Mathematical details of the test statistics used by `kanova`

Rolf Turner

18 July 2024

1 Introduction

This note presents in some 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.

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 $K_{ij}(r)$ ($i = 1, \ldots, g$, $j = 1, \ldots, n_i$) be the (*estimated*) K-function based on pattern X_{ij} in the one-grouping-factor setting, and $K_{ijk}(r)$ ($i = 1, \ldots, a$, $j = 1, \ldots, b$, $k = 1, \ldots, n_{ij}$) be the (*estimated*) K-function based on pattern X_{ijk} in the two-grouping-factor setting. The variances of these quantities are

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

where w_{ij} and w_{ijk} denote (or are proportional to) the number of points in pattern X_{ij} or pattern X_{ijk} respectively.

2 Estimating the variance

Under the null hypothesis of "no group effect(s)" the variance function $\sigma^2(r)$ may be estimated by

$$s^2(r) = \frac{1}{n_{\bullet} - g} \sum_{\ell=1}^{g} \sum_{i=1}^{n_\ell} w_{\ell i} \left(K_{\ell i}(r) - \tilde{K}_{\ell \bullet (r)} \right)^2 \tag{1}$$

where g is the number of groups, n_ℓ is the number of patterns in the ℓth group and $w_{\ell i}$ is (proportional to) the number of points in the ith pattern in the ℓth group. The function $K_{\ell i}(r)$ is the (estimated) K-function estimate corresponding to the ith pattern in the ℓth group, and $\tilde{K}_{\ell \bullet (r)}$ is the "over all" estimate of the K-function for the ℓth group. More detail is given below.
In the one grouping factor setting the number of groups g is the number of levels of the (single) grouping factor In the two grouping factor setting $g = a \times b$ where a is the number of levels of the first grouping factor, and b is the number of levels of the second grouping factor. The quantity $s^2(r)$ is an unbiased estimate of $\sigma^2(r)$. It is related to the error sum of squares that appears in "ordinary" analysis of variance, but the error sum of squares plays no explicit role in the tests used in the current context.
For completeness we now give the explicit expressions for $s^2(r)$ in the single grouping factor (one-way) setting, and in the two grouping factor (two-way)

setting:

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

where n_i is the number of patterns in the ith group (one-way), and

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

where n_{ij} is the number of patterns in the (i, j)th group (two-way). Clearly the foregoing two equations are special cases of (1).

3 Estimates of K-functions

The observed K-function estimate, based on the ith pattern in the ℓth group, is denoted by $K_{\ell i}(r)$. In this setting the estimated K function corresponding to the ℓth group is

$$\tilde{K}_\ell(r) = \sum_{j=1}^{n_\ell} \frac{w_{\ell j}}{w_{\ell\bullet}} K_{\ell j}(r)$$

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

$$\tilde{K}(r) = \sum_{\ell=1}^{g} \sum_{j=1}^{n_\ell} \frac{w_{\ell j}}{w_{\bullet\bullet}} K_{ij}(r) = \sum_{\ell=1}^{g} \frac{w_{\ell\bullet}}{w_{\bullet\bullet}} \tilde{K}_\ell(r) \ .$$

In the two grouping factors setting, it is sometimes necessary to consider the indices i and j explicitly rather than simply considering the index ℓ corresponding to the groups determined by "crossing" the two "main effect" factors. We define:

$$\tilde{K}_{ij}(r) = \frac{1}{w_{ij\bullet}} \sum_{k=1}^{n_{ij}} w_{ijk} K_{ijk} \tag{2}$$

$$\tilde{K}_{i\bullet}(r) = \frac{1}{w_{i\bullet\bullet}} \sum_{j=1,b} \sum_{k=1}^{n_{ij}} w_{ijk} K_{ijk} \tag{3}$$

$$\tilde{K}_{\bullet j}(r) = \frac{1}{w_{\bullet j\bullet}} \sum_{i=1,a} \sum_{k=1}^{n_{ij}} w_{ijk} K_{ijk} \ . \tag{4}$$

In the foregoing, (2) specifies the K-function estimate corresponding to the group with index pair (i, j), (3) specifies the K-function estimate corresponding to the union over j of the groups with index pair (i, j), and (4) specifies the K-function estimate corresponding to the union over i of the groups with index pair (i, j).

4 One-way ANOVA; single grouping factor

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

$$T = \sum_{\ell=1}^{g} n_\ell \int_{r_0}^{r_1} (\tilde{K}_\ell(r) - \tilde{K}(r))^2 / V_\ell(r) \, dr$$

where $V_\ell(r)$ is the (sample) variance of $\tilde{K}_\ell(r) - \tilde{K}(r)$. This variance is given by

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

where $s^2(r)$ is the overall sample variance given by (1).

5 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, in the setting of a two-way additive model, are in effect the same as the test statistics used in section 4. and differ only in their superficial appearance, the difference being due to the double indexing of the groups.

We denote the two grouping factors (main effects) by A and B. The K functions $K_\ell(r)$ are assumed (under the null hypothesis) to have variance equal or proportional to $\sigma^2(r)/w_{\ell j}$ where $w_{\ell j}$ is the number of points in pattern $X_{\ell j}$, the jth pattern in the ℓth group.

In "ordinary" analysis of variance we test for an effect of factor A, allowing for a second factor B, by first calculating the regression sum of squares

$$SSA = \sum_{i=1}^{a} n_i \times (\bar{X}_{i\bullet\bullet} - \bar{X}_{\bullet\bullet\bullet})^2$$

where X_{ijk}, $k = 1, \ldots, n_i$, are the observations in cell (i, j) of the model. Note that in calculating SSA we are in effect ignoring factor B completely and proceeding as if A were the only classification factor. Allowance is made for the B classification factor by means of the way that the *error* sum of squares SSE is calculated. This error sum of squares *does* involve factor B (and the calculations are based on the assumption of an additive model). Testing for the "significance" of factor A involves the comparison of SSA with SSE.

In the context of the analysis of K-function, no error sum of squares is explicitly used. Testing for "significance" of factor A is done by means of permutation tests. If tests are effected by permuting the raw data, then allowance for factor B is made by permuting the data *within* each level of B. I.e. data from different levels of B do not get swapped with each other. If tests are effected by permuting residuals, then allowance for factor B is made by using residuals from the additive model (and *not* from the A-only model. The test statistic, T_A, for testing for A (allowing for B) in the two factor context, is the integral, over r of the Studentized regression sum of squares. It is given by

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

where $V_{Ai}(r)$ is the (sample) variance of $\tilde{K}_{i\bullet}(r) - \tilde{K}(r)$. 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 given by (1).

6 Two-way ANOVA; testing for interaction

Here the test statistic is

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

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

$$V_{ABij}(r) = s^2(r) \left(\frac{1}{w_{ij\bullet}} - \frac{1}{w_{i\bullet\bullet}} + \frac{2w_{ij\bullet}}{w_{i\bullet\bullet} w_{\bullet j\bullet}} - \frac{1}{w_{\bullet j\bullet}} - \frac{1}{w_{\bullet\bullet\bullet}} \right) \tag{5}$$

where, as before, $s^2(r)$ is the overall sample variance given by (1).

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 $\tilde{K}_{ij}(r) - \tilde{K}_{i\bullet}(r) - \tilde{K}_{j\bullet}(r) + \tilde{K}(r)$ as given by (5).

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

Sample calculation: to see that $\mathrm{Cov}(\tilde{K}_{ij}(r), \tilde{K}_{i\bullet}) = \sigma^2/w_{i\bullet\bullet}$, 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 $K_{ijk}(r)$. Since these K functions correspond to independent patterns, they are likewise independent, and so the covariances are 0 except where the indices of the terms coincide. In this 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 $\mathrm{Var}(\tilde{K}_{ij}(r) - \tilde{K}_{i\bullet}(r) - \tilde{K}_{j\bullet}(r) + \tilde{K}(r))$ which is equal to

$$\begin{aligned}
&\mathrm{Var}(\tilde{K}_{ij}(r)) + \mathrm{Var}(\tilde{K}_{i\bullet}(r)) + \mathrm{Var}(\tilde{K}_{\bullet j}(r)) + \mathrm{Var}(\tilde{K}(r)) \\
&- 2\mathrm{Cov}(\tilde{K}_{ij}(r), \tilde{K}_{i\bullet}) - 2\mathrm{Cov}(\tilde{K}_{ij}(r), \tilde{K}_{\bullet j}) + 2\mathrm{Cov}(\tilde{K}_{ij}(r), \tilde{K}) \\
&+ 2\mathrm{Cov}(\tilde{K}_{i\bullet}(r), \tilde{K}_{\bullet j}) - 2\mathrm{Cov}(\tilde{K}_{i\bullet}(r), \tilde{K}) \\
&- 2\mathrm{Cov}(\tilde{K}_{\bullet j}(r), \tilde{K}) \ .
\end{aligned} \tag{6}$$

Using the previously stated expressions for the variances and covariances of the component terms, we see that (6) 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 5, the test that is used by `kanova()` is based on random permutations either of the data or of the residuals from an appropriate model). 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 elaborate a bit on what this means.

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 or equal to $T = 0.2$. 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.