Mathematical details of the test statistics used by `kanova`

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1 Introduction

This note presents in detail the formulae for the test statistics used by the `kanova()` function from the `kanova` package. These statistics are based on, and generalise, the ideas discussed in Diggle et al. (2000) and in Hahn (2012). They consist of sums of integrals (over the argument r of the K-function) of the usual sort of analysis of variance "regression" sums of squares, down-weighted over r by the estimated variance of the quantities being squared. The limits of integration r_0 and r_1 *could* be specified in the software (e.g. in the related `spatstat` function `studpermu.test()` they can be specified in the argument `rinterval`). However there is currently no provision for this in `kanova()`, and r_0 and r_1 are taken to be the min and max of the r component of the `"fv"` object returned by `Kest()`. Usually r_0 is 0 and r_1 is 1/4 of the length of the shorter side of the bounding box of the observation window in question.
There are test statistics for:

- one-way analysis of variance (one grouping factor),
- main effects in a two-way (two grouping factors) additive model, and
- a model with interaction versus an additive model in a two-way context.

In respect of the second item, both the statistic for "testing for A allowing for B" and "testing for B allowing for A" are presented (for the sake of completeness) although the two statistics in fact amount to the same thing.

Under the null hypothesis of "no group effect(s)" the *underlying* variance function $\sigma^2(r)$ of the K-function estimates is the same in each cell of the model. However the variance of the individual K-function estimates changes from pattern to pattern, being inversely proportional to the number of points in the pattern. Explicitly, let $\hat{K}_{ij}(r)$ $(i = 1, \ldots, g,\ j = 1, \ldots, n_i)$ be the estimated K-function based on pattern X_{ij} in the one grouping factor setting, and $\hat{K}_{ijk}(r)$ $(i = 1, \ldots, a,\ j = 1, \ldots, b,\ k = 1, \ldots, n_{ij})$ be the estimated K-function based on pattern X_{ijk} in the two grouping factor setting. The variances of these quantities are

$$\mathrm{Var}(\hat{K}_{ij}(r)) = \frac{\sigma^2(r)}{w_{ij}} \text{ (one grouping factor)}$$
$$\mathrm{Var}(\hat{K}_{ijk}(r)) = \frac{\sigma^2(r)}{w_{ijk}} \text{ (two grouping factors)}$$

where w_{ij} and w_{ijk} denote the number of points in pattern X_{ij} or pattern X_{ijk} respectively.

2 One-way ANOVA; single grouping factor

In this setting the estimated K function corresponding to the ith group is

$$\hat{K}_i(r) = \sum_{j=1}^{n_i} \frac{w_{ij}}{w_{i\bullet}} \hat{K}_{ij}(r)$$

$i = 1, \ldots, g$, and the overall estimate of the K-function (common to all groups under the null hypothesis) is

$$\hat{K}(r) = \sum_{i=1}^{g} \sum_{j=1}^{n_i} \frac{w_{ij}}{w_{\bullet\bullet}} \hat{K}_{ij}(r) = \sum_{i=1}^{g} \frac{w_{i\bullet}}{w_{\bullet\bullet}} \hat{K}_i(r)$$

The test statistic is the integral over r of the Studentized regression sum of squares

$$T = \sum_{i=1}^{g} n_i \int_{r_0}^{r_1} (\hat{K}_i(r) - \hat{K}(r))^2 / V_i(r)\, dr$$

where $V_i(r)$ is the (sample) variance of $\hat{K}_i(r) - \hat{K}(r)$. This variance is given by

$$V_i(r) = s^2(r) \left(\frac{1}{w_{i\bullet}} - \frac{1}{w_{\bullet\bullet}} \right)$$

where $s^2(r)$ is the overall sample variance (an unbiased estimate of σ^2). This quantity is given by

$$s^2(r) = \frac{1}{n_{\bullet} - 1} \sum_{i=1}^{g} \sum_{j=1}^{n_i} w_{ij} \left(\hat{K}_{ij}(r) - \hat{K}(r) \right)^2 \ . \tag{1}$$

3 Two-way ANOVA; testing for main effects in an additive model

In this section we are concerned with testing for a main effect in an additive model, *allowing* for the possibility of there being a second main effect. The test statistics used are in effect the same as the test statistic in section 2. The test statistics are based on the "regression sum of squares", which is the same in a test for a main effect in a two-way ANOVA as it is in a one-way ANOVA. In "ordinary" analysis of variance, the possibility of there being a second main effect is allowed for by adjusting the error sum of squares (making sure that the "error" effect is not augmented by that second main effect).

In the current context, the error sum of squares is not used. The test that is used is based on random permutations (of the data or of the model residuals). Allowing for the possibility of a second main effect is accomplished in different ways depending on whether the permutations are of the data or of residuals from the model. In the former case, the second main effect is allowed for by permuting the data "within" the levels of this second main effect. See Appendix II for further discussion of this idea. In the latter case the residuals are taken to those from the appropriate additive two factor model.

In neither case has the mathematical form of test statistic any real relevance. However the test statistics differ in their superficial appearance from the statistic used in section 2, due to the double indexing of the groups. Consequently the mathematical form of the test statistics are presented in what follows, for the sake of completeness

We denote the two grouping factors (main effects) by A and B. The estimated K functions $\hat{K}_{ijk}(r)$ are assumed (under the null hypothesis) to have variance $\sigma^2(r)/w_{ijk}$ where w_{ijk} is the number of points in pattern X_{ijk}.

3.1 Testing for the first main effect, allowing for the second

We denote the estimated K function corresponding to level i of factor A by $\hat{K}_{i\bullet}$. This function is given by

$$\hat{K}_{i\bullet} = \sum_{j=1}^{b} \sum_{k=1}^{n_{ij}} \frac{w_{ijk}}{w_{i\bullet\bullet}} \hat{K}_{ijk}(r) \ .$$

Here the test statistic is

$$T_A = \sum_{i=1}^{a} n_{i\bullet} \int_{r_0}^{r_1} (\hat{K}_{i\bullet}(r) - \hat{K}(r))^2 / V_{Ai}(r) \, dr$$

where $V_{Ai}(r)$ is the (sample) variance of $\hat{K}_{i\bullet}(r) - \hat{K}(r)$. The function $V_{Ai}(r)$ is given by

$$V_{Ai}(r) = s^2(r) \left(\frac{1}{w_{i\bullet\bullet}} - \frac{1}{w_{\bullet\bullet\bullet}} \right)$$

where $s^2(r)$ is the overall sample variance (an unbiased estimate of σ^2). This quantity is given by

$$s^2(r) = \frac{1}{n_{\bullet\bullet} - 1} \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{n_{ij}} w_{ijk} \left(\hat{K}_{ijk}(r) - \hat{K}(r) \right)^2 \tag{2}$$

(effectively the same as (1)).

3.2 Testing for the second main effect allowing for the first

As pointed out in the introduction, this scenario is really the same as that dealt with in Section 3.1. Here we denote the estimated K function corresponding to level j of factor B by $\hat{K}_{\bullet j}$. This function is given by

$$\hat{K}_{\bullet j} = \sum_{i=1}^{a} \sum_{k=1}^{n_{ij}} \frac{w_{ijk}}{w_{\bullet j \bullet}} \hat{K}_{ijk}(r)$$

and the test statistic is

$$T_B = \sum_{j=1}^{b} n_{\bullet j} \int_{r_0}^{r_1} (\hat{K}_{\bullet j}(r) - \hat{K}(r))^2 / V_{Bj}(r) \, dr$$

where $V_{Bj}(r)$ is the (sample) variance of $\hat{K}_{\bullet j}(r) - \hat{K}(r)$. The function $V_{Bj}(r)$ is given by

$$V_{Bj}(r) = s^2(r) \left(\frac{1}{w_{\bullet j \bullet}} - \frac{1}{w_{\bullet\bullet\bullet}} \right)$$

4 Two-way ANOVA; testing for interaction

Here the test statistic is

$$T_{AB} = \sum_{i=1}^{a} \sum_{j=1}^{b} n_{ij} \int_{r_0}^{r_1} (\hat{K}_{ij}(r) - \hat{K}_{i\bullet}(r) - \hat{K}_{j\bullet}(r) + \hat{K}(r))^2 / V_{ABij}(r)\, dr$$

where $V_{ABij}(r)$ is the (sample) variance of $\hat{K}_{ij}(r) - \hat{K}_{i\bullet}(r) - \hat{K}_{j\bullet}(r) + \hat{K}(r)$. The function $V_{ABij}(r)$ is given by

$$V_{ABij}(r) = s^2(r) \left(\frac{1}{w_{ij\bullet}} - \frac{1}{w_{i\bullet\bullet}} + \frac{2w_{ij\bullet}}{w_{i\bullet\bullet} w_{\bullet j \bullet}} - \frac{1}{w_{\bullet j \bullet}} - \frac{1}{w_{\bullet\bullet\bullet}} \right)$$

where, as before, $s^2(r)$ is the overall sample variance (an unbiased estimate of σ^2) given by (2).

References

Peter J. Diggle, Jorge Mateu, and Helen E. Clough. A comparison between parametric and non-parametric approaches to the analysis of replicated spatial point patterns. *Advances in Applied Probability*, 32:331 – 343, 2000.

Ute Hahn. A studentized permutation test for the comparison of spatial point patterns. *Journal of the American Statistical Association*, 107(498): 754 – 764, 2012. DOI: 10.1080/01621459.2012.688463.

Appendix I

Here are some (terse) details about the variance of $\hat{K}_{ij}(r) - \hat{K}_{i\bullet}(r) - \hat{K}_{j\bullet}(r) + \hat{K}(r)$.

$$
\begin{aligned}
\mathrm{Var}(\hat{K}_{ij}(r)) &= \sigma^2/w_{ij\bullet} \\
\mathrm{Var}(\hat{K}_{i\bullet}(r)) &= \sigma^2/w_{i\bullet\bullet} \\
\mathrm{Var}(\hat{K}_{j\bullet}(r) &= \sigma^2/w_{\bullet j\bullet} \\
\mathrm{Var}(\hat{K}(r)) &= \sigma^2/w_{\bullet\bullet\bullet} \\
\mathrm{Cov}(\hat{K}_{ij}(r), \hat{K}_{i\bullet}) &= \sigma^2/w_{i\bullet\bullet} \\
\mathrm{Cov}(\hat{K}_{ij}(r), \hat{K}_{\bullet j}) &= \sigma^2/w_{\bullet j\bullet} \\
\mathrm{Cov}(\hat{K}_{ij}(r), \hat{K}) &= \sigma^2/w_{\bullet\bullet\bullet} \\
\mathrm{Cov}(\hat{K}_{i\bullet}(r), \hat{K}_{\bullet j}) &= w_{ij\bullet}\sigma^2/w_{i\bullet\bullet}w_{\bullet j\bullet} \\
\mathrm{Cov}(\hat{K}_{i\bullet}(r), \hat{K}) &= \sigma^2/w_{\bullet\bullet\bullet} \\
\mathrm{Cov}(\hat{K}_{\bullet j}(r), \hat{K}) &= \sigma^2/w_{\bullet\bullet\bullet}
\end{aligned}
$$

Sample calculation: to see that $\mathrm{Cov}(\hat{K}_{ij}(r), \hat{K}_{i\bullet}) = \sigma^2/w_{i\bullet\bullet}$, note that the two expressions are weighted sums (with weights $w_{ijk}/wij\bullet$ and $w_{ijk}/w_{i\bullet\bullet}$ respectively) of estimated K functions $\hat{K}_{ijk}(r)$. Since these estimates are independent, the covariances are 0 except where the indices of the terms coincide, in which case the covariance is the product of the weights and the variance of the term. We get

$$
\begin{aligned}
\sum_{k=1}^{n_{ij}} \frac{w_{ijk}}{w_{ij\bullet}} \frac{w_{ijk}}{w_{i\bullet\bullet}} \frac{\sigma^2}{w_{ijk}} &= \frac{\sigma^2}{w_{ij\bullet}w_{i\bullet\bullet}} \sum_{k=1}^{n_{ij}} w_{ijk} \\
&= \frac{\sigma^2}{w_{ij\bullet}w_{i\bullet\bullet}} w_{ij\bullet} \\
&= \frac{\sigma^2}{w_{i\bullet\bullet}}
\end{aligned}
$$

The variance term of interest is $\text{Var}(\hat{K}_{ij}(r) - \hat{K}_{i\bullet}(r) - \hat{K}_{j\bullet}(r) + \hat{K}(r))$ which is equal to

$$\begin{aligned}
&\text{Var}(\hat{K}_{ij}(r)) + \text{Var}(\hat{K}_{i\bullet}(r)) + \text{Var}(\hat{K}_{j\bullet}(r) + \text{Var}(\hat{K}(r)) \\
&- 2\text{Cov}(\hat{K}_{ij}(r), \hat{K}_{i\bullet}) - 2\text{Cov}(\hat{K}_{ij}(r), \hat{K}_{\bullet j}) + 2\text{Cov}(\hat{K}_{ij}(r), \hat{K}) \\
&+ 2\text{Cov}(\hat{K}_{i\bullet}(r), \hat{K}_{\bullet j}) - 2\text{Cov}(\hat{K}_{i\bullet}(r), \hat{K}) \\
&- 2\text{Cov}(\hat{K}_{\bullet j}(r), \hat{K})\ .
\end{aligned} \tag{3}$$

Using the previously stateed expressions for the variances and covariances of the component terms, we see that (3) is equal to

$$\sigma^2 \left(\frac{1}{w_{ij\bullet}} + \frac{1}{w_{i\bullet\bullet}} + \frac{1}{w_{\bullet j\bullet}} + \frac{1}{w_{\bullet\bullet\bullet}} - \frac{2}{w_{i\bullet\bullet}} - \frac{2}{w_{\bullet j\bullet}} + \frac{2}{w_{\bullet\bullet\bullet}} + \frac{2w_{ij\bullet}}{w_{i\bullet\bullet}w_{\bullet j\bullet}} - \frac{2}{w_{\bullet\bullet\bullet}} - \frac{2}{w_{\bullet\bullet\bullet}} \right)$$

which is finally equal to

$$\sigma^2 \left(\frac{1}{w_{ij\bullet}} - \frac{1}{w_{i\bullet\bullet}} + \frac{2w_{ij\bullet}}{w_{i\bullet\bullet}w_{\bullet j\bullet}} - \frac{1}{w_{\bullet j\bullet}} - \frac{1}{w_{\bullet\bullet\bullet}} \right)$$

Appendix II

As indicated in Section 3, the test that is used by `kanova()` is based on random permutations either of the data or of the model residuals). If the permutations are of the data, then allowing for the possibility of a second main effect must be accomplished by permuting the data in such a way that the second main effect does not mask the first main effect. That is, the data must be permuted within the levels of the second main effect. Here we explain what is meant by this idea.
To illustrate this idea in as clear and simple manner as possible, we consider an artificial example of an additive two-factor *scalar* model with factors A and B, have levels A_1, A_2, A_3 and A_4, and B_1, B_2 and B_3 respectively. Suppose the underlying means corresponding to factor A are 0.2, 0.4, 0.6 and 0.8, and those corresponding to factor B are 0, 5 and 10. Note that the B effect is much"larger" than the A effect and would overwhelm the A effect unless appropriate steps were taken.
In an additive model the "cell means" are:

Table 1:

	B_1	B_2	B_3
A_1	0.2	5.2	10.2
A_2	0.4	5.4	10.4
A_3	0.6	5.6	10.6
A_4	0.8	5.8	10.8

When we test for an A effect in this example, we look at a model with 12 cells, three of which correspond to level A_1, of A, three to level A_2, three to level A_3 and three to level A_4. A pseudo test statistic, i.e. a simplified version of the test statistic used in genuine analyses, has the form (for the observed data)

$$T = (5.2 - 5.5)^2 + (5.4 - 5.5)^2 + (5.6 - 5.5)^2 + (5.8 - 5.5)^2 = 0.2$$

where the 5.2, 5.4, 5.6 and 5.8 terms in the foregoing are the means corresponding to the levels of A, 5.5 is the "grand mean", and where we ignore the "noise" that would appear in any real data.

In conducting a test for an A effect we compare the test statistic from the observed data with test statistics T_i^* formed from permutations of the observed data. Since there *is* an A effect, we would hope that the test would reject the null hypothesis, i.e. that T would be large compared with the bulk of the T_i^*.
This will happen if we permute the data "within the levels of B", i.e. if we permute, separately, each of the columns of Table 1. If we permute the data in this manner, then the T_i^* that are produced are all small relative to T. In fact, in this particular (artificial) example all possible T_i^*, that arise from permuting the data within the levels of B, are less than $T = 0.2$.
However if we simply permute the data as if A were the only factor, and ignore B (i.e. proceed as if we were doing a one-way analysis) then from time to time large values will be grouped together, within a level of factor A, with other large values. This phenomenon results in the creation of means, for one or more levels A_i of factor A, which are very different from the overall mean, resulting in large contributions to the calculated statistic. For instance an arbitrary permutation of the 12 data values might result in

Table 2:

A_1	10.4	10.6	5.8
A_2	0.8	10.8	0.2
A_3	5.6	5.2	0.6
A_4	0.4	5.4	10.2

The value of the pseudo test statistic obtained from the data in Table 2, is

$$(8.9333 - 5.5)^2 + (3.9333 - 5.5)^2 + (3.8000 - 5.5)^2 + (5.3333 - 5.5)^2 = 17.16$$

which is much larger than the pseudo test statistic from the observed data shown in Table 1. Generally, the values of the T_i^* resulting from arbitrary permutations will be large in comparison with T and the null hypothesis will not be rejected as it should be.