Mathematical details of the test statistics used by kanova

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4th July 2025

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). (See also Diggle et al. (1991).)

The statistics 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.

2 The data

. In the context of a single classification factor A, with a levels, the data consist of K-functions $K_{ij}(r)$, $i=1,\ldots,a,\ k=1,\ldots,n_i$. The function $K_{ij}(r)$ is constructed (estimated) from an observed point pattern X_{ij} . In the context of two classification factors A and B, with a levels and b levels respectively, the data consist of K-functions $K_{ijk}(r)$, $i=1,\ldots,a,$ $j=1,\ldots,b,\ k=1,\ldots,n_{ij}$. The function $K_{ijk}(r)$ is constructed (estimated) from an observed point pattern X_{ijk} .

2.1 Modelling heteroscedasticity

In order to model the variances of the K-functions that appear in the current context, we need to make the following simplifying assumptions about of the nature of these variances:

- 1. with each cell of the model there is associated an underlying variance function denoted by $\sigma_i^2(r)$ $(i=1,\ldots,a)$ in the case of a one way design, and by $\sigma_{ij}^2(r)$ $(i=1,\ldots,a,j=1,\ldots,b)$ in the case of a two way design
- 2. with each observed pattern there is associated a (positive) weight, depending on the number of points in the pattern and denoted by w_{ij} in the case of a one way design and by w_{ijk} in the case of a two way design

In terms of these assumptions, we assume that the variances of the K-functions are given by:

$$\operatorname{Var}(K_{ij})(r) = \sigma_i^2(r)/w_{ij}$$
 for a one way design $\operatorname{Var}(K_{ijk})(r) = \sigma_{ij}^2(r)/w_{ijk}$ for a two way design

This model has no theoretical basis and is justified only by its simplicity and intuitive appeal.

In the single classification context the weight associated with $K_{ij}(r)$ is specified to be $w_{ij} = m_{ij}^{\eta}$ where m_{ij} is the number of points in the pattern X_{ij} . In the context of two classification factors, the weight associated with $K_{ijk}(r)$ is specified to be $w_{ijk} = m_{ijk}^{\eta}$ where m_{ijk} is the number of points in the pattern X_{ijk} . The exponent η is taken to be a constant, to be specified by the user of the kanova package. In the code η is denoted by expo.

2.2 Homoscedasticity is better

After the package was completed, simulation experiments revealed that expressing the variances in terms of the proposed weights appears to be counterproductive. The power of the tests in questions seems to be maximised when all the weights are 1, i.e. when η (expo) is 0. More importantly, the null distribution of the p-values of the tests appears to deviate from the theoretical ideal, i.e. the U[0,1] distribution, unless the value of expo is 0. Hence the tests appear to be valid only if expo = 0. (More detail will be available in Diggle and Turner (2025).)

The code of the package was designed so as to do all of the relevant calculations in terms of the aforementioned weights. To keep life simple (and to allow for the remote possibility that in some circumstances the use of weights might be called for) the code (and the forthcoming exposition in this vignette) have been left expressed in terms of weights. However the default value of expo has been set equal to 0. Hence, unless the user explicitly changes the value of expo from its default, all of the computations will actually be carried out in an un-weighted manner. I.e. the data will be treated as being homoscedastic.

3 Some details about the weighted means of the observations

The test statistics used are (in general) calculated in terms of various weighted means of the observed K-functions. Explicitly we define:

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

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

$$= \frac{1}{w_{\bullet}} \sum_{i=1}^{a} w_{i\bullet} \tilde{K}_{i\bullet}(r)$$

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

$$\tilde{K}_{i..}(r) = \sum_{j=1}^{b} \frac{w_{ij.}}{w_{i..}} \tilde{K}_{ij.}(r)$$

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

$$\tilde{K}_{.j.}(r) = \sum_{i=1}^{a} \frac{w_{ij.}}{w_{.j.}} \tilde{K}_{ij.}(r)$$

$$= \frac{1}{w_{.j.}} \sum_{i=1}^{a} \sum_{k=1}^{n_{ij}} w_{ijk} K_{ijk}(r) \text{ and}$$

$$\tilde{K}_{...}(r) = \sum_{i=i}^{a} \frac{w_{i..}}{w_{...}} \tilde{K}_{i..}(r)$$

$$= \sum_{j=1}^{b} \frac{w_{.j.}}{w_{...}} \tilde{K}_{.j.}(r)$$

$$= \sum_{i=1}^{a} \sum_{j=1}^{b} \frac{w_{ij.}}{w_{...}} \tilde{K}_{ij.}(r)$$

$$= \sum_{i=1}^{a} \sum_{j=1}^{b} \sum_{k=1}^{n_{ij}} \frac{w_{ijk}}{w_{...}} K_{ijk}(r)$$

4 Estimating the variance functions

The variances of the K-functions are assumed to be proportional to functions which are constant over indices within each cell of the model. In the context of a single classification factor, the variance of $K_{ij}(r)$ is taken to be $\sigma_i^2(r)/w_{ij}$. Under the null hypothesis of "no A effect", it is assumed that the functions $\sigma_i^2(r)$ are all equal to a single function, $\tilde{\sigma}^2(r)$. I.e. they do not vary with i. This function is estimated by

$$s^{2}(r) = \frac{1}{n_{\bullet} - a} \sum_{i=1}^{a} \sum_{j=1}^{n_{i}} w_{ij} (K_{ij}(r) - \tilde{K}_{i\bullet}(r))^{2}.$$

Under the null hypothesisi, this is an unbiased estimate of $\tilde{\sigma}^2(r)$. In the context of two classification factors, the variance of $K_{ijk}(r)$ is taken to be $\sigma_{ij}^2(r)/w_{ijk}$. If we are testing for an A effect, allowing for a B effect, it is assumed that, under the null hypothesis, the functions $\sigma_{ij}^2(r)$ do not vary with i, and for each j are all equal to a single function $\tilde{\sigma}_j^2(r)$ (depending only on the B effect). These $\tilde{\sigma}_j^2(r)$) are estimated by

$$s_j^2(r) = \frac{1}{n_{\bullet j}} \sum_{i=1}^a \sum_{k=1}^{n_{ij}} w_{ijk} (K_{ijk}(r) - \tilde{K}_{ij\bullet}(r))^2 .$$

Under the null hypothesis these are unbiased estimates of the $\tilde{\sigma}_j^2(r)$. In the context of two classification factors, where we are testing for interaction against an additive model (unlikely to arise as these circumstances may be) we need estimates of $\sigma_{ij}^2(r)$. These are given by

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

These are unbiased estimates of the $\sigma_{ij}^2(r)$.

5 The test statistics

The test statistics are (numerical) integrals of certain sums of squares, possibly divided by "normalisation" or "homogenisation" coefficients. The "normalisation" is analogous to the studentisation procedure used by Hahn (2012).

5.1 Single classification factor

In the setting of a single classification factor A, the statistic for testing for an A effect is

$$T = \sum_{i=1}^{a} n_i \int_{r_0}^{r_1} (\tilde{K}_i(r) - \tilde{K}(r))^2 / \mathcal{N}_i(r) dr$$

where $\mathcal{N}_i(r)$ is the normalisation coefficient. If the divByVar argument of kanova() is TRUE, then $\mathcal{N}_i(r)$ is equal to the estimated variance of $\tilde{K}_i(r) - \tilde{K}(r)$ which is given by

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

If divByVar is FALSE then $\mathcal{N}_i(r)$ is taken to be identically equal to 1.

5.2 Two classification factors, testing for A "allowing for B"

In the setting of two classification factors A and B, the statistic for testing for an A effect allowing for a B effect is

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

where $\mathcal{N}_i(r)$ is the normalisation coefficient. If divByVar is TRUE, then $\mathcal{N}_i(r)$ is equal to the estimated variance of $\tilde{K}_{i\bullet}(r) - \tilde{K}(r)$ which is given by

$$\tilde{s}_{i}^{2}(r)\left(\frac{1}{w_{i..}}-\frac{2}{w_{...}}\right)+\frac{1}{w_{...}}\sum_{\ell=1}^{a}\frac{w_{i..}}{w_{...}}\tilde{s}_{\ell}^{2}(r)$$
.

The foregoing expression may be re-written, more compactly, and in a form which makes it more obvious that the quantity is positive, as:

$$\mathcal{N}_i(r) = \frac{1}{w_{\cdot \cdot \cdot}} \left[\sum_{\ell=1}^a \zeta_{i\ell} \times \tilde{s}_{\ell}^2(r) \right]$$

where

$$\tilde{s}_{\ell}^{2}(r) = \sum_{j=1}^{b} \frac{w_{\ell j \bullet}}{w_{\ell \bullet}} s_{j}^{2}(r), \ \ell = 1, \dots, a,$$

$$\zeta_{i\ell} = \begin{cases} \nu_{\ell} & \ell \neq i \\ \frac{(\nu_{i} - 1)^{2}}{\nu_{i}} & \ell = i \end{cases}$$

$$\nu_{\ell} = \frac{w_{\ell \bullet}}{w}, \ \ell = 1, \dots, a.$$

If divByVar is FALSE then $\mathcal{N}_i(r)$ is taken to be identically equal to 1.

5.3 Two classification factors, testing for interaction

In the setting in which there are two classification factors and we are testing for interaction, against an additive models, the test statistic is

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

where $\mathcal{N}_{ij}(r)$ is the normalisation coefficient. If divByVar is TRUE, then $\mathcal{N}_{ij}(r)$ is equal to the (sample) variance of $\tilde{K}_{ij}(r) - \tilde{K}_{i}(r) - \tilde{K}_{j}(r) + \tilde{K}(r)$. The expression for $\mathcal{N}_{ij}(r)$, when divByVar is TRUE, is even messier than the corresponding expression for $\mathcal{N}_{i}(r)$. It is given by

$$s_{ij}^{2}(r) \left(\frac{1}{w_{ij.}} - \frac{2}{w_{i..}} - \frac{2}{w_{.j.}} + \frac{2w_{ij.}}{w_{i..}w_{.j.}} + \frac{2}{w_{...}} \right) + \tilde{s}_{i.}^{2}(r) \left(\frac{1}{w_{i..}} - \frac{2}{w_{...}} \right) + \tilde{s}_{.j}^{2}(r) \left(\frac{1}{w_{.j.}} - \frac{2}{w_{...}} \right) + \frac{\tilde{s}^{2}(r)}{w_{...}}$$

$$(1)$$

where

$$\tilde{s}_{i\bullet}^{2}(r) = \sum_{j=1}^{b} \frac{w_{ij\bullet}}{w_{i\bullet}} s_{ij}^{2}(r)$$

$$\tilde{s}_{\bullet j}^{2}(r) = \sum_{i=1}^{a} \frac{w_{ij\bullet}}{w_{\bullet j\bullet}} s_{ij}^{2}(r) \text{ and}$$

$$\tilde{s}^{2}(r) = \sum_{i=1}^{a} \sum_{j=1}^{b} \frac{w_{ij\bullet}}{w_{\bullet \bullet}} s_{ij}^{2}(r) .$$
(2)

Note that (1) is just (4), and (2) is just (3) (see below) with population quantities replaced by sample (estimated) quantities.

Here are some (terse) details about the variance of \tilde{K}_{ij} $(r) - \tilde{K}_{i}$ $(r) - \tilde{K}_{i}$ $(r) + \tilde{K}(r)$ as given by (4).

$$\operatorname{Var}(\tilde{K}_{ij\bullet}(r)) = \frac{\sigma_{ij}^{2}(r)}{w_{ij\bullet}}$$

$$\operatorname{Var}(\tilde{K}_{i\bullet}(r)) = \frac{\tilde{\sigma}_{i\bullet}^{2}(r)}{w_{i\bullet\bullet}}$$

$$\operatorname{Var}(\tilde{K}_{\bullet j\bullet}(r)) = \frac{\tilde{\sigma}_{\bullet j}^{2}(r)}{w_{\bullet j\bullet}}$$

$$\operatorname{Var}(\tilde{K}_{\bullet i}(r)) = \frac{\tilde{\sigma}^{2}(r)}{w_{\bullet i\bullet}}$$

$$\operatorname{Cov}(\tilde{K}_{ij\bullet}(r), \tilde{K}_{i\bullet}) = \frac{\sigma_{ij}^{2}(r)}{w_{i\bullet}}$$

$$\operatorname{Cov}(\tilde{K}_{ij\bullet}(r), \tilde{K}_{\bullet j\bullet}) = \frac{\sigma_{ij}^{2}(r)}{w_{\bullet j\bullet}}$$

$$\operatorname{Cov}(\tilde{K}_{ij\bullet}(r), \tilde{K}_{\bullet\bullet}) = \frac{\sigma_{ij}^2(r)}{w_{\bullet\bullet}}$$

$$\operatorname{Cov}(\tilde{K}_{i\bullet\bullet}(r), \tilde{K}_{\bullet j\bullet}) = \frac{w_{ij\bullet}\sigma_{ij}^2(r)}{w_{i\bullet\bullet}w_{\bullet j\bullet}}$$

$$\operatorname{Cov}(\tilde{K}_{i\bullet\bullet}(r), \tilde{K}_{\bullet\bullet}) = \frac{\tilde{\sigma}_{i\bullet}^2(r)}{w_{\bullet\bullet}}$$

$$\operatorname{Cov}(\tilde{K}_{\bullet j\bullet}(r), \tilde{K}_{\bullet\bullet}(r) = \frac{\tilde{\sigma}_{\bullet j}^2(r)}{w_{\bullet\bullet}}$$

where

$$\tilde{\sigma}_{i\bullet}^{2}(r) = \sum_{j=1}^{b} \frac{w_{ij\bullet}}{w_{i\bullet}} \sigma_{ij}^{2}(r)$$

$$\tilde{\sigma}_{\bullet j}^{2}(r) = \sum_{i=1}^{a} \frac{w_{ij\bullet}}{w_{\bullet j\bullet}} \sigma_{ij}^{2}(r) \text{ and}$$

$$\tilde{\sigma}^{2}(r) = \sum_{i=1}^{a} \sum_{j=1}^{b} \frac{w_{ij\bullet}}{w_{\bullet \bullet}} \sigma_{ij}^{2}(r) .$$
(3)

Sample calculation: to see that $Cov(\tilde{K}_{ij\bullet}(r), \tilde{K}_{i\bullet\bullet}) = \sigma_{ij}^2/w_{i\bullet\bullet}$, note that $\tilde{K}_{i\bullet\bullet}(r)$ is a weighted sum over ℓ , of terms $\tilde{K}_{i\ell\bullet}(r)$. The K-functions involved correspond to independent patterns, and so are likewise independent. Consequently $\tilde{K}_{ij\bullet}(r)$ is independent of $\tilde{K}_{i\ell\bullet}(r)$, and the corresponding covariances are 0, except when $\ell = j$. We thus get only a single non-zero term from the sum of the covariances, explicitly

$$\operatorname{Cov}(\tilde{K}_{ij\bullet}(r), \frac{w_{ij\bullet}}{w_{i\bullet\bullet}}\tilde{K}_{ij\bullet}) = \frac{w_{ij\bullet}}{w_{i\bullet\bullet}}\operatorname{Var}(\tilde{K}_{ij\bullet}) = \frac{w_{ij\bullet}}{w_{i\bullet\bullet}}\frac{\sigma_{ij}^2}{w_{ij\bullet}} = \frac{\sigma_{ij}^2}{w_{i\bullet\bullet}}.$$

Finally we can obtain the variance term of interest, which is $Var(\tilde{K}_{ij\bullet}(r) - \tilde{K}_{i\bullet}(r) - \tilde{K}_{j\bullet}(r) + \tilde{K}_{\bullet\bullet}(r))$. This expression is equal to

$$Var(\tilde{K}_{ij\bullet}(r)) + Var(\tilde{K}_{i\bullet}(r)) + Var(\tilde{K}_{\bullet j\bullet}(r)) + Var(\tilde{K}_{\bullet \bullet}(r))$$

$$- 2Cov(\tilde{K}_{ij\bullet}(r), \tilde{K}_{i\bullet}(r)) - 2Cov(\tilde{K}_{ij\bullet}(r), \tilde{K}_{\bullet j\bullet}(r)) + 2Cov(\tilde{K}_{ij\bullet}(r), \tilde{K}_{\bullet \bullet}(r))$$

$$+ 2Cov(\tilde{K}_{i\bullet}(r), \tilde{K}_{\bullet j\bullet}) - 2Cov(\tilde{K}_{i\bullet}(r), \tilde{K}_{\bullet \bullet}(r))$$

$$- 2Cov(\tilde{K}_{\bullet j\bullet}(r), \tilde{K}_{\bullet \bullet}(r)).$$

Collecting terms in the foregoing expression, and using the previously stated symbolic representations of these terms, we obtain

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

$$(4)$$

Replacing the population variances by their corresponding estimates (sample quantities) we obtain (1).

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