Kybernetika

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Kybernetika, Vol. 33 (1997), No. 3, 245--258

Persistent URL: http://dml.cz/dmlcz/124711

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KYBERNETIKA — VOLUME 33 (1997), NUMBER 3, PAGES 245–258

DECOMPOSITION IN STEREOLOGICAL UNFOLDING PROBLEMS

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Some new results in an old problem of stereological unfolding in particle systems are presented. Under the conditional independence property of particle section parameters the multivariate unfolding problem can be decomposed into a series of simpler problems. The general idea is applied to the unfolding of trivariate size-shape-orientation distribution of spheroids using the vertical uniform random sampling design.

1. INTRODUCTION

The conditional independence relation plays a key role in a number of topics in probability theory and its applications, cf. van Putten and van Schuppen [14]. In the area of sufficient statistics this relation enters in a natural way. Therefore it is not surprizing that in this context the assumptions of conditional independence appeared in a stereological study Baddeley and Cruz–Orive [1].

We present here another application of conditional independence in stereology, namely in the classical unfolding problem. Consider a system of three-dimensional particles of similar 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 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 (Cruz–Orive [4], Gokhale [6]) or numerically (Ohser and Mücklich [12]).

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 numerical

EM-algorithm (Silvermann et al [13]) 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 R^d is called a particle. Let a fixed particle X be described by n real geometrical parameters $x_1, x_2, \dots, x_n$. 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^{d-1} called a particle section. Let $y_1, \dots, y_m$ be geometrical parameters describing Y, such that $y_1, \dots, y_k$, $k \leq \min(n, m)$ correspond to properties of $x_1, \dots, x_k$, e.g. x_1, y_1 size, x_2, y_2 shape factor etc. Let $p(y_1, \dots, y_m | x_1, \dots, x_n, \uparrow)$ be the conditional probability density of $y_1, \dots, y_m$ given $x_1, \dots, x_n$ 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^d with constant intensity N_d. If particles are still fixed (just translates of X) denote $N_{d-1}(x_1, \dots, x_n)$ the mean (with respect to Q) intensity of particle sections in ρ.

In the following step given N_d let particles are random with probability density $f(x_1, \dots, x_n)$ of parameters $x_1, \dots, x_n$ invariant with respect to translations in R^d. We are interested in particle sections observed in ρ.

Definition 1. The average particle section intensity N_{d-1} and probability density $g(y_1, \dots, y_m)$ of parameters $y_1, \dots, y_m$ are defined by

$$\begin{aligned} & N_{d-1} g(y_1, \dots, y_m) \\ = & \int \cdots \int N_{d-1}(x_1, \dots, x_n) p(y_1, \dots, y_m | x_1, \dots, x_n, \uparrow) f(x_1, \dots, x_n) \, \mathrm{d}x_1 \cdots \mathrm{d}x_n. \end{aligned} \tag{1}$$

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

Proposition 1. The unfolding problem is decribed by an equation

$$N_{d-1} g(y_1, \dots, y_m) = N_d \int \cdots \int k(x_1, \dots, x_n, y_1, \dots, y_m) f(x_1, \dots, x_n) \, \mathrm{d}x_1 \cdots \mathrm{d}x_n, \tag{2}$$

for some nonnegative kernel function k.

Proof. Use Definition 1 and put

$$k(x_1, \dots, x_n, y_1, \dots, y_m) = \frac{N_{d-1}(x_1, \dots, x_n)}{N_d} p(y_1, \dots, y_m | x_1, \dots, x_n, \uparrow). \qquad \square$$

The problems (2) were studied until now for m, n at most 2. They lead to Abel type integral equations which can be solved analytically, cf. Cruz–Orive [4] for size-shape distribution of rotational ellipsoids, Gokhale [6] for size-orientation distribution of circular plates. For situations when the input data form a bivariate histogram equation (2) is discretized and solved by numerical methods, cf. Ohser and Mücklich [12] for size-shape, size-number (number of vertices) distribution of various particular polyhedra. It was shown in the latter paper that even in some cases with complex section classification, when the form of (2) is unknown, the coefficients of its discrete version can be obtained by simulations.

For a greater number of parameters than two, direct analytical or numerical methods are also worth investigation, however, the aim of the present paper is to proceed another way. We observe that when the following property of section parameters is satisfied, the unfolding problem can be decomposed in a series of problems with smaller number of parameters. Each of these subproblems has a kernel function with smaller number of arguments which simplifies the solution.

Definition 2. Random variable y_1 is strongly conditionally independent on $y_2, \ldots, y_m$ given $x_1, \ldots, x_n$ and Q if the kernel function k in (2) satisfies

$$k(x_1, \ldots, x_n, y_1, \ldots, y_m) = k_1(x_1, y_1)\, k_2(x_2, \ldots, x_n, y_2, \ldots, y_m) \tag{3}$$

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

Theorem 1. Let y_1 be strongly conditionally independent on $y_2, \ldots, y_m$. Then there exist nonnegative functions k_1, k_2 and $h(x_1, y_2, \ldots, y_m)$ such that

a) for any $y_2, \ldots, y_m$ fixed

$$N_{d-1} g(y_1, \ldots, y_m) = N_d \int k_1(x_1, y_1)\, h(x_1, y_2, \ldots, y_m)\, \mathrm{d}x_1 \tag{4}$$

b) for each x_1 fixed

$$h(x_1, y_2, \ldots, y_m) = \int \cdots \int k_2(x_2, \ldots, x_n, y_2, \ldots, y_m)\, f(x_1, \ldots, x_n)\, \mathrm{d}x_2 \cdots \mathrm{d}x_n. \tag{5}$$

Proof. Putting (3) into (2) and introducing function h (5) and (4) follows. □

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

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

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

In the rest of the paper we study some special unfolding problems in R^3. The sampling design of vertical uniform random (VUR) sections will be used, which is anisotropic but in practice simpler than commonly used sampling design of isotropic uniform random (IUR) sections.

3. PLATELIKE PARTICLES

We start with a known result which is in fact a special case of subsection 4.1 in this paper on oblate rotational ellipsoid if we reduce the number of parameters by putting there $c = 0$. Let particles are circular plates of zero thickness in R^3 with constant intensity N_V, random radius $a > 0$ and normal orientation (θ, ϕ). Here $\theta \in \langle 0, \frac{\pi}{2} \rangle$ is the colatitude (angle between the plate normal and the fixed vertical axis) and $\phi \in \langle 0, 2\pi)$ the longitude. We denote $f(a,\theta) = \frac{1}{2\pi}\int_0^{2\pi} f_1(a,\theta,\phi)\,\mathrm{d}\phi$ the joint probability density function of the radius a and angle θ. A vertical section plane is such that it is parallel to the vertical axis. In a vertical uniform random section plane particle sections are observed of length $2A > 0$ and orientation angle $\alpha \in \langle 0, \frac{\pi}{2} \rangle$ to the vertical axis. Let $g(A, \alpha)$, N_A be the corresponding probability density function and section intensity in the sense of Definition 1. Gokhale [6] derived an integral equation connecting f and g. First a short proof of his result is presented.

Theorem 2. It holds

$$N_A g(A,\alpha) = N_V \frac{4}{\pi} \int_A^{\infty} \int_{\pi/2-\alpha}^{\pi/2} \frac{A\cos^2\theta \sin\theta f(a,\theta)\,\mathrm{d}a\,\mathrm{d}\theta}{\sin^2\alpha\sqrt{(a^2-A^2)(\sin^2\alpha - \cos^2\theta)}}, \tag{6}$$

for $A > 0$, $\alpha \geq \frac{\pi}{2} - \theta$.

Proof. Let a plate centered in the origin have fixed a, θ, ϕ, and a vertical uniform random section plane hitting the plate have distance d from origin and let the longitude longitude of the normal be ϕ^*. Its probability density is constant

$$q(d, \phi^*) = \frac{1}{L}$$

for $0 \leq \phi^* \leq 2\pi$, $0 \leq d \leq l(\phi^*)$ and

$$q(d, \phi^*) = 0$$

otherwise, where $l(\varphi) = a\sqrt{1 - \sin^2\theta \sin^2(\varphi - \phi)}$ is the support function of the ellipse of particle projection (in vertical direction). The perimeter of this ellipse $L = L(a,\theta) = \pi\bar{b}(a,\theta)$, $\bar{b}(a,\theta)$ being its mean breadth. The basic relations between spatial and planar parameters (derived in Gokhale [6]) are

$$\sin(\phi^* - \phi) = \cot\theta \cot\alpha$$

for $\pi/2 - \theta \leq \alpha \leq \frac{\pi}{2}$ and

$$d = \frac{\cos\theta}{\sin\alpha}\sqrt{a^2 - A^2}$$

for $0 \leq A \leq a$. They define a transformation between (d, ϕ^*) and (A, α) which is one-to-one for $0 \leq \phi^* < \frac{\pi}{2}$ assuming (without loss of generality) that $\phi = 0$. Its Jacobian

$$J = \begin{vmatrix} \frac{\partial d}{\partial A} & \frac{\partial d}{\partial \alpha} \\ \frac{\partial \phi^*}{\partial A} & \frac{\partial \phi^*}{\partial \alpha} \end{vmatrix} = \frac{A}{\sqrt{a^2 - A^2}} \frac{\cos^2\theta}{\sin^2\alpha\sqrt{\sin^2\alpha - \cos^2\theta}}$$

yields the conditional density $p(A, \alpha|a, \theta, \uparrow) = \frac{4}{L}J = 4/(\pi\bar{b}(a,\theta))\, J$ independent of ϕ. Now for a system of fixed particles we have $\bar{b}(a,\theta) = N_A(a,\theta)/N_V$. For system of random particles, we get the result (6) integrating $p(A, \alpha|a, \theta, \uparrow)$ with respect to joint density $f(a,\theta)$ and using (1). □

Formula (6) is a double Abelian integral equation the theoretical solution of which with respect to f is available, see Gokhale [6]. Using Theorem 1 we decompose this problem into series of univariate unfolding problems.

Corollary 1. Denoting

$$k_2(\theta, \alpha) = \frac{2}{\pi}\frac{\cos^2\theta}{\sin^2\alpha\sqrt{\sin^2\alpha - \cos^2\theta}}, \tag{7}$$

the problem (6) can be decomposed as follows:

a) the "outer" problem for each fixed α

$$N_A g(A,\alpha) = 2N_V \int_A^\infty \frac{Ah(a,\alpha)}{\sqrt{a^2 - A^2}}\, \mathrm{d}a, \tag{8}$$

b) the "inner" problem for each fixed $a > 0$

$$h(a,\alpha) = \int_{\pi/2-\alpha}^{\pi/2} k_2(\theta,\alpha)\, f(a,\theta)\sin\theta\, \mathrm{d}\theta. \tag{9}$$

P r o o f. Observe that the strong independence property is fulfilled for the kernel function in (6) with $k_1(a, A) = A/\sqrt{a^2 - A^2}$ and k_2 in (7). Then (8), (9) corresponds to (4), (5) in Theorem 1. □

In practice often the input is a bivariate frequency histogram of lengths and orientations observed in vertical section planes. Then the use of the analytical solution is not comfortable since it requires fitting of the bivariate density followed by numerical differentiation and integration. Therefore a traditional approach of discretization of the integral equation (6) and evaluation of the bivariate histogram of spatial parameters is desired. It can be applied either directly using the techniques of Ohser and Mücklich [12] or in steps using Corollary 1. The latter way, which is preferable especially for problems with more parameters, was developed in Beneš et al [2].

Further aim is to investigate the unfolding problem with three parameters: size, shape factor and orientation (colatitude) of flat particles. It will be shown for the model of oblate ellipsoids that the joint size-shape-orientation distribution can be unfolded from VUR sections.

4. ELLIPSOIDAL PARTICLES

An arbitrary ellipsoid in the Euclidean space R^d can be expressed by means of a symmetric positive-definite square matrix W_d. The ellipsoid E_d centered in the origin of a coordinate system is the set $E_d = \{t \in R^d,\ tW_d^{-1}t' \leq 1\}$, where W^{-1} is the inverse matrix of W and t' is the transposed vector t. It holds $W_d = \mathcal{O}_d L \mathcal{O}'_d$, where $\mathcal{O}_d$ 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 square lengths of the semiaxes of an ellipsoid E_d.

For $d = 3$ consider a three-dimensional ellipsoid $t+E_3$, 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 ρ the plane $x = 0$, and study the intersection of $t + E_3$ with the plane ρ. The following Lemma is a special case of Lemma 2.1 in Møller [11], p. 324:

Lemma 1. The intersection $(t+E_3)\cap\rho$ is non-void if and only if $e = 1 - \frac{x^2}{w_{11}} \geq 0$. Denote

$$U = \begin{pmatrix} y \\ z \end{pmatrix} - \begin{pmatrix} w_{21} \\ w_{31} \end{pmatrix} \frac{x}{w_{11}} \quad \text{and} \quad W_{22.3} = \begin{pmatrix} w_{22} & w_{23} \\ w_{23} & w_{33} \end{pmatrix} - \frac{1}{w_{11}} \begin{pmatrix} w_{21} \\ w_{31} \end{pmatrix} (w_{21}\ w_{31}),$$

then for $e \geq 0$ it is

$$(t + E_3) \cap \rho = \{s \in R^2,\ (s - U)W_{22.3}^{-1}(s - U)' \leq e\} \times o_x, \tag{10}$$

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

4.1. Oblate ellipsoids

Let the particle be a fixed oblate rotational ellipsoid E_3 with semiaxes $a = b > c$ centred in the origin. The orientation of the axis of rotation is θ, ϕ. Let a vertical section plane ρ have normal orientation $\theta^* = \pi/2, \phi^*$ in spherical coordinates and the distance d from the origin. Under the condition that the particle is hit by ρ denote the semiaxes of intersection ellipse (10) by A, C, $A \geq C$ and by α the angle between the semiaxis A and vertical axis (it is correctly defined whenever $C \neq A$).

Definition 3. The shape factors of the particle, its section, are defined as $s = c/a$, $S = C/A$, respectively.

It follows that always $0 < s \leq 1$, $0 < S \leq 1$.

Lemma 2. The spatial and planar parameters of a vertical section of given ellipsoid are related as

$$\sin(\phi^* - \phi) = \cot\theta \cot\alpha \tag{11}$$

$$d = \frac{s\sqrt{a^2 - A^2}}{S} \tag{12}$$

$$A = a\sqrt{1 - \frac{d^2}{w_{11}^*}}, \tag{13}$$

where

$$w_{11}^* = a^2 - (a^2 - c^2)\sin^2\theta\cos^2(\phi^* - \phi). \tag{14}$$

P r o o f. A straightforward algebraic calculation using Lemma 1. □

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

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

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

Proposition 2. Under the vertical uniform random sampling design the conditional distributions of particle section parameters for the size-orientation, size-shape unfolding problem have densities

$$p_1(A, \alpha | a, \theta, s, \uparrow) = \frac{4}{L}\frac{A}{\sqrt{a^2 - A^2}}\frac{\cos\theta}{\sin\alpha}\sqrt{\frac{1 - (1 - s^2)(\sin^2\theta - \cos^2\theta\cot^2\alpha)}{\sin^2\theta - \cos^2\alpha}}, \tag{15}$$

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

$$p_2(A, S | a, \theta, s, \uparrow) = \frac{4}{L}\frac{A}{\sqrt{a^2 - A^2}}\frac{s}{S^2}\left\{\left(1 - \frac{S^2}{s^2}\right)\left[S^2\sin^2\theta + \frac{S^2}{s^2}\cos^2\theta - 1\right]\right\}^{-1/2}, \tag{16}$$

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 vertical direction), $\bar{b}(a, \theta, s)$ its mean breadth.

P r o o f. Consists of the evaluation of Jacobians analogously to the proof of Theorem 2. For the size-orientation problem we start from formula (11) 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 (12) and

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

obtained from (11)–(14). □

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 and 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 3. The size parameter A is strongly conditionally independent on the shape factor S and orientation α and the outer size problem of the decomposition is

$$N_A g(A,\alpha,S) = 2N_V \int_A^{\infty} \frac{A}{\sqrt{a^2-A^2}}\, h(a,\alpha,S)\,\mathrm{d}a \tag{17}$$

for some nonnegative function h and any fixed α, S.

Let $H(a,\alpha,S) = \int_0^{\alpha}\int_0^{S} h(a,\beta,T)\,\mathrm{d}\beta\mathrm{d}T$. The inner shape-orientation problem for any fixed a is

$$H(a,\alpha,S) = \frac{2}{\pi}\int\int K(\alpha,S,\theta,s)\, f(a,\theta,s)\sin\theta\,\mathrm{d}\theta\mathrm{d}s, \tag{18}$$

where

$$K(\alpha,S,\theta,s) = \min(K_1(\alpha,\theta,s), K_2(S,\theta,s)). \tag{19}$$

Here for each fixed θ, s

$$K_1(\alpha,\theta,s) = \mathcal{E}(\arcsin D(\alpha,\theta), B(s,\theta)) \tag{20}$$

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

$$K_2(S,\theta,s) = \mathcal{E}\left(\arcsin\left(\frac{1}{B(s,\theta)}\sqrt{1-\frac{s^2}{S^2}}\right), B(s,\theta)\right) \tag{21}$$

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.

Proof. Proposition 2 yields the strong conditional independence of size on both shape and orientation and formula (17) follows as in Theorem 2 and Corollary 1.

From formulas (11)–(13) in Lemma 2 it follows that for fixed θ, s holds

$$S = S(\alpha) = s\left[1+(s^2-1)(\sin^2\theta - \cos^2\theta\cot^2\alpha)\right]^{-1/2}, \tag{22}$$

which means that 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 fuctions. Observe that the transformation $S(\alpha)$ in (22) is monotone increasing on $\langle 0, \frac{\pi}{2}\rangle$ for each fixed s, θ. Therefore (Mikusinski et al [10]) 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 (19). The functions K_1, K_2 follow from (15), (16):

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

and

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

(18) is thus obtained using the Fubini theorem. □

4.2. Prolate ellipsoids

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 it holds

Proposition 3. In the prolate case the parameter A is not strongly conditionally independent of S and α given a, θ, s.

However, still an analogous way exists, namely to replace in the analysis a, A by the shorter semiaxes c, C. 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 centred in the origin.

Lemma 3. The spatial and planar parameters of a vertical section of given ellipsoid are related as

$$\sin(\phi^* - \phi) = \cot\theta \tan\alpha \tag{23}$$

$$d = \frac{S\sqrt{c^2 - C^2}}{s} \tag{24}$$

$$C = c\sqrt{1 - \frac{d^2}{w_{11}^*}}, \tag{25}$$

where d is the distance of vertical section from origin and

$$w_{11}^* = c^2 + (a^2 - c^2)\sin^2\theta\cos^2(\phi^* - \phi). \tag{26}$$

Proof. A straightforward algebraic calculation using Lemma 1. □

We proceed analogously to the previous subsection, size is represented by smaller semiaxes. Denote

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

Proposition 4. Under the vertical uniform random sampling design the conditional distributions of particle section parameters for the size-orientation, size-shape unfolding problem have densities

$$p_1(C, \alpha | c, \theta, s, \uparrow) = \frac{4}{L}\frac{C}{\sqrt{c^2 - C^2}}\frac{\cos\theta}{\cos\alpha}\sqrt{\frac{1 + (s^{-2} - 1)(\sin^2\theta - \cos^2\theta\tan^2\alpha)}{\sin^2\theta - \sin^2\alpha}}, \tag{27}$$

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

$$p_2(C, S|c, \theta, s, \uparrow) = \frac{4}{L} \frac{C}{\sqrt{c^2 - C^2}} \frac{S^2}{s} \left[(S^2 - s^2)(\sin^2\theta + s^2\cos^2\theta - S^2)\right]^{-1/2}, \quad (28)$$

for $s \leq S \leq \sqrt{s^2\cos^2\theta + \sin^2\theta},\ 0 \leq C \leq c,\ p_2 = 0$ 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.

Proof. Consists of the evaluation of Jacobians analogously to the proof of Theorem 2. For the size-orientation problem we start from formula (23) 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 (24) and

$$\cos(\phi^* - \phi) = \sqrt{\frac{S^2 - s^2}{(1 - s^2)\sin^2\theta}}, \quad (29)$$

obtained from (23) – (26). □

Remark. For the longer semiaxes it holds $d = \frac{S}{s}\sqrt{s^2a^2 - S^2A^2}$, the Jacobian of this transformation (including (29)) cannot be factorized and the negative result of Proposition 3 follows.

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

Theorem 4. The size parameter C is strongly conditionally independent on the shape factor S and orientation α and the outer size problem of the decomposition is

$$N_A g(C, \alpha, S) = 2N_V \int_C^\infty \frac{C}{\sqrt{c^2 - C^2}} h(c, \alpha, S)\,\mathrm{d}c \quad (30)$$

for some nonnegative function h and any fixed α, S.

Let $H(c, \alpha, S) = \int_0^\alpha \int_0^S h(c, \beta, T)\,\mathrm{d}\beta\mathrm{d}T$. The inner shape-orientation problem for any fixed c is

$$H(c, \alpha, S) = \frac{2}{\pi} \int\int K(\alpha, S, \theta, s)\, f(c, \theta, s)\, \sin\theta \mathrm{d}\theta\mathrm{d}s, \quad (31)$$

where

$$K(\alpha, S, \theta, s) = \max\left(0, K_1(\alpha, \theta, s) + K_2(S, \theta, s) - \sqrt{Z(s,\theta)}\,\mathcal{E}(M(s,\theta))\right). \quad (32)$$

Here for each fixed θ, s

$$K_1(\alpha, \theta, s) = \sqrt{Z(s,\theta)}\,\mathcal{E}(\arcsin(\cot\theta\tan\alpha),\ M(s,\theta)) \quad (33)$$

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

$$K_2(S,\theta,s) = \sqrt{Z(s,\theta)}\,\mathcal{E}\left[\arcsin\left(\frac{1}{M(s,\theta)}\sqrt{1-\frac{s^2}{S^2}}\right),\ M(s,\theta)\right] - \sqrt{1-\frac{s^2}{S^2}}\sqrt{Z(s,\theta)-\frac{S^2}{s^2}} \tag{34}$$

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

Proof. Proposition 4 yields the strong conditional independence of size and formula (30) follows as in Theorem 2 and Corollary 1.

From formulas (22)–(24) in Lemma 3 it follows that for fixed θ, s,

$$S = S(\alpha) = \sqrt{s^2 + (1-s^2)(\sin^2\theta - \cos^2\theta\tan^2\alpha)}, \tag{35}$$

Which means that orientation and shape factor are conditionally functionally dependent and the joint conditional density $p(\alpha, S|\theta, s, \uparrow)$ is degenerate. Observe that the transformation $S(\alpha)$ in (35) is monotone decreasing on $\langle 0, \frac{\pi}{2}\rangle$ for each fixed s, θ. Again by Mikusinski et al [10], 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 marginal conditional distribution functions

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

which implies (32). The functions K_1, K_2 follow from (27), (28):

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

and

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

The last integral was found in Gradshtejn and Ryzhik [7], p. 261. □

5. NUMERICAL EXAMPLE

Unfolding problems belong to a class of inverse problems (Coleman [3]) which are often called ill-posed, which means that 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. From reasons described at the end of Section 3, a discretization method is used in our example for the solution of size-shape-orientation problem. It transforms an integral equation onto a system of linear equations. Condition number of the matrix of this system can be used as a criterion for the stability of solution.

Assume that in the model of oblate ellipsoidal particles n particle sections are observed using the VUR sampling design and classified into trivariate histogram with class limits for size, shape factors and orientations, respectively:

$$a_j = A_j = b^j,\ j \in Z; \quad s_i = S_i = \left(1 - \frac{i}{m}\right)^{\nu}, \quad \alpha_i = \theta_i = i\Delta,\ i = 1, \dots, m. \quad (36)$$

Here $b > 1$, $\nu > 0$ are given constants, m the number of classes, $\Delta = \frac{\pi}{2m}$. Notice that classes of colatitude θ in (36) correspond to areas on the hemisphere of spatial orientations proportional to $\cos\theta_{i-1} - \cos\theta_i$.

The unfolding runs in two steps according to Theorem 3. In both of them the iterative EM-algorithm is used, see Silvermann et al [13] for its numerical and statistical properties. The outer problem (17) is in fact the Wicksell [15] corpuscule problem as expected according to results of Kleinwachter and Zähle [9]. $H(a_l, \alpha_j, S_k)$ and N_V are then estimated using any commonly used method, e.g. Beneš et al [2], Ohser and Mücklich [12].

Discretization of the inner bivariate problem (18) is standard, cf. Ohser and Mücklich [12]. For each fixed a it is assumed that s, θ are discrete random variables and $F_{ij} = P(s = s_i, \theta = \theta_j)$. Further

$$H(k,l) = H(a, \alpha_l, S_{k-1}) - H(a, \alpha_l, S_k) - H(a, \alpha_{l-1}, S_{k-1}) + H(a, \alpha_{l-1}, S_k)$$

and

$$\begin{aligned} p_{ijkl} \quad = \quad & \frac{2}{\pi}[K(s_i, \theta_j, S_{k-1}, \alpha_l) - K(s_i, \theta_j, S_k, \alpha_l) \\ & -K(s_i, \theta_j, S_{k-1}, \alpha_{l-1}) + K(s_i, \theta_j, S_k, \alpha_{l-1})] \end{aligned} \quad (37)$$

using (19), i, j, k, $l = 1, \dots, m$. The discrete analogue of (18) is the system of equations

$$H_{kl} = \sum_{i=1}^{m} \sum_{j=1}^{m} p_{ijkl} F_{ij}, \quad (38)$$

which is solved by EM-algorithm with λth iteration step

$$F_{ij}^{(\lambda+1)} = \frac{F_{ij}^{(\lambda)}}{t_{ij}} \sum_k \sum_l \frac{H_{kl} p_{ijkl}}{r_{kl}^{\lambda}}, \quad (39)$$

where $t_{ij} = \sum_k \sum_l p_{ijkl}$, $r_{kl}^{\lambda} = \sum_i \sum_j F_{ij}^{(\lambda)} p_{ijkl}$. As an initial iteration $F_{ij}^{(0)} = H_{ij}$ is sufficient.

In a statistical study, a sample of $n = 10017$ particle sections of a composite material (Beneš et al [2]) was classified according to (36) with $b = 1.756$, $j = 1, \dots, m$; $\nu = 1.5$, $m = 8$. The matrix P of coefficients p_{ijkl} for the inner problem (38) 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 low value (cf. Gerlach and Ohser [5]) justifies the use of the method. Histogram F_{lij} of estimated frequencies of spatial parameters a_l, θ_i, s_j obtained from (39) for each fixed a_l is in Figure 1. It enables further investigation of various kinds of dependencies within the particle system.

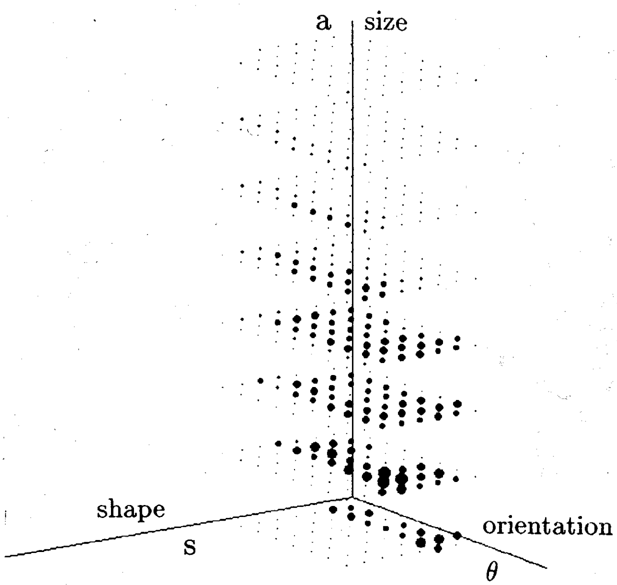

Fig. 1. Histogram of estimated spatial size-shape-orientation distribution. The volume of three-dimensional balls in the Figure is proportional to the estimated values of F_{lij}, $l, i, j = 1, \ldots, 8$. The axes intersect in the point $l = i = j = 1$.

6. DISCUSSION

Møller [11] proved that it is possible to reconstruct an ellipsoid completely from three parallel sections. His method is hardly applicable in quantitative metallography from two reasons. First the preparation of appropriate parallel sections in hard materials with small particles (cf. Beneš et al [2]) is almost impossible, while a vertical plane (e. g. parallel to the deformation axis) is easily obtained. From the same reason also the assumption-free methods of stereology (Karlsson and Cruz–Orive [8]) may sometimes be useless.

Secondly Møller's method works for perfect ellipsoids while in practice the shape assumption is often an approximation, only. Therefore we revisited the 70 years old problem in order to pose a new three-parametric ill-posed problem, the solution of which is, thanks to modern numerical approaches, acceptable for practice.

ACKNOWLEDGEMENTS

The research was supported by the Grant Agency of the Czech Republic, projects No. 201/96/0228, 106/95/1482 and 201/94/0471. We thank to Prof. A. M. Gokhale for sending us a preprint of his paper [6] before its publication.

(Received March 29, 1996.)

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