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MULTIVARIATE UNFOLDING PROBLEMS

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ABSTRACT

The classical stereological unfolding problem for particle systems is studied. While previously at most bivariate problems were solved, here a multivariate version is formulated. Then the unfolding of the joint trivariate distribution of size, shape factor and orientation of spheroidal particles is demonstrated using vertical uniform random sections. The formulation and solution is design-based, first the integral equations are derived, then a numerical solution is discussed. It is emphasized that under the conditional independence property of particle sections, the unfolding problem studied can be decomposed into a series of two simpler problems. The intensity N_V estimator is obtained in the first step which is equivalent to the Wicksell problem of spheres. Finally an application of the results to the study of damage initiation in materials is presented.

Keywords: Conditional independence, size-shape-orientation distribution, stereological unfolding, vertical sections

1 INTRODUCTION

Consider a system of three-dimensional particles of a given shape spread in an opaque base and observe its planar section. The problem may be formulated either in the design-based approach where particles are fixed and the section plane is random or in the model-based approaches where particles form a stationary random process. Defining some geometrical parameters of particles one would like to evaluate their joint distribution from the observed parameters of planar particle sections. The problem typically leads to integral equations between corresponding joint probability densities, which are solved either analytically or numerically. Eventually, the integral equation can be expressed in terms of joint distribution function of particle parameters. Even in cases when the kernel function of the integral equation cannot be derived, Ohser and Mücklich (1995) solved some problems using the simulations of coefficients of the discretized integral equation. The following problems with two particle parameters have been solved: size and shape factor for spheroids (Cruz-Orive, 1976), size and number of edges for polyhedra (Ohser and Mücklich, 1995), size and orientation of platelike particles (Gokhale, 1996).

In the present paper it is shown how multivariate unfolding problems may be investigated using the probabilistic interpretation of the kernel function in the integral equation. When a suitably defined conditional independence property is satisfied the unfolding can be decomposed into a series of simpler problems. The general theory is applied finally to the trivariate size-shape-orientation distribution of ellipsoidal particles. Using the sampling design of vertical uniform random sections the relation between planar and spatial parameters is obtained. In a statistical study, a numerical EM-algorithm (Silverman et al., 1990) is used for the real data evaluation and the stability of solution is discussed.

2 UNFOLDING AND CONDITIONAL INDEPENDENCE

A bounded closed convex set in the l-dimensional Euclidean space R^l is called a particle. Let a fixed particle X be described by n geometrical parameters (real constants) $x_1, x_2, ..., x_n$, which correspond e.g. to the mean caliper diameter, shape factor, orientation, number of vertices etc. A sampling design is represented by a random hyperplane ρ with probability distribution Q on the parametric space of hyperplanes. Assume that the intersection $Y = X \cap \rho \neq \emptyset$, then Y is a random closed convex set in R^{l-1} called a particle section. Let $y_1, ..., y_m$ be geometrical parameters describing Y, such that $y_1, ..., y_k, k \leq \min(n, m)$ correspond to properties of $x_1, ..., x_k$, e.g. x_1, y_1 size, x_2, y_2 shape factor etc. Let $p(y_1, ..., y_m | x_1, ..., x_n, \uparrow)$ be the conditional probability density of $y_1, ..., y_m$ given $x_1, ..., x_n$ and given that the particle is hit by ρ. The upper arrow $\uparrow$ emphasizes that the distribution p depends not only on particle characteristics but also on the sampling design Q.

Further assume that particles are randomly dispersed in R^l with constant intensity N_l. Conditionally that the particles are all the same (just translates of X) denote by $N_{l-1}(x_1, ..., x_n)$ the mean (with respect to Q) intensity of particle sections in ρ.

In the following step given N_l let particles be not all the same, they have a distribution with probability density $f(x_1, ..., x_n)$ of parameters $x_1, ..., x_n$ invariant with respect to translations in R^l. We are interested in particle sections observed in ρ.

The unconditional particle section intensity N_{l-1} and probability density $g(y_1, ..., y_m)$ of parameters $y_1, ..., y_m$ are defined by

$$N_{l-1}g(y_1, ..., y_m) = \int .. \int N_{l-1}(x_1, ..., x_n)p(y_1, ..., y_m | x_1, ..., x_n, \uparrow)f(x_1, ..., x_n)dx_1..dx_n. \quad (1)$$

Integrating both sides of (1) w.r.t. $y_1, ..., y_m$ it is obviously $N_{l-1} = EN_{l-1}(x_1, ..., x_n)$.

The stereological unfolding problem consists in the estimation of unknown probability density f and particle density N_l from the particle section distribution g and N_{l-1}, which can be observed and estimated from realizations of ρ. The first part of the solution is to establish the theoretical relations.

The unfolding problem is described by an equation

$$N_{l-1}g(y_1, ..., y_m) = N_l \int .. \int k(x_1, ..., x_n, y_1, ..., y_m)f(x_1, ..., x_n)dx_1..dx_n, \quad (2)$$

for some nonnegative kernel function k.

To prove this formula we use (1) and put

$$k(x_1, .., x_n, y_1, ..., y_m) = \frac{N_{l-1}(x_1, ..., x_n)}{N_l} p(y_1, ..., y_m | x_1, ..., x_n, \uparrow).$$

The following definition is useful for the simplification of an unfolding problem:

The section parameter y_1 is strongly conditionally independent of $y_2, .., y_m$ given $x_1, ..., x_n$ and Q if the kernel function k in (2) satisfies

$$k(x_1, ..., x_n, y_1, ..., y_m) = k_1(x_1, y_1)k_2(x_2, .., x_n, y_2, .., y_m) \quad (3)$$

for some functions k_1, k_2 and any $y_1, ..., y_m, x_1, ..., x_n$.

It follows that under this property the unfolding problem can be decomposed into a series of problems with smaller numbers of parameters:

Let y_1 be strongly conditionally independent of $y_2, ..., y_m$. Then there exist nonnegative functions k_1, k_2 and $h(x_1, y_2, ..., y_m)$ such that
a) for any $y_2, ..., y_m$ fixed

$$N_{l-1}g(y_1, ..., y_m) = N_l \int k_1(x_1, y_1)h(x_1, y_2, ..., y_m)dx_1 \tag{4}$$

b) for each x_1 fixed

$$h(x_1, y_2, ..., y_m) = \int .. \int k_2(x_2, ..., x_n, y_2, ..., y_m)f(x_1, ..., x_n)dx_2..dx_n. \tag{5}$$

In fact putting (3) into (2) and introducing function h leads (5) and (4) immediately.

The decomposition (4) and (5) of the unfolding problem (2) suggests solving in two steps:

a) given N_{l-1} and g, for each fixed $y_2, ..., y_m$ solve the "outer" univariate problem (4) with respect to unknown N_l and h,

b) for each fixed x_1 investigate the "inner" problem (5) with a simpler kernel function k_2 which could be eventually further decomposed.

Further the aim is to investigate the unfolding problem with three parameters: size, shape factor and orientation (colatitude) of spheroidal particles (either oblate or prolate).

3 SPHEROIDAL PARTICLES

An arbitrary ellipsoid in the Euclidean space R^l can be expressed by means of a symmetric positive-definite square matrix W_l. The ellipsoid E_l centered in the origin of a coordinate system is the set $E_l = \{t \in R^l, tW_l^{-1}t' \leq 1\}$, where W^{-1} is the inverse matrix of W and t' is the transposed vector t. It holds that $W_l = \mathcal{O}_l L \mathcal{O}_l'$, where $\mathcal{O}_l$ is an orthogonal matrix the columns of which correspond to the orientation vectors of principal semiaxes and L is a diagonal matrix with diagonal elements being the squared lengths of the semiaxes of an ellipsoid E_l. $\mathcal{O}_l'$ is the transpose of $\mathcal{O}_l$.

Consider a three-dimensional ellipsoid given by $W_3 = (w_{ij}),\ i,j = 1,2,3$, which is centered in an arbitrary point $t = (x, y, z) \in R^3$. Now denote by ρ the plane $x = 0$, and study the intersection of $t + E_3$ with the plane ρ. The following result is a special case of Moller(1988):

The intersection $(t + E_3) \cap \rho$ is non-void if and only if $e = 1 - \frac{x^2}{w_{11}} \geq 0$. Denote $U = \begin{pmatrix} y \\ z \end{pmatrix} - \begin{pmatrix} w_{21} \\ w_{31} \end{pmatrix} \frac{x}{w_{11}}$ and $W_{22.3} = \begin{pmatrix} w_{22} & w_{23} \\ w_{23} & w_{33} \end{pmatrix} - \frac{1}{w_{11}} \begin{pmatrix} w_{21} \\ w_{31} \end{pmatrix} (w_{21}\ w_{31})$, then for $e \geq 0$

$$(t + E_3) \cap \rho = \{s \in R^2,\ (s - U)W_{22.3}^{-1}(s - U)' \leq e\} \times o_x, \tag{6}$$

where o_x means that a zero x-coordinate is added to (y, z) points and $\times$ refers to cartesian product. Moreover, the length of the orthogonal projection of $t + E_3$ onto the x-axis is equal to $2\sqrt{w_{11}}$.

3.1 Oblate spheroids

Consider spherical coordinates in R^3 where the colatitude is the angle to the vertical axis. Then a vertical section plane ρ has normal orientation colatitude $\theta^* = \pi/2$, longitude ϕ^* and the distance d from the origin. Let the particle be a fixed oblate rotational ellipsoid E_3 with semiaxes $a = b > c$ centered in the origin. The orientation of the main (shorter) axis is θ (colatitude) and ϕ (longitude). Under the condition that the particle is hit by ρ denote the semiaxes of the intersection ellipse by $A, C,\ A \geq C$ and by α the angle between the semiaxis A and vertical axis (it is correctly defined whenever $C \neq A$). The shape factor of the particle, its section, is defined by $s = c/a,\ S = C/A$, respectively. It follows that $0 < s \leq 1,\ 0 < S \leq 1$. For the general setting in Section 2 we have here in particular $n = m = 3$ with $x_1 = a$, $x_2 = s$, $x_3 = \theta$ and $y_1 = A$, $y_2 = S$ $y_3 = \alpha$.

The spatial and planar parameters of a vertical section of a given ellipsoid are related by

$$\sin(\phi^* - \phi) = \cot\theta \cot\alpha \tag{7}$$

$$d = \frac{s\sqrt{a^2 - A^2}}{S} \tag{8}$$

$$A = a\sqrt{1 - \frac{d^2}{w_{11}^*}}, \tag{9}$$

where

$$w_{11}^* = a^2 - (a^2 - c^2)\sin^2\theta\cos^2(\phi^* - \phi). \tag{10}$$

These equations are calculated in a straightforward way from the relation (6).

We proceed by randomizing the sampling design to get conditional densities for the size-orientation and size-shape problems of type (2). Denote by

$$\mathcal{E}(\beta, z) = \int_0^\beta \sqrt{1 - z^2 \sin^2\varphi}\, d\varphi$$

the elliptic integral of the second kind, in particular $\mathcal{E}(\frac{\pi}{2}, z) = \mathcal{E}(z)$.

Under the vertical uniform random sampling design the conditional distributions of particle section parameters for the size-orientation and size-shape unfolding problems have densities

$$p_1(A, \alpha | a, \theta, s, \uparrow) = \frac{4}{L} \frac{A}{\sqrt{a^2 - A^2}} \frac{\cos\theta}{\sin\alpha} \sqrt{\frac{1 - (1 - s^2)(\sin^2\theta - \cos^2\theta\cot^2\alpha)}{\sin^2\theta - \cos^2\alpha}}, \tag{11}$$

for $\pi/2 - \theta \le \alpha \le \pi/2$, $0 \le A \le a$, $p_1 = 0$ otherwise, and

$$p_2(A, S | a, \theta, s, \uparrow) = \frac{4}{L} \frac{A}{\sqrt{a^2 - A^2}} \frac{s}{S^2} \{(1 - \frac{S^2}{s^2})[S^2 \sin^2\theta + \frac{S^2}{s^2}\cos^2\theta - 1]\}^{-1/2}, \tag{12}$$

for $s \le S \le s/\sqrt{s^2\sin^2\theta + \cos^2\theta}$, $0 \le A \le a$, $p_2 = 0$ otherwise, respectively. Here $L = \pi\bar{b}(a, \theta, s) = 4a\mathcal{E}(\sqrt{1 - s^2}\sin\theta)$ is the perimeter of the ellipse of particle projection (in a vertical direction), $\bar{b}(a, \theta, s)$ its mean breadth.

The proof of (11) and (12) consists of the evaluation of Jacobians

$$J_1 = \begin{vmatrix} \frac{\partial d}{\partial A} & \frac{\partial d}{\partial \alpha} \\ \frac{\partial \phi^*}{\partial A} & \frac{\partial \phi^*}{\partial \alpha} \end{vmatrix}, \quad J_2 = \begin{vmatrix} \frac{\partial d}{\partial A} & \frac{\partial d}{\partial S} \\ \frac{\partial \phi^*}{\partial A} & \frac{\partial \phi^*}{\partial S} \end{vmatrix}.$$

For the size-orientation problem we start from formula (7) and

$$d = \sqrt{a^2 - A^2}\sqrt{1 - (1 - s^2)(\sin^2\theta - \cos^2\theta\cot^2\alpha)},$$

for the size-shape problem we start from formula (8) and

$$\sin(\phi^* - \phi) = \sqrt{1 - \frac{\frac{s^2}{S^2} - 1}{(s^2 - 1)\sin^2\theta}},$$

obtained from (7)-(10).

The main result of this Section is the following Theorem concerning the unfolding problem (2) of size-shape-orientation distribution. Let $f(a, \theta, s), g(A, \alpha, S)$ be the probability densities of spatial, planar parameters, respectively. Further denote $D(\alpha, \theta) = \frac{\sqrt{\sin^2\alpha - \cos^2\theta}}{\sin\theta\sin\alpha}$ and $B(s, \theta) = \sin\theta\sqrt{1 - s^2}$.

Theorem 1 *The size parameter A is strongly conditionally independent of the shape factor S and orientation α and the outer size problem of the decomposition is*

$$N_A g(A,\alpha,S) = 2N_V \int_A^\infty \frac{A}{\sqrt{a^2-A^2}} h(a,\alpha,S)da \tag{13}$$

for some nonnegative function h and any fixed α, S. Let $H(a,\alpha,S) = \int_0^\alpha \int_0^S h(a,\beta,T)d\beta dT$. Then the inner shape-orientation problem for any fixed a is

$$H(a,\alpha,S) = \frac{2}{\pi}\int\int K(\alpha,S,\theta,s)f(a,\theta,s)\sin\theta d\theta ds, \tag{14}$$

where

$$K(\alpha,S,\theta,s) = min(K_1(\alpha,\theta,s),K_2(S,\theta,s)). \tag{15}$$

Here for each fixed θ, s

$$K_1(\alpha,\theta,s) = \mathcal{E}(\arcsin D(\alpha,\theta),B(s,\theta)) \tag{16}$$

for $\pi/2-\theta \le \alpha \le \pi/2$, $K_1(\alpha,\theta,s)=0$ for $\alpha < \pi/2-\theta$ and

$$K_2(S,\theta,s) = \mathcal{E}(\arcsin(\frac{1}{B(s,\theta)}\sqrt{1-\frac{s^2}{S^2}}),B(s,\theta)) \tag{17}$$

for $s \le S \le s/\sqrt{s^2\sin^2\theta+\cos^2\theta}$, $K_2(S,\theta,s) = 0$ for $S < s$ and $K_2(S,\theta,s) = \mathcal{E}(B(s,\theta))$ otherwise.

Remark: The unfolding problem is solved in two steps, however, the estimator of N_V is obtained in the first step as a solution of (13).

Proof of Theorem 1: In (11) and (12) we observe the strong conditional independence of size on both shape factor and orientation and formula (13) follows using (4).
From formulas (8)-(10) it holds for fixed θ, s that

$$S = s[1+(s^2-1)(\sin^2\theta-\cos^2\theta\cot^2\alpha)]^{-1/2}, \tag{18}$$

which means that the orientation and shape factor are conditionally functionally dependent. Therefore the joint conditional density $p(\alpha,S|\theta,s,\uparrow)$ is degenerate and we proceed in terms of distribution functions. Observe that the transformation $S(\alpha)$ in (18) is monotone increasing on $\langle 0,\frac{\pi}{2}\rangle$ for each fixed s,θ. Therefore (Mikusinski et al., 1991) the joint conditional distribution function

$$P(\alpha,S|\theta,s,\uparrow) = \frac{K(\alpha,S,\theta,s)}{\mathcal{E}(B(s,\theta))}$$

is equal to the upper Frechet bound of marginal conditional distribution functions

$$\frac{K_1(\alpha,\theta,s)}{\mathcal{E}(B(s,\theta))}, \frac{K_2(S,\theta,s)}{\mathcal{E}(B(s,\theta))},$$

which implies (15). The functions K_1, K_2 follow from (11), (12):

$$K_1(\alpha,\theta,s) = \int_{\frac{\pi}{2}-\theta}^{\alpha} \frac{\cos\theta}{\sin\beta}\sqrt{\frac{1-(1-s^2)(\sin^2\theta-\cos^2\theta\cot^2\beta)}{\sin^2\theta-\cos^2\beta}}d\beta,$$

and

$$K_2(S,\theta,s) = \int_s^S \frac{s}{T^2}\{(1-\frac{T^2}{s^2})[T^2\sin^2\theta+\frac{T^2}{s^2}\cos^2\theta-1]\}^{-1/2}dT.$$

(14) is thus obtained using the Fubini theorem.

3.2 Prolate spheroids

Consider now a system of prolate rotational ellipsoids with semiaxes $a > b = c$ under the same notation as in the previous subsection. The unfolding problem for joint distribution of spatial parameters (a, θ, s) from planar parameters (A, α, S) cannot be derived exactly in the same way as in the oblate case. It will be shown later that in the prolate case the parameter A is not strongly conditionally independent of S and α given a, θ, s.

However, an analogous way exists, by including the shorter semiaxes c, C in the analysis instead of a, A, respectively. In fact the triplet c, θ, s yields the same information as a, θ, s. Therefore solution of the unfolding problem between joint probability densities $f(c, \theta, s)$ and $g(C, \alpha, S)$ of spatial, planar parameters, respectively, is satisfactory for practical statistical purposes.

First let the particle be a fixed prolate rotational ellipsoid E_3 centered in the origin.

The spatial and planar parameters of a vertical section of a given spheroid are related as

$$\sin(\phi^* - \phi) = \cot\theta \tan\alpha \tag{19}$$

$$d = \frac{S\sqrt{c^2 - C^2}}{s} \tag{20}$$

$$C = c\sqrt{1 - \frac{d^2}{w_{11}^*}}, \tag{21}$$

where d is the distance of vertical section from origin and

$$w_{11}^* = c^2 + (a^2 - c^2)\sin^2\theta\cos^2(\phi^* - \phi). \tag{22}$$

Formulas (19)-(22) again follow after some calculation from (6).

Further we proceed analogously to the previous subsection, here size is represented by the smaller semiaxis. Let

$$Z(s, \theta) = 1 + (s^{-2} - 1)\sin^2\theta, \quad M(s, \theta) = \sqrt{\frac{Z(s, \theta) - 1}{Z(s, \theta)}}.$$

Under the vertical uniform random sampling design the conditional distributions of particle section parameters for the size-orientation, size-shape unfolding problem have probability densities

$$p_1(C, \alpha | c, \theta, s, \uparrow) = \frac{4}{L}\frac{C}{\sqrt{c^2 - C^2}}\frac{\cos\theta}{\cos\alpha}\sqrt{\frac{1 + (s^{-2} - 1)(\sin^2\theta - \cos^2\theta\tan^2\alpha)}{\sin^2\theta - \sin^2\alpha}}, \tag{23}$$

for $0 \le \alpha \le \theta$, $0 \le C \le c$, $p_1 = 0$ otherwise, and

$$p_2(C, S | c, \theta, s, \uparrow) = \frac{4}{L}\frac{C}{\sqrt{c^2 - C^2}}\frac{S^2}{s}[(S^2 - s^2)(\sin^2\theta + s^2\cos^2\theta - S^2)]^{-1/2}, \tag{24}$$

for $s \le S \le \sqrt{s^2\cos^2\theta + \sin^2\theta}$, $0 \le C \le c$, $p_2 = 0$ otherwise, respectively. Here $L = \pi\bar{b}(a, \theta, s) = 4cZ(s, \theta)\mathcal{E}(M(s, \theta))$ is the perimeter of the ellipse of particle projection (in vertical direction), $\bar{b}(a, \theta, s)$ its mean breadth.

The proof of formulas (23) and (24) consists of the evaluation of Jacobians

$$J_1 = \begin{vmatrix} \frac{\partial d}{\partial C} & \frac{\partial d}{\partial \alpha} \\ \frac{\partial \phi^*}{\partial C} & \frac{\partial \phi^*}{\partial \alpha} \end{vmatrix}, \quad J_2 = \begin{vmatrix} \frac{\partial d}{\partial C} & \frac{\partial d}{\partial S} \\ \frac{\partial \phi^*}{\partial C} & \frac{\partial \phi^*}{\partial S} \end{vmatrix}.$$

For the size-orientation problem we start from formula (19) and

$$d = \sqrt{c^2 - C^2}\sqrt{1 + (s^{-2} - 1)(\sin^2\theta - \cos^2\theta\tan^2\alpha)},$$

for the size-shape problem we start from formula (20) and

$$\cos(\phi^* - \phi) = \sqrt{\frac{S^2 - s^2}{(1 - s^2)\sin^2\theta}}, \tag{25}$$

obtained from (19)-(23).

Remark: For the longer semiaxes it holds that $d = \frac{S}{s}\sqrt{s^2a^2 - S^2A^2}$, the Jacobian of this transformation (together with (25)) cannot be factorized and the negative result stated at the beginning of this Subsection follows.

Concerning the unfolding problem of size-shape-orientation distribution we get the following result.

Theorem 2 *The size parameter C is strongly conditionally independent of the shape factor S and orientation α and the outer size problem of the decomposition is*

$$N_A g(C, \alpha, S) = 2N_V \int_C^\infty \frac{C}{\sqrt{c^2 - C^2}} h(c, \alpha, S)dc \tag{26}$$

for some nonnegative function h and any fixed α, S. Let $H(c, \alpha, S) = \int_0^\alpha \int_0^S h(c, \beta, T)d\beta dT$. Then the inner shape-orientation problem for any fixed c is

$$H(c, \alpha, S) = \frac{2}{\pi} \int\int K(\alpha, S, \theta, s) f(c, \theta, s) \sin\theta d\theta ds, \tag{27}$$

where

$$K(\alpha, S, \theta, s) = max(0, K_1(\alpha, \theta, s) + K_2(S, \theta, s) - \sqrt{Z(s, \theta)}\mathcal{E}(M(s, \theta))). \tag{28}$$

Here for each fixed θ, s

$$K_1(\alpha, \theta, s) = \sqrt{Z(s, \theta)}\mathcal{E}(\arcsin(\cot\theta \tan\alpha),\ M(s, \theta)) \tag{29}$$

for $0 \leq \alpha \leq \theta$, $K_1(\alpha, \theta, s) = \sqrt{Z(s, \theta)}\mathcal{E}(M(s, \theta))$ for $\alpha > \theta$ and

$$K_2(S, \theta, s) = \sqrt{Z(s, \theta)}\mathcal{E}\left[\arcsin\left(\frac{1}{M(s, \theta)}\sqrt{1 - \frac{s^2}{S^2}}\right),\ M(s, \theta)\right] - \sqrt{1 - \frac{s^2}{S^2}}\sqrt{Z(s, \theta) - \frac{S^2}{s^2}} \tag{30}$$

for $s \leq S \leq \sqrt{s^2\cos^2\theta + \sin^2\theta}$, $K_2(S, \theta, s) = 0$ for $S < s$ and $K_2(S, \theta, s) = \sqrt{Z(s, \theta)}\mathcal{E}(M(s, \theta))$ otherwise.

Proof: In formulas (23) and (24) we observe the strong conditional independence of size on both shape and orientation and formula (26) follows using (4).

From formulas (19)-(21) it follows that for fixed θ, s it holds that

$$S = \sqrt{s^2 + (1 - s^2)(\sin^2\theta - \cos^2\theta\tan^2\alpha)}, \tag{31}$$

which means that orientation and shape factor are conditionally functionally dependent so the joint conditional density $p(\alpha, S|\theta, s, \uparrow)$ is degenerate. Observe that the transformation $S(\alpha)$ in (31) is monotone decreasing on $\langle 0, \frac{\pi}{2}\rangle$ for each fixed s, θ. Again by Mikusinski et al.(1991) the joint conditional distribution function

$$P(\alpha, S|\theta, s, \uparrow) = \frac{K(\alpha, S, \theta, s)}{\sqrt{Z(s, \theta)}\mathcal{E}(M(s, \theta))}$$

is equal to the lower Frechet bound of the marginal conditional distribution functions

$$\frac{K_1(\alpha, \theta, s)}{\sqrt{Z(s, \theta)}\mathcal{E}(M(s, \theta))},\ \frac{K_2(S, \theta, s)}{\sqrt{Z(s, \theta)}\mathcal{E}(M(s, \theta))},$$

which implies (28). The functions K_1, K_2 follow from (23), (24):

$$K_1(\alpha,\theta,s)=\int_0^\alpha \frac{\cos\theta}{\cos\beta}\sqrt{\frac{1+(s^{-2}-1)(\sin^2\theta-\cos^2\theta\tan^2\beta)}{\sin^2\theta-\sin^2\beta}}d\beta,$$

and

$$K_2(S,\theta,s)=\int_s^S \frac{T^2}{s}[(T^2-s^2)(\sin^2\theta+s^2\cos^2\theta-T^2)]^{-1/2}dT.$$

The last integral was found in Gradštejn and Ryžik(1962), p.261.

To summarize the problem of spheroidal particles and match formulas from Sections 2 and 3 observe that the unfolding problem (2) for $n=m=3$ parameters has been decomposed into (4) and (5) (x_1 is the size parameter) which correspond to formulas (13) and (14) (oblate case) or (26) and (27) (prolate case). The inner problem (14) or (27) is formulated in terms of distribution functions instead of in terms of probability densities as (5) since the conditional probability density which forms the kernel function does not exist.

4 NUMERICAL SOLUTION

Unfolding problems belong to a class of inverse problems (Coleman, 1989) which are often called ill-posed, that means a small error in the evaluation of input quantities may cause a large error in the resulting estimator. It is difficult to study this property by functional-analytic methods. Typically a discretization method is used for the solution of unfolding problems. It transforms an integral equation onto a system of linear equations. The condition number of the matrix of this system can be used as a criterion for the stability of solution.

We present the method of solution of unfolding equations which is based on standard discretization techniques (Ohser and Mücklich, 1995). The method is described in terms of oblate spheroids. In the prolate case one can proceed analogously.

Both planar and spatial parameters are classified into a trivariate histogram with some class limits for size, shape factors and orientations $a_i, A_i, \theta_i, \alpha_i, s_i, S_i$, $i=1,...,r$. For simplicity we deal with equal number of classes r. Generally this number need not be the same for each parameter. In the discrete approximation of the distribution of particle parameters it is assumed that $f(i,j,k)=P(a=a_i,\theta=\theta_j,s=s_k)$ with $i,j,k=1,..,r$, are probabilities of discrete values of spatial parameters. We denote by $N_A(i,j,k)$ the input histogram of observed particle section parameters ($A_{i-1}<A\le A_i$, $\alpha_{j-1}<\alpha\le\alpha_j$, $S_k<S\le S_{k-1}$) per unit area using the VUR sampling design. Here $\sum_{ijk}N_A(i,j,k)=N_A$ is the mean particle section number per unit area of section planes observed. In practice the VUR sampling is realized by the use of several vertical section planes with different ϕ^*.

The stereological unfolding involves the estimation of the spatial distribution $f(i,j,k)$ and particle number density N_V given $N_A(i,j,k)$. The problem is solved in two steps corresponding to the procedure in previous section:

a) For each fixed orientation and shape class (j,k) solve the size unfolding problem

$$N_A(i,j,k)=N_V\sum_{l\ge i}p_{li}h(l,j,k),\quad i=1,...,r \tag{32}$$

for unknown N_V and $h(l,j,k)$. E.g. by using $a_i=A_i=b^i$ for a constant $b>1$ we get (cf. Ohser and Mücklich, 1995) $p_{li}=2b^l z_{i-l}$, where $z_i=\sqrt{1-b^{2(i-1)}}-\sqrt{1-b^{2i}}$. The solution of (32) is then obtained by means of the EM-algorithm (Silverman et al., 1990). The estimator of N_V follows from the condition $\sum_{ljk}h(l,j,k)=1$.

b) In the second step denote

$$p_{injk}=\frac{2}{\pi}[K(\alpha_j,S_k,\theta_i,s_n)-K(\alpha_{j-1},S_k,\theta_i,s_n)-K(\alpha_j,S_{k-1},\theta_i,s_n)+K(\alpha_{j-1},S_{k-1},\theta_i,s_n)]. \tag{33}$$

Here $K(\alpha, S, \theta, s)$ is the function defined by (15)-(17).

Now the discrete version of the remaining shape-orientation problem is for each fixed size class l is

$$h(l,j,k) = \sum_{in} p_{injk} f(l,i,n), \tag{34}$$

where $f(l,i,n)$ is the desired histogram of spatial parameters. Use the EM-algorithm with λ-th iteration step

$$f^{(\lambda+1)}(l,i,n) = \frac{f^{(\lambda)}(l,i,n)}{t_{in}} \sum_{jk} \frac{h(l,j,k)p_{injk}}{u_{jk}^{\lambda}}, \tag{35}$$

where $t_{in} = \sum_{jk} p_{injk}$, $u_{jk}^{\lambda} = \sum_{in} f^{(\lambda)}(l,i,n)p_{injk}$. As an initial iteration $f^{(0)}(l,i,n) = h(l,i,n)$ is sufficient. After more than ten steps of iteration in (35) we get the desired estimator $\hat{f}(l,i,n)$, $l,i,n = 1,..,r$ of spatial size-shape-orientation distribution.

5 APPLICATION

The developed method was used for the unfolding of particle size-shape-orientation distribution in a metal matrix composite material. A chill cast Al-1 wt%Si composite made in Pechiney, France, has been heat treated by dissolution annealing at 540°C for 6 h and slow cooling (18°C/h) to 20°C in order to obtain precipitation of platelike Si particles. Aside from a very small number of exceptions the particle shape can be approximated by oblate spheroids or prisms. Uniaxial tensile tests using cylindrical specimens of diameter 8 mm and length 60 mm were carried out. Brittle silicon particles embedded in ductile aluminium matrix do not deform plastically and particle cracking has been expected during deformation. In order to study the damage of Si particles metallographic samples were prepared from both nondeformed and deformed-up-to-fracture (strain 20 %) materials. The samples were cut randomly parallel to the tensile axis to follow the VUR sampling design. Quantitative metallographic analysis has been performed by image analysis technique using IBAS-Kontron analyser connected to a light microscope.

The discretization of parameters used is the following:

$$a_j = A_j = b^j,\ j \in Z; \quad s_i = S_i = (1 - \frac{i}{r})^{\kappa}, \quad \alpha_i = \theta_i = i\triangle,\ i = 1,..,r. \tag{36}$$

Here $b = 1.756$, $\kappa = 1.5$ are chosen constants, $r = 8$ the number of classes, and $\triangle = \frac{\pi}{2r}$. The matrix P of coefficients p_{ijkl} for the inner problem (34) has size 64×64 and condition number $cond(P) = ||P||\,||P^{-1}|| = 75.75$ using the norm $||P|| = \sqrt{\sum_{ijkl} p_{ijkl}^2}$. This relatively acceptable value (cf. Gerlach and Ohser, 1986) justifies the use of the method.

Fig. 1 presents spatial trivariate size-shape-orientation histograms evaluated according to the developed methods. The histogram on the left results from the input sample S1 of size $n = 10017$ of all particle sections, while the histogram on the right was evaluated from the sample S2 of $n = 1058$ particles on the same area with observed cracks in the deformed-up-to-fracture state. The estimated number densities $N_V = 210.10^{-6}\,\mu m^{-3}$ for S1 and $N_V = 14.5.10^{-6}\,\mu m^{-3}$ for S2 yield an estimator of the probability of damage $P = 14.5/210 = 0.07$ for the whole population of particles. (It should be mentioned that not all cracks are observed in the section plane, therefore for S2 it holds $N_V = kN_V^u$, where N_V^u is obtained from the unfolding procedure. Under the assumptions of platelike particles and at most one crack per particle it is $k = 2$, see Beneš et al.(1997) for a discussion of k when these assumptions are not valid.)

The goal of the trivariate unfolding method for the present application is that we are able to refine the analysis of crack initiation in particles to each subclass of histograms in Fig.1. Thus we obtain a histogram of probabilities of damage which is an input to parameter estimation of statistical models for damage initiation such as the Weibull formula, cf. Beneš et al.(1997).

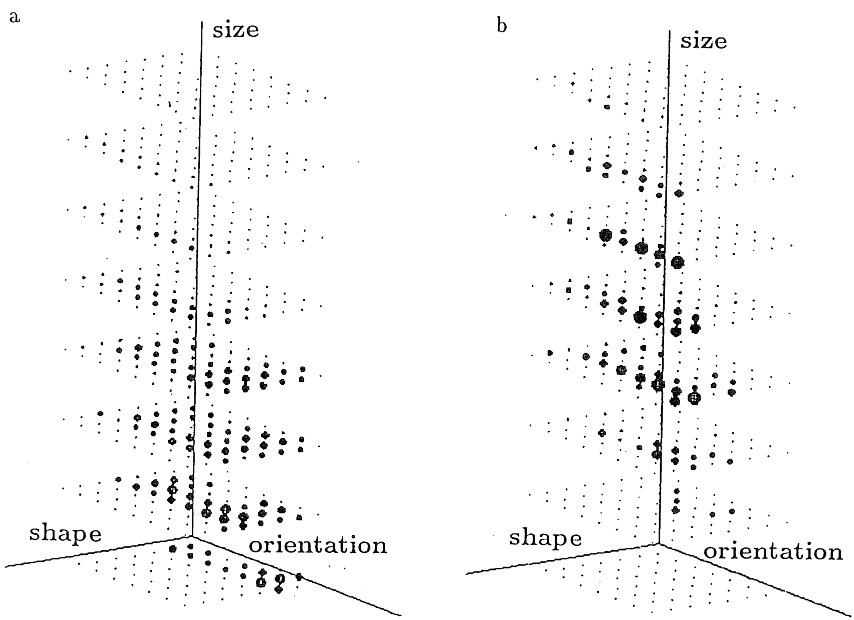

Fig.1: Estimated spatial size-shape-orientation histograms estimated from samples $S1$ (a), $S2$ (b). The volume of three-dimensional balls observed is proportional to $N_V f(i,j,k)$ values. The axes are scaled according to formula (36) and they intersect in the point corresponding to $i = j = k = 1$.

6 DISCUSSION

Moller(1988) proved that it is possible to reconstruct an ellipsoid completely from three parallel sections. His result is very useful, but it does not close the discussion about the spheroidal problem. E.g. his method is not generally applicable in quantitative metallography for two reasons. First the preparation of appropriate parallel sections in hard materials with small particles is difficult and in some cases impossible. For the same reason also the excellent assumption-free methods of stereology (Karlsson and Cruz-Orive, 1992) cannot be used in all metallographic applications. On the other hand a vertical plane is easily obtained and may have a physical meaning (e.g. being parallel to deformation axis, cf. Beneš et al., 1997).

Secondly Moller's method works for perfect ellipsoids only, while in practice the shape assumption is often an approximation. There is an empirical evidence that the presented unfolding solution is more robust against the assumption of shape. Therefore we revisited the 70 years old problem to pose a new three-parametric ill-posed problem, the solution of which is acceptable for practice when using modern numerical techniques.

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