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SECOND-ORDER STEREOLOGY

Eva Bjørn Jensen, Kien Kiêu and Hans Jørgen G. Gundersen

Institute of Mathematics, University of Aarhus, Institut National de la Recherche Agronomique, Montfavet and Stereological Research Laboratory, University of Aarhus

ABSTRACT

Stereological methods of estimating the K-function for d-dimensional particles in \mathbb{R}^n (d = 0,1,...,n) with respect to a process of reference points are reviewed and unified. The general theory is first presented in \mathbb{R}^n and then followed by an explicit treatment of the planar and spatial cases.

Keywords: disector, geometric measure theory, interaction, K-function, particles, stereology, vertical sections. 1. INTRODUCTION

Second-order stereology deals with stereological methods of making inference about parameters describing variability and interaction in spatial structures. The most simple example is a spatial point process where the object is to examine whether the points show clustering or inhibition. Here, the homogeneous Poisson point process serves as a reference, representing the complete random arrangement. If the points are indeed centers of particles, it could also be of interest to study whether there is an interaction between position and size. Here, the null hypothesis may be independence between position and size. For two spatial structures, the question could be whether there is an attraction or inhibition between the two structures.

The East German School of Stochastic Geometry has developed stereological estimators of second-order properties of random spatial structures in the last decade, cf. e.g. Hanisch (1985), Hanisch and Stoyan (1981), Schwandtke (1988), Stoyan (1981, 1984, 1985a, 1985b). In the present paper we will give a review of some of these developments and show that they can be derived from a single formula in geometric measure theory. Related results can be found in Miles (1979), Jensen et al. (1989) and Zähle (1989).

In the present paper, we will take a model-based approach. Thus, the probes (lines, planes and disectors) are fixed while the spatial structures are regarded as random. The design-based theory, where the randomness is on the probes, is somewhat easier to formulate and does not pose restrictions (stationarity, isotropy,...) on the structures. However, for many statisticians, the model-based approach is more appealing, because it

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allows the formulation of stochastic models for the spatial structures, including a model describing a complete random arrangement.

In Section 2, we define the K-function which is the second-order quantity to be studied. In Section 3, we formulate the geometric measure decomposition which is needed for constructing the stereological estimators of the K-functions. In Section 4, the estimators of the K-functions are presented.

2. THE K-FUNCTION

In this and the following sections we will formulate the theory for \mathbb{R}^n and then, as a rule, treat the planar (n = 2) and spatial (n = 3) cases explicitly.

The situation we will concentrate on, is the following. We consider a point process in \mathbb{R}^n , $\psi_0 = \{x_i\}$, which will be a process of reference points. Together with this process we have a process of d-dimensional particles, where d can take the value 0,1,...,n. We will be interested in studying the distribution of the particles around the reference points.

The particle process will be represented by a marked point process $\psi_1 = \{ [y_j; \Xi_j] \}$, where $y_j \in \mathbb{R}^n$ is a point and $\Xi_j \subseteq \mathbb{R}^n$ is a bounded subset of \mathbb{R}^n . Here, y_j is the 'center' of the j'th particle $Y_j = y_j + \Xi_j$, cf. Fig. 1. If $\{x_i\} = \{y_j\}$, we look at the particles from the particle centres. If, in addition, $\Xi_j = \{0\}$ for all j, we simply have a single point process. We assume that ψ_0 and ψ_1 are jointly stationary and that ψ_1 is isotropic.



Fig. 1. Illustration of the particle model.

We will concentrate on a particular type of second-order characteristic, the so-called K-function, cf. Stoyan et al. (1987) and Stoyan & Ohser (1982). Let v_n^d denote the d-intensity of particles, i.e. the total d-volume of particles per unit volume reference space. In particular, with standard stereological notation,

$$\begin{aligned}
 \nu_2^0 &= N_A & \nu_3^0 &= N_V \\
 \nu_2^1 &= L_A & \nu_3^1 &= J_V \\
 \nu_2^2 &= A_A & \nu_3^2 &= S_V \\
 \nu_3^3 &= V_V
 \end{aligned}$$

Then, the K-function K_d of the d-dimensional particles with respect to the reference points is defined by

$$\nu_{n}^{d} \kappa_{d}(R) = E_{0}\left(\sum_{j=1}^{\infty} I\left(|Y_{j}| \leq R\right) \lambda_{n}^{d}(Y_{j})\right)$$
(2.1)

where E_0 is the mean operator under the Palm distribution of ψ_1 w.r.t. ψ_0 , I denotes indicator function and λ_n^d denotes d-volume in \mathbb{R}^n . The quantity $v_n^d K_d(\mathbb{R})$ can be interpreted as the expected total d-volume of particles sitting at a distance at most R from a typical reference point.

If we let $\omega_n = \pi^{n/2} / \Gamma(\frac{n}{2}+1)$ be the volume of the unit ball in \mathbb{R}^n , then

$$\nu_{n}^{d}(K_{d}(R_{2})-K_{d}(R_{1}))/\omega_{n}(R_{2}^{n}-R_{1}^{n})$$
(2.2)

can be interpreted as the local d-intensity for particles at a distance between R_1 and R_2 from a typical reference point. If ψ_0 and ψ_1 are independent, the local d-intensity equals the global d-intensity v_n^d .

3. THE MEASURE DECOMPOSITION

It is possible to construct an estimator of the K-function for d-dimensional particles based on measurements on or in the neighbourhood of a p-subspace of \mathbb{R}^n (a p-dimensional linear subspace of \mathbb{R}^n), if d+p-n \geq 0. Some of the estimators are based on measurements on a p-subspace, containing a fixed r-subspace, $0 \leq r < p$. These can be applied under the less restrictive assumption that the distribution of the particles are invariant only under rotations which keep the r-subspace in question fixed. Let $L_{p(r)}^{n}$ denote a p-subspace of \mathbb{R}^{n} , containing a fixed r-subspace, $0 \leq r \leq p \leq n$. In particular, $L_{1(0)}^{2}$ is a line through 0 in the plane and

$$L_{1(0)}^{3} = \text{line in } \mathbb{R}^{3} \text{ through } 0$$

$$L_{2(1)}^{3} = \text{plane in } \mathbb{R}^{3} \text{ containing a fixed line}$$

$$L_{2(0)}^{3} = \text{plane in } \mathbb{R}^{3} \text{ through } 0,$$



Fig. 2. Parametrization of
$$\mathscr{L}_{1(0)}^{3}$$
, $\mathscr{L}_{2(0)}^{3}$ and $\mathscr{L}_{2(1)}^{3}$.

cf. Fig. 2. Let $\mathscr{L}_{p(r)}^{n}$ be the set of all $L_{p(r)}^{n}$ and let $dL_{p(r)}^{n}$ be the (differential) element of the measure on $\mathscr{L}_{p(r)}^{n}$ which is invariant under rotations in \mathbb{R}^{n} which keep a particular r-subspace $L_{r(00)}^{n}$, say, fixed. The measure is unique up to multiplication with a positive constant and it is here scaled such that

$$\int_{\mathcal{L}_{p}^{n}} dL_{p(r)}^{n} = \sigma_{n-r} \cdots \sigma_{n-p+1} / \sigma_{1} \cdots \sigma_{p-r}$$
$$= d(n, p, r) \qquad (3.1)$$

say, where

$$\sigma_{n} = 2\pi^{n/2} / \Gamma(n/2)$$
 (3.2)

is the surface area of the unit ball in \mathbb{R}^n . In particular,

$$dL_{1(0)}^{3} = \sin\theta \ d\theta \ d\phi$$
$$dL_{2(1)}^{3} = d\phi$$
$$dL_{2(0)}^{3} = \sin\theta \ d\theta \ d\phi$$

where the notation is as shown in Fig. 2.

The estimators of the K-functions are based on a geometric measure decomposition which will now be presented. Let Y_j be a d_j -dimensional bounded manifold in \mathbb{R}^n , $j = 1, \ldots, q$. Let $L^n_{r(00)}$ be a fixed r-subspace and let p = q+r. We assume that $d_j-n+p \ge 0$, $j = 1, \ldots, q$. In section 4, we shall consider the case where the Y's are particles and thereby random sets. For

the moment, they are regarded as non-random. Let $y_j^{d_j} \in Y_j$, j = 1,...,q. The superscript of $y_j^{d_j}$ is used to indicate the dimension of the space within which the point is regarded to lie. For brevity, we write, when convenient, $dy_j^{d_j}$ instead of $\lambda_n^{d_j}(dy_j^{d_j})$ in what follows. Consider the mapping

$$(y_1^{d_1}, \dots, y_q^{d_q}) \rightarrow L_{p(r)}^n$$
 (3.3)

where $L_{p(r)}^{n}$ is the p-subspace spanned by $y_{1}^{d_{1}}, \ldots, y_{q}^{d_{q}}$ and $L_{r(00)}^{n}$. For an illustration with n = 3, q = 1, r = 1, p = 2, $d_{1} = d = 1$, see Fig. 3. An explicit expression of the Jacobian of this mapping can be found, cf. Jensen and Kiêu (1989). Related results have been given by Zähle (1989). The result is

$$v_{p(r)}^{-(n-p)}(y_{1}, \dots, y_{q}) \stackrel{q}{=} a_{j}^{a_{j}, p}(y_{j}) \stackrel{q}{=} a_{j}^{a_{j}} d_{j}^{j}$$

$$= \prod_{j=1}^{q} a_{j}^{a_{j}^{j}-n+p} d_{p(r)}^{n} .$$

$$(3.4)$$

Here, $v_{p(r)}$ is p! times the p-volume of a simplex spanned $d_1 \qquad d_q$ by y_1, \ldots, y_q and r orthonormal vectors in $L_{r(00)}^n$. In particular

$$v_{1(0)} = \text{distance of } y_1$$
 to the origin
 $v_{2(1)} = \text{distance of } y_1$ to $L_{1(00)}$
 $v_{2(0)} = 2 \times \text{area of triangle with vertices } 0, y_1, y_2$,



Fig. 3. Illustration relevant for the geometric measure decomposition.





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see Fig. 4. Furthermore, $G_n^{d_j;p}(Y_j)$ is the (n-p)-volume of the projection onto $L_{p(r)}^{nl}$ of a unit cube in $T_j \cap (T_j \cap L_{p(r)}^n)^l$ where T_j is the tangent space to Y_j at Y_j^j . In Table 1, values of $G_n^{d;p}(y)$ are given for all interesting cases in \mathbb{R}^2 and \mathbb{R}^3 . Note that the G-factors depend on the local geometry of the manifolds considered and require local n-dimensional measurements.

The measure decomposition will be used in two different ways. In the first case, we let r = p-1 and q = 1. Only one manifold Y of dimension d, say, is then involved. We get

$$v_{p(p-1)}^{-(n-p)}(y)G_{n}^{d;p}(y)dy^{d} = dy^{d-n+p} dL_{p(p-1)}^{n}$$
(3.5)

or

$$\lambda_{n}^{d}(Y) = \int_{\substack{\mathcal{Q}^{n} \\ p(p-1)}} m(Y, L_{p(p-1)}^{n}) \frac{dL_{p(p-1)}^{n}}{d(n, p, p-1)}$$
(3.6)

where

$$m(Y, L_{p(p-1)}^{n}) = d(n, p, p-1) \int_{\substack{Y \cap L_{p(p-1)}^{n} (p-1)}}^{y n-p} (y) / G_{n}^{d;p}(y) dy^{d-n+p} . (3.7)$$

Therefore, if Y is a random set with a distribution invariant under rotations that keep $L_{p-1(00)}^{n}$ fixed, the distribution of $m(Y, L_{p(p-1)}^{n})$ does not depend on $L_{p(p-1)}^{n}$. In that case, $\lambda_{n}^{d}(Y)$ and $m(Y, L_{p(p-1)}^{n})$ have the same first-order properties. Therefore, unbiased stereological estimators of the K-function, ACTA STEREOL 1990; 9/1

<u>Table 1</u>

The factor $G_2^{d;p}$: Planar case

d/p	1	2
1	sin a _{ll}	1
2	1	1

 α_{11} = angle between tangent line of planar curve and line probe.

The factor G₃^{d;p}: Spatial case

_d\ ^p	11	2	_3
1	-	$\sin \alpha_{12}$	1.
2	sin ^a 21	sin a ₂₂	1
3	1	1	1

- a₁₂ = angle between tangent line of spatial curve and plane
 probe
- α_{21}^{21} = angle between tangent plane of spatial surface and line probe
- α_{22} = angle between tangent plane of spatial surface and plane probe

cf. (2.1), can be constructed by replacing $\lambda_n^d(Y_j)$ with the measurement $m(Y_j, L_{p(p-1)}^n)$, cf. Section 4.

This approach does not cover all cases of interest. For instance, the estimation of the K-function for 2-dimensional particles in \mathbb{R}^3 , based on measurements on an arbitrary plane.

For simplicity, we will concentrate on constructing estimators based on measurements at $L_{2(0)}^{n}$. This correspond to p = 2 and r = 0, cf. Fig. 2. Let $Y_{1} = b(0,1)$, the unit ball in \mathbb{R}^{n} , and $Y_{2} = Y$, a bounded manifold of dimension $d_{2} = d$. Then, we get from (3.4)

$$v_{2(0)}^{-(n-2)}(y_{1}, y_{2})G_{n}^{d;2}(y_{2})dy_{1}^{n}dy_{2}^{d}$$
$$= dy_{1}^{2}dy_{2}^{d-n+2}dL_{2(0)}^{n}. \qquad (3.8)$$

Since $\omega_n^{-1} \int_{b(0,1)} dy_1^n \equiv 1$, we have

$$\begin{split} \lambda_{n}^{d}(Y) &= \int_{Y} dy_{2}^{d} \\ &= \omega_{n}^{-1} \int_{Y} \int_{b(0,1)} dy_{1}^{n} dy_{2}^{d} \\ &= \omega_{n}^{-1} \int_{\mathcal{L}_{2}^{n}(0)} \int_{Y \cap L_{2}^{n}(0)} \int_{b(0,1) \cap L_{2}^{n}(0)} \\ &= \omega_{n}^{-2} \int_{\mathcal{L}_{2}^{n}(0)} \int_{Y \cap L_{2}^{n}(0)} \int_{b(0,1) \cap L_{2}^{n}(0)} \\ &= \frac{r(\frac{n-1}{2})}{\frac{n-1}{12}} \int_{\mathcal{L}_{2}^{n}(0)} \int_{Y \cap L_{2}^{n}(0)} v_{1(0)}^{n-2}(y_{2}) / G_{n}^{d;2}(y_{2}) dy_{2}^{d-n+2} dL_{2}^{n}(0) \end{split}$$

$$= \int_{\substack{\mathcal{G} \\ \mathcal{G}_{2}(0)}} m(Y, L_{2}^{n}(0)) \frac{dL_{2}^{n}(0)}{d(n, 2, 0)}$$
(3.9)

where

$$m(Y, L_{2(0)}^{n}) = \omega_{n-2} \int_{Y \cap L_{2(0)}^{n}} v_{1(0)}^{n-2}(Y_{2}) / G_{n}^{d;2}(Y_{2}) dy_{2}^{d-n+2} .$$
(3.10)

Therefore, $\lambda_n^d(Y_j)$ can be replaced by the measurement $m(Y_j, L_{2(0)}^n)$ when constructing estimators of K-functions on the basis of an arbitrary planar section.

4. ESTIMATORS OF K-FUNCTIONS

Any of the estimators of K-functions are obtained by first collecting a sample of reference points and then, with each sampled point as origin, determining an estimate of the total d-volume of particles at a distance at most R from the reference point in question. The estimate can be based on information at a p-subspace $L_{p(r)}^{n}$ containing a fixed r-subspace, $0 \leq r < p$, provided that $d+p-n \geq 0$.

For $d \ge 1$, we can use the measure decomposition described in the previous section. If we sample all reference points in a box B, we have the following estimate of $\nu_n^d \times K_d(R)$:

$$N^{-1} \sum_{\substack{X_{i} \in B Y_{j}}} \sum I(|Y_{j}-X_{i}| \leq R) m(Y_{j}, X_{i}+L^{n}_{p(r)}), \qquad (4.1)$$

where N is the number of sampled reference points and $m(Y_j, x_i + L_p^n(r))$ is an estimate of the d-volume of the particle Y_j , based on measurements at the p-flat $x_i + L_p^n(r)$ through x_i . In all cases of practical interest, the actual form of the measurements can be derived from (3.7) and (3.10) and is presented in Table 2 and Table 3.

Many of the cases described in Table 2 and Table 3 have previously been treated separately in further detail: Stoyan (1981) (Table 2a), Jensen & Gundersen (1987) (Table 2a,b and Table 3c,f), Cruz-Orive (1987) (Table 3f,g), Stoyan (1984) (Table 3a).

It still remains to treat the case of 0-dimensional particles which is not covered by the measure decomposition from the previous section. The solution to this problem is due to Evans, cf. Gundersen et al. (1988). For simplicity, we will concentrate on the spatial case n = 3.

Let us first present a simple result about sampling points by means of two parallel planes, a distance h apart, viz. a disector, cf. Sterio (1984). The points $\{Y_j\}$ are for the moment regarded as fixed. One of the planes $L_{2(r)}^3$ in the disector is either an isotropic random plane through the origin or a vertical random plane through the origin depending on whether r = 0 or 1. A particular point y is sampled if it lies between the two planes. It is easy to show that the sampling probability is

isotropic disector:
$$p_{y,h} = h/[2d_0(y)], h \le d_0(y)$$

= 1/2, h > d_0(y) (4.2)

<u>Table 2</u>. Estimates of the d-volume of a particle, based on measurements at p-flat containing a fixed r-flat. For details, see Section 4.

d\ ^{p,r}	p = 1, r = 0
	line
1	m = a = m = a = m = a = m = a = m = a = m = a = m = a = a
2	$\frac{\frac{\pi}{2}\sum_{k=1}^{\infty}h_2(y_{k-}, y_{k+})}{k}$

Planar case

- a: The intersection points between a one-dimensional particle Y and a line $x+L_{1(0)}^2$ are numbered by index k, d_{0k} denotes the distance between the k'th intersection point and the reference point x and α_k the angle between the tangent line to the particle and the line $x+L_{1(0)}^2$. In the general formula (3.4), the distances are denoted by v.
- b: The intersection between a 2-dimensional particle and a line $x+L_{1(0)}^2$ is divided into intercepts

$$Y \cap (x+L_{1(0)}^{2}) = \bigcup_{k=1}^{M} [Y_{k-}, Y_{k+}]$$
.

The measurements depend on the function h_2 where for general n

 $h_{n}(y_{-},y_{+}) = \begin{cases} |y_{-}x|^{n} + |y_{+}-x|^{n}, & \text{if } x \text{ is between} \\ & y_{-} \text{ and } y_{+} \end{cases}$ $||y_{-}x|^{n} - |y_{+}-x|^{n}|, \text{ otherwise} \end{cases}$

ർ Estimates of the d-volume of a particle, based on measurements at p-flat containing fixed r-flat. For details, see Section 4 Table 3.

Spatial case

d\ ^{P, r}	p = 1, r = 0	p = 2, r = 1	p = 2, r = 0
	line	plane containing fixed line	plane
1	l	$ \begin{array}{c} m \\ \pi & \Sigma \\ k=1 \end{array} d_{1k}/sin \alpha_{12k} \\ \end{array} $	$\begin{array}{c} m\\ 2 & \Sigma\\ k=1 \end{array} d_{0k}/sin \alpha_{12k} \end{array} b$
2	$2\pi \begin{array}{c} m\\ k=1 \end{array} \begin{array}{c} a_{0k}^{2}/\sin \alpha_{21k} \\ k=1 \end{array} \begin{array}{c} \pi \int \\ Y_{0l} \end{array}$	$\pi \int_{Y\cap(x+L_{2(1)})} d_{1}(y)/\sin \alpha_{22}(y) dy$	$\begin{bmatrix} J \\ Y^{(K+L_{2(1)})} d_{1}(Y)/\sin \alpha_{22}(Y) d_{Y} \end{bmatrix} \begin{bmatrix} 2 & J \\ Y^{(K+L_{2(0)})} d_{0}(Y)/\sin \alpha_{22}(Y) d_{Y} \end{bmatrix}$
3	$\frac{2\pi}{3} \begin{array}{c} M \\ k=1 \end{array} h_3 (Y_{k-}, Y_{k+}) \end{array}$	π ∫ d1(Y)dY g	2 f Yn(x+L ₂₍₀₎)d ₀ (Y)dY

Table 3 (continued)

- a,b,c: The intersection between particle and probe has dimension 0. The intersection points are numbered by k. The distance from the k'th intersection point to a reference point x is denoted d_{0k} , while the distance to a fixed line is denoted d_{1k} . The notation for the corresponding angles can be found in Table 1.
- d,e: Only integral representations are available. Here, d_i(y) denotes the distance from y to a reference point or to a fixed line, depending on whether i = 0 and 1. The nota-tion for the angle can be found in Table 1.
- f: The notation is as for the planar case b.

g,h: The notation for the distance is as for case d and e.

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vertical disector:
$$p_{y,h} = Arcsin(h/d_1(y))/\pi$$
, $h \leq d_1(y)$
= 1/2, $h > d_1(y)$, (4.3)

where the notation for the distances $d_0(y)$ and $d_1(y)$ is as for Table 3.

This simple result can be used to estimate the K-function of the point process $\{Y_j\}$ with respect to the point process $\{x_i\}$. We therefore change to the model-based approach. As in the previous cases, we first collect a sample of reference points and then, with each sampled point as origin, determine an estimate of the total number of Y_j 's at a distance at most R from the reference point in question. This estimate is obtained by sampling all points between the two planes of a disector centered at the reference point and summing up the inverse sampling probabilities. The final estimator of $N_V K_0(R)$ is

$$N^{-1} \sum_{\substack{x_i \in B \\ y_j \text{ sampled} \\ at x_i}} \Sigma I(|y_j - x_i| \le R) p_{y_j - x_i,h}^{-1} .$$
(4.8)

REGULARITY CONDITIONS

The present paper has been written with the purpose of presenting a unified theory of second-order stereology in an informal way. For that reason, the emphasis has not been on technical matters.

It is, however, important to emphasize that regularity conditions are needed on the sets involved.First of all, the

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sets are assumed to λ_n^d -rectifiable and λ_n^d -measurable, cf. Federer (1969). This assumption ensures that a d-dimensional tangent space can be defined almost everywhere. Secondly, we assume that the mapping (3.3) is well-defined and that the Jacobian (3.4) is non-zero almost everywhere. A more detailed discussion of these regularity conditions will be presented in Jensen and Kieu (1989).

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