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Published in:
Journal of Computational and Graphical Statistics

DOI:
10.1198/106186007X208966

Published: 01/06/2007

Document Version:
Peer reviewed version

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Abstract

For a spatial point pattern observed in a bounded window, we propose to use discrepancies, which are measures of uniformity in the Quasi-Monte Carlo method, to test the complete spatial randomness hypothesis. Tests using these discrepancies are in fact goodness-of-fit tests for uniform distribution. The discrepancies are free from edge effects and, unlike the popular maximum absolute pointwise difference statistic of a summary function over a suitably chosen range, do not have an arbitrary parameter. Simulation studies show that they are often more powerful when a given pattern is a realization of a process with long range interaction or a non-stationary process.

Keywords: Complete spatial randomness, Discrepancy, Quasi-Monte Carlo method, Spatial point process.

1 Introduction

Problems arising in geosciences, biology, astrophysics and medicine often require analyses of spatial point patterns. Many such studies have involved in testing the complete spatial randomness (CSR) hypothesis of a given point pattern, because "rejection of CSR is a minimal prerequisite to any serious attempt to model an observed pattern" (Diggle, 2003, p.12). Several summary functions such as the nearest neighbour

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distance distribution G, the empty space function F, Ripley's reduced second order moment function K and its variance-stablized version L are typical tools for such a purpose.

Basically, there are two ways to test CSR, namely, confidence envelopes (Møller and Waagepetersen, 2004, pp. 40–43) and Monte Carlo tests (Diggle, 1979; Ripley, 1979).

To construct confidence envelopes of a summary function, we simulate m independent realizations of a conditional Poisson process with the same number of points as the number of observed points, and then we take the pointwise $100(1-\alpha/2)$-th and $100\alpha/2$-th percentile of estimates of that summary function to form pointwise $100(1-\alpha)\%$ confidence upper and lower envelopes, provided that m is large. If the estimate of that summary function of a given point pattern is not contained entirely in the confidence envelopes, we reject the CSR hypothesis. However, the significance level of the test is unknown.

A possible way to have significance tests is to use Monte Carlo tests (Davison and Hinkley, 1997, Chapter 4), sometimes also known as Diggle's tests (Diggle, 1979) in this context. Two popular test statistics are the maximum absolute pointwise difference between the estimated and the theoretical form of a summary function, generically denoted by H, and the integrated version, i.e.

$$\sup_{r \le r_0} \left| H(r) - \hat{H}(r) \right|, \qquad \text{and} \qquad \int_0^{r_0} \left| H(r) - \hat{H}(r) \right|^p \mathrm{d}r, \tag{1}$$

where r_0 is a suitably chosen upper limit. Ripley (1979) suggested that r_0 should be proportional to the mean nearest neighbour distance in a Poisson process in such a way that for 25 points observed in a unit square $r_0 = 0.25$, and for 100 points in a unit square $r_0 = 0.125$, whilst Diggle (1979) used $r_0 = 0.25$ for his simulation studies with 100 points in a unit square. However, the choice of this upper limit r_0 is crucial for testing CSR (Ho and Chiu, 2006; Thönnes and van Lieshout, 1999; Yamada and Rogerson, 2003). One explanation is that the variance of $\hat{H}(r)$ usually increases as r increases, because the estimation of these summary functions is hampered by the edge effects; the larger the value r, the more severe the edge effects. Naturally, different edge correction methods will lead to different estimates. Although the choice of edge correction method does not affect the validity of a Monte Carlo test, the standard errors of the estimates and hence the power of the test depend on the choice (Gignoux et al., 1999; Haase, 1995; Ho and Chiu, 2006; Yamada and Rogerson, 2000).

These two approaches are in fact applications of the parametric bootstrap and require simulating independent realizations of a conditional Poisson process with a fixed number of points, which is known as the binomial process, where each of a fixed number of points is independent and uniformly distributed in the sampling window. However, in the estimation of the above summary functions, we usually assume that what we have observed is a part of a realization of a stationary spatial point process operating on the whole plane and hence sometimes we also have to estimate its intensity; it is because we have edge-corrected unbiased estimators for, e.g., $\lambda^2 K$ and λG (see Stoyan et al., 1995, pp. 134 and 139) and so estimators for λ^2 and λ are needed in the estimation of K and G, respectively. As shown in Ho and Chiu (2006) and Stoyan and Stoyan (2000), different intensity estimators will lead to different powers in testing CSR and different standard errors of the estimates of the summary functions. It is counterintuitive because the Monte Carlo test requires simulated patterns with exactly the same fixed number of points, but the intensity estimator plays a role.

This paper suggests that the CSR hypothesis can be replaced by the uniformity hypothesis, i.e. the hypothesis that the coordinates of the points are independent and uniformly distributed, so that we may simply perform goodness-of-fit tests for the uniform distribution. The advantages of the approach suggested here are (i) there are no edge effects, (ii) there are no arbitrary, user-chosen parameters such as r_0, (iii) intensity estimators do not play a role, and (iv) as we can see below, the powers of our proposed statistics, in most cases of our simulation study, are higher than the maximum absolute pointwise difference statistics given in (1). The only drawback is that if the sampling window is not a union of squares, we have to approximate the discrepancies. The idea of testing uniformity of a planar point pattern first appeared in Zimmerman (1993), in which he used the L_2-star discrepancy (see the next section for details). He showed that his test is more powerful when used to test against non-stationary processes but is less powerful against regular or clustered alternatives. In this paper, we introduce more sophisticated measures of uniformity, and compare them with other statistics.

2 Measures of uniformity: Discrepancy

Denote by Φ and N the random set and the random counting measure of a spatial point process, and by ν the Lebesgue measure in $\mathbb{R}^d$. Suppose we observed $\Phi \cap W = \Phi_W = \{\mathbf{x_1}, \ldots, \mathbf{x_n}\}$ in the unit square sampling window $W = [0,1)^d$. The empirical distribution of the locations is

$$U_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} \mathbf{1}(\mathbf{x_i} \leq \mathbf{x}),$$

where the partial order $\leq$ in $\mathbb{R}^d$ is defined componentwise. There are many statistics available to test the hypothesis that the true distribution of the locations is the uniform distribution U and the classical two are the Kolmogorov–Smirnov statistic and the Cramér–von Mises statistic, which are special cases of the so-called L_p-star discrepancy, defined by

$$LD_p^*(\Phi_W) = \left\{ \int_{[0,1)^d} |U(\mathbf{x}) - U_n(\mathbf{x})|^p \mathrm{d}\mathbf{x} \right\}^{\frac{1}{p}}.$$

Let $[\mathbf{0}, \mathbf{x}) = [0, x_1) \times \cdots \times [0, x_d)$, where $\mathbf{x} = \{x_1, \ldots, x_d\}$. Then, we have

$$LD_p^*(\Phi_W) = \left\{ \int_W \left| \nu([\mathbf{0}, \mathbf{x})) - \frac{N([\mathbf{0}, \mathbf{x}))}{n} \right|^p \mathrm{d}\mathbf{x} \right\}^{\frac{1}{p}}.$$

For $p \to \infty$,

$$LD_\infty^*(\Phi_W) = \sup_{\mathbf{x} \in W} \left| \nu([\mathbf{0}, \mathbf{x})) - \frac{N([\mathbf{0}, \mathbf{x}))}{n} \right| = \sup_{\mathbf{x} \in W} |U(\mathbf{x}) - U_n(\mathbf{x})|.$$

The idea of discrepancy, which first appeared in Weyl (1916), came from the quasi-Monte Carlo method in numerical integration (Hua and Wang, 1981; Niederreiter, 1992). Consider the following approximation

$$I(f) = \int_{[0,1)^d} f(\mathbf{x})\mathrm{d}\mathbf{x} \approx Q(f) = \frac{1}{n}\sum_{i=1}^{n} f(\mathbf{x}_i),$$

where $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ is a finite set of points in $[0,1)^d$. The Koksma–Hlawka inequality (Niederreiter, 1992, Theorem 2.11) gives an upper bound for the error in this approximation

$$\|I(f) - Q(f)\| \leq D(\{\mathbf{x}_1, \ldots, \mathbf{x}_n\})V(f),$$

where $V(f)$ is the variation of the function f and $D(\cdot)$ is a function defined according to the definition of the variation $V(\cdot)$ and its value depends on the distribution of the point set $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$. This function $D(\cdot)$

is called the discrepancy, and the smaller the discrepancy, the smaller the upper bound of the error; it is a measure of uniformity of points. Statistically speaking, the discrepancy $D(\{\mathbf{x}_1, \ldots, \mathbf{x}_n\})$ can be regarded as a goodness-of-fit test (Hickernell, 1999a) for testing the uniform distribution, where $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ are the data. In addition to the star discrepancy, a number of other discrepancies were proposed by e.g. Hickernell (1998a, b; 1999a, b), Niederreiter (1992) and Warnock (1972), and in this paper we investigated five discrepancies that have simple formulae for computation when $p = 2$.

In the following, let $S = \{1, 2, \ldots, d\}$ and for $u \subset S$ and $\mathbf{y} = (y_1, \ldots, y_d) \in \mathbb{R}^d$, let $\mathbf{y}^u$ denote a $|u|$-dimensional vector formed by the components of $\mathbf{y}$ that are indexed by the elements of u, and let $\tilde{\mathbf{y}}^u$ denote the vector $(\tilde{y}_1, \ldots, \tilde{y}_d)$, where $\tilde{y}_j$ is equal to y_j if $j \in u$ and equal to 1 otherwise. Furthermore, let $[0,1)^u$ denote the $|u|$-dimensional unit cube that is the projection of $[0,1)^d$ into the coordinates indexed by the elements of u. Let $\mathbf{x} = (x_1, \ldots, x_d)$ and $\mathbf{x}' = (x'_1, \ldots, x'_d)$ denote two generic points in Φ_W, which has n distinct points.

The centre $(\frac{1}{2}, \ldots, \frac{1}{2})$ of the cube $[0,1)^d$ with each of the 2^d vertices forms a sub-cube in such a way that for $\mathbf{y} \in [0,1)^d$, $\mathbf{y}$ must be contained in one of these sub-cubes. Denote by $\mathbf{v}_{\mathbf{y}}$ the vertex of $[0, 1)^d$ belonging to the sub-cube containing $\mathbf{y}$.

The discrepancies we considered in this paper are as follows.

(i) The L_2-star discrepancy (Warnock, 1972):

$$LD_2^*(\Phi_W) = \left\{ \frac{1}{3^d} - \frac{2}{n} \sum_{\mathbf{x} \in \Phi_W} \prod_{j=1}^{d} \left(\frac{1 - x_j^2}{2} \right) + \frac{1}{n^2} \sum_{\mathbf{x}, \mathbf{x}' \in \Phi_W} \prod_{j=1}^{d} [1 - \max(x_j, x'_j)] \right\}^{\frac{1}{2}},$$

which considers the uniformity of the points in the d-dimensional cube.

To measure not only the uniformity in the d-dimensional cube, but also the uniformity of the projection of the points onto lower dimensional cubes, a straightforward generation of the L_p-star discrepancy has been proposed:

(ii) The modified L_2-star discrepancy (Hickernell, 1998a, b, 1999b):

$$
\begin{aligned}
MD_2^*(\Phi_W) &= \left\{ \sum_{\emptyset \subset u \subseteq S} \int_{[0,1)^u} \left| \nu([\mathbf{0}, \tilde{\mathbf{y}})) - \frac{N([\mathbf{0}, \tilde{\mathbf{y}}^u))}{n} \right|^2 \mathrm{d}\mathbf{y}^u \right\}^{\frac{1}{2}} \\
&= \left\{ \left(\frac{4}{3}\right)^d - \frac{2}{n} \sum_{\mathbf{x} \in \Phi_W} \prod_{j=1}^d \left(\frac{3 - x_j^2}{2} \right) \right. \\
&\quad \left. + \frac{1}{n^2} \sum_{\mathbf{x}, \mathbf{x}' \in \Phi_W} \prod_{j=1}^d \left[2 - \max(x_j, x_j') \right] \right\}^{\frac{1}{2}}.
\end{aligned}
$$

The zero $(0, 0, \ldots, 0)$ in the L_p-star discrepancy and the modified L_p-star discrepancy is arbitrarily chosen but has a special role. The next discrepancy moves this special point to the center $(\frac{1}{2}, \ldots, \frac{1}{2})$ so that the discrepancy value will be invariant under reflection:

(iii) The L_2-centred discrepancy (Hickernell, 1998a, b, 1999b):

$$
\begin{aligned}
CD_2^*(\Phi_W) &= \left\{ \sum_{\emptyset \subset u \subseteq S} \int_{[0,1)^u} \left| \nu([\mathbf{v}_{\mathbf{y}}^u, \mathbf{y}^u)) - \frac{N([\mathbf{v}_{\mathbf{y}}^u, \mathbf{y}^u))}{n} \right|^2 \mathrm{d}\mathbf{y}^u \right\} \\
&= \left\{ \left(\frac{13}{12}\right)^d - \frac{2}{n} \sum_{\mathbf{x} \in \Phi_W} \prod_{j=1}^d \left(1 + \frac{1}{2}\left|x_j - \frac{1}{2}\right| - \frac{1}{2}\left|x_j - \frac{1}{2}\right|^2 \right) \right. \\
&\quad + \frac{1}{n^2} \sum_{\mathbf{x}, \mathbf{x}' \in \Phi_W} \prod_{j=1}^d \left[1 + \frac{1}{2}\left|x_j - \frac{1}{2}\right| + \frac{1}{2}\left|x_j' - \frac{1}{2}\right| \right. \\
&\quad \left. \left. - \frac{1}{2}\left|x_j - x_j'\right| \right] \right\}^{\frac{1}{2}}.
\end{aligned}
$$

The special role of $(\frac{1}{2}, \ldots, \frac{1}{2})$ in the L_p-central discrepancy can be easily got rid of, if we replace the vertices by another $\mathbf{y}^u$:

(iv) The L_2-unanchored discrepancy (Niederreiter, 1992, Definition 2.2; Hickernell, 1998b, 1999b):

$$
\begin{aligned}
UD_2(\Phi_W) &= \left\{ \sum_{\emptyset \subset u \subseteq S} \int\int_{[0,1)^u \times [0,1)^u,\ \mathbf{y}_1^u \le \mathbf{y}_2^u} \left| \nu([\mathbf{y}_1^u, \mathbf{y}_2^u)) - \frac{N([\mathbf{y}_1^u, \mathbf{y}_2^u))}{n} \right|^2 \mathrm{d}\mathbf{y}_1^u \mathrm{d}\mathbf{y}_2^u \right\}^{\frac{1}{2}} \\
&= \left\{ \left(\frac{13}{12}\right)^d - \frac{2}{n} \sum_{\mathbf{x} \in \Phi_W} \prod_{j=1}^d \left[1 + \frac{x_j(1 - x_j)}{2} \right] \right. \\
&\quad \left. + \frac{1}{n^2} \sum_{\mathbf{x}, \mathbf{x}' \in \Phi_W} \prod_{j=1}^d \left[1 + \min(x_j, x_j') - x_j x_j' \right] \right\}^{\frac{1}{2}},
\end{aligned}
$$

which is still invariant under reflection.

The L_2-unanchored discrepancy integrates over $\mathbf{y}_1^u \leq \mathbf{y}_2^u$ only. If we use the periodic boundary condition, this restriction can be removed:

(v) The L_2-wrap-round discrepancy (Hickernell, 1998a, b, 1999b):

$$\begin{aligned} WD_2(\Phi_W) &= \left\{ \sum_{\emptyset \subset u \subseteq S} \int_{[0,1)^u} \int_{[0,1)^u} \left| \nu(J(\mathbf{y}_1^u, \mathbf{y}_2^u)) - \frac{N(J(\mathbf{y}_1^u, \mathbf{y}_2^u))}{n} \right|^2 \mathrm{d}\mathbf{y}_1^u \mathrm{d}\mathbf{y}_2^u \right\}^{\frac{1}{2}} \\ &= \left\{ -\left(\frac{4}{3}\right)^d + \frac{1}{n^2} \sum_{\mathbf{x}, \mathbf{x}' \in \Phi_W} \prod_{j=1}^{d} \left[\frac{3}{2} - |x_j - x_j'|(1 - |x_j - x_j'|) \right] \right\}^{\frac{1}{2}}, \end{aligned}$$

where

$$\begin{aligned} J(y_j', y_j) &= \begin{cases} [y_j', y_j), & y_j' \leq y_j, \\ [0, y_j) \cup [y_j', 1), & y_j < y_j', \end{cases} \\ J(\mathbf{y}', \mathbf{y}) &= \bigotimes_{j=1}^{d} J(y_j', y_j). \end{aligned}$$

If the sampling window is not a square, we can approximate the window by a union of non-overlapping squares and take a weighted or unweighted sum of the discrepancies over the squares as the discrepancy over the sampling window.

The points of a binomial process are independent and uniformly distributed over the sampling window; a large value of a discrepancy may indicate that the point pattern is not a realization of a binomial process. Moreover, since the points of a pattern are not necessarily independent, a very small value of a discrepancy may also indicate that points are located too uniformly, or regularly, in the sampling window, meaning that the point pattern may be a realization of a process that generates regular patterns. Thus, we have two-sided critical regions for these goodness-of-fit test statistics in our context.

3 Summary Statistics for Diggle's test

Diggle's test given in equation (1) considers the difference between the theoretical form and the estimate of a summary function. Popular summary functions of a stationary point process in $\mathbb{R}^d$ with intensity λ include

(i) the nearest neighbour distance distribution function

$$G(r) = \mathbf{P}(\text{distance from an arbitrary point to the nearest point} \leq r),$$

(ii) the empty space function

$$F(r) = \mathbf{P}(\text{distance from an arbitrary location to the nearest point} \leq r),$$

(iii) the K-function

$$K(r) = \frac{\mathbf{E}(\text{number of further points within distance } r \text{ of an arbitrary point})}{\lambda},$$

(iv) the L-function

$$L(r) = \sqrt[d]{\frac{K(r)}{w_d}},$$

where $w_d = \frac{\sqrt{\pi}^d}{\Gamma(1+d/2)}$ is the volume of a unit ball in $\mathbb{R}^d$.

Under the periodic boundary condition, for the binomial point process in a unit square $W = [0,1)^2$, we have

$$\begin{aligned} G(r) &= 1-(1-\pi r^2)^{n-1}, & F(r) &= 1-(1-\pi r^2)^n, \\ K(r) &= \tfrac{n-1}{n}\pi r^2, & L(r) &= r\sqrt{\tfrac{n-1}{n}}, \end{aligned}$$

for $r \leq 0.5$, where n is the number of points in W.

Denote by d_i the distance from the ith point to the nearest other points in W and e_{ij} the distance between points i and j under the periodic boundary condition. The empirical G and K are given by

$$\hat{G}(r) = \frac{1}{n}\sum_{i=1}^{n}\mathbf{1}(d_i \leq r), \quad \text{and} \quad \hat{K}(r) = \frac{1}{n^2}\sum_{i=1}^{n}\sum_{i\neq j}^{n}\mathbf{1}(e_{ij} \leq r).$$

To obtain an estimator of $F(r)$, we consider a regular grid over the sampling window, and let u_i be the distance from the ith grid point to the nearest point in W under the periodic boundary condition, then the empirical F is given by

$$\hat{F}(r) = \frac{1}{m}\sum_{i=1}^{m}\mathbf{1}(u_i \leq r),$$

where m is the number of the grid points. Diggle (1979; 2003, p. 21) suggested that $m \approx n$ may be adequate and in the following simulation study we always used a 50×50 regular lattice and so $m = 2500$ for both $n = 25$ and $n = 100$, much more than the number suggested by Diggle.

Periodic boundary condition is one edge correction method, but it is restricted to a rectangular window. There are many other edge correction methods and, as a comparison, in this paper we also consider the isotropic edge correction for the K-function

$$\hat{K}_{\mathrm{iso}}(r) = \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{i \neq j}^{n} w_{ij}^{-1} \mathbf{1}(d_{ij} \leq r),$$

where d_{ij} is the distance between points i and j and w_{ij} is the proportion of circumference of the circle centred at the ith point with the radius d_{ij} which lies within W. In this case a CSR point pattern should be considered as a realization of a Poisson process, whose K-function is $K(r) = \pi r^2$.

4 Simulations

4.1 Alternative models

Four models, namely, the Matérn cluster process, the Strauss process and two non-stationary process (to be specified below), were used to investigate the powers of the above statistics in testing the CSR hypothesis.

To obtain a clustered point pattern with exactly n points in a unit square from a Matérn cluster process, we generate a prescribed number n_{parent} of independent parent points which are uniformly distributed in a unit torus and then n daughter points are assigned randomly to these parents in such a way that each daughter is located independently and uniformly in the disk centred at her parent with radius R.

A Strauss process (Kelly and Ripley, 1976; Strauss, 1975) is a particular Markov point process (van Lieshout, 2000; Møller and Waagepetersen, 2004, Chapter 6); it is a pairwise interaction point process producing, by self-inhibiting, patterns in which points are more spread out than they would be in CSR; such patterns exhibit regularity. We start with a Poisson process in a bounded region and then define the Strauss process by giving a probability density with respect to the Poisson process. The probability density of the Strauss process is proportional to $\prod_{\mathbf{x}_i, \mathbf{x}_j} c^{\mathbf{1}(\|\mathbf{x}_i - \mathbf{x}_j\| \leq R)}$ so that the parameter c controls the strength of inhibition and the parameter R determines the range of inhibition in such a way that $c = 0$ and $c = 1$ correspond to the hard core process with hard core distance R and the Poisson process, respectively; for $0 < c < 1$ we have a self-inhibiting point process. In the simulation below we use the built-in function for generating Strauss process in the `R` library `spatial` (Venables and Ripley, 2002).

We also consider two non-stationary finite point processes in $[0, 1)^2$. One is that points are independent, and the x-coordinate and the y-coordinate are independently and normally distributed with means and variances μ_x and σ_x^2, and μ_y and σ_y^2, respectively. The other one is that points are independent, and the y-coordinate of each point is uniformly distributed, whilst the x-coordinate has a density proportional to x^{s+1}.

4.2 Test statistics

For each test statistic the Monte Carlo test was performed 100 times independently to estimate the power in testing CSR at the 0.05 significance level against the cluster process, the Strauss process or the non-stationary processes specified above. We employed the maximum absolute pointwise difference statistic of each of the three popular functions G, F and L, where L would be estimated by two different edge-corrected estimators $\hat{L} = \sqrt{\hat{K}/\pi}$ and $\hat{L}_{\text{iso}} = \sqrt{\hat{K}_{\text{iso}}/\pi}$, i.e. we have four statistics

$$\begin{aligned} d_G &= \max_{r \le r_0} \left| \hat{G}(r) - [1 - (1 - \pi r^2)^{n-1}] \right|, \\ d_F &= \max_{r \le r_0} \left| \hat{F}(r) - [1 - (1 - \pi r^2)^{n}] \right|, \\ d_L &= \max_{r \le r_0} \left| \hat{L}(r) - r\sqrt{\frac{n-1}{n}} \right|, \\ d_{L_{\text{iso}}} &= \max_{r \le r_0} \left| \hat{L}_{\text{iso}}(r) - r \right|, \end{aligned}$$

and the discrepancies LD_2^*, MD_2^*, CD_2^*, UD_2 and WD_2 as our test statistics. The CSR hypothesis would be rejected whenever a test statistic calculated from a pattern generated according to the alternative model, when pooled with the values of the statistic calculated from 99 independent realizations of the binomial process with the same number of points, has been ranked in the top 5% if the statistic is a maximum absolute pointwise difference statistic or ranked in the bottom or top 2.5% if the statistic is a discrepancy.

4.3 Technical Remarks

The values of LD_2^* and MD_2^* depend on the arbitrary choice of the zero $(0, \ldots, 0)$. Thus, for a pattern observed in a square, there are four possible values for each LD_2^* and MD_2^*, which can be obtained by simple transformations of the coordinates: (I) (x, y), (II) $(1-x, y)$, (III) $(x, 1-y)$ and (IV) $(1-x, 1-y)$. However, since we are testing the uniformity hypothesis, we do not expect any substantial difference in the powers.

Sometimes data are not observed in square windows. In such cases, we suggest to approximate the sampling window by a union of non-overlapping squares, and the test statistics are just a weighted or unweighted sum of the discrepancies in these squares. In the following simulation, we consider the rectangular window [0,1)×[0,3), which is the union of three unit squares.

For a unit square window in $\mathbb{R}^2$, Diggle (2003) suggested that the value of the upper limit r_0 in the maximum absolute pointwise difference should be at most 0.25, and Ripley (1979) proposed that the value r_0 should be inversely proportional to $\sqrt{n}$. However, for non-square windows, to the best of our knowledge, no value for r_0 has been recommended. In the following simulation studies, the sample sizes are $n = 25$ and $n = 100$ in $[0, 1)^2$, and $n = 75$ and $n = 300$ in [0, 1)×[0, 3), and for the unit square, we follow Ripley's recommendation, i.e. $r_0 = 0.25$ for $n = 25$ and $r_0 = 0.125$ for $n = 100$, and for the rectangular window, in the same spirit as Ripley's, we try $r_0 = \frac{1.25}{\sqrt{n}} = 0.14434$ and $r_0 = 0.25$ for $n = 75$, and $r_0 = \frac{1.25}{\sqrt{n}} = 0.07217$ and $r_0 = 0.125$ for $n = 300$.

5 Simulation results

5.1 Square sampling window

The results of the simulation experiments were depicted in Tables 1, 2, 3 and 4, from which we can see that the powers of test statistics LD_2^* and MD_2^*, as expected, do not depend on the direction of the coordinate axes. However, for an individual given pattern, the conclusion does depend on the directions.

Table 1 about here

Table 2 about here

Table 3 about here

Table 4 about here

We can observe that, for the cluster process, UD_2 and WD_2 perform better than the others in the majority of cases. When the radius of clusters is large, the estimated powers of the discrepancies are higher than those of the maximum absolute pointwise difference statistic of any one of the three summary functions considered, no matter what the sample size is. For a fixed n and n_{parent}, it is clear that the power of a statistic testing CSR will decrease as R increases. Nevertheless, we can observe that discrepancies have lower decrease rates. We expect that in general using UD_2 and WD_2 would lead to more powerful tests against clustered patterns with long range interaction.

For the Strauss process, the points are more uniformly distributed over the area of interest. Table 2 shows that for small values of R, discrepancies do not work better than the summary functions, no matter what the value of c is. Because discrepancies are measures of uniformity and are positive, their distributions are quite skewed. Thus, the left critical value is so small that the powers of the tests against regular patterns, which are supposed to have small values of discrepancies, are low. Nevertheless, when R is larger than some unknown threshold value, discrepancies, especially UD_2 and WD_2, become powerful. This agrees with our conclusions above that discrepancies are more able to detect long range interaction.

Figure 1 about here

In particular, we focus on the cases that (n, c, R) are $(25, 0.6, 0.5)$ and $(100, 0.8, 0.3)$; in these two cases UD_2 and WD_2 are very powerful. A plausible explanation of the remarkable difference in the powers at small and large values of R can be suggested by investigating Figure 1, which gives a simulated realization for each case. We can see that the point patterns look more clumped, even though the points are generated by the Strauss process. As a result, that patterns are similar to clustered processes with long range interaction and the discrepancy values are large, and consequently we are also able to use the right critical value to reject the CSR hypothesis. However, we are not suggesting that we should use only the right tail to test. Consider the Strauss process $(25, 0, 0.1)$, the estimated powers of the left-tailed test at the 5% level using

LD_2^*, MD_2^*, CD_2^*, UD_2 and WD_2 are 37, 32, 33, 33 and 34, respectively, indicating that the discrepancies of about 30% of realizations of the Strauss process $(25, 0, 0.1)$ are small enough to conclude rejection at the 0.05 level at the left tail.

$\boxed{\text{Figure 2 about here}}$

Figure 2 shows the estimated powers of the maximum absolute pointwise difference statistic of each summary function in testing CSR against the Strauss process (n, c, R) as a function of r_0, see equation (1). Ho and Chiu (2006), Thönnes and van Lieshout (1999), and Yamada and Rogerson (2003) showed that the choice of the upper limit r_0 is crucial. From Figure 2, we can see that statistics based on summary functions have higher powers as r_0 increases, and they, especially $\hat{L}_{\text{iso}}$, do not attain their maxima at the r_0-value recommended by Ripley (1979). This can be explained by Figure 3, which plots $\hat{L}_{\text{iso}}(r) - r$ of a realization of the Strauss $(25, 0.6, 0.5)$ against r, together with upper and lower envelops obtained from taking the pointwise maximum and minimum of the estimates of $L(r) - r$ of 99 independently simulated realizations of the binomial process. The figure shows that $\hat{L}_{\text{iso}} - r$ of this realization of the Strauss process $(25, 0.6, 0.5)$ lies within the envelopes for $0 \le r \le 0.4$ and so if $r_0 = 0.25$ only, there is no strong evidence against the CSR hypothesis. On the other hand, the discrepancies are not functions of r_0 and so their powers do not depend on the arbitrarily chosen value of r_0.

$\boxed{\text{Figure 3 about here}}$

Furthermore, consider only the results from the L-function. Tables 1 and 2 and Figure 2 reveal that even $\hat{L}$ works better (has higher power) than $\hat{L}_{\text{iso}}$ in many cases; the latter works better in cases where the parameter R of the Strauss process is small. Thus, even if we use the power of Diggle's test statistic as the only criterion, there is still no uniformly best edge correction method. On the other hand, each discrepancy is free from the edge effects and so has only one formula; users do not have to choose an edge correction method.

For the non-stationary process with identically normally distributed coordinates, we can observe that UD_2 and WD_2 work better than the maximum absolute pointwise difference, and the bigger the variance of the normal distribution, the bigger the advantage of using UD_2 and WD_2.

Furthermore, for the non-stationary process with intensity proportional to x^{s+1}, we can see that the discrepancies are more powerful than the maximum absolute pointwise difference statistics, especially when $n = 100$.

5.2 Rectangular sampling window

The results of simulation experiments with $r_0 = r_0' = 0.11547$ and $r_0 = r_0'' = 0.25$ for $n = 75$, and $r_0 = r_0' = 0.05774$ and $r_0 = r_0'' = 0.125$ for $n = 300$ were shown in Tables 5, 6, 7 and 8, from which the same conclusions as those stated above can be drawn. Moreover, consider the powers of the statistics based on summary functions. The powers are usually higher when we choose $r_0 = r_0''$; the reason may be that the r_0'' is closer to the range of interaction. This observation reinforces the advantage of using test statistics, such as the discrepancies considered here, that are free from user-chosen parameters.

Table 5 about here

Table 6 about here

Table 7 about here

Table 8 about here

6 Conclusion

In conclusion, we recommend the use of discrepancies as test statistics in testing the CSR hypothesis because users do not have to choose an edge correction method or a value for the upper bound r_0, and in quite a number of cases considered above, their powers are higher than the maximum absolute pointwise difference statistics. Among the discrepancies considered, we suggest to use either UD_2 or WD_2, because in the simulation study they give higher power when used to test against the Strauss process with long range interaction, the cluster process and the non-stationary process with normally distributed coordinates; although the other discrepancies are more powerful when used to test against the non-stationary process in which the x-coordinates have a density proportional to x^{s+1}, UD_2 or WD_2 still performs better than the maximum absolute pointwise difference statistics in most cases. Moreover, the values of UD_2 and WD_2, unlike LD_2^* and MD_2^*, do not depend on the arbitrary choice of the directions of the coordinate axes.

When the sampling window is not a square, we can use a union of nonoverlapping squares to approximate the sampling window and take a weighted or unweighted sum of their discrepancies as the overall discrepancy.

Finally, as pointed out by an associate editor and a referee, a CSR test is a basic tool in exploratory analysis for understanding spatial structure but not taken as an end in itself. We agree with Diggle (2003, p.12) that "tests are used to explore a set of data and to assist in the formulation of plausible alternatives to CSR". However, although large and small values of the discrepancies suggest clustering and regularity, respectively, they do not offer any fine details of the clustering or regularity as the summary functions may do, because each discrepancy is not a function of distance but a constant. Thus, these discrepancies cannot replace summary functions in modelling observed patterns after the CSR hypothesis is rejected.

Acknowledgements

We thank an associate editor and the referees for helpful comments. This research was supported by grants from the Research Grants Council of the Hong Kong Special Administrative Region, China (Project Numbers HKBU2048/02P and HKBU200503) and an FRG grant from the Hong Kong Baptist University.

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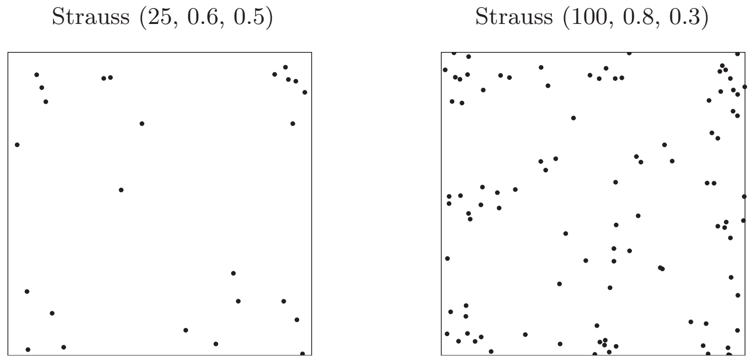

Figure 1: Simulated realizations of the Strauss process $(n,\, c,\, R)$.

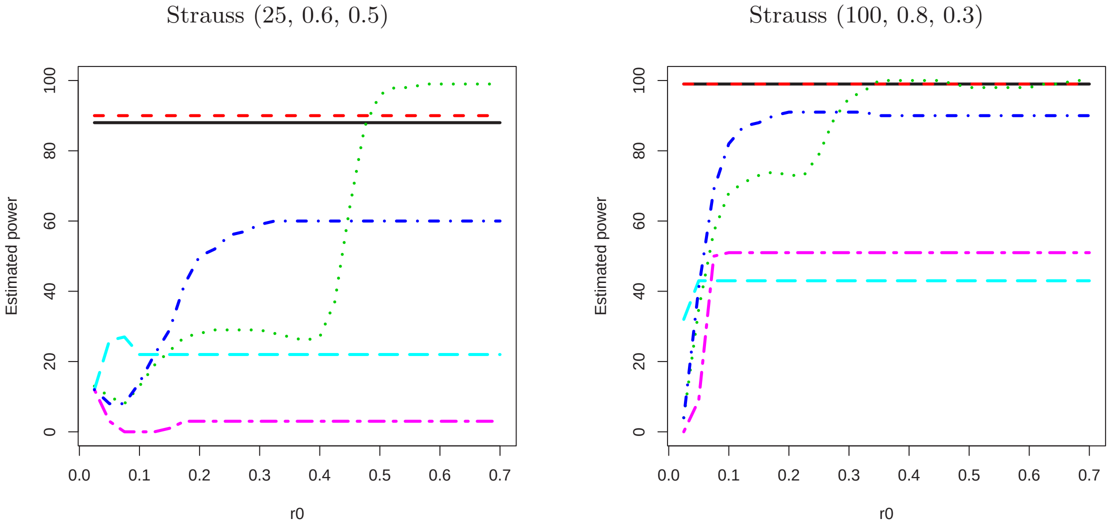

Figure 2: Estimated powers of testing CSR against the Strauss process $(n,\, c\ ,\, R)$ as a function of r_0. *Key:* —, UD_2; - - -, WD_2; $\cdots$, $\hat{L}_{\mathrm{iso}}$; - · -, $\hat{L}$; — —, $\hat{G}$; – - –, $\hat{F}$.

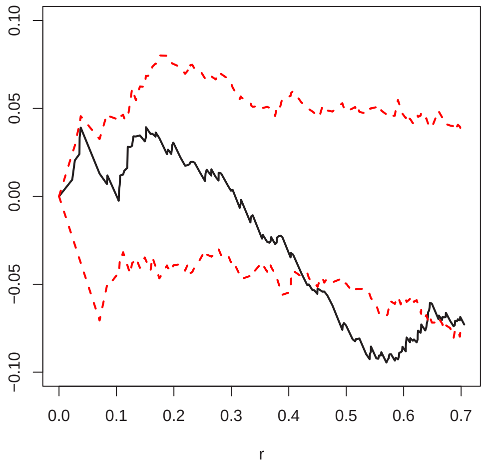

Figure 3: Plot of $\hat{L}_{\text{iso}}(r) - r$ (solid curve) of a realization of the Strauss process $(25, 0.6, 0.5)$, together with upper and lower envelops (dashed curves) obtained by taking the pointwise maximum and minimum of the estimated $L(r) - r$, using the isotropic edge correction, from 99 independently simulated realizations of the binomial process with 25 points.

Table 1: Estimated powers (in percentage) of testing CSR against the cluster process in $[0,1)^2$.

							LD_2^*				MD_2^*						
n	n_{parent}	R	d_F	d_G	d_L	$d_{L_{\text{iso}}}$	I	II	III	IV	I	II	III	IV	CD_2^*	UD_2	WD_2
25	12	0.2	1	12	21	25	15	19	15	18	28	26	23	29	27	33	34
		0.3	4	9	9	11	15	7	8	12	15	15	15	16	17	20	19
	8	0.15	16	61	75	72	31	35	31	34	45	43	38	45	45	72	74
		0.2	10	24	46	37	22	17	18	22	28	27	29	26	30	44	47
		0.3	7	8	6	11	15	8	11	9	18	13	10	14	16	21	20
	5	0.1	95	100	100	100	58	56	56	57	67	65	69	66	69	93	95
		0.2	7	55	72	68	39	36	27	41	52	53	49	57	52	71	72
		0.3	4	20	32	30	27	15	18	25	32	31	30	31	31	53	54
100	50	0.1	70	57	80	86	30	23	34	35	41	38	41	41	39	56	57
		0.15	21	22	38	38	23	16	20	17	31	30	32	30	30	39	39
		0.2	7	7	17	14	14	13	12	10	20	18	20	16	18	32	32
	20	0.2	33	22	56	57	39	35	41	37	55	51	56	54	57	69	68
		0.3	17	12	18	17	33	17	17	22	29	27	26	27	30	45	45
	10	0.2	83	59	87	86	59	64	58	59	67	69	65	68	68	80	81
		0.3	36	22	43	43	43	40	42	37	50	51	50	47	52	76	76
	5	0.25	94	71	94	94	74	72	77	78	82	82	81	83	83	91	91
		0.3	75	44	80	81	55	63	60	56	74	74	73	73	75	91	92
		0.4	15	15	29	28	33	29	29	26	49	43	43	45	48	68	68

Table 2: Estimated powers (in percentage) of testing CSR against the Strauss process in $[0,1)^2$.

							LD_2^*				MD_2^*						
n	c	R	d_F	d_G	d_L	$d_{L_{\text{iso}}}$	I	II	III	IV	I	II	III	IV	CD_2^*	UD_2	WD_2
25	0	0.1	82	94	92	100	15	18	15	16	14	12	15	15	14	17	16
	0.2	0.1	51	71	54	62	9	12	9	15	12	11	11	14	14	8	12
	0.4	0.1	21	30	23	32	6	8	10	8	9	9	9	8	9	12	12
	0.6	0.1	21	22	23	25	6	3	6	7	9	6	7	8	8	8	8
		0.3	3	5	5	9	1	0	1	3	2	1	2	3	2	2	1
		0.5	0	28	56	31	3	2	3	2	6	5	6	2	10	83	83
		0.6	33	49	92	76	20	20	18	20	43	39	38	40	55	100	100
	0.8	0.1	9	10	11	8	2	3	8	4	5	4	4	6	5	6	7
		0.3	11	11	4	10	8	5	5	5	4	3	5	3	5	5	6
		0.5	2	2	7	8	2	3	3	6	2	1	4	1	4	20	21
		0.6	4	15	26	16	2	4	1	5	4	4	3	4	6	51	49
100	0	0.05	100	100	100	100	33	29	34	29	30	29	32	30	31	29	32
	0.2	0.05	70	100	100	99	22	17	19	18	20	21	19	16	18	25	26
	0.4	0.05	41	92	82	92	17	6	16	7	10	7	10	11	11	9	9
	0.8	0.05	10	16	8	10	5	3	6	6	2	1	1	4	3	6	5
		0.2	5	7	5	4	2	2	0	0	0	0	0	0	0	7	4
		0.3	56	40	82	73	11	17	7	6	21	17	20	15	22	95	95
	0.9	0.05	8	12	6	9	5	3	3	3	4	6	5	5	4	2	2
		0.2	3	5	4	5	5	1	4	9	2	4	3	3	2	3	3
		0.3	8	10	13	13	0	1	0	1	0	0	0	0	0	40	36
		0.5	93	50	99	98	86	84	85	89	96	97	96	96	97	100	100

Table 3: Estimated powers (in percentage) of testing CSR against the non-stationary process with independently and identically normally distributed coordinates with mean $\mu_x = \mu_y = 0.5$ and variance $\sigma_y^2 = \sigma_x^2 = \sigma^2$ in $[0, 1)^2$.

						LD_2^*				MD_2^*						
n	σ^2	d_F	d_G	d_L	$d_{L_{\mathrm{iso}}}$	I	II	III	IV	I	II	III	IV	CD_2^*	UD_2	WD_2
25	0.125	100	99	100	100	98	100	100	99	100	100	100	100	100	100	100
	0.15	89	88	100	100	93	92	85	94	99	97	94	98	94	100	100
	0.175	54	69	98	99	63	68	61	64	80	80	76	74	71	100	100
	0.2	16	38	83	82	32	33	32	29	39	38	39	41	32	99	95
	0.25	1	12	30	32	10	9	7	6	11	10	8	7	6	79	74
100	0.225	98	76	100	100	100	97	100	99	100	100	100	100	100	100	100
	0.25	86	49	96	96	89	85	85	84	96	94	92	95	91	100	100
	0.275	58	31	84	83	61	65	65	71	78	80	80	80	79	100	100
	0.325	22	12	40	42	24	23	20	23	28	28	29	24	23	95	93
	0.35	17	9	29	27	16	19	25	20	23	21	29	26	24	82	80
	0.4	12	6	10	8	10	6	11	8	10	6	8	7	7	48	46

Table 4: Estimated powers (in percentage) of testing CSR against the non-stationary process in which the x-coordinates have a density proportional to x^{s+1} in $[0, 1)^2$.

						LD_2^*				MD_2^*						
n	s	d_F	d_G	d_L	$d_{L_{\text{iso}}}$	I	II	III	IV	I	II	III	IV	CD_2^*	UD_2	WD_2
25	0.2	5	4	5	6	10	5	6	10	8	6	9	12	7	7	8
	0.4	3	5	3	4	11	9	6	17	15	16	14	20	15	8	8
	0.6	7	4	8	7	16	20	14	26	29	28	24	30	27	12	12
	0.8	2	9	12	22	26	42	27	33	48	58	50	50	55	23	22
	1	1	7	8	24	34	42	36	39	55	63	54	55	60	30	32
100	0.2	6	6	9	7	10	15	10	16	17	16	17	19	18	11	11
	0.4	7	7	8	14	45	42	45	52	60	60	5	63	59	32	31
	0.6	8	9	14	32	78	73	82	83	92	92	94	92	94	70	72
	0.8	29	18	37	67	95	92	96	90	100	99	100	100	100	86	85
	1	45	23	63	83	100	99	99	98	100	100	100	100	100	98	99

Table 5: Estimated powers (in percentage) of testing CSR against the cluster processes in $[0,\ 1)\times[0,\ 3)$.

			d_F		d_G		d_L		$d_{L_{\mathrm{iso}}}$						
n	n_{parent}	R	r_0'	r_0''	r_0'	r_0''	r_0'	r_0''	r_0'	r_0''	LD_2^*	MD_2^*	CD_2^*	UD_2	WD_2
75	35	0.2	45	47	41	41	50	73	51	73	32	47	52	68	70
		0.3	7	11	16	16	11	27	11	27	26	33	30	42	41
	20	0.2	86	90	77	77	87	98	85	96	65	75	79	88	88
		0.3	33	42	34	34	40	64	37	65	48	61	65	66	66
	15	0.2	98	98	95	95	98	100	97	100	85	92	91	94	95
		0.3	53	58	56	56	55	74	59	73	58	71	71	75	79
		0.4	20	22	27	27	23	44	25	49	40	51	52	54	54
	12	0.3	76	81	63	63	71	87	70	82	69	80	82	88	88
		0.4	35	39	32	32	37	53	35	53	40	53	56	63	65
	8	0.3	96	97	92	92	91	98	89	95	86	92	93	100	99
		0.4	58	60	50	50	51	73	48	73	61	77	78	85	83
300	150	0.1	100	100	92	92	99	99	98	99	60	66	69	86	89
		0.2	42	47	14	14	23	46	21	46	36	50	52	69	70
	100	0.2	72	73	32	32	48	79	47	79	52	66	68	81	81
		0.3	18	20	9	9	10	19	11	19	18	29	33	41	44
	75	0.2	90	91	46	46	63	89	64	86	66	83	87	90	90
		0.3	32	38	9	9	18	39	15	42	41	54	56	66	64
	50	0.2	100	100	80	80	93	100	91	99	83	96	96	99	99
		0.3	64	66	25	25	30	64	31	65	59	71	71	84	83
		0.4	36	41	14	14	16	35	19	38	44	53	54	52	53
	20	0.3	99	99	82	82	95	99	96	99	93	99	99	99	99
		0.5	48	51	15	15	16	45	14	42	54	59	58	57	57

Table 6: Estimated powers (in percentage) of testing CSR against the Strauss processes in [0, 1)×[0, 3).

			d_F		d_G		d_L		$d_{L_{\mathrm{iso}}}$						
n	c	R	r_0'	r_0''	r_0'	r_0''	r_0'	r_0''	r_0'	r_0''	LD_2^*	MD_2^*	CD_2^*	UD_2	WD_2
75	0	0.1	100	100	100	100	100	100	100	100	37	38	41	60	63
	0.2	0.1	67	67	97	97	95	95	99	99	20	20	18	29	27
	0.4	0.1	37	37	77	77	68	66	73	70	10	11	13	21	22
	0.6	0.1	19	19	26	26	17	17	18	18	6	6	5	9	11
		0.3	4	4	6	6	5	5	5	23	7	2	2	2	1
		0.5	81	81	81	80	94	97	87	92	33	60	68	100	100
		0.6	100	100	99	99	100	100	100	100	95	99	100	100	100
	0.8	0.1	15	15	12	12	11	11	9	8	7	7	5	8	9
		0.3	6	6	6	6	10	9	10	6	5	3	6	4	4
		0.5	5	5	14	14	12	19	13	14	5	10	13	41	41
		0.6	31	37	37	37	41	66	41	52	21	30	43	92	92
300	0	0.05	100	100	100	100	100	100	100	100	52	59	57	76	78
	0.2	0.05	100	100	100	100	100	100	100	100	29	33	37	48	51
	0.4	0.05	92	92	100	100	100	100	100	100	18	21	24	30	30
	0.8	0.05	9	9	31	32	19	20	21	22	5	6	6	7	8
		0.2	7	7	4	4	6	7	8	10	2	2	3	3	2
		0.3	99	99	83	83	98	100	95	98	48	77	78	100	100
	0.9	0.05	13	13	13	13	8	8	9	8	4	10	8	3	3
		0.2	8	7	7	7	5	6	6	8	7	6	8	4	4
		0.3	21	22	10	10	10	21	9	14	3	4	6	47	44

Table 7: Estimated powers (in percentage) of testing CSR against the non-stationary process with independent and normally distributed coordinated in [0, 1)×[0, 3) with means $\mu_x = 0.5$, $\mu_y = 1.5$ and variances $\sigma_y^2 = 3\sigma_x^2$.

		d_F		d_G		d_L		$d_{L_{\mathrm{iso}}}$						
n	σ_x^2	r_0'	r_0''	r_0'	r_0''	r_0'	r_0''	r_0'	r_0''	LD_2^*	MD_2^*	CD_2^*	UD_2	WD_2
75	0.15	100	100	100	100	100	100	100	100	100	100	100	100	100
	0.2	98	98	78	78	99	100	98	100	96	100	99	100	100
	0.25	37	44	31	31	51	88	52	87	59	78	78	92	92
	0.275	27	32	22	22	29	62	28	65	41	59	59	78	77
	0.3	15	17	20	20	23	47	22	52	37	46	44	65	65
300	0.25	100	100	92	92	100	100	100	100	100	100	100	100	100
	0.275	99	99	79	79	96	100	96	100	100	100	100	100	100
	0.3	97	99	39	39	74	100	73	100	95	100	100	100	100
	0.35	67	73	25	25	29	68	26	71	67	87	90	98	98
	0.375	43	46	15	15	16	43	17	44	55	69	71	92	91
	0.4	24	30	6	6	10	20	10	22	41	57	58	76	76

Table 8: Estimated powers (in percentage) of testing CSR against the non-stationary process in which the x-coordinates have a density proportional to x^{s+1} in [0, 1)×[0, 3).

		d_F		d_G		d_L		$d_{L_{\text{iso}}}$						
n	s	r_0'	r_0''	r_0'	r_0''	r_0'	r_0''	r_0'	r_0''	LD_2^*	MD_2^*	CD_2^*	UD_2	WD_2
75	0.2	2	2	3	3	3	3	3	4	7	8	8	7	8
	0.4	5	5	8	8	6	7	6	11	13	22	30	15	16
	0.6	6	7	11	11	10	12	13	23	40	62	60	27	26
	0.8	7	8	12	12	9	13	17	33	67	87	88	49	48
	1	12	13	16	16	15	24	22	52	79	98	99	71	69
300	0.2	4	4	9	9	6	5	7	7	25	37	43	16	17
	0.4	20	23	13	13	10	13	13	24	86	99	99	68	69
	0.6	57	62	21	21	12	39	21	72	99	100	100	96	96
	0.8	85	88	35	35	45	80	61	100	100	100	100	100	100
	1	97	98	63	63	76	98	88	99	100	100	100	100	100