NUMERICAL AND ANALYTICAL COMPUTATION OF SOME SECOND-ORDER CHARACTERISTICS OF SPATIAL POISSON–VORONOI TESSELLATIONS

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We describe and discuss the explicit calculation of the pair correlation function of the point process of nodes associated with a three-dimensional stationary Poisson–Voronoi tessellation. Moreover, the precise asymptotics for the variance of the number of nodes in an expanding region and the variance of the number of vertices of the typical Poisson–Voronoi polyhedron are obtained. This gives rise to an asymptotically exact confidence interval for the number of nodes and cells when the sampling region is large enough. A geometric interpretation of our formulae shows that, among others, an essential problem is to calculate the mean volume of a tetrahedron whose vertices are uniformly distributed on a circular domain of the unit sphere.

Keywords: Stationary Poisson point process; Voronoi and Delaunay tessellation; point process of nodes; pair correlation function; typical Voronoi polyhedron; mean volume of a tetrahedron; asymptotic confidence interval

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1. BASIC DEFINITIONS AND PRELIMINARIES

Throughout in this paper we are concerned with Voronoi (or Dirichlet, or Thiessen) tessellations $V_x(\Psi) = \{C_i(\Psi), i \geq 0\}$ of the three-dimensional Euclidean space $\mathbb{R}^3$ generated by a stationary spatial Poisson
process $\Psi = \sum_{i \geq 0} \delta_{X_i}$ of intensity $\lambda$. Here $\delta_x(\cdot) = 1_A(x)$ denotes the Dirac measure concentrated in $x \in \mathbb{R}^3$ and $\Psi$ is a locally finite random counting measure over a hypothetical probability space $\mathcal{F}, \mathcal{U}, P$ acting on $\mathbb{R}^3$ and satisfying the well-known properties that the number $\Psi(B)$ of atoms (called nuclei in what follows) in a Borel set $B \subset \mathbb{R}^3$ with Lebesgue measure $|B|$ has a Poisson distribution with parameter $\lambda|B|$; and, if $B_1, \ldots, B_k$ are disjoint such subsets, $\Psi(B_1), \ldots, \Psi(B_k)$ are mutually independent, see [5].

A cell $C_i(\Psi)$ of the spatial Poisson-Voronoi tessellation (briefly: PVT) is defined to be the set of all points in $\mathbb{R}^3$ which are closest to the nucleus $X_i$, i.e.,

$$C_i(\Psi) = \{x \in \mathbb{R}^3 : \|x - X_i\| < \|x - X_j\|, j \neq i\},$$

($\|\cdot\|$ = Euclidean norm).

By this construction the cells $C_i(\Psi)$, $i \geq 0$ form a countable family of pairwise disjoint, space-filling random (open) convex polyhedra, where the Lebesgue null set of cell boundaries $\partial V_\lambda(\Psi) = \bigcup_{i \geq 0} \partial C_i(\Psi)$ is a stationary random closed set consisting of the polygonal faces, the edges and vertices of the cells. Such divisions of the space turn up in several fields of application like material sciences (crystallization of metals), pattern recognition, statistical data analysis, numerical interpolation, and many other subjects.

Geometrical properties of general $d$-dimensional (not necessarily Poisson-) Voronoi tessellations are studied in [11, 19, 20, 25 and 27]. In several papers R. E. Miles and his co-workers developed basic techniques and derived many fundamental results for (mostly planar) PVT's, see e.g. [15, 18]. For recent results on distributional properties related to the typical cell we refer to [21, 22, 23]. Large-scale simulations of planar and spatial PVT's are suitable to find good numerical approximations of their moment and distributional characteristics, see e.g. [1, 9, 13 and 7]. Relationships between mean values of stationary (not necessary Voronoi) tessellations and characteristics of the corresponding typical cell are well-studied in great generality, see [14, 26, 19 and 27], while second-order quantities (such as product densities of the nodes (= vertices of cells) and the associated geometrical point processes of edges and facets) were rarely investigated so far, see [6, 11 and 4]. Variances and covariances of some characteristics of the typical 2-D and 3-D Poisson-Voronoi cell
were determined by numerical integration in two unpublished papers by K. A. Brakke [2, 3].

For further details and the historical background the reader is referred to the monographs [20], Okabe et al. [25] and Stoyan et al. [27] (in particular Chapter 10 and references therein).

It is well-known that a spatial PVT is normal, that is each edge resp. vertex lies in the boundaries of three resp. four cells for \( \mathbb{P} \)-almost all realizations of \( \Psi \).

Closely connected with a spatial PVT \( V_\lambda(\Psi) \) is its associated spatial Poisson–Delaunay tessellation \( D_\lambda(\Psi) = \{ C_i^*(\Psi), i \geq 0 \} \); each cell \( C_i^*(\Psi) \) is a random tetrahedron the four vertices of which are atoms of the Poisson process \( \Psi \) such that its circumball contains no further atom of \( \Psi \). By definition of the PVT, the circumcentre of the Delaunay cell \( C_i^*(\Psi) \) is a vertex of \( V_\lambda(\Psi) \) that belongs to the four Voronoi cells generated by the vertices of \( C_i^*(\Psi) \). In this way the point process \( \Psi_{V,\lambda} \) of the nodes of \( V_\lambda(\Psi) \) coincides (\( \mathbb{P}\)-a.s.) with the set of circumcentres of the associated Delaunay cells.

The main goal of this paper is to calculate the pair correlation function \( g_{V,\lambda}(r) \) of the point process \( \Psi_{V,\lambda} \) of nodes of the 3-D PVT \( V_\lambda(\Psi) \) by numerical integration of a set of multiple parameter integrals derived in [10, 11] for any dimension \( d \geq 2 \).

Furthermore, the asymptotic variance \( \sigma_{V,\lambda}^2 = \lim_{n \to \infty} \text{Var} \Psi_{V,\lambda}(0, n^3)/n^3 \) and the variance \( \text{Var}(N_0) \) of the number of vertices of the typical Poisson–Voronoi cell are obtained by numerical evaluation of integral formulae also proved in [10] for any \( d \geq 2 \). Note that \( \text{Var}(N_0) \) was already calculated in [2]; unfortunately, the sketch of the formulae and procedures used there is very condensed but apparently Brakke's way is quite different from ours.

The paper is organized as follows. In Section 2 we are concerned with the mean volume of a tetrahedron whose vertices are independent uniformly distributed on a circular domain on the unit sphere \( S^2 \) in dependence of its spherical radius. As pointed out in [10, 11], this is the key to determine \( g_{V,\lambda}(r) \) and, on the other hand, this integral-geometric problem seems to be of interest in itself. Sections 3 and 4 are devoted to a detailed interpretation and calculation of \( g_{V,\lambda}(r) \) for \( \lambda = 1 \). Section 5 gives as asymptotic confidence interval for the intensity of nodes resp. of cells for which the variance \( \sigma_{V,\lambda}^2 \) is needed. As a by-product the variance \( \text{Var}(N_0) \) is evaluated.
2. MEAN VOLUME OF A TETRAHEDRON WITH UNIFORMLY DISTRIBUTED VERTICES ON $S^2$

First let us represent the points on the 3-D unit sphere $S^2$ by spherical coordinates $(\theta, \vartheta)$ as follows: $s(\theta, \vartheta) = (\sin \theta \sin \vartheta, \cos \theta \sin \vartheta, \cos \theta)$ for $-\pi \leq \theta \leq \pi, 0 \leq \vartheta \leq \pi$.

An orientation-preserving rotation of $S^2$ which shifts $s(0, 0)$ to $s(\theta, \vartheta)$ can be represented by the following orthogonal matrix $R(\theta, \vartheta)$:

$$R(\theta, \vartheta) = \begin{pmatrix} \cos \theta & \sin \theta \cos \vartheta & \sin \theta \sin \vartheta \\ -\sin \theta & \cos \theta \cos \vartheta & \cos \theta \sin \vartheta \\ 0 & -\sin \vartheta & \cos \vartheta \end{pmatrix}$$

From linear algebra it is well-known that the volume $V(x_1, x_2, x_3, x_4)$ of a tetrahedron spanned by four points $x_i = (x_i^{(1)}, x_i^{(2)}, x_i^{(3)}) \in \mathbb{R}^3, (i = 1, 2, 3)$ can be calculated by the formula

$$V(x_1, x_2, x_3, x_4) = \frac{1}{6} \left| \det \begin{pmatrix} 1 & x_1^{(1)} & x_1^{(2)} & x_1^{(3)} \\ x_2^{(1)} & x_2^{(2)} & x_2^{(3)} \\ x_3^{(1)} & x_3^{(2)} & x_3^{(3)} \\ x_4^{(1)} & x_4^{(2)} & x_4^{(3)} \end{pmatrix} \right|.$$

For later applications to second-order characteristics of a spatial PVT we need to compute the parameter integral

$$J_0(\alpha) = \int_{[0, \pi]^4} \int_{[-\pi, \pi]^4} \left| \det \begin{pmatrix} 1 & s(\phi_1, \varphi_1) \\ \vdots & \vdots \\ 1 & s(\phi_4, \varphi_4) \end{pmatrix} \right| \prod_{i=1}^{4} \sin \varphi_i \, d(\phi_1, \ldots, \phi_4) \times d(\varphi_1, \ldots, \varphi_4).$$

for $0 \leq \alpha \leq \pi$.

First note that, if we replace the cube $[\alpha, \pi]^4$ in the latter integral by the cube $[0, \alpha]^4$, the corresponding integral coincides with $J_0(\pi - \alpha)$. The function $J_0(\pi - \alpha)$ has an obvious probabilistic interpretation; it is equal (up to the norming factor $6 (2\pi (1 - \cos \alpha))^4$) to the mean volume $V(\alpha)$ of a tetrahedron whose vertices are independent and uniformly distributed on the “cap” $S^2(\alpha) = \{s(\theta, \vartheta): -\pi \leq \theta \leq \pi, 0 \leq \vartheta \leq \alpha\}$ of
the 3-D unit sphere, i.e.,

$$V(\alpha) = \frac{J_0(\pi - \alpha)}{6(2\pi (1 - \cos \alpha))^4}.$$ 

In the particular case $\alpha = \pi$ (i.e., the four vertices are uniformly distributed on the entire sphere $S^2$) the problem was solved (even for $d$-simplices in any dimension $d \geq 2$ with $d + 1$ independent and uniformly distributed vertices on $S^{d-1}$) by R. E. Miles in [16], see also Møller [20]. For $d = 3$ the general formula yields

$$V(\pi) = \frac{J_0(0)}{6(4\pi)^4} = \frac{4\pi}{105} \approx 0.11968.$$ 

It should be noted that in the planar case an explicit expression for the mean area $A(\alpha)$ of a triangle whose three vertices are independent and uniformly distributed on $S^1(\alpha) = \{(\sin \theta, \cos \theta): -\alpha \leq \theta \leq \alpha\}$ was derived in [11]:

$$A(\alpha) = \frac{3}{2\alpha^3}(\alpha^2 + \alpha \sin \alpha \cos \alpha - 2 \sin^2 \alpha) \quad \text{for} \quad 0 \leq \alpha \leq \pi.$$ 

For $d \geq 3$ such elementary solution seems to be quite impossible. The severest obstacle in evaluating the integral $J_0(\alpha)$ is that there is no possibility to factorize the inner determinant in an appropriate way in order to carry out the multiple integration over the absolute value of the determinant. So we have to resort to numerical integration procedures after reducing the number of integrals in the expression $J_0(\alpha)$ to a minimum.

For doing this an important step towards simplification is based on the following integral transformation:

**Lemma 1** (Miles [17]) Let $f: S^2 \times S^2 \times S^2 \to [0, \infty)$ be a measurable function. Then

$$\int_{[-\pi, \pi]^3} \int_{[0, \pi]^3} f(s^T(\phi_1, \varphi_1), s^T(\phi_2, \varphi_2), s^T(\phi_3, \varphi_3)) \times$$

$$\times \prod_{i=1}^3 \sin \varphi_i d(\varphi_1, \varphi_2, \varphi_3) d(\phi_1, \phi_2, \phi_3)$$
\[
\int_{\theta} \int_{\phi} \int_{\theta_1} \int_{\phi_1} \int_{\theta_2} \int_{\phi_2} \int_{\theta_3} \int_{\phi_3} \int_{\phi_4} \int_{\phi_5} \int_{\phi_6} f(R(\phi, \varphi)s^T(\theta_1, \tau), R(\phi, \varphi)s^T(\theta_2, \tau) , R(\phi, \varphi)s^T(\theta_3, \tau)) \times \sin^3 \tau \sin \varphi \sigma(\theta_1, \theta_2, \theta_3) d\tau d\varphi d\phi d\theta_1 d\theta_2 d\theta_3
\]

where

\[
\sigma(\theta_1, \theta_2, \theta_3) = \left| \begin{array}{ccc}
1 & \sin \theta_1 & \cos \theta_1 \\
1 & \sin \theta_2 & \cos \theta_2 \\
1 & \sin \theta_3 & \cos \theta_3 \\
\end{array} \right| = 4 \sin \frac{\theta_2 - \theta_1}{2} \sin \frac{\theta_3 - \theta_1}{2} \sin \frac{\theta_3 - \theta_2}{2}
\]

Since the volume of a tetrahedron is invariant under rotation and

\[
I_{\theta_1}(\varphi_i) = I_{\theta_2}(\varphi_i) = I_{\theta_3}(\varphi_i) = I_{\theta_4}(\varphi_i), \quad i = 1, 2, 3,
\]

the integral \( J_0(\alpha) \) is equal to

\[
2\pi \int_{\alpha}^{\pi} \int_{[-\pi, \pi]^3} \int_{[0, \pi]^3} \left| \begin{array}{ccc}
1 & s(\phi_1, \varphi_2) \\
1 & s(\phi_2, \varphi_2) \\
1 & s(\phi_3, \varphi_3) \\
1 & s(0, \varphi_0) \\
\end{array} \right| \prod_{i=1}^{3} (\sin \varphi_i I_{[-1, \cos \alpha]}(\cos \varphi_i)) \times d(\varphi_1, \varphi_2, \varphi_3) d(\phi_1, \phi_2, \phi_3) \sin \varphi_0 d\varphi_0.
\]

In order to evaluate the inner six-fold integral we apply Lemma 1 to the function

\[
f(x_1^T, x_2^T, x_3^T) = \left| \begin{array}{ccc}
1 & x_1^T \\
1 & x_2^T \\
1 & x_3^T \\
\end{array} \right| \prod_{i=1}^{3} I_{[-1, \cos \alpha]}(x_i^{(3)}).
\]

Since \( R(\phi, \varphi) \) is an orthogonal matrix we can verify the identity

\[
\left| \begin{array}{ccc}
1 & 1 & 1 \\
R(\phi, \varphi)s^T(\theta_1, \tau) & R(\phi, \varphi)s^T(\theta_2, \tau) & R(\phi, \varphi)s^T(\theta_3, \tau) \\
1 & 1 & 1 \\
\end{array} \right| = \left| \begin{array}{ccc}
1 & 1 & 1 \\
1 & 1 & 1 \\
R(\phi, \varphi)s^T(\theta_1, \tau) & R(\phi, \varphi)s^T(\theta_2, \tau) & R(\phi, \varphi)s^T(0, \varphi_0) \\
\end{array} \right| = \sin^2 \tau |\cos \phi \sin \varphi \sin \varphi_0 + \cos \varphi \cos \varphi_0 - \cos \tau | \sigma(\theta_1, \theta_2, \theta_3).
\]

This identity and Lemma 1 together with \( (R(\phi, \varphi)s^T(\theta_1, \tau))_3 = \cos \varphi \times \cos \tau - \cos \theta_1 \sin \varphi \sin \tau \) (where \( (\cdot)_3 \) denotes the projection on the third
component of (·)) lead to

\[ J_0(\alpha) = 2\pi \int_{\alpha}^{\pi/2} \int_{0}^{\pi/2} \int_{0}^{\pi} \left| \cos \phi \sin \phi \sin \phi_0 + \cos \phi \cos \phi_0 - \cos \tau \right| \times \]
\[ \times T(\alpha, \phi, \tau) \sin^5 \tau \sin \phi \sin \phi_0 \times \]
\[ \times d\phi \ d\phi \ d\tau \ d\phi_0, \]

where

\[ T(\alpha, \phi, \tau) = \frac{3}{\prod_{i=1}^{3} \left| \cos \phi \cos \tau - \cos \theta_i \sin \phi \sin \tau \right| \ d(\theta_1, \theta_2, \theta_3).} \]

The latter integral can be given in closed form. For this purpose we introduce the function

\[ S(\gamma) = \int_{\gamma, \gamma}^{\gamma, \gamma} \sigma^2 (\theta_1, \theta_2, \theta_3) d(\theta_1, \theta_2, \theta_3) = 12 \gamma^3 - \]
\[ 3 \gamma \sin^2 2 \gamma - 24 \gamma \sin^2 \gamma + 12 \sin 2 \gamma \sin^2 \gamma. \]

for \(0 \leq \gamma \leq \pi\). Since \(\sigma(\theta_1, \theta_2, \theta_3)/2\) equals the area of a triangle spanned by the points \((\sin \theta_i, \cos \theta_i), i = 1, 2, 3\), the function \(S(\alpha)/32 \alpha^3\) is just the second moment of the area of a triangle whose three vertices are independently and uniformly distributed on \(S^1(\alpha) = \{(\sin \theta, \cos \theta) : -\alpha \leq \theta \leq \alpha\}\).

By elementary manipulations it is easily verified that

\[ \mathbf{1}_{[-1, \cos \alpha]} (\cos \phi \cos \tau - \cos \theta_i \sin \phi \sin \tau) \]
\[ = \begin{cases} 
0 & \text{if } \cos (\phi + \tau) \geq \cos \alpha \\
1 & \text{if } \cos (\phi - \tau) \leq \cos \alpha \\
1 & \text{if } \frac{\cos \phi \cos \tau - \cos \alpha}{\sin \phi \sin \tau} < \cos \theta_i.
\end{cases} \]

In the most relevant third case the angle \(\theta_i\) moves in the open interval \((0, \pi)\). This gives

\[ T(\alpha, \phi, \tau) \]
\[ = \begin{cases} 
0 & \text{if } 0 \leq \phi + \tau \leq \alpha \text{ or } 2\pi - \alpha \leq \phi + \tau \\
12 \pi^3 & \text{if } |\phi - \tau| \geq \alpha \\
S \left( \arccos \left( \frac{\cos \phi \cos \tau - \cos \alpha}{\sin \phi \sin \tau} \right) \right) & \text{otherwise.}
\end{cases} \]
Since \((s(\phi, \varphi_0) \cdot R(0, \varphi))_3 = \cos \phi \sin \varphi \cdot \sin \varphi_0 + \cos \varphi \cdot \cos \varphi_0\) and \((s(\phi, \varphi_0))_3 = \cos \varphi_0\), we obtain by substituting \(s(\phi, \varphi_0) = s(\phi_1, \varphi_1) \cdot R(0, \varphi))_3 = \cos \varphi \cdot \cos \varphi_1 - \sin \varphi \cdot \sin \varphi_1 \cdot \cos \varphi_1\) that

\[
J_0(\alpha) = 2\pi \int_0^\pi \int_0^{\pi/2} \int_0^\pi \int_0^\pi I_{[-1,\cos \alpha]}(\cos \varphi \cdot \cos \varphi_1 - \\
\sin \varphi \cdot \sin \varphi_1 \cdot \cos \varphi_1) \times \\
\times |\cos \varphi - \cos \tau| T(\alpha, \varphi, \tau) \sin^5 \tau \sin \varphi \sin \varphi_1 \, d\varphi \, d\phi_1 \, d\tau \, d\varphi_1.
\]

Clearly, the integration w.r.t. \(\phi_1\) can be carried out. Finally, summarizing the above formulae we arrive at

**Lemma 2** We have

\[
J_0(\alpha) = 2\pi \int_0^\pi \int_0^{\pi/2} \int_0^\pi |\cos \psi - \cos \tau| T(\alpha, \varphi, \tau) \times \\
U(\alpha, \varphi, \psi) \sin^5 \tau \sin \varphi \sin \psi \, d\tau \, d\varphi \, d\psi,
\]

where \(T(\alpha, \varphi, \tau)\) is defined by (2.1) and

\[
U(\alpha, \varphi, \psi) = \int_{-\pi}^{\pi} I_{[-1,\cos \alpha]}(\cos \varphi \cdot \cos \psi - \sin \varphi \cdot \sin \psi \cdot \cos \varphi_1) \, d\phi_1
\]

\[
= \begin{cases} 
0 & \text{if } 0 \leq \varphi + \psi \leq \alpha \text{ or } 2\pi - \alpha \leq \varphi + \psi \\
2\pi & \text{if } |\varphi - \psi| \geq \alpha \\
2 \arccos \left( \frac{\cos \varphi \cdot \cos \psi - \cos \alpha}{\sin \varphi \cdot \sin \psi} \right) & \text{otherwise.}
\end{cases}
\]

Numerical integration results for the three-fold integral in Lemma 2 and the plot of the function \(\tilde{V}(\alpha) = J_0(\pi - \alpha)/(96\pi^4(1 - \cos \alpha)^4)\) are presented in Table I and Figure 1, respectively.

**3. ADDITIVE DECOMPOSITION OF THE PAIR CORRELATION FUNCTION OF NODES IN A SPATIAL POISSON–VORONOI TESSELLATION**

The pair correlation function \(g(r), r > 0\), of an arbitrary second-order stationary point process \(\Phi = \sum_{i \geq 0} \delta_{Y_i}\) with intensity \(\lambda > 0\) can be
TABLE I

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<td>3.1416</td>
<td>0.1196</td>
</tr>
</tbody>
</table>

FIGURE 1 Plot of the function $\tilde{V}(\alpha)$. 
explained as the limit

\[
g(r) = \lim_{\epsilon \to 0} \frac{\mathbb{E}(\Phi(b(o, r + \epsilon) \setminus b(o, r))|\Phi(\{o\}) > 0)}{\mathbb{E}(b(o, r + \epsilon) \setminus b(o, r))} = \lim_{\epsilon \to 0} \frac{\mathbb{P}(\Phi(b(o, r + \epsilon) \setminus b(o, r)) > 0 | \Phi(\{o\}) > 0)}{\lambda |b(o, r + \epsilon) \setminus b(o, r)|}. \tag{3.1}
\]

A rigorous definition of the conditional probability and conditions for the existence of the right-hand limits can be found in [5] and [27]. Loosely spoken, \( \lambda g(r) \) characterizes the frequency or, more correctly, the density of pairs \((Y_i, Y_j)\) of \(\Phi\) with a distance \(\|Y_i - Y_j\| = r\). In case \(\Phi\) is additionally isotropic, \(g(\cdot)\) and \(\lambda\) describe the second-order properties of \(\Phi\) completely.

In [10] a general representation formula for the pair correlation function of the point process of vertices of a \(d\)-dimensional PVT was proved. In the planar case the parameter integrals occurring in this formula could be calculated in [0] by comparatively simple numerical procedures while the computational expenditure grows drastically in higher dimensions. By the scale transformation

\[
g_{\nu, \lambda}(r) = g_\nu(\lambda^{1/3} r) \quad \text{for} \quad r > 0 \tag{3.2}
\]

we only need to consider the standard case \(\lambda = 1\), where the index \(\lambda\) is omitted.

**Theorem 1** (see [10, 11]). The pair correlation function \(g_\nu\) of the point process of vertices (or nodes) induced by a spatial PVT \(V(\Psi)\) of unit intensity takes the form

\[
g_\nu(r) = \frac{g_0^*(r) + g_0(r)}{576} + \frac{g_1(r)}{36} + \frac{g_2(r)}{8} + \frac{g_3(r)}{6} \quad \text{for} \quad r > 0, \tag{3.3}
\]

where the functions \(g_0(r), \ldots, g_3(r)\) are multiple parameter integrals given by

\[
g_j(r) = \left(\frac{35}{96\pi^2}\right)^2 \left(\frac{r^3}{4}\right)^{6-j} \int_1^\infty \int_0^1 \exp\{-r^3 \nu(\rho_1, \rho_2)\} \left(\rho_2^2 - \rho_1^2\right)^{8-j} \Delta_j(\rho_1, \rho_2) \, d\rho_1 \, d\rho_2,
\]
where

\[
\nu(\rho_1, \rho_2) = |b(o, (\rho_1 + \rho_2)/2) \cup b(x, (\rho_2 - \rho_1)/2)| \quad \text{with} \quad \|x\| = 1
\]

\[
= \frac{\pi}{12} (2\rho_2(3\rho_1^2 + \rho_2^2) + 3(\rho_1^2 + \rho_2^2 + \rho_1^2 \rho_2^2) - 1)
\]

and the functions \(g_0^*(r)\) has the relatively simple form

\[
g_0^*(r) = 288 \int_0^4 r^3 f \left( \left[ \left( \frac{4\pi}{3} \right)^{1/3} r - \rho^{1/3} \right] \right) e^{-\rho} \rho^2 d\rho \quad (3.4)
\]

where \(f(x) = 1 - e^{-x} (1 + x + (x^2/2))\). Furthermore, \(\Delta_0(\rho_1, \rho_2) = J_0(\alpha(\rho_1, \rho_2)) J_0(\alpha(-\rho_1, \rho_2))\) and, for \(j = 1, 2, 3\), the functions \(\Delta_j(\cdot, \cdot)\) are defined by

\[
\Delta_j(\rho_1, \rho_2) = \int_{[-\pi, \pi]^j} J_j(\alpha(\rho_1, \rho_2), \psi_1, \ldots, \psi_j) J_j(\alpha(-\rho_1, \rho_2), \psi_1, \ldots, \psi_j) d(\psi_1, \ldots, \psi_j),
\]

where the angles \(\alpha(\pm\rho_1, \rho_2) = \arccos[(1 \pm \rho_1 \rho_2)/(\rho_2 \pm \rho_1)]\) lies in the interval \([0, \pi]\) and

\[
\cos \alpha(\rho_1, \rho_2) = \frac{1 + \rho_1 \rho_2}{\rho_2 + \rho_1} \quad \text{and} \quad \sin \alpha(\rho_1, \rho_2) = \frac{\sqrt{(1 - \rho_1^2)(\rho_2^2 - 1)}}{\rho_2 + \rho_1}.
\quad (3.5)
\]

The function \(J_0(\alpha)\) is that studied in Section 2 and the other \(J_j\)'s are defined in a similar way:

\[
J_1(\alpha, \psi_1) = \int_{[-\pi, \pi]^3} \int_{[\tau, \pi]^3} \left| \det \begin{pmatrix} 1 & s(\phi_1, \varphi_1) \\ 1 & s(\phi_2, \varphi_2) \\ 1 & s(\phi_3, \varphi_3) \end{pmatrix} \right| \times \\
\prod_{i=1}^{3} \sin \varphi_i \ d(\varphi_1, \varphi_2, \varphi_3) \ d(\phi_1, \phi_2, \phi_3)
\]
\[ J_2(\alpha, \psi_1, \psi_2) = \int_{[\alpha, \pi]^2} \int_{[-\pi, \pi]^2} \det \begin{pmatrix} 1 & s(\phi_1, \varphi_1) \\ 1 & s(\phi_2, \varphi_2) \\ 1 & s(\psi_1, \alpha) \\ 1 & s(\psi_2, \alpha) \end{pmatrix} \begin{vmatrix} \sin \varphi_1 & \sin \varphi_2 \\ d(\varphi_1, \varphi_2) & d(\phi_1, \phi_2) \end{vmatrix} \]

\[ J_3(\alpha, \psi_1, \psi_2, \psi_3) = \int_{[\alpha, \pi]} \int_{[-\pi, \pi]} \det \begin{pmatrix} 1 & s(\phi_1, \varphi_1) \\ 1 & s(\psi_1, \alpha) \\ 1 & s(\psi_2, \alpha) \\ 1 & s(\psi_3, \alpha) \end{pmatrix} \begin{vmatrix} \sin \varphi_1 & \sin \varphi_2 \\ d(\varphi_1, \varphi_2) & d(\phi_1, \phi_2) \end{vmatrix} \]

**Remark** Keeping in mind the statistical interpretation of the limits in (3.1), one can explain the geometrical meaning of the summands in (3.3). Up to the normalizing constant, \( g_j(r) \) equals the density of pairs of nodes of the PVT \( V(\Psi) \) with distance \( r \) which are circumcentres of two neighbouring Delaunay cells with exactly \( j \) common vertices, \( j = 1, 2, 3 \). Correspondingly, for \( j = 0 \) (that is, the two Delaunay cells are not adjacent) we distinguish between intersecting and disjoint circumballs leading to \( g_0(r) \) and \( g_0^*(r) \), respectively.

By some algebraic manipulations or simply by the fact that the volume is rotation-invariant one confirms without difficulties that \( J_1(\alpha, \psi_1) = J_1(\alpha, 0) \), \( J_2(\alpha, \psi_1, \psi_2) = J_2(\alpha, 0, \psi_2-\psi_1) \) and \( J_3(\alpha, \psi_1, \psi_2, \psi_3) = J_3(\alpha, 0, \psi_2-\psi_1, \psi_3-\psi_1) \) for any \(-\pi \leq \psi_1, \psi_2, \psi_3 \leq \pi \). For convenience we omit the \( \psi_1 \)-component and obtain

\[
\Delta_1(\rho_1, \rho_2) = 2\pi J_1(\alpha(\rho_1, \rho_2)) J_1(\alpha(-\rho_1, \rho_2))
\]

\[
\Delta_2(\rho_1, \rho_2) = 2\pi \int_{-\pi}^{\pi} J_2(\alpha(\rho_1, \rho_2), \psi) J_2(\alpha(-\rho_1, \rho_2), \psi) d\psi
\]

\[
\Delta_3(\rho_1, \rho_2) = 2\pi \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} J_3(\alpha(\rho_1, \rho_2), \psi, \varphi) J_3(\alpha(-\rho_1, \rho_2), \psi, \varphi) d\psi d\varphi.
\]

Taking into account the geometric-statistical interpretation of the integral \( J_0(\alpha) \) in the fore-going section, the quantity \( J_j(\alpha, \psi_1, \ldots, \psi_j) \) \((j = 1, 2, 3)\) is nothing but (up to a norming factor depending on \( \alpha \)) the conditional mean value of the volume of a tetrahedron spanned by \( 4-j \) uniformly distributed vertices on \( S^2 \setminus S^2(\alpha) \) and given \( j \) vertices \( s(\psi_1, \alpha), \ldots, s(\psi_j, \alpha) \).
This interpretation suggests in particular for \( j = 3 \) how to evaluate the integral \( J_3(\alpha, \psi, \varphi) \). Having in mind the volume interpretation of the above determinants or formally by applying well-known transformation rules for determinants we recognize that

\[
\begin{vmatrix}
1 & s(\phi_1, \varphi_1) \\
1 & s(\psi, \alpha) \\
1 & s(\varphi, \alpha)
\end{vmatrix} = \sin^2 \alpha (\cos \alpha - \cos \varphi_1) \begin{vmatrix}
1 & \sin \psi \cos \psi \\
1 & \sin \varphi \cos \varphi \\
1 & 0
\end{vmatrix},
\]

for \( \alpha \leq \varphi_1 \leq \pi \) and any \(-\pi \leq \phi_i \leq \pi\), whence, since the determinant on the rhs equals \( \sigma(\psi, \varphi, 0) \), it follows by the definition of the function \( S(\gamma) \) in Section 2 that

\[
\Delta_3(\rho_1, \rho_2) = 4\pi^2 S(\pi) \sin^2 \alpha(\rho_1, \rho_2) \sin^2 \alpha(-\rho_1, \rho_2) I(\rho_1, \rho_2) I(-\rho_1, \rho_2),
\]

where, by (3.5),

\[
I(\rho_1, \rho_2) = \int_0^\pi (\cos \alpha(\rho_1, \rho_2) - \cos \varphi_1) \sin \varphi_1 \, d\varphi_1 = \frac{(1 + \cos \alpha(\rho_1, \rho_2))^2}{2}.
\]

Finally, by \( S(\pi) = 12\pi^3 \) and (3.5),

\[
\Delta_3(\rho_1, \rho_2) = 12\pi^5(1 - \rho_1^2)^4 (1 + \rho_2)^4 (\rho_2^2 - 1)^2 (\rho_2^2 - \rho_1^2)^{-4}. \quad (3.6)
\]

For later applications in Section 5 we are interested in the limits \( \gamma_j = \lim_{r \to 1} r^{j-1} g_j(r) \) and the integrals \( I_j = \int_0^\infty g_j(r) \, r^2 \, dr \) for \( j = 0, 1, 2, 3 \).

**Lemma 3** We have

\[
\gamma_j = \frac{2}{3} \left( \frac{35}{24 \pi^2} \right)^2 \left( \frac{3}{4 \pi} \right)^{(17-2j)/3} \Gamma \left( \frac{17 - 2j}{3} \right) \int_0^1 \Delta_j(\rho, \infty) \, d\rho \quad (3.7)
\]

\[
I_j = \frac{(6 - j)!}{12} \left( \frac{35}{24 \pi^2} \right)^2 \int_0^\infty \int_1^1 \frac{(\rho_2^2 - \rho_1^2)^{8-j}}{(4 \nu(\rho_1, \rho_2))^{7-j}} \Delta_j(\rho_1, \rho_2) \, d\rho_1 \, d\rho_2 \quad (3.8)
\]
for \( j = 0,1,2,3 \). In particular,
\[
\gamma_3 = \frac{700}{81 \pi^2} \Gamma\left(\frac{2}{3}\right) \left(\frac{3}{4 \pi}\right)^{2/3} \approx 0.45624 \quad \text{and} \quad \lim_{r \to 0^+} r^2 g(r) = \frac{\gamma_3}{6} \approx 0.07604.
\]

In order to proof (3.8) we first integrate the integrand of the double integral \( g_j(r) \) from Theorem 1 multiplied by \( r^2 \) and use then that
\[
\int_0^\infty e^{-a r^3} r^{2a-3} dr = \frac{(6-a)!}{3} a^{j-7} \quad \text{for} \quad a > 0.
\]

4. COMPUTATION OF THE PAIR CORRELATION FUNCTION OF NODES

4.1. The Functions \( g_0(r) \) and \( g_0^\#(r) \)

From Theorem 1 it follows directly that
\[
g_0(r) = r^{18} \left(\frac{35}{6144 \pi^2}\right)^2 \int_0^\infty r^1 \int_0^1 \exp\{-r^3 \nu(\rho_1, \rho_2)\} (\rho_2^2 - \rho_1^2)^5 \times 
\]
\[\times J_0(\alpha(\rho_1, \rho_2)) J_0(\alpha(-\rho_1, \rho_2)) d\rho_1 d\rho_2.
\]

Using the highly precise numerical integration results for the function \( J_0(\alpha) \), a second numerical double integration based on suitable Gauss quadrature formulae is applied to obtain \( g_0(r) \) for a sufficiently dense grid of \( r \)-values in \([0, 3]\). Figure 2 at the end of Section 4 presents the graph of \( g_0(r)/576 \) in \([0, 3]\) calculated for \( r_k = k \cdot 10^{-2}, k = 1, \ldots, 300 \).

The integrals on the rhs of (3.7) and (3.8) for \( j = 0 \) can be evaluated analogously giving
\[
I_0 \approx 495.977
\]
\[
\gamma_0 = \frac{11}{2 \pi^3} \left(\frac{35}{24 \pi^2}\right)^3 \left(\frac{3}{4 \pi}\right)^{2/3} \Gamma\left(\frac{2}{3}\right) \times \int_0^{\pi/2} J_0(\alpha) J_0(\pi - \alpha) \sin \alpha d\alpha 
\]
\[
\approx 2.9819 \cdot 10^{-4} \times 92908.95 \approx 27.7045.
\]
The function $g_0^*(r)$ defined by (3.4) can be rewritten as follows:

$$
g_0^*(r) = f(R) - \frac{3}{2} R^2 e^{-R/4} \int_0^1 e^{-3R^3x^2} dx \\
\times \left(1 + R(1 - x)^3 + \frac{R^2}{2} (1 - x)^6\right) dx,$$

where $R = 4\pi r^3/3$. Furthermore, the integral on the rhs can be expressed as linear combination of incomplete $\Gamma$-functions which are available in MATHEMATICA. This facilitates to determine $g_0^*(r)/576$ in Figure 2.

4.2. The Function $g_1(r)$

Since $\Delta_1(\rho_1, \rho_2) = 2\pi J_1(\alpha(\rho_1, \rho_2)) J_1(\alpha(-\rho_1, \rho_2))$, we may write

$$
g_1(r) = r^{15} 2\pi \left(\frac{35}{3072 \pi^2}\right)^2 \int_0^\infty \int_0^1 \exp\{-r^3\nu(\rho_1, \rho_2)\} (\rho_2^2 - \rho_1^2)^7 \times \\
\times J_1(\alpha(\rho_1, \rho_2)) J_1(\alpha(-\rho_1, \rho_2)) d\rho_1 d\rho_2.
$$

The inner integral $J_1(\alpha)$ can be treated in a similar way as $J_0(\alpha)$ in Section 2 which gives

$$
J_1(\alpha) = \int_{[-\pi, \pi]^3} \int_{[-\pi, \pi]^3} \left| \begin{array}{ccc}
1 & s(\phi_1, \varphi_1) \\
1 & s(\phi_2, \varphi_2) \\
1 & s(\phi_3, \varphi_3) \\
1 & s(0, \alpha)
\end{array} \right| \\
\prod_{i=1}^3 \sin \varphi_i d(\varphi_1, \varphi_2, \varphi_3) d(\phi_1, \phi_2, \phi_3) \\
= \int_0^{\pi/2} \int_{-\pi}^{\pi} \int_0^\pi |\cos \phi \sin \varphi \sin \alpha + \cos \varphi \cos \alpha - \cos \tau| \\
\times T(\alpha, \varphi, \tau) \sin^5 \tau \sin \varphi d\varphi d\phi d\tau,
$$

where as in Section 2

$$
T(\alpha, \varphi, \tau) = \begin{cases} 
0 & \text{if } 0 \leq \varphi + \tau \leq \alpha \\
12\pi^3 & \text{if } 2\pi - \alpha \leq \varphi + \tau \\
S(\arccos \left(\frac{\cos \varphi \cos \tau - \cos \alpha}{\sin \varphi \sin \tau}\right)) & \text{if } |\varphi - \tau| \geq \alpha
\end{cases}
$$

(4.1)
By elementary integral calculus,

\[ V(\alpha, \varphi, \tau) = \int_{-\pi}^{\pi} |\cos \phi \sin \varphi \sin \alpha + \cos \varphi \cos \alpha - \cos \tau| d\phi \]

\[ = 2\pi (\cos \tau - \cos \varphi \cos \alpha) + \]

\[ \begin{cases} 0 & \text{if } |\varphi - \alpha| \geq \tau \\ 4\pi (\cos \varphi \cos \alpha - \cos \tau) & \text{if } \alpha \leq \tau - \varphi \text{ or } 2\pi - \alpha \leq \tau + \varphi \\ 4 \left[ (\cos \varphi \cos \alpha - \cos \tau) \arccos \left( \frac{\cos \tau - \cos \varphi \cos \alpha}{\sin \varphi \sin \alpha} \right) \right] & \text{otherwise.} \\ + \sqrt{(\cos (\varphi - \alpha) - \cos \tau)(\cos \tau - \cos (\varphi + \alpha))} \end{cases} \]

(4.2)

Thus, we arrive at

**Lemma 4** The function \( J_1(\alpha) \) can be represented by the double integral

\[ J_1(\alpha) = \int_{0}^{\pi/2} \int_{0}^{\pi} T(\alpha, \varphi, \tau) \sin \varphi \sin^5 \tau \, d\varphi \, d\tau, \]

where \( T(\alpha, \varphi, \tau) \) and \( V(\alpha, \varphi, \tau) \) are defined by (4.1) and (4.2), respectively.

Note that, by the very definition of \( J_0(\alpha) \) and \( J_1(\alpha) \), both these functions are connected by the relations

\[ \frac{d}{d\alpha} J_0(\alpha) = -8\pi \sin \alpha J_1(\alpha) \quad \text{and} \quad J_1(0) = \frac{J_0(0)}{4\pi} = \frac{512\pi^4}{35} \approx 1424.9558. \]

By numerical integration we calculate for the double integral \( J_1(\alpha) \) on a sufficiently dense grid of \( \alpha \)-values. Further, to obtain the values of \( g_1(r) \) we repeat the comments made above in case of \( g_0(r) \). The resulting graph of \( g_1(r)/36 \) is seen in Figure 2. In the same way we can compute the subsequent values of (3.7) and (3.8) for \( j = 1 \):

\[ I_1 \approx 28.1166 \]
\[ \gamma_1 = \frac{3}{2} \left( \frac{315}{96\pi^2} \right)^2 \times \int_0^{\pi/2} J_1(\alpha) J_1(\pi - \alpha) \sin \alpha \, d\alpha \]

\[ \approx 1.702 \times 10^{-3} \times 4850.04 = 8.255 \]

### 4.3. The Function \( g_2(r) \)

The computational determination of the function

\[ g_2(r) = r^{12} \left( \frac{35}{1536\pi^2} \right)^2 \int_1^{\infty} \int_0^1 \exp\{-r^3 \nu(\rho_1, \rho_2)\} (\rho_2^3 - \rho_1^3) \Delta_2(\rho_1, \rho_2) \, d\rho_1 \, d\rho_2 \]

is somewhat more involved and of greater complexity than the computation of \( g_0(r) \) and \( g_1(r) \). The reason for this is the fact that the nine-fold integral

\[ \Delta_2(\rho_1, \rho_2) = 2\pi \int_{-\pi}^{\pi} J_2(\alpha(\rho_1, \rho_2), \psi) J_2(\alpha(-\rho_1, \rho_2), \psi) \, d\psi \]

is needed for a sufficiently dense lattice of pairs \((\rho_1, \rho_2)\). For this we first compute formally the determinants \( J_2(\pm \rho_1, \rho_2) \), \( J_2(\rho_1, \rho_2) \) and then change the variables such that

\[ \Delta_2(\rho_1, \rho_2) = 256 \pi^6 \left( \frac{1 - \rho_1^2}{\rho_2^2 - \rho_1^2} \right)^{9/2} (\rho_2^3 - 1) (1 + \rho_2^3) \Delta_2^*(\rho_1, \rho_2), \]

where

\[ \Delta_2^*(\rho_1, \rho_2) = \int_0^1 \int_{[0,1]^d} \int_{[0,1]^d} \sin^2 \left( \frac{\pi u_4}{2} \right) \left| u_2 \sqrt{1 - u_1^2 - (1 - u_1)^2} A(\rho_1, \rho_2) \times \right. \]

\[ \times \cos(\pi u_3) - u_1 \sqrt{1 - u_2^2 - (1 - u_2)^2} A(\rho_1, \rho_2) \cos(\pi u_4) \]
\[ + \sqrt{1 - A(\rho_1, \rho_2)} \left( u_1 - u_2 \right) \cos \left( \frac{\pi \theta}{2} \right) \times \]
\[ \times v_2 \sqrt{1 - v_1^2 - (1 - v_1)^2 A(-\rho_1, \rho_2) \cos (\pi v_3)} - \]
\[ v_1 \sqrt{1 - v_2^2 - (1 - v_2)^2 A(-\rho_1, \rho_2) \cos (\pi v_4)} + \]
\[ + \sqrt{1 - A(-\rho_1, \rho_2)} (v_1 - v_2) \cos \left( \frac{\pi \theta}{2} \right) d(u_1, \ldots, u_4) \]
\[ \times d(v_1, \ldots, v_4) d\theta \]

with

\[ A(\rho_1, \rho_2) = \frac{1 + \rho_1 \rho_2}{\rho_1 + \rho_2} \quad \text{for} \quad -1 \leq \rho_1 \leq 1, \quad \rho_2 \geq 1. \]

The function \( \Delta_2(\rho_1, 1/\rho_2) \) is calculated on an equidistant grid of 300 \( \times \) 300 points \((\rho_1, \rho_2) \in [0, 1]^2\) by MC-techniques (with sample size 500,000) followed by the numerical evaluation of the double integral

\[ g_2(r) = r^{12} \left( \frac{35 \pi}{96} \right)^2 \int_0^1 \int_0^1 \exp \{-r^3 \nu(\rho_1, 1/\rho_2)\} \rho_2^{-14} (1 - \rho_1^2 \rho_2^2)^{3/2} \times \]
\[ \times (1 - \rho_1)^{10/2} (1 - \rho_2^2) (1 + \rho_2)^7 \Delta_2^*(\rho_1, 1/\rho_2) \ d\rho_1 \ d\rho_2. \]

The plot of the function \( g_2(r)/8 \) is drawn in Figure 2. In this way we also get the following values of (3.7) and (3.8) for \( j=2^1 \):

\[ l_2 = \frac{1}{2} \left( \frac{35 \pi}{24} \right)^2 \int_0^1 \int_0^1 \frac{\Delta_2^*(\rho_1, 1/\rho_2)}{\left( \nu(\rho_1, 1/\rho_2) \right)^5} \rho_2^{14} (1 - \rho_1^2 \rho_2^2)^{3/2} (1 - \rho_2^2) \times \]
\[ \times (1 + \rho_2)^7 \ d\rho_1 \ d\rho_2 \]

\(^1\text{The evaluation of the eleven-fold integral } l_2 \text{ was checked by a Quasi-MC-technique with } 10^8 \text{ quasirandom points in } [0, 1]^{11}.\)
\[ \gamma_2 = \frac{1}{\pi} \left( \frac{35}{3} \right)^3 \left( \frac{3}{4\pi} \right)^{4/3} \Gamma \left( \frac{4}{3} \right) \times \int_0^1 (1 - \rho^2)^{9/2} \Delta_*(\rho, \infty) \, d\rho \]

\[ \simeq 66.841 \times 0.0321 \simeq 2.146. \]

| TABLE II Values of the function \( g_*(r) \) |
|---|---|---|---|---|---|---|---|
| \( r \) | \( g_*(r) \) | \( r \) | \( g_*(r) \) | \( r \) | \( g_*(r) \) | \( r \) | \( g_*(r) \) |
| 0.01 | 764.2737 | 0.36 | 1.4646 | 0.71 | 0.8681 | 1.11 | 0.9165 | 1.81 | 1.0424 |
| 0.02 | 200.9507 | 0.37 | 1.4204 | 0.72 | 0.8645 | 1.13 | 0.9256 | 1.83 | 1.0389 |
| 0.03 | 91.7819 | 0.38 | 1.3795 | 0.73 | 0.8612 | 1.15 | 0.9350 | 1.85 | 1.0354 |
| 0.04 | 52.9982 | 0.39 | 1.3416 | 0.74 | 0.8583 | 1.17 | 0.9446 | 1.87 | 1.0320 |
| 0.05 | 34.8261 | 0.40 | 1.3064 | 0.75 | 0.8557 | 1.19 | 0.9544 | 1.89 | 1.0287 |
| 0.06 | 24.8361 | 0.41 | 1.2737 | 0.76 | 0.8534 | 1.21 | 0.9641 | 1.91 | 1.0257 |
| 0.07 | 18.7362 | 0.42 | 1.2433 | 0.77 | 0.8515 | 1.23 | 0.9738 | 1.93 | 1.0228 |
| 0.08 | 14.7276 | 0.43 | 1.2149 | 0.78 | 0.8498 | 1.25 | 0.9835 | 1.85 | 1.0201 |
| 0.09 | 11.9455 | 0.44 | 1.1884 | 0.79 | 0.8484 | 1.27 | 0.9929 | 1.97 | 1.0176 |
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| 0.11 | 8.4236 | 0.46 | 1.1406 | 0.81 | 0.8465 | 1.31 | 1.0109 | 2.01 | 1.0133 |
| 0.12 | 7.2635 | 0.47 | 1.1190 | 0.82 | 0.8459 | 1.33 | 1.0194 | 2.03 | 1.0114 |
| 0.13 | 6.3503 | 0.48 | 1.0988 | 0.83 | 0.8456 | 1.35 | 1.0274 | 2.05 | 1.0098 |
| 0.14 | 5.6177 | 0.49 | 1.0799 | 0.84 | 0.8455 | 1.37 | 1.0348 | 2.07 | 1.0083 |
| 0.15 | 5.0201 | 0.50 | 1.0621 | 0.85 | 0.8457 | 1.39 | 1.0417 | 2.09 | 1.0070 |
| 0.16 | 4.5259 | 0.51 | 1.0455 | 0.86 | 0.8461 | 1.41 | 1.0479 | 2.11 | 1.0059 |
| 0.17 | 4.1120 | 0.52 | 1.0299 | 0.87 | 0.8468 | 1.43 | 1.0534 | 2.13 | 1.0049 |
| 0.18 | 3.7616 | 0.53 | 1.0153 | 0.88 | 0.8476 | 1.45 | 1.0582 | 2.15 | 1.0040 |
| 0.19 | 3.4621 | 0.54 | 1.0016 | 0.89 | 0.8487 | 1.47 | 1.0623 | 2.17 | 1.0033 |
| 0.20 | 3.2039 | 0.55 | 0.9888 | 0.90 | 0.8500 | 1.49 | 1.0657 | 2.19 | 1.0027 |
| 0.21 | 2.9796 | 0.56 | 0.9768 | 0.91 | 0.8515 | 1.51 | 1.0683 | 2.21 | 1.0022 |
| 0.22 | 2.7834 | 0.57 | 0.9655 | 0.92 | 0.8532 | 1.53 | 1.0702 | 2.23 | 1.0018 |
| 0.23 | 2.6108 | 0.58 | 0.9549 | 0.93 | 0.8551 | 1.55 | 1.0714 | 2.25 | 1.0014 |
| 0.24 | 2.4579 | 0.59 | 0.9450 | 0.94 | 0.8572 | 1.57 | 1.0718 | 2.27 | 1.0011 |
| 0.25 | 2.3219 | 0.60 | 0.9358 | 0.95 | 0.8594 | 1.59 | 1.0717 | 2.29 | 1.0009 |
| 0.26 | 2.2004 | 0.61 | 0.9271 | 0.96 | 0.8619 | 1.61 | 1.0709 | 2.31 | 1.0007 |
| 0.27 | 2.0912 | 0.62 | 0.9190 | 0.97 | 0.8645 | 1.63 | 1.0695 | 2.33 | 1.0006 |
| 0.28 | 1.9929 | 0.63 | 0.9115 | 0.98 | 0.8673 | 1.65 | 1.0677 | 2.35 | 1.0004 |
| 0.29 | 1.9039 | 0.64 | 0.9045 | 0.99 | 0.8703 | 1.67 | 1.0654 | 2.37 | 1.0003 |
| 0.30 | 1.8231 | 0.65 | 0.8980 | 1.00 | 0.8734 | 1.69 | 1.0628 | 2.39 | 1.0003 |
| 0.31 | 1.7495 | 0.66 | 0.8919 | 1.01 | 0.8767 | 1.71 | 1.0598 | 2.41 | 1.0002 |
| 0.32 | 1.6824 | 0.67 | 0.8863 | 1.03 | 0.8837 | 1.73 | 1.0566 | 2.43 | 1.0001 |
| 0.33 | 1.6209 | 0.68 | 0.8812 | 1.05 | 0.8912 | 1.75 | 1.0532 | 2.45 | 1.0001 |
| 0.34 | 1.5644 | 0.69 | 0.8764 | 1.07 | 0.8992 | 1.77 | 1.0496 | 2.47 | 1.0001 |
| 0.35 | 1.5125 | 0.70 | 0.8721 | 1.09 | 0.9076 | 1.79 | 1.0460 | 2.49 | 1.0001 |
4.4. The Function $g_3 (r)$

By virtue of (3.6), the function $g_3 (r)$ from Theorem 1 takes the form

$$
g_3 (r) = r^9 \frac{\pi}{3} \left( \frac{35}{128} \right)^2 \int_1^\infty \int_0^1 \exp \left\{ -r^3 \nu (\rho_1, \rho_2) \right\} \left( 1 - \rho_1^2 \right)^4 \left( \rho_2^2 - \rho_1^2 \right) \times \left( 1 + \rho_2^2 \right)^4 \left( \rho_2^2 - 1 \right)^2 \, d\rho_1 \, d\rho_2.
$$

This parameter integral is treated again by the above numerical methods.

Since $\Delta_3 (\rho_1, \rho_2)$ and $\nu (\rho_1, \rho_2)$ are polynomials in two variables, it is indeed possible to compute analytically the values of $\gamma_3$ and $I_3$, see
(3.9) and

\[ I_3 = \frac{35}{4\pi^3} \approx 0.2822. \]

Now, we are in a position to calculate the PCF \( g_\nu(r) \) according to the additive decomposition (3.3). In Table II the numerical values of \( g_\nu(r) \) are summarized and Figure 2 shows the graph of \( g_\nu(r) \) together with its local extremal points and the points of level 1.

5. CONFIDENCE INTERVAL FOR THE NUMBER OF NODES IN A LARGE CUBE AND THE VARIANCE OF THE NUMBER OF VERTICES OF THE TYPICAL POISSON–VORONOI POLYHEDRON

Our goal is to construct a 100(1-\(\alpha\))% confidence interval \( \hat{K}_n(\alpha) \) for the intensity \( \mu_{V,\lambda} = \mathbb{E}[\Psi_{V,\lambda}(0,1)^3] \) of nodes (= vertices of cells) in a 3-D PVT \( V_\lambda(\Psi) \) based only on the number of nodes \( \Psi_{V,\lambda}(W_n) \) in a cube \( W_n = [0, n]^3 \). Moreover, the interval \( \hat{K}_n(\alpha) \) is required to be asymptotically exact (as \( n \to \infty \)) and its end-points may not depend on the unknown parameter \( \lambda \).

We first note that \( \mu_{V,\lambda} = \kappa_3 \lambda \) with \( \kappa_3 = 24 \pi^2/35 \approx 6.7677 \), see e.g. [20]. Next we will establish a central limit theorem for the number \( \Psi_{V,\lambda}(W_n) \) which includes the evaluation of the limit

\[ \sigma^2_{V,\lambda} = \lim_{n \to \infty} \frac{\text{Var} \Psi_{V,\lambda}(W_n)}{|W_n|}. \]

Using the relationship between the second factorial moment measure and the PCF of a stationary and isotropic spatial point process, see [5], it is easily checked that

\[ \text{Var} \Psi_{V,\lambda}(W_n) = \mu_{V,\lambda} |W_n| + \mu^2_{V,\lambda} \int_0^\infty \gamma(r, W_n) (g_{V,\lambda}(r) - 1) r^2 dr, \]

where

\[ \gamma(r, W_n) = \int_{-\pi}^\pi \int_0^\pi |W_n \cap (W_n + rs(\theta, \vartheta))| \sin \vartheta \, d\vartheta \, d\theta. \]
Since \( \lim_{n \to \infty} \gamma(r, W_n)/|W_n| = 4\pi \) and from (3.2), we deduce that

\[
\sigma_{V, \lambda}^2 = \mu_{V, \lambda} \left( 1 + 4\pi \mu_{V, \lambda} \int_0^\infty (g_{V, \lambda}(r) - 1) r^2 dr \right) = \kappa_3 (1 + \kappa_3 \sigma_3^2) \lambda, \tag{5.1}
\]

where the number

\[
\sigma_3^2 = 4\pi \int_0^\infty (g_{V}(r) - 1) r^2 dr
\]

does not depend on \( \lambda \). In view of (3.3) and the relation

\[
4\pi \int_0^\infty \left( 1 - \frac{8\delta^*_0(r)}{576} \right) r^2 dr = 6 + \frac{2240\pi}{243\sqrt{3}} \simeq 22.71980. \tag{5.2}
\]

\( \sigma_3^2 \) can be expressed in terms of the integrals \( I_0, \ldots, I_3 \) (see Lemma 3) as follows:

\[
\sigma_3^2 = \frac{\pi}{144} (I_0 + 16 I_1 + 72 I_2 + 96 I_3) - \left( 6 + \frac{2240\pi}{243\sqrt{3}} \right) \simeq 0.90274. \tag{5.3}
\]

The latter number results from (5.2) and the numerically calculated values of \( I_0, \ldots, I_3 \) in Section 4. Finally, from (5.1),

\[
\sigma_{V, \lambda}^2 \simeq 48.11517 \lambda.
\]

Making use of the exponential decay of the absolute regularity mixing coefficient of a stationary PVT, see [8] (Theorem 2.1), we may deduce from Corollary 2.3 in [8] that the estimator \( \hat{\mu}_n = \Psi_{V}(W_n)/|W_n| \) is asymptotically normally distributed as \( n \to \infty \) with mean \( \mu_{V, \lambda} \) and a variance which is asymptotically equal to \( \sigma_{V, \lambda}/|W_n| \).

In other words, together with (5.1),

\[
\frac{1}{\sqrt{|W_n|}} (\Psi_{V, \lambda}(W_n) - \kappa_3 \lambda |W_n|) \Rightarrow \mathcal{N}(0, \kappa_3 (1 + \kappa_3 \sigma_3^2) \lambda) \quad \text{as} \quad n \to \infty, \tag{5.4}
\]

where \( \mathcal{N}(\mu, \sigma^2) \) denotes a Gaussian random variable with mean \( \mu \) and variance \( \sigma^2 \).
Hence, using (5.4) and some simple facts from the theory of weak convergence,

\[
\sqrt{|W_n|} \left( \sqrt{\tilde{\mu}_n} - \sqrt{\mu_{V, \lambda}} \right) = \sqrt{|W_n|} \left( \hat{\mu}_n - \mu_{V, \lambda} \right) \over \sqrt{\tilde{\mu}_n + \sqrt{\mu_{V, \lambda}}} \\
\implies \mathcal{N} \left( 0, \frac{1 + \kappa_3 \sigma_3^2}{4} \right) \quad \text{as} \quad n \to \infty,
\]

whence it follows immediately.

**Theorem 2**  
*The symmetric confidence interval*

\[
\hat{K}_n (\alpha) = \left[ \left( \sqrt{\tilde{\mu}_n} - \frac{z_{n/2}}{2} \sqrt{\frac{1 + \kappa_3 \sigma_3^2}{|W_n|}} \right)^2, \left( \sqrt{\tilde{\mu}_n} + \frac{z_{n/2}}{2} \sqrt{\frac{1 + \kappa_3 \sigma_3^2}{|W_n|}} \right)^2 \right]
\]

covers the intensity \( \mu_{V, \lambda} = \kappa_3 \lambda \) (as \( n \to \infty \)) with probability \( 1 - \alpha \), where the quantile \( z_{n/2} \) is chosen such that \( \mathbb{P}(|\mathcal{N}(0,1)| \geq z_{n/2}) = \alpha \). In particular, together with \( z_{0.025} = 1.96 \),

\[
\hat{K}_n (0.05) \approx \left[ \left( \sqrt{\tilde{\mu}_n} - \frac{2.613}{\sqrt{|W_n|}} \right)^2, \left( \sqrt{\tilde{\mu}_n} + \frac{2.613}{\sqrt{|W_n|}} \right)^2 \right].
\]

The study of the point process \( \Psi_{V, \lambda} \) reveals a tight connection between its (factorial) moment measures and the (factorial) moments of the number \( N_0 \) of vertices of the typical Voronoi polyhedron. The precise formulation of this fact makes use of (higher-order) Palm distributions and is carried out in detail in [10]. As a quite simple consequence we confirm the classical relation \( \mathbb{E} N_0 = 4 \kappa_3 = 96 \pi^2/35 \approx 27.0709 \), see [14]. Moreover, we are able to derive the formula

\[
\mathbb{E} N_0 (N_0 - 1) = \frac{64 \pi^5}{1225} (I_1 + 9I_2 + 18I_3), \quad (5.5)
\]

where \( I_1, I_2, I_3 \) are the same integrals as in (5.3). Using their numerical values obtained in Section 4 yields

\[
\mathbb{E} N_0 (N_0 - 1) \approx 750.261.
\]
This value has already been found by Brakke [3] (in fact: \( \text{Var}(N_0) \approx 44.49833 \)). However, his analytic approach is hard to compare with ours.

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References


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Germany
New and more precise numerical results for $J_0(\alpha), J_1(\alpha), \bar{V}(\alpha)$

by L. Muche (October 9, 2012)

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