

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

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Abstract The test of Scott-Knott is a clustering algorithm used as one of the alternatives where multiple comparison procedures are applied, in the ANOVA context, with a very important characteristic: it does not present any treatment overlapping in its grouping results. We wrote a code, in R, that performs this algorithm starting from `vectors`, `data.frame` or `aov` objects. The results are presented in the usual way as well as in graphical way using different colors to differentiate among the distinct groups.

Introduction

A common problem in ANOVA is the experiment designed to compare treatments. In the situation where it leads to a significant *F*-test for the difference among treatment means, there is the problem of isolating those treatments that do not appear to be different.

All multiple comparison procedures proposed to solve that problem (*t*-test, Tukey, Duncan, Newman-Keuls procedures), usually divide the set of treatment means in groups which are not completely distinct, many treatments end up belonging to different groups simultaneously, this is called overlapping (Calinski and Corsten, 1985).

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

The possibility of using cluster analysis in place of multiple comparison procedures was suggested by O'Neill and Wetherill (1971) since the results of cluster analysis type of solution would divide the treatments into distinct groups.

The Scott and Knott (SK) algorithm is a hierarchical cluster analysis approach used to partition the treatments into distinct groups. Many other hierarchical cluster analysis approaches have been proposed since Scott, A.J. and Knott, M. (Scott and Knott, 1974) published their results, as for example Jolliffe (1975), Cox and Spjøtvoll (1982), and Calinski and Corsten (1985). However, the SK approach has been the most widely used due to the simple intu-

itive appeal of its idea, and also the good results it always gives (Gates and Bilbro, 1978; Bony et al., 2001; Dilson et al., 2002; Jyotsna et al., 2003).

The SK procedure uses a clever algorithm of cluster analysis, where, starting from the whole group of observed mean effects, it divides, and keep dividing the sub-groups in such a way that the intersection of any two groups formed in that manner is empty. Using A. J. Scott and M. Knott own words: "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" (Scott and Knott, 1974).

Simulation studies show that the performance of the SK procedure, compared to the multiple comparison procedures cited above, is very good, and in many cases even superior to them.

It should be noted that in spite of Hierarchical Cluster Analysis and Multiple Comparison being different type of statistical procedures, the SK is used by experimenters either one or the other way.

This paper illustrates the use of the **ScottKnott** R package, which implements the SK procedure (Scott and Knott, 1974). The package is available on the Comprehensive R Archive Network (CRAN) website at <http://CRAN.R-project.org/package=ScottKnott>.

The R Package **ScottKnott** is composed of two methods, `SK` and `SK.nest`. The method `SK` performs the algorithm on treatments of main factors and `SK.nest` does the same on nested designs of factorial, split-plot and split-split-plot experiments. They return objects of class `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, where the groups are indicated by their colors.

The SK clustering algorithm

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 a problem finding out how many homogeneous groups there are and which are the treatment means contained in each group.

It should be noted that we follow (Calinski and Corsten, 1985) 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 nonrejection of equality. Nor it should 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 which attempts to find out those groups without overlapping.

Let k be the number of treatments. As it starts, the SK procedure will either find two distinct groups dividing the treatment means or will declare those k treatment means a homogeneous belonging to just one group. To do so it should look at the $2^{k-1} - 1$ possible partitions of the k means into two nonempty groups, but it is enough to look at the $k - 1$ partitions formed by ordering the treatment means and dividing them between two successive ones (Scott and Knott, 1974). 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 (Ramalho et al., 2000).

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_0 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 separated and stop until all the groups formed up to then are homogeneous.

The statistics used for the likelihood ratio test is:

$$\lambda = \frac{\pi}{2(\pi - 2)} \times \frac{B_0}{\sigma_o^2}$$

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 $\frac{\sigma^2}{r}$, v be degrees of freedom associated with that estimator, then

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

λ is asymptotically a χ^2 distributed random variable with $v_o = \frac{k}{\pi-2}$ 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 chosen type I error (α value) 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, while if α is too large, the process will go too far and split homogeneous sets of means" (Scott and Knott, 1974).

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 group formed in this way is either homogeneous or just contains one observed mean.

It is important to emphasize the fact that the α value defined above is not the nominal error rate of the type I error of the algorithm as a whole. If we set the α value to be 5% then every test the SK procedure performs to divide or not a sub-group has a type I error rate of 5% but 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.

In performance studies among statistical tests is often very difficult to obtain analytically their rate of type I error and power. The most usual way to get that information is through simulation using Monte Carlo methods. Boardman and Moffit (1971) show that the difference between analytical values and Monte Carlo's is very small therefore making its use an optimal way to get the necessary information. Their results are similar to those found by Bernhardson (1975).

In spite of the SK being 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.

Comparative performance of SK method

It is very difficult to compare the type I error rates (Carmer and Swanson, 1971) in multiple comparisons procedures. Two of the most common measures 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* (Carmer and Swanson, 1971; Steel and Torrie, 1980).

Two simulation studies (Boardman and Moffit, 1971; Bernhardtson, 1975) conducted at the Universidade Federal de Lavras, Brazil, used Monte Carlo methods to evaluate the performance of the SK method. One Da Silva et al. (1999) has shown that it possesses high power and error rate almost always in accordance with the nominal levels using both comparisonwise and experimentwise error rates. That is, the rates are not far from α value cited above. The other, Borges and Ferreira (2003) 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. 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 1%, 10%, 20% and 30%.

The ScottKnott package

The package **ScottKnott** was written in R language (R Development Core Team, 2010). It's results are objects of the class `list`, `SK` and `SK.nest`, which are used as input to the generic functions `summary` and `plot`.

The ScottKnott package performs the clustering algorithm on three designs and three experiments. It must be emphasized again that the two functions `SK` and `SK.nest` **work only 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 package ScottKnott has two main functions, `SK` and `SK.nest`. The function `SK` is used for clustering treatment means of a main factor. The function `SK.nest` is used for clustering treatment means of interaction 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. The function `SK.nest` supports at most two nestings as shown above.

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

The main algorithm is the function `MaxValue` which builds groups of means according to the

method of SK. Basically it is an algorithm for 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 form a group of means. At the end all the leaves of the tree are the groups of homogeneous means.

The functions `SK` and `SK.nest` are methods for objects of class `vector`, `matrix` or `data.frame` joined as default, and `aov` and `aovlist` 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 necessary to inform this parameter only if `x` represent 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. Used only in case 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.
- `fl2`: A vector of length 1 giving the level of the second factor in nesting order tested.
- `fl3`: A vector of length 1 giving the level of the third factor in nesting order tested.
- `id.trim`: The number of characters to trim the label of the factor levels.
- `...`: Further arguments (required by generic).

The function `SK` returns an object of class `SK`, the function `SK.nest` returns an object of class `SK.nest`, respectively, containing the groups of means plus other necessary variables for `summary` and `plot`.

The generic functions `summary` and `plot` are used to obtain and print a summary and a plot of the results.

The method `plot.SK` plots both: `SK` and `SK.nest` objects. The parameters are:

- `x`: A `SK` object.
- `pch`: A vector of plotting symbols or characters.
- `col`: A vector of colors for the means representation.
- `xlab`: A label for the x axis.
- `ylab`: A label for the y axis.
- `xlim`: The x limits of the plot.
- `ylim`: The y limits of the plot.

- `id.lab`: Factor level names at x-axis if the user wants them changed, otherwise it will appear as specified at the original data.
- `id.las`: Factor level names written either horizontally or vertically.
- `rl`: Horizontal line connecting the circle to the y-axis.
- `rl.lty`: Line type of `rl`.
- `rl.col`: Line color of `rl`.
- `mm`: Vertical line through the circle (mean value) linking the minimum to the maximum of the factor level values corresponding to that mean value.
- `mm.lty`: Line type of `mm`.
- `title`: A title for the plot.
- `...`: Optional plotting parameters.

All data used in the examples are in data set of the **ScottKnott** package.

Using ScottKnott package

The following are some examples on how to use the **ScottKnott** package. All the following examples show how to run the `SK` (`SK.nest`) function from an `aov` object.

Completely Randomized Design (CRD)

`CRD2` is the object containing the data set of completely randomized design. It can be called using the command below:

```
> library(ScottKnott)
> data(CRD2)
```

It is a simulated data to model a CRD of 45 levels (treatments) and 4 repetitions.

```
> sk0 <- with(CRD2, SK(x = x, y = y,
+   model = "y ~ x", which = "x",
+   id.trim = 5))
> plot(sk0, id.las = 2, rl = FALSE,
+   title = "")
```

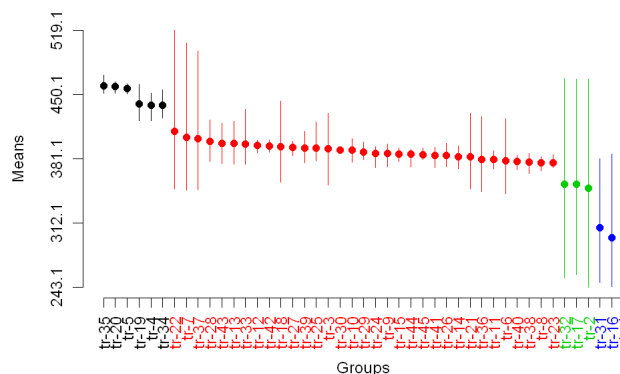


Figure 1: Completely Randomized Design (CRD), $\alpha = 5\%$.

Randomized Completely Block Design (RCBD)

RCBD is the object containing the data set of randomized completely block design. It can be called using the command below:

```
> data(RCBD)
```

It is a simulated data to model a RCBD of 5 factor levels and 4 blocks.

```
> av1 <- with(RCBD, aov(y ~ blk + tra,
+   data = dfm))
> skl <- SK(x = av1, which = "blk")
> summary(skl)
```

Levels	Means	SK(5%)
1	145.496	a
2	143.916	a
3	143.264	a
4	139.994	a

```
> plot(skl, pch = 15, id.lab = paste("Block",
+   1:length(skl$groups), sep = "_"),
+   rl = FALSE, title = "")
```

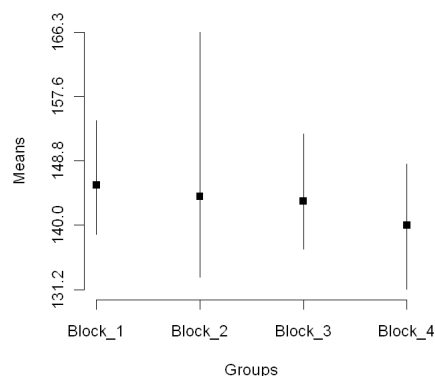


Figure 2: Randomized Completely Block Design (RCBD). Main factor is block, $\alpha = 5\%$.

```
> sk2 <- SK(x = av1, which = "tra",
+   sig.level = 0.1)
> summary(sk2)
```

Levels	Means	SK(10%)
E	155.3700	a
A	142.9325	b
D	140.3950	b
B	138.5750	b
C	138.5650	b

```
> plot(sk2, xlab = "", rl = FALSE, title = "")
```

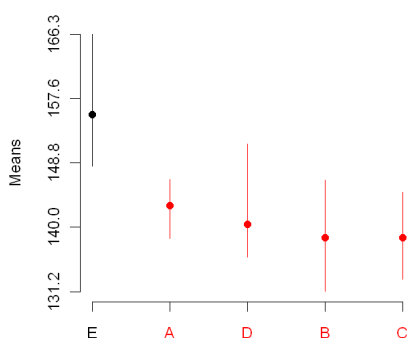


Figure 3: Randomized Completely Block Design (RCBD). Main factor is treatment, $\alpha = 10\%$.

Factorial Experiment (FE)

FE is the object containing the data set of a factorial experiment. It can be called using the command below:

```
> data(FE)
```

It is a simulated data set to model a FE with 3 factors, 2 levels per factor and 4 blocks.

```
> nav1 <- with(FE, aov(y ~ blk + N *
+   P * K, data = dfm))
```

Main factors

```
> nsk1 <- SK(nav1, which = "N")
> summary(nsk1)
```

Levels	Means	SK(5%)
n1	2.750000	a
n0	2.306875	b

```
> plot(nsk1, rl = FALSE, title = "")
```

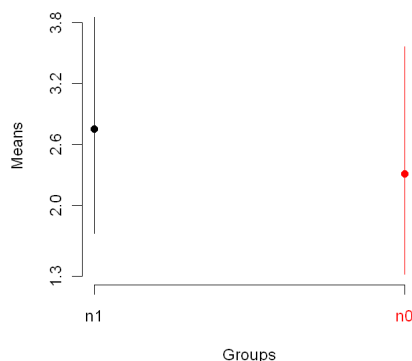


Figure 4: Factorial Experiment (FE). Main factor is N, $\alpha = 5\%$.

Nested factors

When comparison among means of a factor nested in another one, the function `SK.nest` must be used. In this case the two parameters fl_2 (factor level 2) and fl_3 (factor level 3) take values depending on which level we choose to study. Figure 5 shows that the factor P is nested in factor K, and it is desired to compare the means of P when $K = 2$ ($fl_2 = 2$). In that case K is factor 2. By default, whenever the number of nestings is just one, $fl_3 = 0$.

```
> nsk2 <- SK.nest(nav1, which = "P:K",
+   fl2 = 2)
> summary(nsk2)
```

```
Nested: P/K
Levels Means SK(5%)
P_1/K_2 2.83375 a
P_2/K_2 2.62125 a
```

```
> plot(nsk2, rl = FALSE, title = "")
```

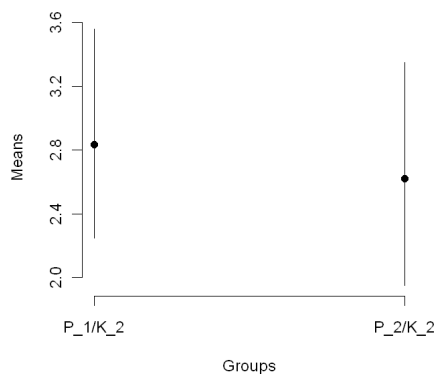


Figure 5: Factorial Experiment (FE). Factor P is nested into level 2 of factor K, $\alpha = 5\%$.

Figure 6 shows factor N nested in factor P which is nested in factor K, and it is desired to compare the

means of N when $P = 1$ ($fl_2 = 1$) and $K = 2$ ($fl_3 = 2$). In that case P is factor 2 (fl_2) and K is factor 3 (fl_3).

```
> nsk3 <- SK.nest(nav1, which = "N:P:K",
+   fl2 = 1, fl3 = 2)
> plot(nsk3, rl = FALSE, title = "")
```

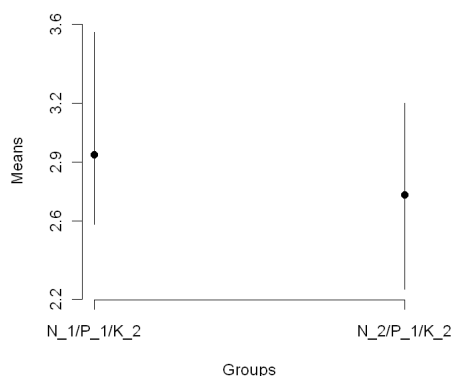


Figure 6: Factorial Experiment (FE). Nesting factor N into level 1 of factor P which is nested into level 2 of factor K , $\alpha = 5\%$.

Changing the nesting order of factors, the following is the way to do it:

```
> nav2 <- with(FE, aov(y ~ blk + K *
+   N * P, data = dfm))
> nsk4 <- SK.nest(nav2, which = "K:N:P",
+   fl2 = 1, fl3 = 1)
> summary(nsk4)
```

```
Nested: K/N/P
Levels Means SK(5%)
K_2/N_1/P_1 2.9375 a
K_1/N_1/P_1 1.8850 b
```

```
> plot(nsk4, rl = FALSE, title = "")
```

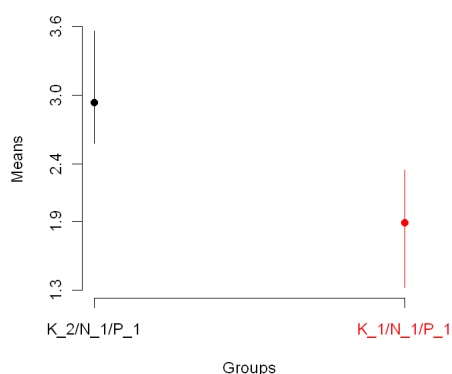


Figure 7: Factorial Experiment (FE). Nesting factor K into level 1 of factor N which is nested into level 1 of factor P , $\alpha = 5\%$.

Split-Split-Plot Experiment (SSPE)

SSPE is the object containing the data set of a Split-Split-Plot Experiment (SSPE). It can be called using the command below:

```
> data(SSPE)
```

It is a simulated data to model a SSPE with 3 plots, each one split 3 times, each split, split again 5 times and 4 repetitions per split-split.

From aovlist object:

```
> nav3 <- with(SSPE, aov(y ~ blk + ssp *
+   sp * p + Error(blk/p/sp), data = dfm))
```

Nested, sp/p=2

The factor sp is nested in factor p .

```
> nsk5 <- SK.nest(nav3, which = "sp:p",
+   error = "blk:p:sp", fl2 = 2)
> plot(nsk5, rl = FALSE, title = "")
```

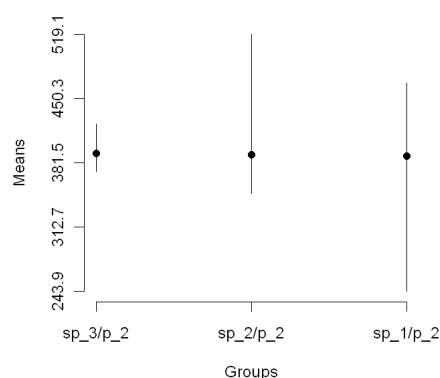


Figure 8: Split-Split-Plot Experiment (SSPE), nested analysis ($sp/p=2$), $\alpha = 5\%$.

Nested, ssp/sp=1/p=1

The factor ssp is nested in factor sp which is nested in factor p . The value 1 of the parameter fl_2 and 1 of parameter fl_3 mean that the first level of factor p and factor 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.

```
> nsk6 <- SK.nest(nav3, which = "ssp:sp:p",
+   error = "Within", fl2 = 1, fl3 = 1)
> summary(nsk6)
```

```
Nested: ssp/sp/p
Levels Means SK(5%)
ssp_5/sp_1/p_1 456.3500 a
ssp_4/sp_1/p_1 438.9850 a
ssp_3/sp_1/p_1 392.0725 a
ssp_2/sp_1/p_1 349.3500 b
ssp_1/sp_1/p_1 294.6800 b
```

```
> plot(nsk6, rl.col = c(rep("black",
+ 3), rep("red", 2)), title = "")
```

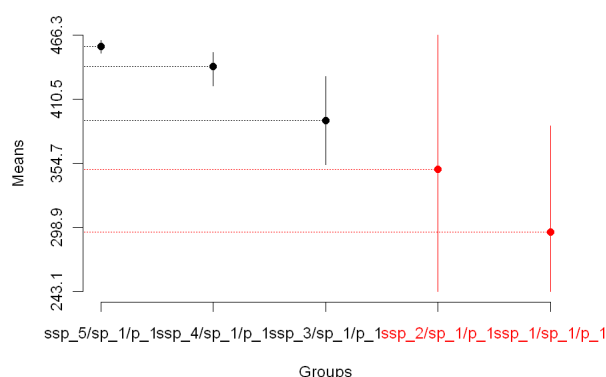


Figure 9: Split-Split-Plot Experiment (SSPE). Nested analysis ($ssp/sp=1/p=1$), $\alpha = 5\%$.

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

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