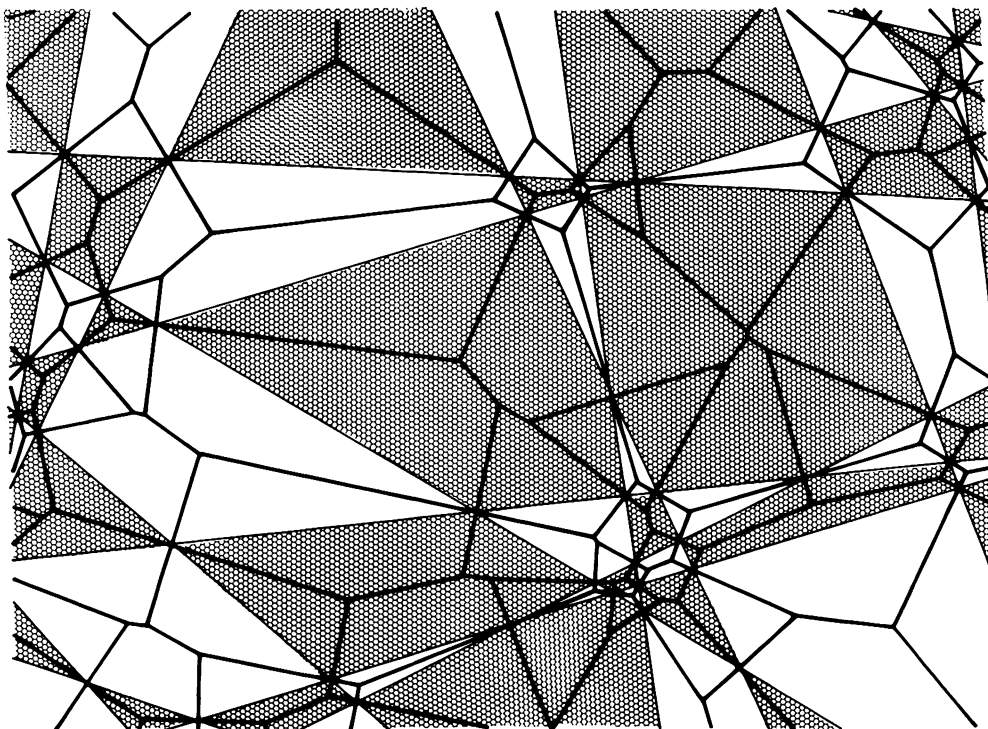


Journal of Microscopy

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Stereology and Stochastic Geometry (II)



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Front cover. Line process, chequer-board pattern and associated skeleton tessellations which, wherever they cross, cross at a right angle. (Courtesy R. E. Miles, *J. Microsc.* 151, 191.)

Exact formulae for the precision of systematic sampling

by ALBRECHT M. KELLERER, *Institut für Med. Strahlenkunde der Universität Würzburg, Versbacher Strasse 5, D-8700 Würzburg, F.R.G.*

KEY WORDS. Systematic sampling, variance of volume estimator, Zitterbewegung, Euler's summation formula, point-pair distance distribution, chord-length density, covariogram.

SUMMARY

A formula is given for the variance of the intersection of two geometric objects, S and T , under uniform, i.e. translation invariant, randomness. It involves an integral of the product of the point-pair distance distributions of S and T . In systematic sampling S is the specimen and T is the test system, for example a system of planes, lines, or dots in \mathbb{R}^3 or \mathbb{R}^2 . The general n -dimensional integral (or sum) is difficult to use, but for systematic sectioning, i.e. for a test system of parallel hyperplanes (planes in \mathbb{R}^3 or lines in \mathbb{R}^2) it can be reduced to a one-dimensional expression: this leads to Matheron's treatment in terms of 'covariograms' of the specimens. Under the condition of isotropy analogous simplifications lead to equations involving the distributions of scalar point-pair distances and to the approach developed by Matérn for sampling with point grids. The equations apply to arbitrary test systems, but they include fluctuating functions that require high precision in the numerical evaluation and make it difficult to predict undamped variance oscillations of the volume estimator which occur for some specimen shapes but not for others. A generalized Euler method of successive partial integrations removes this difficulty and shows that, for a convex specimen, the undamped oscillations result from discontinuities in its chord-length density. The periodicities equal the ratios of the critical chord-lengths to the periodicities of the test system. Analogous relations apply to the covariogram. The formulae for the variance are extended also to the covariance of the volume estimators of paired specimens.

1. INTRODUCTION

Systematic sampling is a common stereological procedure to estimate volumes of certain specimens. When the specimen is cut by a system of planes, lines, or points, the variance of the resulting estimator depends on specimen shape. Matheron (1965, 1971) has developed a theory of 'regionalized variables' that provides relations for the variance of systematic sampling. His methods have been extensively used to obtain approximations in terms of the 'covariograms' of the specimens (see Gundersen, 1986, and the general overview by Gundersen & Jensen, 1987). The approximations disregard the fluctuating dependences of the variance on the spatial resolution of the test system, e.g. the distance between sectioning planes. Matheron has termed this phenomenon 'Zitterbewegung (terme fluctuant)'. Exact solutions have been obtained for sampling with regular point grids by Kendall (1948) and Kendall & Rankin (1953) who have

linked their results to the classical point-lattice problem of number theory (Hardy & Landau, 1924). Matérn (1960, 1985) has treated systematic sampling with point grids, and has derived formulae which express the variance of the estimators in terms of the point-pair distance distributions of the specimen and the point grid. These and analogous exact studies (Kellerer, 1986; Matérn, 1988; Mattfeldt, 1988) provide examples, but no general criteria, for the presence or absence of undamped oscillations, i.e. the Zitterbewegung, for different specimens.

For systematic planar sectioning Cruz-Orive (1985) has reduced the ellipsoid-ellipsoid problem in the estimation of volume ratios to that of spheres, and he and Mattfeldt provide the exact analytical expression for the Zitterbewegung in these cases (Mattfeldt, 1987, 1988; Cruz-Orive, 1988). The present study deals with some further aspects of the problem, and links the fluctuating dependences to discontinuities of the chord-length distributions or the covariograms of the specimens.

2. VARIANCE OF RANDOM INTERSECTIONS

Systematic sampling can be regarded as intersecting at random a specimen, S , with a test system, T . To deal with this process we need formulae for the first and second moment of the measure (volume) of the intersection, $S \cap T$. These formulae will first be given in a general form. Simplifications will then be considered that lead to formulations either in terms of the covariogram or in terms of scalar point-pair distance distributions. The reader is referred to the surveys of these two approaches by Cruz-Orive (1988) and Matérn (1988). The comparison includes also related notions utilized in radiation physics and microdosimetry. The variety of approaches makes it necessary to employ a somewhat varied notation and a number of different but closely linked quantities.

As a first step, formulae will be given that apply to bounded domains S and T . Subsequent modifications will make the relations applicable also to actual test systems, T , which are unbounded.

If q is the measure of the intersection $S \cap T$ ($\neq 0$) under uniform, i.e. translation invariant, randomness, the mean value, Eq , is given as a special case of the formula of Blaschke-Santaló (Blaschke, 1937; Santaló, 1953):

$$Eq = V(S)V(T)/\gamma \quad (2.1)$$

$V(S)$ and $V(T)$ are the contents of S and T , respectively, and γ is the content of the Minkowski sum $S \oplus T$.

Let $p_{n,x}(x)$ be the probability density function of vectorial distances, x , between pairs of uniform and independent random points in a bounded region $X \subset \mathbb{R}^n$. The second moment, Eq^2 , can then be expressed as an integral over the point-pair distance densities of S and T :

$$Eq^2 = Eq V(S)V(T) \int_{\mathbb{R}^n} p_{n,S}(x) p_{n,T}(x) dx. \quad (2.2)$$

This relation can be obtained from the theorem of Robbins (1944); the derivation is analogous to the one employed under the assumption of isotropy (Kellerer, 1986). From Eq. (2.2) we obtain the coefficient of variance:

$$\begin{aligned} CV^2(q) &= Eq^2/(Eq)^2 - 1 \\ &= \frac{V(S)V(T)}{Eq} \int_{\mathbb{R}^n} p_{n,S}(x) p_{n,T}(x) dx - 1. \end{aligned} \quad (2.3)$$

Eqs. (2.1) to (2.3) cannot be applied to an unbounded T , for which $p_{n,T}(x)$ and $V(T)$ are not defined.

Matheron (1965, 1971) uses, instead of $p_{n,x}(x)$, the covariogram:

$$g_{n,x}(x) = \int_{\mathbb{R}^n} f(x+z) f(z) dz \quad (2.4)$$

where $f(x)$ is the indicator function of a bounded domain $X \subset \mathbb{R}^n$, i.e. the function that equals 1 for $x \in X$ and 0 otherwise. For a bounded specimen, X , of volume $V(X)$ the probability density function, $p_{n,x}(x)$, of (vectorial) distances between pairs of uniform random points in X is related to $g_{n,x}(x)$ as follows:

$$g_{n,x}(x) = p_{n,x}(x) V(X)^2. \quad (2.5)$$

In subsequent considerations there will be further reference to the covariogram, but it is readily seen from Eq. (2.4) that it, too, cannot be applied to unbounded volumes.

The covariogram and the point-pair distance density differ by the normalization factor $V(X)^2$. The different normalization factor $V(X)$ leads to a function which can be extended naturally to an unbounded test system, because $V(X)p_{n,x}(x)$ is the mean spatial density of the content of X at vectorial distance x from a 'typical' point, i.e. a uniform random point, of X . Alternatively one can say that $V(X)p_{n,x}(x)$ is, as seen from Eq. (2.4), the probability for $(z+x) \in X$, if z is a typical point of X .

In systematic sampling, the volume estimator, q , is the content of $S \cap T$ multiplied by a factor, c , which depends on the test system. For example in \mathbb{R}^3 , we assign the measure cA to an area A of the test system of parallel planes, if c is the distance between adjacent planes.

According to these considerations we associate with the test system a function $t_n(x)$, which equals the density of the measure of T (containing the scaling factor c) at vectorial distance x from a typical point of T . An analogous function is used in microdosimetry to characterize the microscopic random patterns of energy transferred to irradiated matter by ionizing particles (Kellerer & Chmelevsky, 1975; ICRU, 1983); it is termed 'proximity function'.

Replacing $V(S)/Eq$ by c and $cV(T)p_{n,T}(x)$ by $t_n(x)$ we obtain from Eq. (2.3):

$$CV^2(q) = \int_{\mathbb{R}^n} p_{n,S}(x) t_n(x) dx - 1. \quad (2.6)$$

This is the general relation for the coefficient of variance in systematic sampling. Its validity in trivial cases is evident. Let T be equal to \mathbb{R}^n ; due to $t_n(x) = 1$ and $\int p_{n,S}(x) dx = 1$ we obtain then $CV^2(q) = 0$. As a second example, let T be a stationary random set of independently distributed points with intensity λ points per unit volume; we have then $t_n(x) = \delta(x)/\lambda + 1$ (where $\delta(x)$ is the Dirac delta function), and with $p_{n,S}(0) = 1/V(S)$ (see Eqs. 2.4 and 2.5) obtain the familiar result $CV^2(q) = 1/[\lambda V(S)]$.

Equation (2.6) and subsequent results remain valid, even if the probe can miss the specimen. However, the values $q=0$ must then be included, in order to have $cEq = V(S)$.

In general Eq. (2.6) is difficult to use, except by numerical integration or by simulations. It is, therefore, necessary to use simplifying assumptions based on symmetries in the functions $p_{n,S}(x)$ or $t_n(x)$.

3. REDUCTION TO THE ONE-DIMENSIONAL CASE

3.1. Use of the covariogram

If the sampling probe, T , is a set of parallel planes, $t_n(x)$ depends only on the coordinate orthogonal to the planes. One can then integrate out the other coordinates to obtain from $f(x)$ the 'graded' one-dimensional function $f_1(x)$ where x is now a scalar (Matheron, 1965, 1971; Cruz-Orive, 1988). $f_1(x)$ is the 'cross-section' of the specimen. Similarly one obtains from $p_{n,S}(x)$ or $g_{n,S}(x)$ the graded functions $p_1(x)$ and $g_1(x)$ with scalar argument x . However, these

latter functions can also be derived from $f_1(x)$:

$$g_1(x) = p_1(x) V(S)^2 = \int f_1(x+s) f_1(s) ds. \quad (3.1)$$

$p_1(x)$ is the density of point-pair distances of S projected onto the normal to the planes; it is the normalized covariogram. With these conventions Eq. (2.6) reduces to the one-dimensional integral:

$$\begin{aligned} CV^2(q) &= \int_{-\infty}^{\infty} p_1(x) t_n(x) dx - 1 \\ &= \frac{1}{V(S)^2} \int_{-\infty}^{\infty} g_1(x) t_n(x) dx - 1. \end{aligned} \quad (3.2)$$

These and subsequent integrals and sums are written with open boundaries, but they terminate at maximum values of x determined by the specimen size. The dimensionless function $t_n(x)$ is the same as in the preceding section, but x is the coordinate orthogonal to the sectioning planes.

The simplest example (although one of no practical interest) is that of independently positioned parallel sectioning planes with mean spacing c . One has then $t_n(x) = c \delta(x) + 1$ and obtains with $g_1(0) = \int f_1(x)^2 dx$ and $V(S) = \int f_1(x) dx$:

$$\begin{aligned} CV^2(q) &= c g_1(0) / V(S)^2 \\ &= [1 + CV^2(f_1)] / m \end{aligned} \quad (3.3)$$

where $CV^2(f_1)$ is the coefficient of variance of the 'cross-section' of S , and m is the mean number of sections.

For the practically important case of equidistant sectioning planes one has:

$$t_n(x) = c \sum_{i=-\infty}^{\infty} \delta(x - ic) \quad (3.4)$$

which yields the basic relation for Matheron's approach:

$$\begin{aligned} CV^2(q) &= c \sum_{i=-\infty}^{\infty} p_1(ic) - 1 \\ &= \frac{c}{V(S)^2} \sum_{i=-\infty}^{\infty} g_1(ic) - 1. \end{aligned} \quad (3.5)$$

Cruz-Orive (1988) gives a concise overview of the resulting theory and its application to systematic planar sectioning and to stepwise sampling by planes, lines, and dots. The exact evaluation of Eq. (3.5) in terms of the Bernoulli polynomials—an alternative to Matheron's approach in terms of Fourier transforms—is explained in Appendix 1; it is largely analogous to the method subsequently described for isotropic systematic sampling with general probes.

3.2. Assumption of isotropy

Isotropy is another condition that reduces Eq. (2.6) to a one-dimensional relation. It applies if the specimens have spherical symmetry, or if specimens of arbitrary shape are isotropically orientated relative to the test system. One can then integrate Eq. (2.6) over spherical surfaces centred at the origin, and one obtains the result which has been derived by Matérn (1960, 1985, 1988) for point sampling and 'stratified' point sampling:

$$CV^2(q) = \int_0^{\infty} \frac{p(x) t(x)}{nC_n x^{n-1}} dx - 1 \quad (3.6)$$

where C_n is the volume of the n -sphere of unit radius. The limit 0 in this and subsequent integrals stands for -0 . The functions $p(x)$ and $t(x)$ are the integrals of $p_{n,s}(z)$ and $t_n(z)$ over the spherical surface of radius $x=|z|$ which has the area $nC_n x^{n-1}$. These functions, too, can be regarded as 'graded' functions in the sense of Matheron; but the 'integrating out' of $(n-1)$ coordinates is performed in a spherical coordinate system. $p(x)$ is the density of scalar point-pair distances in S , and $t(x)$ is the analogous non-normalized function, i.e. the (graded) proximity function, for T . For parallel planar sectioning under the condition of isotropy Eqs. (3.5) and (3.6) are equally applicable, and are, as shown in Appendix 2, equivalent.

For a regular point lattice in \mathbb{R}^n the proximity function, $t(x)$, reduces to a sum of Dirac delta functions:

$$t(x) = \sum_{i=0}^{\infty} t_i \delta(x - x_i) \quad (3.7)$$

where t_i is the number of points at distance x_i from a typical lattice point divided by the mean number, λ , of points per unit volume ($x_0=0$ and $t_0=1/\lambda$). Instead of Eq. (3.6) one obtains then the equation which is given—with somewhat different notation—by Matérn (1988, eq. 1):

$$CV^2(q) = \sum_{i=0}^{\infty} \frac{p(x_i) t_i}{nC_n x_i^{n-1}} - 1. \quad (3.8)$$

4. EVALUATION OF THE INTEGRAL

4.1. The geometric reduction factor, $U(x)$, and the functions $Z_i(x)$ for the test system

The functions $t(x)$ for typical test systems vary rapidly (see example in Eqs. 3.7 or 5.2); the numerical evaluation may, therefore, require high precision, and analytical solutions are complicated. However, we can use successive integrations by parts to obtain more manageable expressions, and to establish criteria for the presence of undamped fluctuations of the variance. This treatment will involve a function $U(x)$ (related to S) and its derivatives, and a function $Z_1(x)$ (related to T) and its integrals.

For the evaluation of Eq. (3.6) it is practical to use, instead of the point-pair distribution, $p(x)$, the dimensionless quantity:

$$U(x) = \frac{V(S) p(x)}{nC_n x^{n-1}}, \quad (4.1)$$

namely the product of $V(S)$ times the average value of $p_n(z)$ over the spherical surface of radius $x=|z|$; it has been termed 'geometric reduction factor' by Berger (1971) who has established applications to dosimetry calculations for radionuclides.* $U(x)$ is the probability that the translate of a typical point of S by distance x in isotropic random direction is contained in S ; accordingly $U(0)=1$. Although $U(x)$ is not defined for negative x , it is convenient to set $U(x)=1$ for $x<0$.

In the integrations by parts we obtain contributions due to any discontinuities, $\delta U^{(i)}(x_j)$, ($=U^{(i)}(x_j+0)-U^{(i)}(x_j-0)$), of the derivatives, $U^{(i)}(x)$. For sufficiently regular specimens, $U(x)$ and $U'(x)$ have no discontinuities, except:

$$\delta U'(0) = U'(0) = -\frac{P}{aV} \quad (a = nC_n/C_{n-1} = 2, \pi, 4 \text{ for } \mathbb{R}^1, \mathbb{R}^2, \mathbb{R}^3) \quad (4.2)$$

where V is the content (length, area, volume) of the specimen, and P is its boundary measure

* Enns & Ehlers (1978) use the notation $\Omega(x)$ for this quantity. Matérn (1960, 1985) who has given solutions for standard configurations in \mathbb{R}^2 uses the notation $j(x)$. The symbol $U(x)$ is here utilized because it is employed in microdosimetry (see e.g. Kase *et al.*, 1985) where the quantity has special importance. For various relations linking $U(x)$, $p(x)$, and the chord-length distributions and for numerical expressions see for example Kendall & Moran (1963), Coleman (1969, 1981), Enns & Ehlers (1978), Kellerer (1984, 1986), and Stoyan *et al.* (1987).

(number of end points, perimeter, surface). To simplify notation the symbol V is used hereafter, instead of $V(S)$. Equation (4.2) has been obtained by Serra (1969) and Enns & Ehlers (1978), who have also given the relation between $U''(x)$ and the probability density function, $c(x)$, of chord lengths for a convex specimen under uniform, isotropic randomness (μ -randomness):

$$c(x) = \frac{aV}{P} U''(x). \quad (4.3)$$

It will, furthermore, be practical to use, instead of $t(x)$ and its integral the following functions:

$$Z_1(x) = t(x) - nC_n x^{n-1} \quad (4.4)$$

$$Z_2(x) = T(x) - C_n x^n \quad \left[\text{with } T(x) = \int_0^x t(s) ds \right]$$

as well as the subsequent integrals, $Z_i(x)$ ($i \geq 3$), which oscillate around zero, and are chosen to average zero. $T(x)$ is the 'integral' proximity function, i.e. the expected content of T within a sphere of radius x centred at a typical point of T . The terms $nC_n x^{n-1}$ and $C_n x^n$ can be considered as the differential and integral proximity functions of the entire space, \mathbb{R}^n ; consequently the functions $Z_i(x)$ vanish in the trivial case $T = \mathbb{R}^n$.

4.2. Repeated integrations by parts

Integrating by parts the right-hand side of Eq. (3.6) and using the preceding definitions, we get:

$$VCV^2(q) = \int_0^\infty U(x) Z_1(x) dx \quad (4.5)$$

$$= - \int_0^\infty U'(x) Z_2(x) dx. \quad (4.6)$$

Formally we can use the expression $c(x)$ from Eq. (4.3) also for non-convex specimens. With Matérn's notation $\varepsilon^2 = CV^2(q) V^2/P$ and the symbol Z_3 for $Z_3(0)$ we obtain with Eq. (4.2) and through further integrations by parts:

$$a\varepsilon^2 = -Z_3 + \int_0^\infty c(x) Z_3(x) dx \quad (4.7)$$

$$= -Z_3 - \sum_j \delta c(x_j) Z_4(x_j) - \int_0^\infty c'(x) Z_4(x) dx \quad (4.8)$$

$$= -Z_3 - \sum_j \delta c(x_j) Z_4(x_j) + \sum_j \delta c'(x_j) Z_5(x_j) + \int_0^\infty c''(x) Z_5(x) dx \quad (4.9)$$

$= \dots$

$\delta c^{(i)}(x_j) = c^{(i)}(x_j+0) - c^{(i)}(x_j-0)$ are the discontinuities in $c(x)$ and its derivatives.

Equation (4.7) applies generally, Eq. (4.8) applies if $c(x)$ has no singularities, and the subsequent relations apply if the derivatives have no singularities.

The constant term, $-Z_3$, determines the trend, $-Z_3 P/(aV^2)$, of $CV^2(q)$. The remainder determines an oscillatory component and terms of decreasing order; the first oscillatory component, i.e. the undamped 'Zitterbewegung', is absent if $c(x)$ has no discontinuities, $\delta c(x_j)$.

From Eqs. (4.7)–(4.9) it is apparent that the fluctuations in the dependence of ε^2 on specimen size are linked to the oscillatory functions $Z_i(x)$ ($i \geq 3$), that their amplitudes are determined by the discontinuities or singularities (at $x > 0$) of the chord-length density and its

derivatives, and that their periodicities equal the ratios of the critical chord lengths, x_j , to the grid periods.

We can derive the functions $Z_i(x)$ for different test systems, to use them in computations for different specimens. The problem of the precision of systematic sampling is thus reduced to two distinct and simplified computational steps. A compilation of the functions $Z_i(x)$ for various point and line grids, the exploration of their order, and the assessment of the discontinuities and singularities of $c(x)$ for different specimen shapes in \mathbb{R}^2 and \mathbb{R}^3 are outside the scope of the present article. However, the example of planar systematic sectioning will illustrate some of the main points.

5. APPLICATIONS

5.1. The functions $Z_i(x)$ for systematic planar sectioning

To derive the functions $Z_i(x)$ for a system of parallel sectioning planes with unit spacing in \mathbb{R}^3 , one can first consider the integral, $T(x)$, of $t(x)$ which is the expected content of T within a sphere of radius x centred at a typical point of T . In the unbounded system of planes all points are equivalent, and designating the integer and the fractional parts of x by I and Δ , respectively, one has:

$$T(x) = \pi x^2 + 2\pi \sum_{i=1}^I (x^2 - i^2) \quad (5.1)$$

$$t(x) = 2\pi x + 4\pi x I \quad (5.2)$$

whereby:

$$Z_i(x) = 4\pi [-x B_i(x)/i! + (i-1) B_{i+1}(x)/(i+1)!] \quad (5.3)$$

where the $B_i(x)$ are the Bernoulli polynomials (see Appendix 1) which average zero, depend only on the fractional part of x , and are linked by the relation $dB_i(x)/dx = i B_{i-1}(x)$.

The explicit expressions for $i=1, \dots, 5$ are:

$$\begin{aligned} Z_1(x) &= 4\pi \left[-x \left(\Delta - \frac{1}{2} \right) \right] \\ Z_2(x) &= 4\pi \left[-x \left(\Delta^2 - \Delta + \frac{1}{6} \right) / 2 + \left(\Delta^3 - \frac{3}{2} \Delta^2 + \frac{\Delta}{2} \right) / 6 \right] \\ Z_3(x) &= 4\pi \left[-x \left(\Delta^3 - \frac{3}{2} \Delta^2 + \frac{\Delta}{2} \right) / 6 + \left(\Delta^4 - 2\Delta^3 + \Delta^2 - \frac{1}{30} \right) / 12 \right] \\ Z_4(x) &= 4\pi \left[-x \left(\Delta^4 - 2\Delta^3 + \Delta^2 - \frac{1}{30} \right) / 24 + \left(\Delta^5 - \frac{5}{2} \Delta^4 + \frac{5}{3} \Delta^3 - \frac{1}{6} \Delta \right) / 40 \right] \\ Z_5(x) &= 4\pi \left[-x \left(\Delta^5 - \frac{5}{2} \Delta^4 + \frac{5}{3} \Delta^3 - \frac{1}{6} \Delta \right) / 120 + \left(\Delta^6 - 3\Delta^5 + \frac{5}{2} \Delta^4 - \frac{1}{2} \Delta^2 + \frac{1}{42} \right) / 180 \right] \\ &\dots \end{aligned} \quad (5.4)$$

Using the notation $Z_i = Z_i(0)$ we have:

$$Z_1 = Z_2 = 0, Z_3 = -\pi/90, Z_4 = 0 \quad \text{and} \quad Z_5 = \pi/1890.$$

5.2. The sphere, and other simple geometrical objects

The probability-density function of the length of isotropic uniform random chords of a sphere of diameter d is:

$$c(x) = 2x/d^2, \quad 0 \leq x \leq d. \quad (5.5)$$

Here, as in subsequent examples, it is understood that the function is zero outside the stated range.

The discontinuities are:

$$\delta c(d) = -c(d) = -2/d, \quad \delta c'(0) = c'(0) = 2/d^2, \quad \delta c'(d) = -c'(d) = -2/d^2. \quad (5.6)$$

From Eq. (4.9) we obtain, therefore, the solution for the sphere which applies to any test system:

$$a\varepsilon^2 = \frac{\pi d^4}{9} CV^2(q) = -Z_3 + 2Z_4(d)/d + 2Z_5/d^2 - 2Z_6(d)/d^2. \quad (5.7)$$

The explicit form for planar sectioning is then, according to Eqs. (5.4):

$$\begin{aligned} CV^2(q) &= \frac{1}{10d^4} - \frac{3B_4(\Delta)}{d^4} + \frac{12B_5(\Delta)}{5d^5} + \frac{1}{105d^6} - \frac{2B_6(\Delta)}{5d^6} \\ &= \left[\frac{1}{5} - 3\Delta^2(1-\Delta)^2 \right] d^{-4} - \frac{2}{5} \Delta(1-\Delta)(1-2\Delta)(1+3\Delta-3\Delta^2) d^{-5} \\ &\quad + \frac{1}{5} \Delta^2(1-\Delta)^2(1+2\Delta-2\Delta^2) d^{-6}. \end{aligned} \quad (5.8)$$

The result is in agreement with the solution obtained by Cruz-Orive (1985, 1988) and by Mattfeldt (1987, 1988). The second and last term is, as seen in Fig. 1, of no importance, even for small values of d . The coefficient of variance is, therefore, essentially determined by the first term. The oscillatory function has maxima, $1/(5d^4)$, at integer values of d and minima, $1/(80d^4)$, at $\Delta = 0.5$.

Cruz-Orive (1985) points out that the results for the sphere apply equally to the ellipsoid, if it is sectioned in fixed direction; the variance depends then merely on the mean number of sections. For isotropic sampling the mean number of sections varies, and the 'Zitterbewegung' is averaged out. The absence of undamped oscillations for ellipsoids has also been found for systematic sampling with point grids (Kellerer, 1986). It is in agreement with Eq. (4.9) and the fact that the chord-length density for ellipsoids (Enns & Ehlers, 1978; Kellerer, 1984) has no discontinuities. Numerical values for oblate spheroids are given in the right panel of Fig. 2; these values have been obtained numerically by using Eq. (4.8) in the convenient form:

$$a\varepsilon^2 = -Z_3 - \int_0^{x_{\max}} Z_4(x) dc(x). \quad (5.9)$$

The left panel of Fig. 2 compares the result for the sphere of diameter d (dotted curve) with that for the cube of side length d . At $x=d$ there is a discontinuity of the chord-length density for the sphere of $-2/d$ and of $2/d$ for the cube (Coleman, 1969); the undamped oscillations of ε^2 are, therefore, equal but of opposite sign for the cube and the sphere. This has the interesting implication that the leading term for the cube vanishes for integer d :

$$CV^2(q) = 3\Delta^2(1-\Delta^2)^2 d^{-4} + O(d^{-5}). \quad (5.10)$$

The ratio of the maxima at $\Delta = 0.5$ and the minima at $\Delta = 0$ increases, therefore, with increasing values of d . The chord-length density for a box (Coleman, 1981) has positive discontinuities at the values of x equal to the side lengths; in the general case one obtains, therefore, superposition of undamped oscillations with three different periodicities. The hemisphere is an example of a configuration with edges (i.e. with $c(0) > 0$), but with no discontinuities in $c(x)$ for $x > 0$; accordingly, and as also shown in the left panel of Fig. 2, there is no undamped 'Zitterbewegung'.

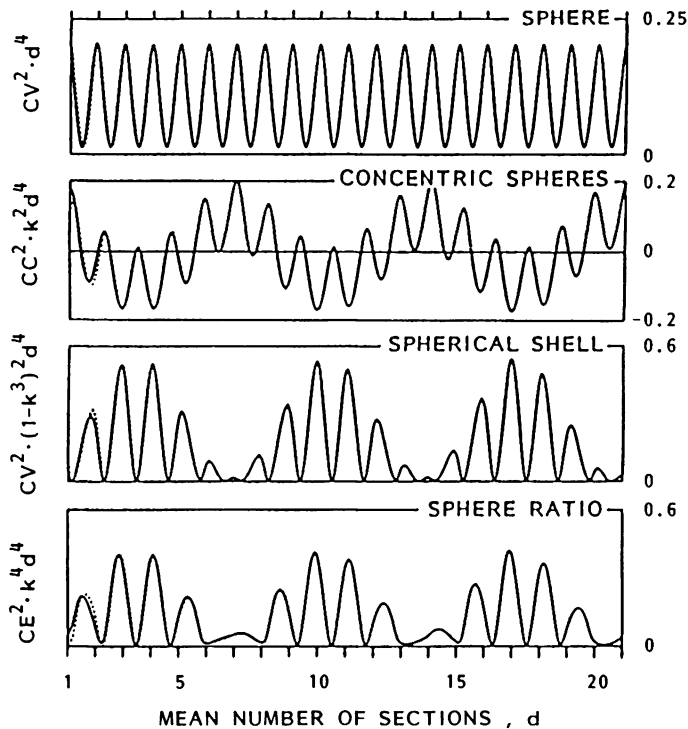


Fig. 1. Coefficients of variance and related quantities that result for systematic planar sectioning with unit spacing between planes. From top to bottom panel: Coefficient of variance, CV^2 , of the volume estimator for the sphere (Eq. 5.8). Relative covariance, CC^2 , of the volume estimators of two concentric spheres with ratio $k=0.71$ of diameters (Eq. 6.3). The coefficient of variance, CV^2 , of a spherical shell with ratio $k=0.71$ of inner to outer diameter (Eq. 6.6 or 6.7). The coefficient of error, CE^2 , of the volume-ratio estimator of two concentric spheres with diameter ratio $k=0.71$ (Eq. 6.10 or 6.11). The diagrams are normalized by suitable terms containing the mean number, d , of sections and the ratio, k , of diameters. The dotted lines indicate the contribution of the leading terms with trend d^{-4} , and show that the remaining terms are inconsequential, even at small d .

The oscillations are also suppressed, with increasing d , if there are size variations in the specimens that are comparable to the spacing of the sampling planes.

6. RELATIONS FOR PAIRED SPECIMENS

A spherical shell is a further configuration for which all derivatives of $U(x)$ exist. One could, therefore, again use Eq. (4.9) to derive the variance of the volume estimator. However, it is somewhat simpler and more instructive to utilize the fact that the equations for the variance can readily be generalized to those for the covariance of the volume estimators of two objects. The treatment will be brief and incomplete, but may indicate the general nature of possible extensions of the results. The work of Gundersen & Jensen (1987, section 7) can be consulted for general reference.

6.1. Covariance of two volume estimators

Let S_1 and S_2 be two specimens in fixed relative position, and q_1 and q_2 the volumes of their intersections with T . Arguments entirely analogous to those in Sections 2 and 3 (and for this reason here omitted) show that Eqs. (2.3), (2.6), (3.2, first line) and (3.6) turn into equations for the coefficient of covariance, if $p_{n,s}(x)$, $p_1(x)$, and $p(x)$ are replaced by the densities of (vectorial,

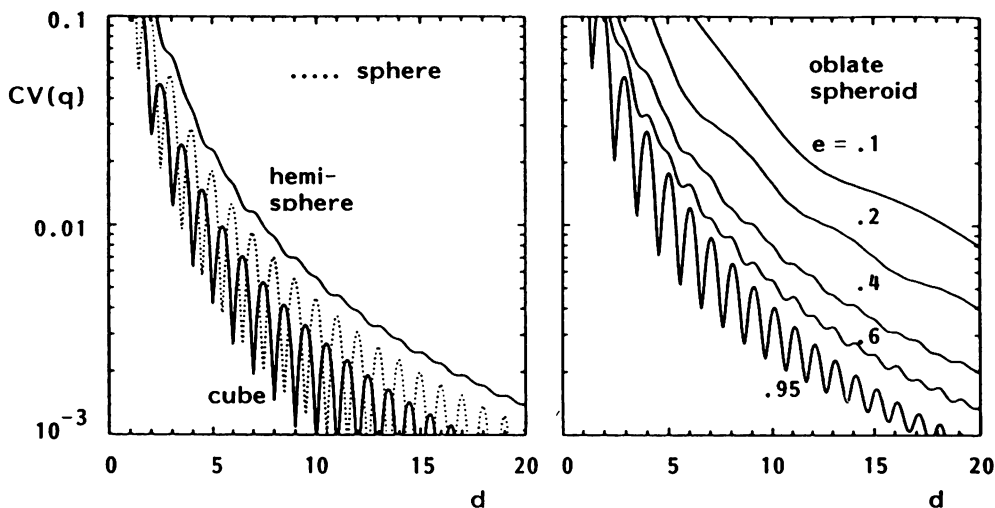


Fig. 2. The fractional standard error, $CV(q)$, of the volume estimator from isotropic systematic planar sections (with unit spacing). Left panel: lower solid curve: cube of side length d ; upper solid curve: hemisphere of diameter d ; dotted curve: sphere of diameter d . Right panel: oblate spheroids of two larger axes d and smaller axis ed (from bottom to top, $e=0.95, 0.6, 0.4, 0.2, 0.1$).

projected, or scalar) distances between independent uniform random points in S_1 and S_2 . This is merely an extension of the earlier case $S_1=S_2=S$.

We can then use the generalized geometric reduction factor $U_{12}(x)=V(S_2)p(x)/nC_n x^{n-1}$. It equals the probability that the translate of a typical point of S_1 by x (in uniform random direction) belongs to S_2 . In analogy to Eq. (4.5) we have:

$$V(S_1)CC^2(q_1, q_2)=Eq_1q_2/(Eq_1Eq_2)-1=V(S_1)\int_0^\infty U_{12}(x)Z_1(x)dx \quad (6.1)$$

and further relations corresponding to Eqs. (4.6)–(4.9).

For two concentric spheres S_1 and S_2 of smaller and larger diameter kd and d we have (Kellerer & Hahn, 1987):

$$U_{12}(x)=\begin{cases} 1 & \text{for } 0 < x < d(1-k)/2 \\ \frac{3}{d^3k^3} [d^3(1+k^3)/2 - d^2(1-k^2)/32x - d^2(1+k^2)x/4 + x^3/6] & \text{for } d(1-k)/2 < x < d(1+k)/2. \end{cases} \quad (6.2)$$

With elementary arithmetic we obtain from the extended Eq. (4.6):

$$\begin{aligned} CC^2(q_1, q_2) = & -3 \left[B_4 \left(\frac{1-k}{2} d \right) + B_4 \left(\frac{1+k}{2} d \right) \right] / k^2 d^4 \\ & - \frac{6}{5} \left[(1-k) B_5 \left(\frac{1-k}{2} d \right) - (1+k) B_5 \left(\frac{1+k}{2} d \right) \right] / k^3 d^5 \\ & + \frac{2}{5} \left[B_6 \left(\frac{1-k}{2} d \right) - B_6 \left(\frac{1+k}{2} d \right) \right] / k^3 d^6. \end{aligned} \quad (6.3)$$

All contributions from discontinuities of the fifth and higher derivatives of $U_{12}(x)$ cancel.

Equation (6.3) reduces to Eq. (5.8) for $k=1$. For $k<1$ the result appears complicated because it is the superposition of a slow oscillation with the period $2/(1-k)$ in d , and a fast oscillation with period $2/(1+k)$. According to the basic property of the Bernoulli polynomials the contributions average zero over the periods. This implies that the average covariance is zero if the variations of d are large. It is usually sufficient to consider only the leading terms which have the general magnitude $1/k^2 d^4$ (see example in Fig. 1).

6.2. Application to the spherical shell

The formula for the covariance can be applied to derive the variance of the volume estimator of a configuration, S , that is the difference of two simple configurations, S_2 and S_1 . The variance of the intercept, q , of S with the sectioning planes can then be expressed in terms of the variances and the covariance of the intercepts, q_1 and q_2 , of S_1 and S_2 with the sectioning planes:

$$\text{Var}(q) = \text{Var}(q_1) + \text{Var}(q_2) - 2 \text{Cov}(q_1, q_2). \quad (6.4)$$

The coefficient of variance is, therefore:

$$CV^2(q) = [V(S_2)^2 CV^2(q_2) + V(S_1)^2 CV^2(q_1) - 2 V(S_2) V(S_1) CC^2(q_1, q_2)] / [V(S_2) - V(S_1)]^2 \quad (6.5)$$

where $CV^2(q_2)$ and $CV^2(q_1)$ are the coefficients of variance of q_2 and q_1 , and $CC^2(q_1, q_2)$ is the relative covariance. If S is the sum of S_1 and S_2 , the minus signs are replaced by plus signs.

A spherical shell is the difference of a larger sphere with diameter d and a smaller sphere with diameter kd . In this case the relation can be written in the form:

$$CV^2(q) = [CV^2(q_2) + k^6 CV^2(q_1) - 2k^3 CC^2(q_1, q_2)] / (1-k^3)^2. \quad (6.6)$$

Combining the leading terms of Eqs. (5.8) and (6.3) we obtain the coefficient of variance of the volume estimator of the spherical shell:

$$CV^2(q) = \left\{ \frac{1+k^2}{10} - 3[B_4(d) + k^2 B_4(kd)] + 6k \left[B_4\left(\frac{1-k}{2}d\right) + B_4\left(\frac{1+k}{2}d\right) \right] \right\} / (1-k^3)^2 d^4. \quad (6.7)$$

Figure 1 illustrates this dependence and shows that the omitted terms are of minor importance for sufficiently large values of d .

6.3. Variance of the estimate of volume ratios

Let $r = q_2/q_1$ be the estimator of the ratio of the volumes, $V(S_2)$ and $V(S_1)$, of S_2 and S_1 . Utilizing the relative deviations, $x_1 = q_1/V(S_1) - 1$ and $x_2 = q_2/V(S_2) - 1$, of the volume estimators we have:

$$\frac{r}{V(S_2)/V(S_1)} = \frac{1+x_2}{1+x_1}. \quad (6.8)$$

When the deviations are small, i.e. $x_2 \ll 1$ and $x_1 \ll 1$ (see Cruz-Orive, 1985, table I) we can approximate this by:

$$r/[V(S_2)/V(S_1)] = 1 + x_2 - x_1 \quad (6.9)$$

and obtain the coefficient of error of the volume-ratio estimator:

$$\begin{aligned} CE^2(r) &= \text{Var}(r) / [V(S_2)/V(S_1)]^2 = E(x_2^2) + E(x_1^2) - 2E(x_1 x_2) \\ &= CV^2(q_2) + CV^2(q_1) - 2CC^2(q_1, q_2). \end{aligned} \quad (6.10)$$

With the leading terms of Eqs. (5.8) and (6.3) we obtain for two concentric spheres of outer

diameter d and ratio k of diameters, and again for sectioning with planes of unit spacing:

$$CE^2(r) = \left\{ \frac{1+k^4}{10} - 3[k^4 B_4(d) + B_4(kd)] + 6k^2 \left[B_4\left(\frac{1-k}{2}d\right) + B_4\left(\frac{1+k}{2}d\right) \right] \right\} / (kd)^4. \quad (6.11)$$

As in Eq. (6.7), the general trend, represented by the first term, is simple. The four oscillatory terms have different periodicities and produce, therefore, a complicated superposition. Again, the higher order terms are inconsequential. For Eqs. (6.3) and (6.11) the two spheres need not be concentric, provided the sectioning planes are parallel to the connection of their centres.

The considerations at the end of Section 5.2 apply equally to the various results for spherical shells or pairs of spheres, i.e. the results can be applied to ellipsoids, and, for isotropic sampling, the oscillatory terms become negligible as d increases.

7. CONCLUSION

Equation (2.2) links the second moment, and therefore also the variance, of the intersection of two geometric objects under uniform, i.e. translation invariant, randomness to the point-pair distance distributions within these objects. The equation is based on Robbins' theorem (1944) and is connected to wider results of stochastic geometry (see e.g. Weil, 1983; Stoyan *et al.*, 1987). In a variety of modifications it is linked not only to systematic sampling (Matérn, 1960; Matheron, 1965, 1971), but also to problems arising in radiation physics and microdosimetry (Kellerer & Chmelevsky, 1975; Kase *et al.*, 1985).

In its application to systematic sampling the equation can be reduced to a one-dimensional integral or sum. Matheron has developed the treatment in terms of the covariogram; it applies to parallel sectioning planes in \mathbb{R}^3 or parallel sectioning lines in \mathbb{R}^2 . This treatment permits approximations which are adequate for most practical purposes. As explained by Cruz-Orive (1988), the approach can also be utilized (with fair approximations) for point grids in \mathbb{R}^2 or for point or line grids in \mathbb{R}^3 .

Isotropy is another condition which permits reduction to a one-dimensional integral. Real specimens are often anisotropic and exhibit some degree of alignment, but, as shown by Gundersen & Jensen (1987), the 'design approach' can usually achieve sufficient isotropy for the position of the test system hitting the specimen. If isotropy pertains, we need only one comparatively simple function, the point-pair distance distribution, for the specimen and an analogous function for the test system, and we obtain exact solutions even for complex test systems, as shown by Matérn (1960, 1985, 1988) who has developed the approach not only for sampling with regular point grids, but also for 'stratified' point sampling.

The relation for the variance of the volume estimator contains an oscillating and, in some cases, complicated function for the test system. This requires high precision in the numerical evaluation. Furthermore it is difficult to predict the undamped oscillations that result for certain specimens, but not for others.

Evaluation of the integral or, for dot grids, of the corresponding sum in terms of a generalized Euler method of successive partial integrations leads to a separation of the solution into the term that represents the general trend and a far more manageable integral that determines the fluctuating term. The simplified integral contains, for convex bodies, the probability density of chord-lengths. Undamped fluctuations occur when there are discontinuities in the chord-length density; this happens for the sphere, the cylinder, or for any polyhedron with parallel opposing faces. The periods of the fluctuations equal the ratio of the chord lengths for which discontinuities occur (e.g. distance between opposing parallel faces or diameter of a sphere) to the periods of the test system (e.g. distances between sectioning planes or between adjacent dots). The relations have here been exemplified for planar sectioning, but the extension to other grid systems is apparent. Appendix 1 contains an analogous treatment in

terms of the covariograms; this is a simple and, in some cases, more efficient alternative to the use of the Fourier transform.

It will be of particular interest to investigate the functions $Z_i(x)$ for different test systems, and especially for regular point grids. These functions are linked to the classical, and still partly unsolved, lattice problem in number theory.

The generalized formulae relate not only to the variance of a volume estimator but also to the covariance of the volume estimators of paired specimens. This permits the treatment of geometries which are the union or difference of simpler structures, and it implies that the results for the variance of volume estimators can be extended to analogous relations for the estimation of volume ratios.

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APPENDIX 1. THE BERNOULLI POLYNOMIALS AND THE USE OF THE COVARIOGRAMS

The Bernoulli polynomials, $B_i(x)$, are periodic functions with mean value zero and, for $i > 1$, with no discontinuities (see Fig. 3):

$$\begin{aligned}
 B_1(x) &= \Delta - \frac{1}{2} & [\text{with } \Delta = \text{Frac}(x)] \\
 B_2(x) &= \Delta^2 - \Delta + \frac{1}{6} \\
 B_3(x) &= \Delta^3 - \frac{3}{2}\Delta^2 + \frac{1}{2}\Delta \\
 B_4(x) &= \Delta^4 - 2\Delta^3 + \Delta^2 - \frac{1}{30} \\
 B_5(x) &= \Delta^5 - \frac{5}{2}\Delta^4 + \frac{5}{3}\Delta^3 - \frac{1}{6}\Delta \\
 B_6(x) &= \Delta^6 - 3\Delta^5 + \frac{5}{2}\Delta^4 - \frac{1}{2}\Delta^2 + \frac{1}{42} \\
 &\dots
 \end{aligned} \tag{A1.1}$$

or generally for $i > 0$:

$$B_i(x) = \sum_{k=0}^i \binom{i}{k} B_k \Delta^{i-k} \tag{A1.2}$$

with the Bernoulli numbers $B_0=1$, $B_1=-1/2$, $B_2=1/6$, $B_4=-1/30$, $B_6=1/42$, $B_8=-1/30$, ..., $B_3=B_5=\dots=0$.

In accord with the relation:

$$B_i(x) = \frac{dB_{i+1}(x)}{dx} / (i+1) \tag{A1.3}$$

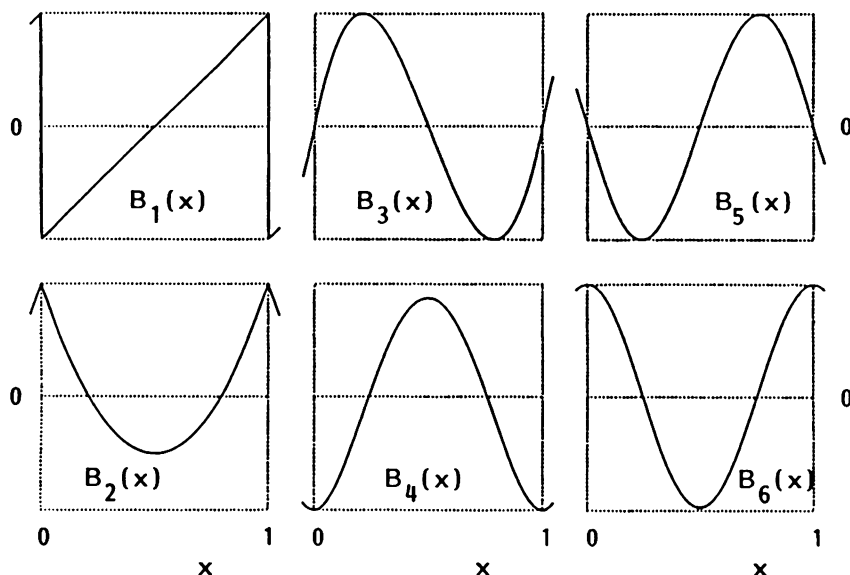


Fig. 3. The first six Bernoulli polynomials (Eq. A1.1). The diagrams are normalized to the maximal absolute values of the functions (0.5, 0.166, 0.0481, 0.0333, 0.0244 and 0.0238).

we use the additional convention:

$$B_0(x) = 1 - \sum_{i=-\infty}^{\infty} \delta(x-i) = 1 - \delta(\Delta) \quad (\text{A1.4})$$

where $\delta(x)$ is the Dirac delta function.

Assuming unit distance, c , between sections we can write Eq. (3.5) in the form:

$$CV^2(q) = - \int_{-\infty}^{\infty} p_1(x) B_0(x) dx \quad (\text{A1.5})$$

and through integration by parts we obtain:

$$\begin{aligned} CV^2(q) = & \sum_j \delta p_1(x_j) B_1(x_j) - \frac{1}{2} \sum_j \delta p_1'(x_j) B_2(x_j) + \dots \\ & - \frac{(-1)^i}{i!} \sum_j \delta p_1^{(i-1)}(x_j) B_i(x_j) - \frac{(-1)^i}{i!} \int_{-\infty}^{\infty} p_1^{(i)}(x) B_i(x) dx. \end{aligned} \quad (\text{A1.6})$$

The solution for systematic sectioning, i.e. for a test system of equidistant hyperplanes, can thus be formulated purely in terms of the Bernoulli polynomials which determine the oscillatory terms and occur whenever there are discontinuities (at $x > 0$) of the (normalized) covariogram $p_1(x)$ and its derivatives. The analogous treatment in terms of the functions $Z_i(x)$ (see Eq. 4.9) requires isotropy but, given this condition, it has the advantage to apply to any test system, including, for example, point grids in \mathbb{R}^2 and \mathbb{R}^3 .

Matheron (1965, 1971) has employed the Euler–MacLaurin formula to obtain the non-oscillatory terms which correspond to the discontinuities at $x_0 = 0$. For the example $p_1(x) = a(b^2 - x^2)^k$ and by methods of Fourier transformation and serial expansion he has derived the explicit solution.

To illustrate the application of Eq. (A1.6) one can utilize the covariogram of the sphere which is readily derived (see Eq. A2.3):

$$p_1(x) = \frac{6}{d} \left[\frac{1}{5} - \left(\frac{x}{d} \right)^2 + \left| \frac{x}{d} \right|^3 - \frac{1}{5} \left| \frac{x}{d} \right|^5 \right] \quad (-d \leq x \leq d). \quad (\text{A1.7})$$

Equation (5.8) is then immediately obtained.

Mattfeldt (1987, 1988) has, partly by direct integration and partly by Fourier methods, derived explicit solutions for different geometries, expressed in terms of the function $f_1(x)$, i.e. the ‘cross-section’ of the specimen (see Section 3.1). From the variety of interesting models we choose an example for further illustration of the straightforward applicability of Eq. (A1.6). Mattfeldt (1988) treats the case which relates to systematic angular sampling of ‘Buffon’s needle’; the normalized density is:

$$f_1(x) = \frac{\pi}{2d} \sin \left(\pi \frac{x}{d} \right) \quad (0 \leq x \leq d). \quad (\text{A1.8})$$

The corresponding (normalized) covariogram:

$$\begin{aligned} p_1(x) &= \int f_1(s) f_1(s+x) ds \\ &= \frac{1}{8} \left(\frac{\pi}{d} \right)^2 \left[\left(1 - \frac{x}{d} \right) \cos \left(\pi \frac{x}{d} \right) + \frac{1}{\pi} \sin \left(\pi \frac{x}{d} \right) \right] \quad (-d \leq x \leq d) \end{aligned} \quad (\text{A1.9})$$

has discontinuities (at $x=0$ and equal discontinuities at $x=-d$ and $x=d$) for derivatives of

uneven order, i ($i \geq 3$):

$$\begin{aligned}\delta p_1^{(3)}(-d) + \delta p_1^{(3)}(d) &= \frac{1}{2} \left(\frac{\pi}{d} \right)^4 = \delta p_1^{(3)}(0) \\ \delta p_1^{(5)}(-d) + \delta p_1^{(5)}(d) &= - \left(\frac{\pi}{d} \right)^6 = \delta p_1^{(5)}(0) \\ \delta p_1^{(7)}(-d) + \delta p_1^{(7)}(d) &= \frac{3}{2} \left(\frac{\pi}{d} \right)^8 = \delta p_1^{(7)}(0) \\ &\dots\end{aligned}\tag{A.10}$$

Therefore, according to Eq. (A1.6):

$$\begin{aligned}CV^2(q) &= - \{ [B_4 + B_4(d)] / 48 \} \left(\frac{\pi}{d} \right)^4 \\ &\quad + \{ [B_6 + B_6(d)] / 720 \} \left(\frac{\pi}{d} \right)^6 \\ &\quad - \{ [B_8 + B_8(d)] / 60,480 \} \left(\frac{\pi}{d} \right)^8 \\ &\quad \dots\end{aligned}\tag{A1.11}$$

Even at low values of d , it is sufficient to use only the first term, $2 \cdot 03 [1/15 - \Delta^2(1 - \Delta)^2]/d^4$, which resembles that for the sphere Eq. (5.8). The solution agrees with Mattfeldt's result, although it is of quite different form. As Mattfeldt points out, it would be very tedious to derive a solution by familiar methods, other than Fourier transform and expansion.

APPENDIX 2. EQUIVALENCE OF EQUATIONS (3.5) AND (3.6)

The equivalence of Eqs. (3.5) and (3.6) for isotropic sampling with parallel planes can be readily shown.

The normalized covariogram, $p_1(x)$, can, under assumption of isotropy, be expressed in terms of the point-pair distance density, $p(s)$, and the conditional density, $h(x|s)$:

$$p_1(x) = \int_x^\infty h(x|s) p(s) ds.\tag{A2.1}$$

In \mathbb{R}^3 we obtain:

$$h(x|s) = \frac{1}{2s}, \quad -s < x < s\tag{A2.2}$$

therefore:

$$p_1(x) = \int_x^\infty \frac{p(s)}{2s} ds, \quad p_1(-x) = p_1(x).\tag{A2.3}$$

Inserting this expression for $p_1(x)$ into Eq. (3.5) and using $t(x)$ from Eq. (5.2) we obtain Eq. (3.6). Alternatively we can insert $p(x) = -2x p'(x)$ and $t(x)$ into Eq. (3.6) to obtain, through integration by parts, Eq. (3.5).