THE VARIANCE OF A NEW CLASS OF $N$-POINT CORRELATION ESTIMATORS IN POISSON AND BINOMIAL POINT PROCESSES

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Abstract

We describe a set of new estimators for the $N$-point correlation functions of point processes. The variance of these estimators is calculated for the Poisson and binomial cases. It is shown that the variance of the unbiased estimator converges to the continuum value much faster than with any previously used alternative, all terms with slower convergence exactly cancel. We compare our estimators with Ripley’s $\hat{K}_0$ and $\hat{K}_2$.

1. Introduction

Estimation of correlation functions from a set of points is a classical problem of spatial statistics. The two-point correlation functions are the most widely used, but there is an increasing interest in estimating higher order correlation functions as well. A new class of estimators was introduced in astrophysics [11] which pertains to most methods currently applied to data sets of galaxy positions. We present the

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rigorous calculation of the variances of these new estimators for Poisson and binomial point processes. It will be shown in the next sections that for these processes the estimators have smaller variance than any estimator previously used for the same statistics. While the results are completely general, they were motivated by future astrophysical applications, therefore all the examples will be taken from there. Higher order correlation functions from galaxy catalogs are routinely estimated since the 70’s. With a new generation of galaxy catalogs coming on line in the next five years, understanding the estimators is an important and timely problem.

A unique feature of spatial statistics is that errors of a measurement are often dominated by geometrical terms, like edge effects \[9\]. Thus ever since correlation functions were estimated, corrections for edge effects have played a central role. The estimators for correlation functions in the astrophysical literature is reviewed in \[11\], here we only quote a few selected additional references \[6, 1, 8, 4\]. It is generally accepted that the most efficient estimator for the two-point function is that of \[8\], or its relative \[4\].

The new estimator can be approximated in the continuum limit (achieved when the number density of data points \(\to \infty\)) as \(\hat{w}_2 = \langle \delta_1 \delta_2 \rangle\), where \(\langle \rangle\) denotes ensemble average, and \(\delta\) is the fluctuation of the continuous (galaxy) density field \(\rho\). It is defined as \(\rho = \langle \rho \rangle (1 + \delta)\), thus \(\langle \delta \rangle = 0\). The Monte Carlo representation of this estimator is often written symbolically as \((DD - 2DR + RR)/RR\), with \(DD\), \(DR\), and \(RR\) representing the respective pair counts. The important point is that the above estimator contains only the most necessary terms in the continuous limit, while all others, such as \(DD/RR - 1 \to \langle (1 + \delta_1)(1 + \delta_2) \rangle - 1 = \langle \delta_1 \delta_2 + \delta_1 + \delta_2 \rangle\), have extra terms. These extra terms do not affect the ensemble average of the unbiased estimator, but increase the variance. The deceptively simple look of the second estimator in terms of \(D\) and \(R\) was the reason for its popularity.

Ripley \[9\] has discussed extensively the variance of second order estimators for Poisson and binomial point processes. He has shown, that the \(O(n^{-1})\) term in the variance of the simple estimator, \(\hat{K}_0\), is proportional to \(u\), the perimeter for a two dimensional domain. This implies that the effect is due to inadequate edge corrections, in agreement with Hewett’s \[6\] suggestion. The subtraction of the appropriate \(DR\)
terms is equivalent to an edge correction.

The effect of the extra terms on the variance is even more pronounced for the higher order functions, since there will be a lot more terms arising through various combinatorial expressions. We proposed intuitively that the obvious generalization for higher order correlations is to create higher order equivalents of the estimator \[ \hat{w} \]. With \( \delta_i \approx (D_i - R_i)/R_i \) this corresponds to \( \langle \delta_1 \cdots \delta_N \rangle \). In symbolic notation, this estimator can be written as

\[
\hat{w}_N = \frac{(D_1 - R_1)(D_2 - R_2) \cdots (D_N - R_N)}{R_1 \cdots R_N}.
\]

This corresponds to the Monte-Carlo approximation of the continuum limit of the \( N \)-point correlation function of fluctuations; the exact meaning is discussed later. The most significant result is that the correlations of the fluctuations automatically correct for edge effects for Poisson and binomial point processes.

Different approaches to edge effects exist; for a review see \[10, 7\]. It remains to be seen whether these geometrically motivated estimators, or their generalization for higher order \[5\] fare better than the \[8\] estimator, or the related estimator introduced by \[3\].

The main goal of this article is to rigorously derive the variance of the estimator for Poisson and binomial processes. The next section presents the analytic calculation of the variance for arbitrary \( N \). Section 3 compares the second order estimator with that of the related Ripley’s \( K \) function. The last section summarizes the results.

2. Variance of the Edge Corrected Estimators in the Poisson and Binomial Point Processes

Many interesting statistics, such as the \( N \)-point correlation functions and their Fourier analogs, can be formulated as functions over \( N \) points from the catalog. The covariance of a pair of such estimators will be calculated for Poisson and binomial point processes. They correspond to the cases, where the number of detected objects is varied or fixed a priori. The general case, where correlations are non-negligible is left for future work. The following calculations heavily rely on the elegant formalism...
outlined in Ripley [9], which can be consulted for details.

Let $D$ be a catalog of data points to be analyzed, and $R$ randomly generated over the same area, with averages $\lambda$, and $\rho$ respectively. The role of $R$ is to perform a Monte Carlo integration compensating for edge effects, therefore eventually the limit $\rho \to \infty$ will be taken. $\lambda$ on the other hand is assumed to be externally estimated with arbitrary precision. We also assume that the correlations in the point process are weak, i.e. we operate in the Poisson limit.

Let us define symbolically an estimator $D^p R^q$, with $p + q = N$ for a function $\Phi$ symmetric in its arguments

$$D^p R^q = \sum \Phi(x_1, \ldots, x_p, y_1, \ldots, y_q),$$

with $x_i \neq x_j \in D, y_i \neq y_j \in R$. For example for the two point correlation function $\Phi(x, y) = [x, y \in D, r \leq d(x, y) \leq r + dr]$, where $d(x, y)$ is the distance between the two points, and [condition] equals 1 when condition holds, 0 otherwise. Ensemble averages can be estimated via factorial moment measures, $\nu_s$ [2, 9]. In the Poisson limit $\nu_s = \lambda^s \mu_s$, where $\mu_s$ is the $s$ dimensional Lebesgue measure.

The general covariance of a pair of estimators is

$$\langle D^p R^q D^{p_1} R^{q_1} D^{p_2} R^{q_2} \rangle = \sum_{i,j} \binom{p_1}{i} \binom{p_2}{j} i! j! S_{i+j} \lambda^{p_1+p_2-i} \rho^{q_1+q_2-j},$$

with $p_1 + q_1 = p_2 + q_2 = N$, and

$$S_k = \int \Phi_a(x_1 \ldots x_k, y_{k+1} \ldots y_N) \Phi_b(x_1 \ldots x_k, z_{k+1} \ldots z_N) \mu_{2N-k}.$$

Throughout the paper we use the convention that $\binom{k}{l}$ is nonzero only for $k \geq 0, l \geq 0$, and $k \geq l$. Here $\Phi_a$ and $\Phi_b$ denote two different functions, for instance corresponding to two radial bins. The expression simply describes the fact that out of the $p_1$ and $p_2$ different data points in $D$ we have an $i$-fold degeneracy, as well as a $j$-fold degeneracy in the random points drawn from $R$. For each of these configurations the geometric phase-space $S_{i+j}$ is different, and we sum their contributions. The dependence of $S_k$ on $a, b$, and $N$ is not noted for convenience, but they will be assumed throughout the paper. An estimator for the generalized N-point correlation function is

$$\hat{w}_N = \frac{1}{S} \sum_i \binom{N}{i} (-)^{N-i} \left( \frac{D}{\lambda} \right)^i \left( \frac{R}{\rho} \right)^{N-i},$$
where $S = \int \Phi \mu_N$ (without subscript). This definition can be expressed as $(\hat{D} - \hat{R})^N$, where ^ means normalization with $\lambda, \rho$ respectively. In this symbolic $N$th power, each factor is evaluated at a different point. Simple calculation in the limit of zero correlations yields $\langle \hat{w}_N \rangle = 0$.

**Theorem 1** The asymptotic covariance between two estimators of the above form for a Poisson point process in the limit of $\rho \to \infty$ is

$$\text{(co)}\text{Var}_\lambda \hat{w}_N = \langle \hat{w}_a,N \hat{w}_b,N \rangle = \frac{S_N \lambda^N}{S^2 \lambda^N}. \quad (6)$$

**Proof.** According to Eq. 3 the covariance can be written as

$$\langle \hat{w}_a,N \hat{w}_b,N \rangle = \sum_{i_1, i_2, i, j} \binom{N}{i_1} \binom{N}{i_2} \binom{i_1}{i} \binom{i_2}{j} \binom{N - i_1}{j} \binom{N - i_2}{j} j! i! \frac{S_{i+i} \lambda^{-i} \rho^{-j} (-)^{2N-i_1-i_2}}{S^2}. \quad (7)$$

In the interesting limit, where $\rho \to \infty$ only $j = 0$ survives. Changing the order of summation yields

$$\langle \hat{w}_a,N \hat{w}_b,N \rangle = \frac{1}{S^2} \sum_i S_i \lambda^{-i} i! f_{Ni}^2, \quad (8)$$

with

$$f_{Ni} = \sum_j \binom{N}{j} \binom{j}{i} (-1)^{N-j}. \quad (9)$$

This latter can be identified as the coefficients of $\sum (xy)^N$, therefore $f_{Ni} = \delta_{Ni}$. This in turn proves the theorem noting that $\langle \hat{w}_N \rangle = 0$. This formula represents both variance and covariance depending on whether in the definition of $S_N$ the implicit indices $a$ and $b$ are equal or not.

While in the Poisson model the total number of points in the domain can vary, it is fixed in the binomial model. This latter case corresponds to surveys, that detect a certain number of galaxies, and use that to estimate the mean density as well. In a sense, this would be the conditional estimator of the correlations given the number of galaxies. The normalization of the estimator changes slightly: $\lambda^i \to (n)_i / v^i$, where $n$ is the total number of objects in the survey, and $(n)_i = n(n-1) \ldots (n-i+1)$ is the
\[ \hat{w}_N = \frac{1}{S} \sum_i \binom{N}{i} (-1)^{N-i} \frac{(Dv)^i}{(n)_i} \left( Rv \right)^{N-i} \frac{(Rv)^{N-i}}{(n_r)_{N-i}}, \]

where \( n_r \) is the number of points in the auxiliary random process \( R \).

For a binomial process the factorial moment measure is \((n)_N v^{-N} \mu_N\), with \( v \), the volume of the survey. This fact enables the proof of the following theorem.

**Theorem 2** The asymptotic covariance of two estimators for a binomial point process in the limit of \( n_r \to \infty \) is

\[ \text{(co)Var}_n \hat{w}_N = \frac{1}{S^2} \binom{n}{N}^{-1} \sum_i S_i v^i \binom{N}{i} (-1)^{N-i}. \]

**Proof.** First it is convenient to prove the following lemma

**Lemma 1** For all possible integer values of \( N, n, \) and \( i \)

\[ \sum_{i_1, i_2} \binom{n-i_2}{N-i_2} \binom{n-i_1}{i_2-i} \binom{N-i}{i_1-i} (-1)^{i_1+i_2} = (-1)^{N-i}, \]

where the summation is over all possible values of \( i_1 \) and \( i_2 \).

**Proof.** It follows by induction over \( N \). For \( N = i \) it is true, since \( N = i = i_1 = i_2 \) are the only possible values. Thus

\[ \binom{n-i}{0} \binom{n-i}{0} \binom{0}{0} (-1)^{2i} = (-1)^{0} \]

for any \( n \) and \( i \). Assume it is true for a particular \( N \) for any \( n \) and \( i \). Then for \( N + 1 \)

\[ \sum_{i_1, i_2} \binom{n-i_2}{N+1-i_2} \binom{n-i_1}{i_2-1} \binom{N+1-i}{i_1-1} (-1)^{i_1+i_2} = (-1)^{N+1-i}. \]

By introducing \( m = n - 1, k = i - 1, k_1 = i_1 - 1, \) and \( k_2 = i_2 - 1 \) this reads

\[ \sum_{k_1, k_2} \binom{m-k_2}{N-k_2} \binom{n-k_1}{k_2-1} \binom{N-k}{k_1-1} (-1)^{k_1+k_2} = (-1)^{N-k}, \]

which is true by induction.
Now to prove the theorem consider the equation for the covariance using the appropriate factorial moment measure for binomial point process. After \( n_r \to \infty \)

\[
\langle \hat{w}_{a,N} \hat{w}_{b,N} \rangle = \frac{1}{S^2} \sum_{i,i_1,i_2} S_i v^{i_1!} \left( \begin{array}{c} N \\ i_1 \end{array} \right) \left( \begin{array}{c} N \\ i_2 \end{array} \right) (i_1) (i_2) (n_{i_1+i_2-i})(-)^{i_1+i_2}.
\]

Applying the lemma for each \( i \) separately, the theorem is proven.

\[
\sum_{i_1,i_2} \left( \begin{array}{c} N \\ i_1 \end{array} \right) \left( \begin{array}{c} N \\ i_2 \end{array} \right) (i_1) (i_2) (-)^{i_1+i_2} (n-i_1)_{N-i_1} (n-i_2)_{N-i_2} (n_{i_1+i_2-i})! = N! (n) N \left( \begin{array}{c} N \\ i \end{array} \right) (-)^{N-i}.
\]

For \( N = 2 \) the theorem coincides with \[\frac{S^2}{S_0} \simeq (S_2 v^2)^2.\]

3. Discussions

For practical applications the function \( \Phi \) has to be specified. For instance, \( \Phi = 1 \) when the \( N \)-tuplet satisfies a certain geometry (with a suitable bin width), and 0 otherwise yields the total (or disconnected) \( N \)-point correlations of the fluctuations of the process. See \[\text{[11]}\] for detailed discussion of possible choices for the function \( \Phi \) to render popular statistics for the distribution of galaxies, such as power spectra, cumulant correlators, etc. Here we concentrate on the comparison with other second order estimators.

The number of neighbors from a point within a distance of \( \leq t \) is defined as \( \lambda K(t) \)
\[\text{[9]}\]. A family of estimators denoted by \( \hat{K}_i \) was introduced \[\text{[9]}\] with subtle differences in edge correction. It was found that Ripley’s \( \hat{K}_2 \) has the smallest variance of all. Similar conclusions were reached in a numerical setting motivated by potential astrophysical applications \[\text{[7]}\]. The difference between these estimators and ours is twofold: first, the normalization is different, second, they estimate the moments of the full point process while \( \hat{w}_N \) deals with the moments of the fluctuations. The former point is trivial, while the latter is crucial, as shown later. When \( \hat{w}_2 \) is used to extract the (differential) two-point correlation function, the connection with Ripley’s cumulative
$K$ can be expressed as $K(t) = \lambda \int_0^t dr (1 + w_2(r))$. Note that in astrophysics the prevailing choice is $w$, and $K$ for the most part would be estimated for the purpose of eventually obtaining $w$ from it. Nevertheless, in other disciplines, or perhaps even for certain aspects of astrophysics, $K$ could be more advantageous.

Next we show that $\hat{w}_2$ has smaller variance than any of the $\hat{K}_i$. For a pair-estimator $\hat{T} = \sum_{x \neq y} \Phi(x, y)$ the variance for a Poisson process can be expressed in a quite general fashion. Using the notation of the previous section, the variance is $\text{Var}_{\lambda} \hat{T} = 4\lambda^3 S_1 + 2\lambda^2 S_2$. Ripley has derived an approximation of this formula for the “naive” estimator $\hat{K}_0(t) = a T/n^2$, $\text{Var}_{\lambda} \hat{K}_0(t) = \frac{1}{\lambda^2} \left[ \frac{\pi a^2}{6} - 2 \frac{ut^3}{a^3} + 1.34 \lambda \frac{ut^3}{a^3} \right]$, where $a$ is the area of the two-dimensional domain, and $u$ is its perimeter.

In order to compare the variance $\hat{w}_2$ and $\hat{T}$ ($\hat{K}_0$ up to normalization), we scale $\hat{T}$ by $S\lambda^2$

$$\text{Var}_{\lambda} \hat{w}_2 = \frac{2S_2}{S^2 \lambda^2},$$

$$\text{Var}_{\lambda} \left( \frac{\hat{T}}{S\lambda^2} \right) = \frac{2S_2}{S^2 \lambda^2} + \frac{4S_1}{S^2 \lambda}.$$ (18)

The Poisson terms in the number of pairs, $\simeq \lambda^{-2}$, are identical, while the $O(1/\lambda)$ terms are missing from the variance of $\hat{w}_2$. The latter can be appreciable when $\lambda$ is small for the estimator $\hat{K}_0$ based on $T$.

The most clever estimators of $K$, such as Ripley’s $\hat{K}_2$, suppress this term considerably, nevertheless it is always present. E.g., the variance of $\hat{K}_2$ for a Poisson process is $\text{Var}_{\lambda} \hat{K}_2(t) = \frac{1}{\lambda^2} \left[ \frac{\pi a^2}{6} + 0.96 \frac{ut^3}{a^3} + 0.13 \lambda \frac{ut^3}{a^3} \right]$.

In general for any $N$, all contributions $O(\lambda^{-k})$, $k < N$, exactly cancel for $\hat{w}_N$. Since terms higher than $O(\lambda^{-N})$ are absent, the asymptotic behavior of our estimator is optimal: the only possible improvement for Poisson (or binomial) processes is perhaps to decrease the multiplicative factor.

In fact $\hat{K}_2$ suppresses the $\lambda^{-1}$ term at the expense of boosting the coefficient of $\lambda^{-2}$ compared to $\hat{K}_0$. In contrast, for $\hat{w}_2$ no such boost is present according to Equation (18) the coefficients of the Poisson term are identical to that of the $\hat{K}_0$ estimator. This suggests that the estimator $\hat{w}_N$ is probably close to optimal for Poisson (and binomial) processes. We conjecture that this is approximately true for many correlated point
processes as well, although for extreme cases, such a line segment process, a small bias was noted by the numerical investigations of [7] for both \( \hat{w}_2 \), and for other estimators related to the \( K \) function.

The intuitive meaning of the results for binomial process is clear from Theorem 2.: the variance of the estimators is \( \propto \left( \frac{n}{N} \right)^{-1} \), i.e. Poisson in the number of \( N \)-tuplets, with multiplicative factors depending on the available geometric phase space. For the Poisson process, Theorem 1. is identical up to discreteness effects: it is inversely proportional to the probability density of finding \( N \)-points in the domain, \( \propto (\lambda^N)^{-1} \approx (n/v)^{-N} \).

Our approach to suppressing the offending non-Poisson terms involves an auxiliary Poisson process \( R \), for which the average density is assumed to be infinity \( \rho \to \infty \). The limit is not possible in practice, therefore it is desirable to evaluate the speed of convergence. A calculation analogous to the proof of Theorem 1. shows that

\[
\text{(co)}\text{Var}_{\lambda, \rho} \hat{w}_N = \frac{S_N N!}{S^2 N^N} \left\{ 1 + \frac{1}{N} \left( \frac{\lambda}{\rho} \right) + O(\lambda/\rho)^2 \right\}.
\]

(19)

This generalization of Theorem 1. clearly shows that for a finite auxiliary Poisson process \( R \), there is indeed a term with \( 1/\lambda \), but suppressed by a large factor. For instance, the relative non-Poisson correction is \( \lambda/(2\rho) \) for \( N = 2 \), giving less than a percent contamination when the auxiliary process is more than fifty times the original process to be measured. This is fairly convenient, since, unlike for the original process, we have full control over the artificially introduced process. Note that the above considerations assume exact knowledge of the average count \( \lambda \), thus no conditioning on the number of points is assumed.

For a binomial process the argument is exactly analogous to the previous one, therefore we only outline it briefly. The variance for a general estimator \( T \) is

\[
\text{Var}_n T = 4n(n-1)(n-2)a^3 S_1 - n(n-1)(4n-6)a^{-1}S^2 + 2n(n-1)a^{-2}S_2.
\]

This is to be compared with Theorem 2. \( \text{Var}_n \hat{w}_2 = 2[S_0 - 2S_1 a + S_2 a^2]/S^2 n(n-1) \) (replacing \( v \) with \( a \) for two dimensions). Again \( T(n(n-1))^{-2}a^4 \) has to be considered because of the normalization. The first two terms in the previous equation will yield \( n^{-1} \) terms, while the variance of \( \hat{w}_2 \) is again Poisson in terms of the number of pairs. Finally, the convergence properties are expected to be similar to the Poisson process, although
we have not performed the calculations.

It is worth to emphasize again that, while both are two-point measures, \( w \) and \( K \) are slightly different objects. In astrophysics \( w \) is the desired quantity, but in some cases \( K \) might be more advantageous; then Ripley’s \( \hat{K}_2 \) is still the preferred estimator. Clearly, these findings remain true for \( N > 2 \) as well.

4. Summary

In summary we have calculated the variance of a new class of estimators \( \hat{w}_N \) for the \( N \)-point correlation functions for Poisson and binomial point processes. The results were compared with variances concerning a different class of estimators based on the \( K \) function. The main difference is that \( \hat{w}_N \) estimates the \( N \)-point correlation function of the fluctuations of the point process, while \( \hat{K}_i \) estimate the (cumulative) moments of the full point process. This property apparently renders the edge effect correction in \( \hat{w}_N \) exact, leaving only the Poissonian contribution to the variance in terms of \( N \)-tuplets, i.e. terms \( \propto 1/\lambda^N \), or \( 1/(\binom{n}{N}) \) for Poisson and binomial processes, respectively. All lower order terms, dominating for sparse processes, exactly cancel. This is not true for any of the estimators for \( K \), although the best ones achieve a significant suppression of the offending non-Poisson terms at the price of boosting the constant factor multiplying the Poisson terms with respect to \( \hat{K}_0 \), the naive estimator. The speed of convergence was calculated for the new estimator \( \hat{w}_N \), which assumed an auxiliary Poisson process \( R \), with the average \( \rho \rightarrow \infty \). The leading order non-Poisson term in the variance was found to be suppressed by a large factor \( \lambda/\rho N \), thus the convergence is controllable in practice when \( \rho \) is finite.

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