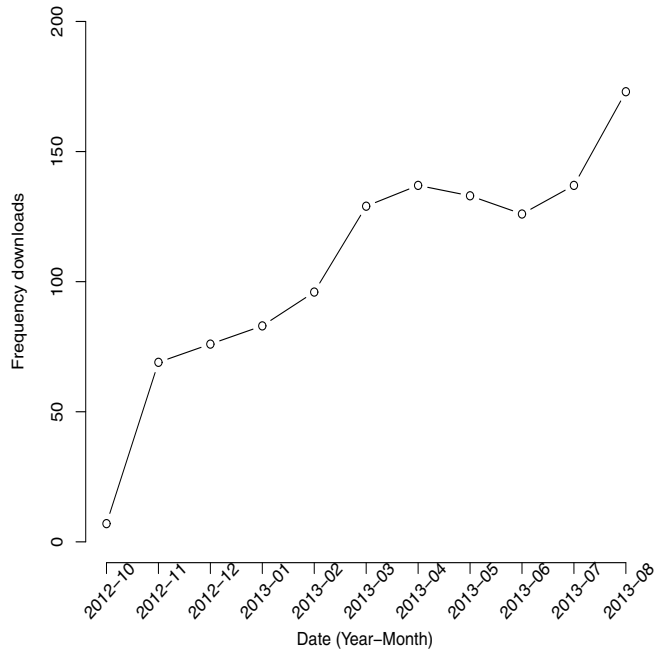


Figure 6: Number of downloads of the ScottKnott package between October 1, 2012 and August 30, 2013.

6 CONCLUSION

The Scott and Knott (SK) algorithm is a very useful methodology in the practice of statistical analysis of experiments involving analysis of variance. It has been widely used by researchers who wish to compare the group means of treatments, since it divides groups without any overlapping, a feature that makes the algorithm very useful. The R package ScottKnott provides an easy-to-use framework for performing the SK algorithm. In comparison with other software or Rpackages, this one is unique unto itself, since it allows for easily interpreting of graphics results, what greatly facilitates the interpretation of analyses. As explained in the article, it also makes possible various designs and experiments.

ScottKnot is still undergoing active development. Planned extensions include extension of the method to factorial up to fifth order, methods using poisson distribution, dendrogram graphic option with p-values obtained for each group, and an alternative method of the Scott-Knott test proposed by [1].

RESUMO. O Scott-Knott é um algoritmo de agrupamento hierárquico utilizado na aplicação da ANOVA, quando o pesquisador está comparando as médias dos tratamentos, com uma característica muito importante: ele não apresenta qualquer sobreposição em seus resultados de agrupamento. Nós escrevemos um código em R, que executa este algoritmo a partir de objetos das classes `vectors`, `matrix`, `data.frame`, `aov` ou `aov.list`. Os resultados são apresentados com letras que representam os grupos, bem como por meio de

gráficos usando cores diferentes para diferenciar os grupos distintos. Este pacote do R, nomeado *ScottKnott* é o principal tema deste artigo.

Palavras-chave: Scott-Knott, comparações múltiplas, R core team.

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