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A note on the null distribution of the local spatial heteroscedasticity (LOSH) statistic

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Abstract Recently, Ord and Getis (Ann Reg Sci 48:529–539, 2012) developed a local statistic H_i , called local spatial heteroscedasticity statistic, to identify boundaries of clusters and to describe the nature of heteroscedasticity within clusters. Furthermore, in order to implement the hypothesis testing, Ord and Getis suggested a chi-square approximation method to approximate the null distribution of H_i , but they said that the validity of the chi-square approximation remains to be investigated and some other approximation methods are still worthy of being developed. Motivated by this suggestion, we propose in this paper a bootstrap procedure to approximate the null distribution of H_i and conduct some simulation to empirically assess the validity of the bootstrap methods. The results demonstrate that the bootstrap method can provide a more accurate approximation than the chi-square method at the cost of more computation time. Moreover, the power of H_i in identifying boundaries of clusters is empirically examined using the proposed bootstrap method to compute p values of the tests, and the multiple comparison issue is also discussed.

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1 Introduction

With the increasing availability of spatially extensive geo-referenced data and due to the geological and geographical diversity of different regions, it is in general unrealistic to assume that the values of a variable are of spatial homogeneity (Fotheringham 1977; Unwin and Unwin 1998). Therefore, much attention has been paid to exploring local patterns in spatial data using local forms of statistics among which Anselin's LISAs (Anselin 1995) and Getis and Ord's G_i or G_i^* statistic (Getis and Ord 1992; Ord and Getis 1995) are perhaps the most popular local statistics for identifying local patterns of spatial association.

In order to implement the confirmatory inference on the significance of local spatial patterns, it is essential to find out the null distribution of a local statistic. Currently, there are mainly two methodologies on this topic. One methodology uses random permutation technique to derive the moments of the local statistic and then to approximate the null distribution of the standardized local statistic using the standard normal distribution (see, for example, Getis and Ord 1992; Anselin 1995). However, many studies have found that the normal approximation is sometimes problematic (see, for example, Anselin 1995; Bao and Henry 1996; Boots and Tiefelsdorf 2000; Bivand et al. 2009). The other methodology assumes that the observations are independently drawn from a normal distribution. Then, the local statistic is re-expressed as a ratio of quadratic forms and the exact or the approximate null distribution is derived using the distributional results about a quadratic form in normal variables (see, for example, Tiefelsdorf and Boots 1997; Tiefelsdorf 1998, 2002; Boots and Tiefelsdorf 2000; Leung et al. 2003). Although the latter methodology generally performs better than the normal approximation does, it largely depends on the assumption that the observations are normally distributed. This assumption might be invalid in some real-world data sets.

Most of the existing local statistics focus on identifying spatial association at the mean level of the observations. Recently, Ord and Getis (2012) developed a new local statistic H_i , called local spatial heteroscedasticity (LOSH), to uncover the nature of LOSH, which is also one of the important issues in spatial data analysis. As pointed out by Ord and Getis (2012), the usefulness of LOSH includes exploring differential rates, such as disease rates, within a disease cluster; finding the degree of homogeneity or heterogeneity within an already delimited cluster; identifying trends in the homogeneity or heterogeneity surrounding a given observation; and identifying and testing for the existence of boundaries between districts.

For the local statistic H_i , its null distribution is also essential to the significance test for LOSH. Based on the mean and variance of H_i derived by the random permutation technique, Ord and Getis (2012) suggested a chi-square method to approximate the null distribution of H_i . That is, the null distribution of H_i is approximated by a properly scaled chi-square distribution. Ord and Getis (2012) pointed out that "following Box (1953), the use of the permutations moments will better account for non-normality in the data so that a chi-square approximation might provide a satisfactory approximation to the distribution of H_i ," but they said that "this is clearly an area for further research." That is to say, the validity of the chi-square approximation remains to be investigated and some other approximation methods are still worthy of being developed. Motivated by the suggestion made by Ord and Getis (2012), we propose in this paper a bootstrap procedure as an alternative to approximate the null distribution of H_i and perform an empirical evaluation on the validity of both the bootstrap and the chi-square methods. The simulation results demonstrate that, at the cost of more computation time, the bootstrap method performs much better than the chi-square approximation. Moreover, the power of H_i in detecting the boundary of two homogeneous clusters is investigated by simulation, and the multiple comparison issue is also discussed.

2 The local spatial heteroscedasticity (LOSH) statistic and a bootstrap approximation to its null distribution

In this section, we first give a brief description on the LOSH statistic developed by Ord and Getis (2012). Then, a bootstrap procedure is suggested to approximate the null distribution of the statistic.

Let $x_1, x_2, ..., x_n$ be the observations of a random variable X at the given n geographical units or locations and $\mathbf{W}(d) = (w_{ij}(d))_{n \times n}$ be a symmetric spatial link matrix, where d is a pre-specified distance threshold value. For each i = 1, 2, ..., n, as defined by Ord and Getis (2012), $w_{ij}(d)(j = 1, 2, ..., n)$ are positive for all j within distance d of the location i and are zero for other j's. Based on the observations $x_1, x_2, ..., x_n$ of X and the spatial link matrix $\mathbf{W}(d)$, Ord and Getis (2012) developed a LOSH statistic to study the nature of the homogeneity of the observation groups. Given a reference location i, the construction of the local statistic H_i can be described in what follows. Without loss of generality, we drop the distance threshold d in the weights $w_{ij}(d)(j = 1, 2, ..., n)$ for notational simplicity.

Firstly, the local mean of the observations at the reference location i is defined as

$$\bar{x}_i = \frac{\sum_{j=1}^n w_{ij} x_j}{\sum_{j=1}^n w_{ij}}.$$
(1)

In fact, \bar{x}_i is the weighted mean of the observations of X in the neighborhood of the location *i*. The neighborhood is determined by the positive weights among w_{ij} (j = 1, 2, ..., n) and is denoted by N(i). Then, the local residuals are

$$e_j = x_j - \bar{x}_i, \, j \in N(i), \tag{2}$$

and the LOSH statistic at the location i is defined as

$$\tilde{H}_{i} = \frac{\sum_{j=1}^{n} w_{ij} |e_{j}|^{a}}{\sum_{j=1}^{n} w_{ij}},$$
(3)

where *a* is a given positive constant. In particular, when a = 1, \tilde{H}_i is an absolute deviation measure; when a = 2, \tilde{H}_i is a variance measure. If the local residuals $e_i(j \in N(i))$ are extended to be defined at all of the locations, that is,

$$e_j = x_j - \bar{x}_i, \, j = 1, 2, \dots, n$$
 (4)

and the average of the absolute errors is defined by

$$h_1 = \frac{1}{n} \sum_{j=1}^n |e_j|^a,$$
(5)

a scaled version of the LOSH statistic is

$$H_{i} = \frac{\sum_{j=1}^{n} w_{ij} |e_{j}|^{a}}{h_{1} \sum_{j=1}^{n} w_{ij}}.$$
(6)

In order to carry out the confirmatory inference on the basis of the scaled LOSH statistic H_i , it is essential to derive the distribution of H_i under the null hypothesis that the observations of X are spatially homoscedastic over the region. Ord and Getis (2012) suggested a chi-square approximation to the null distribution of H_i on the basis of the permutations moments. We briefly introduce this approximation approach in what follows.

Assuming the set of *n*! possible permutations of $|e_1|^a$, $|e_2|^a$, ..., $|e_n|^a$ as equally likely, Ord and Getis (2012) computed the permutation mean and variance of H_i as

$$\mathcal{E}_{\mathbf{p}}(H_i) = 1 \tag{7}$$

and

$$v_i = \operatorname{Var}_{p}(H_i) = \frac{1}{n-1} \left(\frac{1}{h_1 W_{i1}}\right)^2 (h_2 - h_1^2) (n W_{i2} - W_{i1}^2),$$
(8)

respectively, where $h_1 = \frac{1}{n} \sum_{j=1}^{n} |e_j|^a$, $h_2 = \frac{1}{n} \sum_{j=1}^{n} (|e_j|^a)^2$, $W_{i1} = \sum_{j=1}^{n} w_{ij}$ and $W_{i2} = \sum_{j=1}^{n} w_{ij}^2$. Let the distribution of H_i be approximated by that of $b\chi_r^2$, where χ_r^2 is the random variable following the chi-square distribution with *r* degrees of freedom and *b* is a constant. The probability density function of $b\chi_r^2$, which we denote by $f_{H_i}^{(c)}(x)$, shows

$$f_{H_i}^{(c)}(x) = \begin{cases} \frac{x^{\frac{r}{2}-1}}{(2b)^{\frac{r}{2}}\Gamma(\frac{r}{2})} e^{-\frac{x}{2b}}, & \text{if } x > 0; \\ 0, & \text{if } x \le 0. \end{cases}$$
(9)

In the chi-square approximation, b and r are determined in such a way that the permutation mean and variance are made to match the mean and variance of $b\chi_r^2$, respectively, which results in $b = \frac{v_i}{2}$ and $r = \frac{2}{v_i}$.

Considering the fact that Ord and Getis (2012) said that the validity of chi-square approximation remains to be investigated, we conducted some simulation to evaluate the performance of the chi-square approximation (see the next section) and found that, although the approach can basically approximate the null distribution of H_i , there is obviously much room for improvement.

It has been well known in statistics that the bootstrap method, originally proposed by Efron (1979), is a powerful tool to approximate the distribution of a statistic and is in general free of the assumption that the observations are drawn from a normal population. We thus propose in this paper a bootstrap procedure to approximate the null distribution of H_i and expect that this method can achieve a more accurate approximation.

Given a reference location *i* and the observations $x_1, x_2, ..., x_n$ of *X* with the spatial link matrix $\mathbf{W} = (w_{ij})_{n \times n}$, the bootstrap procedure for approximating the null distribution of H_i can be summarized in the following steps:

Step 1. Draw with replacement a bootstrap sample $x_1^*, x_2^*, \ldots, x_n^*$ from the observations x_1, x_2, \ldots, x_n and compute the bootstrap value H_i^* of H_i according to

$$H_i^* = \frac{\sum_{j=1}^n w_{ij} |e_j^*|^a}{h_1^* \sum_{j=1}^n w_{ij}},$$
(10)

where $e_j^* = x_j^* - \frac{\sum_{j=1}^n w_{ij} x_j^*}{\sum_{j=1}^n w_{ij}} (j = 1, 2, ..., n)$ and $h_1^* = \frac{1}{n} \sum_{j=1}^n |e_j^*|^a$.

Step 2. Repeat step 1 for *m* times and obtain *m* bootstrap values of H_i which are denoted by $H_i^*(1), H_i^*(2), \ldots, H_i^*(m)$.

Step 3. Compute the empirical distribution function of $H_i^*(1), H_i^*(2), \ldots, H_i^*(m)$ as

$$F_{H_i}^*(x) = \frac{1}{m} \sum_{k=1}^m I(H_i^*(k) \le x), \tag{11}$$

where $I(\cdot)$ is the indicator function. $F_{H_i}^*(x)$, called the bootstrap distribution function of H_i , is then used as an estimator of the null distribution of H_i at the reference location *i*.

Based on the bootstrap values $H_i^*(1)$, $H_i^*(2)$, ..., $H_i^*(m)$, we can also estimate the bootstrap density function by, for example, the kernel smoothing method (Parzen 1962). The bootstrap kernel density estimator is

$$f_{H_i}^*(x) = \frac{1}{mh} \sum_{k=1}^m K\left(\frac{H_i^*(k) - x}{h}\right),$$
(12)

where $K(\cdot)$ is a kernel function and h is a bandwidth. $K(\cdot)$ is generally taken to be the probability density function of the standard normal distribution (i.e., the Gaussian kernel), and h is determined by a few of methods such as the cross-validation method (Bowman 1984) and the plug-in method (Wand and Jones 1995). In this paper, the bandwidth is chosen by a rule-of-thumb method (Silverman 1986) where the optimal value is $h = 1.059s^*m^{-\frac{1}{5}}$ with s^* being the standardized sample variance of $H_i^*(1), H_i^*(2), \ldots, H_i^*(m)$. The bootstrap density function in Eq. (12), as an approximation of the true probability density function of H_i , will be used in the next section for evaluating the validity of the bootstrap procedure.

In the H_i -based hypothesis test, since a large value of H_i tends to reject the null hypothesis that the observations are spatially homoscedastic over the region, the p value is

$$p = P_0(H_i > h_i^{(0)}), \tag{13}$$

where $h_i^{(0)}$ is the observed value of H_i computed from Eq. (6), and P₀ means that the probability is computed with the null distribution of H_i . Particularly, if the chi-square approximation is used, the *p* value is

$$p = P_0(H_i > h_i^{(0)}) = \int_{h_i^{(0)}}^{+\infty} f_{H_i}^{(c)}(x) dx$$
(14)

with $f_{H_i}^{(c)}(x)$ shown in Eq. (9); if the bootstrap method is used, the *p* value can be computed by

$$p = P_0(H_i > h_i^{(0)}) = \frac{1}{m} \sharp \{H_i^*(k) > h_i^{(0)}, k = 1, 2, \dots, m\},$$
(15)

where $\sharp A$ stands for the number of the elements in set A.

3 Simulation studies

In this section, we will conduct some simulation to assess the performance of the bootstrap and the chi-square methods in approximating the null distribution of H_i . Moreover, the power of H_i in identifying the boundary between two homogenous clusters is also examined.

3.1 Spatial layout for the simulation experiments

The spatial region for the simulation experiments is chosen as a square with 20 units in each side. The observations of the variable X are collected on the 20×20 regular grid cells by equally dividing the whole region into 20×20 small squares. These 20×20 square cells are labelled by 1–400 with the order from left to right and from bottom to top. Each observation of X is located at the center of the corresponding small square, and the sample size of the observations is n = 400.

The following two types of spatial link matrix $\mathbf{W} = (w_{ij})_{n \times n}$ are considered:

- (1) the rook scheme. That is, cells *i* and *j* are neighbors if they share a common edge.
- (2) the queen scheme. That is, cells *i* and *j* are neighbors if they have a common edge or vertex.

The binary coding scheme is assumed for the spatial link matrix $\mathbf{W} = (w_{ij})_{n \times n}$. That is, $w_{ij} = 1$ if cell *i* is a neighbor of cell *j* or vice versa; $w_{ij} = 0$ in other situations. Since the local mean defined by Eq. (1) includes the observation of *X* at the reference location, we define $w_{ii} = 1$ for i = 1, 2, ..., n. 3.2 Validity of the bootstrap approximation and the chi-square approximation for the null distribution of H_i

In order to assess the performance of the bootstrap and the chi-square methods for the data from a normal distribution and those from a non-normal distribution, we, respectively, consider the following two populations from which the observations of X are drawn:¹

- (1) standard normal distribution N(0, 1);
- (2) uniform distribution $U(-\sqrt{3},\sqrt{3})$.

The observations of X are independently drawn from one of the two populations and are randomly allocated to the n cells so that the null hypothesis is guaranteed.

We mainly consider three typical reference locations at i = 1, 2, and 190, which represent the corner cells, the boundary cells, and the inner cells of the square region, respectively. For these three reference locations, the numbers of their neighbors are, respectively, 2, 3, and 4 under the rook scheme and are 3, 5, and 8 under the queen scheme. In the following simulation, we set a = 2.

For each combination of the two populations, the two spatial linkage schemes and the three reference locations, the true probability density function of H_i is also estimated by the kernel method in order to achieve the task of comparison. Specifically, draw independently a sample x_1, x_2, \ldots, x_n of size n = 400 from the given population and compute the value of H_i by Eq. (6). Repeat this process for N = 5,000 times and obtain N values $H_i(1), H_i(2), \ldots, H_i(N)$ of H_i on which the estimator of the probability density function of H_i , which we denote by $f_{H_i}(x)$, is computed by the same formula as that in Eq. (12) with m and $H_i^*(k)$ replaced by N and $H_i(k)$, respectively. Since the sample size N = 5,000 for estimating $f_{H_i}(x)$ is large enough, we can take $f_{H_i}(x)$, called the empirical density function of H_i hereinafter, as the true probability density function of H_i and use it as a benchmark for evaluating the accuracy of the bootstrap and the chi-square approximations. In the simulation, the kernel function K(t) in density estimation is always taken as the Gaussian kernel, i.e., $K(t) = \frac{1}{\sqrt{2\pi}}e^{-\frac{t^2}{2}}$.

It is noted that each sample x_1, x_2, \ldots, x_n drawn from the given population can generate a bootstrap density function $f_{H_i}^{(c)}(x)$ in Eq. (9). In order to make a comprehensive comparison among $f_{H_i}(x)$, $f_{H_i}^*(x)$ and $f_{H_i}^{(c)}(x)$, we randomly choose 100 samples from those used for estimating the empirical density function $f_{H_i}(x)$ and obtain 100 bootstrap density functions and 100 chi-square density functions, respectively, where each bootstrap density function is estimated with m = 5,000 bootstrap replications. For the considered two populations and three reference locations, we depict these 100 bootstrap density functions with the empirical density function $f_{H_i}(x)$ in Fig. 1 for the rook scheme and in Fig. 2 for the queen scheme. Similarly, we depict the 100 chi-square

¹ According to one of the reviewer's suggestion, we further considered the heavy-tailed distribution t(3) and the skew distribution lognormal(1,1) when we revised the manuscript. It was found that the results are all similar to those for the normal and the uniform distributions.



Fig. 1 The 100 bootstrap density functions and the empirical density function for the rook spatial linkage scheme

density functions with the empirical density function $f_{H_i}(x)$ in Fig. 3 for the rook scheme and in Fig. 4 for the queen scheme.

It can be observed from Figs. 1 and 2 that the bootstrap method works quite well in approximating the null distribution of H_i for all the combinations of the two populations, the two spatial linkage schemes and the three reference locations. In particular, very accurate approximation is observed around the right tail of the empirical density function in various settings, which is important to derive the valid p values of the hypothesis tests. For the fixed sample size, although the bootstrap method seems to perform better for the normal observations, it still results in a satisfactory approximation to the null distribution of H_i for non-normal observations. Furthermore, with the increase of the neighbors of the reference locations, the approximation accuracy improves obviously especially for the non-normal observations.



Fig. 2 The 100 bootstrap density functions and the empirical density function for the queen spatial linkage scheme

In contrast, it can be seen from Figs. 3 and 4 that the chi-square method can only provide a rough approximation to the null distribution of H_i . Although this approximation indeed shows non-sensitivity to the non-normal observations and the accuracy of the approximation improves as the number of the neighbors of the reference locations increases, there is a systematic deviation from the empirical density function in all of the settings. In particular, the chi-square density functions show a heavier right tail than the empirical density function, which would lead to a larger p value for rejecting the null hypothesis and consequently a conservative test result.

The simulation results demonstrate that the bootstrap method provides a much better approximation to the null distribution of H_i than the chi-square approximation. In this sense, the proposed bootstrap method is a promising alternative to the chi-square approximation. However, it should be noted that the bootstrap method requires more



Fig. 3 The 100 chi-square density functions and the empirical density function for the rook spatial linkage scheme

computation time in comparison with the relatively simple chi-square approximation. In practice, the choice between the two methods should depend upon the computational cost or the approximation accuracy being of more concerns.

3.3 Power of H_i in detecting the boundary of homogeneous clusters

In this subsection, we empirically examine the power of H_i in identifying the boundary between two homogenous clusters, where the bootstrap method is used to compute the *p* values of the tests.

The same spatial layout as that in Sect. 3.1 is used to conduct the simulation. Here, only the queen spatial linkage scheme is considered. Let I be the set of the central 10×10 cells of the whole region and S be the set of the surrounding cells. The observations of X are generated by the following way:



Fig. 4 The 100 chi-square density functions and the empirical density function for the queen spatial linkage scheme

(1) when $j \in I$, $x_j = 1 + c + \varepsilon_j$;

(2) when
$$j \in S, x_j = 1 + \varepsilon_j$$
,

where the noises ε_j (j = 1, 2, ..., n) are independently drawn from $U(-\frac{\sqrt{3}}{4}, \frac{\sqrt{3}}{4})$, and c is a constant taking the values of 1, 3, 5, and 7, respectively. With the value of c increasing, the difference between the two clusters of the observations becomes larger and more significant boundary between the two clusters would be expected.

Given a value of c, a set of the observations x_1, x_2, \ldots, x_n of X is generated according to the above experiment design. Then, take each of the 20×20 cells as a reference location and compute the p value at this location according to Eq. (15), where the bootstrap replications are m = 1,000. The results are shown in Fig. 5 by the maps of the p values.



Fig. 5 Maps of the p values for $\mathbf{a} c = 1$; $\mathbf{b} c = 3$; $\mathbf{c} c = 5$; $\mathbf{d} c = 7$

It can be observed from Fig. 5 that the p values on the boundary of the two homogeneous clusters are relatively smaller than those in the inside and the outside areas. As the difference between the two clusters of the observations becomes larger (that is, with the increase of the value of c), a more significant boundary is identified. This result demonstrates that the statistic H_i with its bootstrap procedure for computing the p values is of reasonable power in identifying the boundaries of homogeneous clusters of observations.

We further conduct the above simulations for a = 1. The results are similar to those of a = 2 except that some p values on the boundary become somewhat larger. This might be reasonable since the statistic H_i is more robust when a = 1. To save the space, the results are omitted here, but are available from the authors.

4 Some discussion on the multiple comparison issue

In order to explore the LOSH in the observations of a variable, the test is generally conducted at all of the locations where the observations are collected, which leads to multiple tests. Therefore, it is reasonable to make an adjustment for the overall significance level. Although a Bonferroni adjustment could readily be applied by adjusting the overall significance level to be compared with the p values, such

procedure tends to be very conservative (Ord and Getis 2012). In the literature of nonparametric regression, Chaudhuri and Marron (1999) proposed a concept, socalled effective sample size, to locally measure the effective number of the data inside a kernel window and to determine the number of independent blocks for the adjustment of the overall significance level in the simultaneous inferences. For the present case, the effective sample size is in fact the number of observations in the neighborhood of a reference location if the binary coding scheme is used in the spatial link matrix **W**. Therefore, according to the method for determining the number of independent blocks in Chaudhuri and Marron (1999), if we denote by d_0 the average number of observations in the neighborhoods of all the reference locations, the adjusted significance level is $\frac{d_0}{n_0}\alpha$, where n_0 is the number of the total tests performed and α is the overall significance level. For example, for the spatial layout with the queen spatial linkage scheme in the foregoing simulation, there are totally 324, 72, and 4 reference locations having 9, 6, and 4 neighbors, respectively. Therefore, $d_0 = (324 \times 9 + 72 \times 6 + 4 \times 4)/400 = 8.41$. Given an overall significance level α , the adjusted level is $\frac{8.41}{400}\alpha = 0.021\alpha$. In fact, the similar idea has been proposed by Getis and Ord (2000) to address the problem of multiple tests in spatial data analysis. McLaughlin and Boscoe (2007) have used the similar adjustment to deal with the multiple comparison issue in the local Moran's I_i -based test.

The aforementioned adjustment can overcome, to some extent, the conservativeness of the Bonferroni method in the sense that $\frac{d_0}{n_0}\alpha$ is generally larger than the Bonferroni's adjusted significance level $\frac{\alpha}{n_0}$. Nevertheless, the above adjustment method seems to be still too conservative for the simulation experiment in Sect. 3.3, as the designed significant boundary of the two observation clusters is ignored even if the overall significance level α is set to be 0.1. Given its less conservativeness than the Bonferroni method, the above adjustment might be useful in other situations.

5 Concluding remarks

In this paper, a bootstrap procedure is proposed as an alternative method to approximate the null distribution of H_i . The simulation results have demonstrated that the bootstrap method performs better than the chi-square approximation. Although the bootstrap procedure is more time-consuming, it can still easily be implemented with the help of modern computers.

The LOSH statistic is in fact a local estimator of the deviation of observations. This statistic, as shown by the foregoing simulation, is of reasonable power in detecting the boundary of homogeneous clusters of the observations. Furthermore, as demonstrated in Ord and Getis (2012), the LOSH statistic H_i , accompanied with the mean level local statistic G_i^* (Ord and Getis 1995), offers deep understanding and comprehensive explanation of spatial patterns of the observations. This inspires us to explore in the future the possibility that a combination of the LOSH statistic with other mean level local statistics such as the Anselin's LISAs and Ord and Getis' G_i^* might generate more powerful statistics for detecting LOSH and some spatial patterns of interest in the observations.

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