Simulating stochastic geometries: morphology of overlapping grains

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Abstract

Integral geometry furnishes a family of morphological descriptors known as Minkowski functionals which are related to curvature integrals. We present an exact algorithm for the calculation of Minkowski functionals for overlapping grains each with arbitrary location, orientation and shape (Boolean model). The method is numerically robust even for small samples, independent of statistical assumptions, and yields global as well as local morphological information. We illustrate the method by applying it to distributions of overlapping and hard disks. © 2002 Elsevier Science B.V. All rights reserved.

The effective modeling of spatial structures becomes more and more important in statistical physics, particularly on mesoscopic scales in order to bridge different length and time scales. For instance, overlapping disks and spheres serve as standard models of stochastic geometries for many physical applications, e.g., for porous media, complex fluids (see Fig. 1), or even for the large-scale structure in the universe [1]. The morphology of patterns may be characterized by the covered volume (or area), the surface area (or boundary length), and the Euler characteristic, i.e. connectivity of the penetrating grains. Such geometric functionals which are known as Minkowski functionals in integral geometry [2] may be introduced as integrals of curvatures. Let A be a compact domain in \( \mathbb{R}^d \) with regular boundary \( \partial A \in C^2 \) and \( d - 1 \) principal radii of curvature \( R_i \) (\( i = 1, \ldots, d - 1 \)). The functionals \( M_\nu(A) \), with \( \nu \geq 1 \), can be defined by the surface integrals

\[
M_{\nu+1}(A) = \frac{1}{(\nu + 1)(\nu + 1)} \int_{\partial A} S_{\nu} \left( \frac{1}{R_1}, \ldots, \frac{1}{R_{d-1}} \right) dS,
\]

where \( S_{\nu} \) denotes the \( \nu \)th elementary symmetric function and \( dS \) the \( (d - 1) \)-dimensional surface element.

A remarkable theorem in integral geometry is the completeness of the so-called Minkowski functionals [2]. The theorem asserts that any additive, motion invariant and conditional continuous functional \( M(A) = \sum_{\nu=0}^{d} c_\nu M_\nu(A) \) on subsets \( A \subset \mathbb{R}^d \) is a linear combination of the \( d + 1 \) Minkowski functionals \( M_\nu \) with real coefficients \( c_\nu \) independent of \( A \). Here, we propose a novel algorithm to compute exactly these additive morphological measures.

Let us consider a configuration \( A_N = \bigcup_{i=1}^{N} K_i \) of \( N \) overlapping grains \( K_i \) in two dimensions. The bod-
ies \( K_i \) can have any distribution of size and shape. Our aim is to calculate analytically the Minkowski measures \( M_\nu(A) \) which are unambiguously determined by the borderline \( \partial A = \bigcup_{i=1}^{N} \partial A_i \). Here, \( \partial A_i \) denotes the uncovered part of the grain boundary \( \partial K_i \) which is connected at singular points of \( \partial A \) (see Fig. 1).

Since more than four particles may intersect, the determination of the functionals by using additivity is very time-consuming so that for Monte Carlo simulations another algorithm is necessary. First, we focus on the two-dimensional volume \( M_0 \), whose determination succeeds with the help of Gauss’ formula \( \int_{A} \nabla \cdot F \, d^d x = \int_{\partial A} F \cdot n \, dS \) where \( F \) denotes a continuous differentiable vector field and \( n : \partial V \to \mathbb{R}^d \) the outer normal of \( \partial A \). Using \( F(x) = x = (x_1, x_2) \in \mathbb{R}^2 \) and applying a piecewise parametrization \( \hat{x}'(t), t_{\text{st}} \leq t \leq t_{\text{en}} \) of the boundary \( \partial A_i \), one finds for the volume:

\[
M_0(A) = \frac{1}{d} \sum_{i} \int_{\partial A_i} x \cdot n \, dS
= \frac{1}{2} \sum_{i} \int_{\partial A_i} (x_1^i(t)\dot{x}_2^i(t) - x_2^i(t)\dot{x}_1^i(t)) \, dt,
\]

(2)

where \( \dot{x}^i(t) \) denotes the tangent vector and \( t_{\text{st}}^i \) and \( t_{\text{en}}^i \) the start and end point of \( A_i \) where the continuous pieces of \( \partial A \) are connected. The boundary length \( M_1(A) \) is directly given by integrating along the boundaries \( \partial A_i \) and the Euler characteristic \( \chi(A) = \pi M_2(A) \) equals the integral of the curvature \( \kappa_i(t) \), i.e.

\[
M_1(A) = \sum_{i} \int_{\partial A_i} |\hat{x}'(t)| \, dt,
M_2(A) = \sum_{i} \int_{\partial A_i} \kappa_i(t) |\hat{x}'(t)| \, dt + \sum_{j} \chi_j,
\]

(3)

where \( \chi_j \) is a contribution at the intersection points of two adjacent pieces \( \partial A_j \) and \( \partial A_{j+1} \) of the boundary \( \partial A \) where the parametrization is discontinuous (see Fig. 1). and (3). For two overlapping disks of radius \( R \) at \( \hat{x}_1^m \) and \( \hat{x}_2^m \) one finds, for instance, \( t_{\text{st}}^i = \arcsin(|\hat{x}_m^i - \hat{x}_1^m|/(2R)) \), \( t_{\text{end}}^i = 2\pi - t_{\text{st}}^i \), \( t_{\text{st}}^j = t_{\text{st}}^i \), \( t_{\text{end}}^j = t_{\text{end}}^i - \pi \), \( t_{\text{st}}^j = -t_{\text{st}}^i \), \( \kappa_i = 1/R \), and the local curvature \( 2\pi \chi_j = \pi + (t_{\text{st}}^i - t_{\text{en}}^i) \) by applying the Gauss–Bonnet theorem, since the parameter \( t \) equals the angle \( \alpha \) shown in Fig. 1. In general, the Minkowski functional \( M_\nu \), i.e. the curvature integrals given by Eq. (1) where \( \partial A \) is the union of the uncovered borderlines of the disks, reads

\[
M_1 = \sum_{i} \frac{R}{2\pi} (t_{\text{en}}^i - t_{\text{st}}^i).
\]
\[ M_2 = \frac{M_1}{\pi R} + \sum_j \chi_j, \]
\[ M_0 = \sum_i R^2(t_{\text{en}}^i - t_{\text{st}}^i) \]
\[ + R^2(x_1^i \sin t_{\text{en}}^i - x_2^i \cos t_{\text{en}}^i) \]
\[ + x_2^i \cos t_{\text{st}}^i - x_1^i \sin t_{\text{st}}^i. \]

Thus, to compute \( M_\nu \) one has only to determine the parameters \( t_{\text{en}} \) and \( t_{\text{st}} \) and the local Euler characteristics \( \chi_j \) of the intersection points not covered. In order to test the accuracy of the method we apply the algorithm first to a Poissonian ensemble of overlapping disks where analytical results are known [3,4]. Simulating equilibrium distributions \( A \) of disks and measuring the Minkowski functionals \( M_\nu(A) \) one can compare the results which are shown in Fig. 2. In the case of hard disks, an exact result for Minkowski functionals is not known so that one relies on an accurate algorithm to evaluate the morphological measures, in particular, the Euler–Poincaré characteristic. Equilibrium data were generated in the following manner: disks where chosen sequentially, moved and checked whether they overlap other disks or not. For each density \( \rho \) more than 10,000 steps per particle were performed by a standard Monte Carlo procedure. Depending on the ratio \( \kappa \) of the outer and inner radius (see Fig. 1) it is possible to have multiple overlaps of disks.

In particular, two disks can overlap iff \( \kappa < 1 \) and three iff \( \kappa < \sqrt{3}/2 \sim 0.866 \), but if \( \kappa < 1/2 \) a proliferation of possible overlaps occurs. In this limit an expansion of the Minkowski functionals in density or applying the additivity property is not useful anymore and the above algorithm is necessary. The data points in Fig. 2 can be well fitted by polynomials

\[ m_0(n) = 0.987n - 0.3265n^2 + 0.0361n^3, \]
\[ m_1(n)R = 0.9994n - 0.8626n^2 + 0.2432n^3 \]
\[ - 0.02211n^4, \]
\[ m_2(n)R^2 = 0.9422n - 1.747n^2 + 0.8417n^3 \]
\[ - 0.12210n^4. \]

The standard error for all three polynomial regressions is less than or equal to \( 10^{-3} \). Although the qualitative behaviour of the morphological measures does not change, the differences to an ensemble of fully penetrable disks increases with density \( \rho = \pi R^2 \). The calculation of mean values and variances of random disk systems is only one example of the utility of integral geometry and of Minkowski functionals. Since many physical phenomena depend essentially on the geometry of spatial structures, models for stochastic geometries and algorithms to characterize the morphology may help to elucidate physical properties in future work.

Fig. 2. Mean values \( m_\nu(n) \) (left) and variances \( m_{\nu\nu}(n) \) (right) of Minkowski functionals \( M_\nu \) for Poisson-distributed fully overlapping disks of density \( n = \pi R^2 \rho \) (dashed line) and for partially overlapping hard disks of ratio \( \kappa = 0.4 \) (circles: area; squares: boundary length; triangles: Euler characteristic). The dashed lines also represent the analytical results \( m_0 = 1 - e^{-n}, m_1 = \pi R e^{-n}, m_2 = \pi (1 - n) e^{-n} \) for the mean values [3] and for the variances [4] which cannot be distinguished from the numerically evaluated values since error bars are much smaller than the symbol size. The solid lines give the fitted polynomials in Eq. (5).
References


