Sci. Form 1 (1): 49-58 , 1985

On Mathematical Principles of Stereological Estimation

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Key words : anisotropy, internal structure, stereology, sphere

Stereological procedures are classified according to the type of estimation, and their mutual relationships are discussed. Then, estimation of sphere size distribution from observation of material cross-sections is discussed from the viewpoint of numerical analysis, i.e., discrete approximation of the basic integral equation of Abel type. Finally, methods of estimating structural anisotropy due to internal distribution of line tissues and surfaces are considered. The anisotropy of structure is characterized by the distribution density, which is expressed in terms of what is called the "fabric tensors." The distribution density is related to observed data by what is called the "Buffon transform," and estimation is done by computing its inversion. Main emphasis is placed on the role played by mathematics.

INTRODUCTION

"Stereology" can be defined as a study of methods to estimate "geometrical characteristics" of the space (of any dimensionality, mostly 2 and 3 dimensions) from "partial observations" such as observations of material cross-sections or thin slices. Hence, definite solutions can not be obtained, and the problem is statistical in its nature. Hence, statistical models are employed with appropriate probabilities assigned, and the solution has a meaning only in the statistical sense. In the following, we classify and summarize various techniques obtained so far. In view of the interdisciplinary nature of stereology, we make clear the role played by mathematics and underlying mathematical thinking. This may help researchers in different areas to understand stereology from a unified rational viewpoint.

AVERAGE DENSITY ESTIMATION

Mathematical structure of stereological estimation differs according to the object of estimation. A simplest one is the estimation of "density" such as V_V (the volume of a specific phase per unit volume of the material), A_V (the area of a specific surface per unit volume) and L_V (the length of specific

Accepted for Publication : June 15, 1985.

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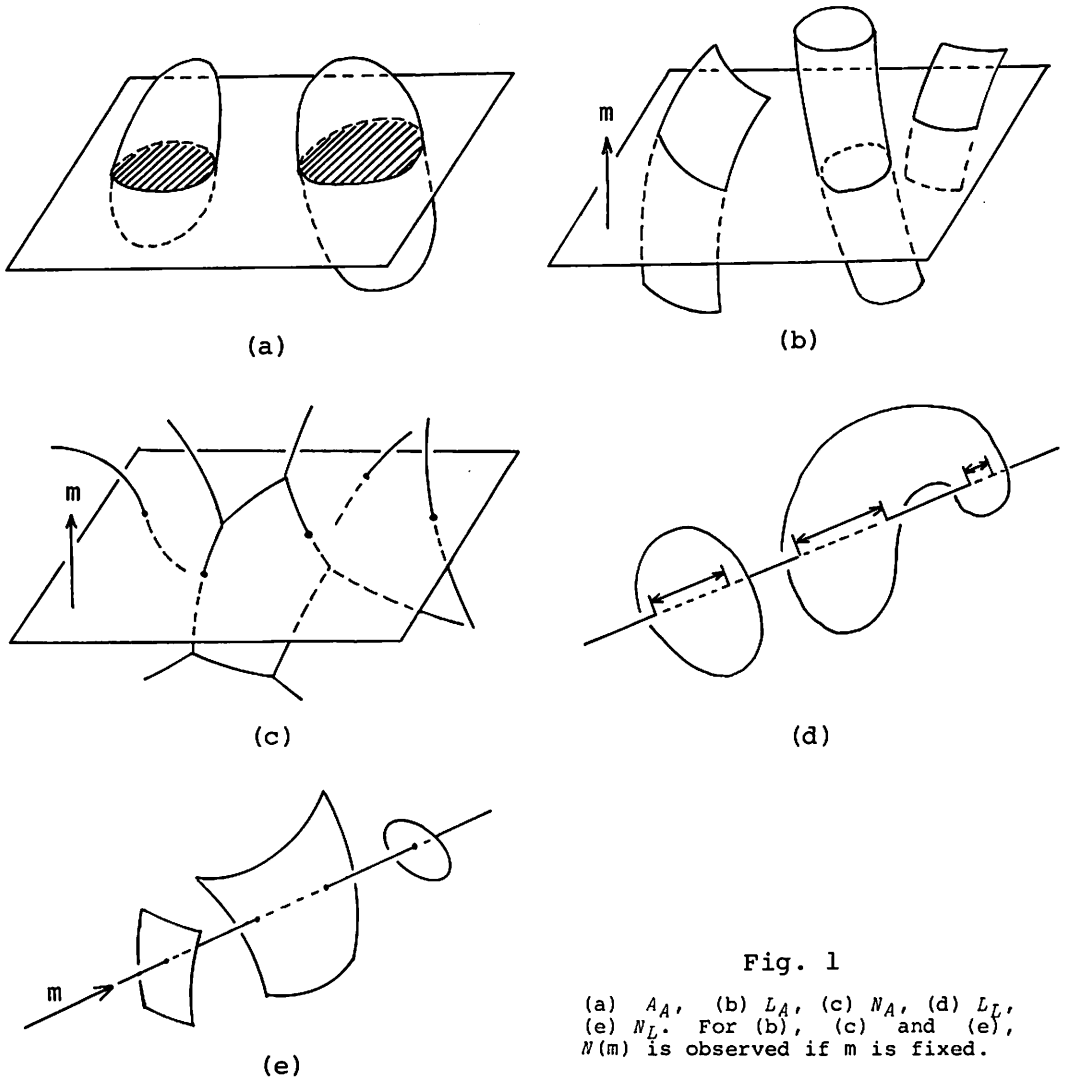

Fig. 1

(a) A_A, (b) L_A, (c) N_A, (d) L_L, (e) N_L. For (b), (c) and (e), $N(m)$ is observed if m is fixed.

tissues per unit volume). Observations are made on planes cutting the material, measuring A_A (the area of a specific phase per unit area of the cutting plane, Fig. 1(a)), L_A (the length of intersections with surfaces per unit area of the cutting plane, Fig. 1(b)), N_A (the number of intersections with line tissues per unit area of the cutting plane, Fig. 1(c)) or on probe lines piercing the material, measuring L_L (the length of intercepts of a specific phase per unit length of the probe line, Fig. 1(d)) or N_L (the number of intersections with surfaces per unit length of the probe line, Fig. 1(e)).

Densities like V_V, A_V, L_V, A_A, L_A, N_A, L_L and N_L all have meanings in the sense of average. This type of estimation has been extensively studied in biology, medicine, metallurgy and geology in order to examine the internal biological tissues, inclusions in metals, underground minerals, etc, and mathematical relations among those densities are listed in many books (e.g., DeHoff and Rhines: 1968, Underwood: 1970, Weibel: 1979, 1980).

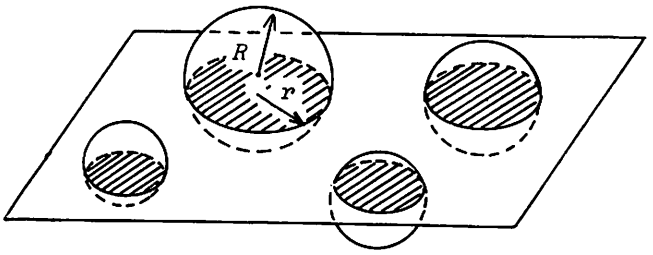

Fig. 2: Distribution of spheres in the material and their corss-sections on a cutting plane.

SIZE DISTRIBUTION ESTIMATION

At times we want to know not only average densities but also their "distributions." For example, if many objects of the same shape but of different sizes are distributed in the material, we often need to know the size distribution. Most extensively studied is the case of spherical inclusions. Although other shapes such as ellipsoids and cubes are also important, the assumption of sphere makes the theory simple and elegant. Moreover, spherical particles often play a significant role in biology, medicine, metallurgy and geology (e.g., DeHoff and Rhines: 1968, Underwood: 1970, Weibel: 1979, 1980).

Let the "distribution density" $F(R)$ be defined in such a way that $F(R)dR$ is the number of spheres of radii between R and $R + dR$ in unit volume of the material. The spheres are assumed to be distributed randomly. Suppose we place a cutting plane randomly in the material and observe particle cross-sections on the cutting plane (Fig. 2). Let the observed distribution density $f(r)$ be defined in such a way that $f(r)dr$ is the number of circular cross-sections of radii between r and $r + dr$ in unit area of the cutting plane. Then, $F(R)$ and $f(r)$ are shown to be related by the integral equation of the form

$$f(r) = 2r\int_r^{R_{max}} \frac{F(R)dR}{\sqrt{R^2 - r^2}} , \qquad (1)$$

where R_{max} is the maximum particle radius. A small change of variables reduces this equation to an integral equation of Abel type, and it can be analytically inverted to express $F(R)$ in terms of $f(r)$ in the form

$$F(R) = \frac{R}{\pi} \int_R^{R_{max}} \frac{d(f(r)/r)}{\sqrt{r^2 - R^2}} . \qquad (2)$$

Many numerical schemes are also proposed to compute this process from a finite number of observed data. Various other effects such as a thin slice instead of a cutting plane (the "Holmes effect" or "overprojection"), the "resolution threshold" and the "capping effect" are also incorporated (DeHoff and Rhines: 1968, Underwood: 1970, Weibel: 1979, 1980, Cruz-Orive: 1983, Coleman: 1982, 1983 and many others).

Thus, the estimation problem is completely solved in principle. However, there are several points that should be pointed out. First, most numerical schemes were devised on the basis of some discrete distribution models. For example, each particle is assumed to belong to one of prefixed classes of the particle size. The schemes are then evaluated only by the numerical outcomes of actual or synthetic examples. However, we should recall that exact integral equation (1) or (2) is already obtained. Hence, every numerical scheme must be a discrete

approximation of (1) or (2) in some sense, and it should be evaluated from the viewpoint of how well it approximates the exact integral equation.

Kanatani and Ishikawa (1985) showed that the familiar schemes due to Scheil, Schwartz or Saltykov (cf. DeHoff and Rhines: 1968, Underwood: 1970, Weibel: 1979, 1980) are poor approximations to the exact integral equation. They divided the interval $[0, R_{\max}]$ into n subintervals and formulated various discrete approximations. Each of them was evaluated by analyzing the discrepancy between the approximation and the original integral equation asymptotically in terms of n. Schemes of Scheil, Schwartz or Saltykov, for example, are shown to have errors of $O(1/n)$. Such an asymptotic analysis provides not simply a general criterion to compare different numerical schemes but also various numerical techniques to improve accuracy such as the "acceleration" (cf. Kanatani and Ishikawa: 1985).

Next thing to note is the use of the (cumulative) "distribution functions" $\Phi(R)$, the number of spheres of radii smaller than R in unit volume of the material, and $\phi(r)$, the number of cross-sections of radii smaller than r in unit area of the cutting plane, rather than the use of the "distribution densities" $F(R)$ and $f(r)$. This is because $\Phi(R)$ and $\phi(r)$ alone are well defined functions both from a practical point of view and from a mathematical point of view, while densities $F(R)$ and $f(r)$ can be obtained only through "differentiation," their definitions involving "infinitesimals" like dR and dr. Making a discrete histogram is nothing but one process of numerical differentiation of measured data, and this process is very susceptible to noise.

In many books, not only $F(R)$ and $f(r)$ are used but also they are used in the sense of "probability," i.e., they are normalized so that the total becomes unity. However, there is no physical sense to interpret them as probabilities, since they express "geometrical" characteristics, describing distributed quantities "per unit volume" or "per unit area." Normalization only complicates mathematical treatment. These facts should be well known among mathematicians and engineers, but it seems that many researchers of biology and medicine may not be aware of this.

In terms of distribution functions $\Phi(R)$ and $\phi(r)$, equations (1) and (2) are integrated into the form of

$$\phi(r) = 2\bar{R}N - 2\int_r^{R_{\max}} \sqrt{R^2 - r^2}\, d\Phi(R), \tag{3}$$

$$\Phi(R) = N - \frac{1}{\pi}\int_R^{R_{\max}} \frac{d\phi(r)}{\sqrt{r^2 - R^2}}, \tag{4}$$

where N is the "numerical density," i.e., the number of particles per unit volume, and $\bar{R}$ is the "mean radius" of the particles, and the integration is in the sense of Stieltjes. The discrete approximation is made as follows. First, we take discrete radii $(0 =)\ a_0 < a_1 < \ldots < a_n\ (= R_{\max})$. If the integration of equation (3) is approximated by appropriate summation, we obtain a discrete scheme of the form

$$\phi(a_i) = \sum_{j=1}^{n} A_{ij}\Phi(a_j), \quad i = 1, 2, \ldots, n. \tag{5}$$

Formulae of this type were called "implicit formulae" by Kanatani and Ishikawa (1985). If we compute the inverse matrix $B = (B_{ij})$

$(= A^{-1})$ of $A = (A_{ij})$, we obtain a formula of the form

$$\Phi(a_i) = \sum_{j=1}^{n} B_{ij}\phi(a_j), \quad i = 1, 2, \ldots, n. \tag{6}$$

which converts observed data $\phi(a_1)$, $\phi(a_2)$, ..., $\phi(a_n)$ into desired distribution $\Phi(a_1)$, $\Phi(a_2)$, ... , $\Phi(a_n)$. Another type of approach is to approximate equation (4) directly by a discrete equation in the form of (6). Formulae of this type were called "explicit formulae" by Kanatani and Ishikawa (1985). They analyzed various schemes and concluded that implicit formulae give in general better approximation to the exact integral equation.

Another thing to keep in mind is the distinction of error sources. The accuracy of estimation increases if observations are repeated many times and accurate measurement is done. This is because "sampling errors" are reduced. On the other hand, the use of accurate formulae also increases the accuracy. This is because "computational errors" are reduced. These two error sources are different in their nature and should not be mixed up. So far, many estimation schemes have been tested experimentally and evaluated according to the overall accuracy. However, good overall accuracy does not imply that the formula is accurate. Different error sources should be examined separately, and the computational accuracy should be studied from the viewpoint of numerical analysis.

Kanatani and Ishikawa (1985) pointed out that the computational accuracy of the formulae of the form of equations (5) and (6) depends dominantly on the treatment of "singularities" in equations (3) and (4). The reason that explicit formulae give poor accuracy is that the order of singularity is higher for (4) than for (3). This fact is not affected when other factors such as the Holmes effect, the resolution threshold and the capping effect are taken into account. Kanatani and Ishikawa (1985) also studied the numerical stability in terms of the "condition number" of matrices $A = (A_{ij})$ and $B = (B_{ij})$.

ESTIMATION OF STRUCTURAL ANISOTROPY

Geometrical characteristics of the material in which objects are distributed are not restricted to average densities and their size distributions. Sometimes, the extent of "anisotropy" of the distribution may be an important concern. If the distribution is not isotropic, the same observation process yields different results for different orientations of the material. Hence, there have been proposed various observation processes which depend on the material orientation, and many "indices of anisotropy" are devised out of these observations (cf. DeHoff and Rhines: 1968, Underwood: 1970, Weibel: 1979, 1980).

Although this type of approaches are often taken in biology, medicine, metallurgy and geology, they cannot be called truly "scientific." The rational way should be as follows. (I) We first try to define a definite "model" of anisotropy in mathematical terms and determine the parameters by which it is completely specified "irrespective of whether or not there exists a means to measure them." (II) Then, we try to devise means of measurement. If they cannot be measured directly by any available means, they should be "estimated" by some approximation

schemes. The philosophy is the same as in the above case of particle size distribution where schemes are evaluated from the view point of how well they approximate the exact integral equation.

Consider two cases of anisotropy due to internal structure. One is the case where line tissues are distributed in the material. The line tissues may be straight or curved. They may be dissected into separate "needles" or linked to form a connected "network." Let the line tissues be hypothetically dissected into infinitesimally small line segments. Let each line segment be assigned an orientation by a unit vector n randomly with a probability of 1/2 out of the two possibilities. Let the "distribution density" $f(\mathrm{n})$ be defined in such a way that $f(\mathrm{n})\mathrm{d}\Omega(\mathrm{n})$ is the total length of those line segments, in unit volume of the material, whose orientations are inside the differential solid angle $\mathrm{d}\Omega(\mathrm{n})$ around n. By definition, $\int f(\mathrm{n})\mathrm{d}\Omega(\mathrm{n})$ equals L_V, the length of the line tissues per unit volume. If the distribution is isotropic, $f(\mathrm{n})$ = const..

The other is the case where surfaces are distributed in the material. The surfaces may be planar or curved. They may be dissected into separate "disks" or linked to form a connected "cell walls." Let the surfaces be hypothetically dissected into infinitesimally small surface segments. Let each surface segment be assigned a unit normal vector n randomly with a probability 1/2 out of the two possibilities. Let the "distribution densities" $f(\mathrm{n})$ be defined in such a way that $f(\mathrm{n})\mathrm{d}\Omega(\mathrm{n})$ is the total area of those surface segments, in unit volume of the material, whose normals are inside the differential solid angle $\mathrm{d}\Omega(\mathrm{n})$ around n. By definition, $\int f(\mathrm{n})\mathrm{d}\Omega(\mathrm{n})$ equals A_V, the area of the surface per unit volume. If the distribution is isotropic, $f(\mathrm{n})$ = const..

Our aim has been now formulated in mathematical terms in either case as estimating the distribution density $f(\mathrm{n})$. Next, let us consider how to parameterize $f(\mathrm{n})$. Since it is regarded as a function on a unit sphere defined by the unit vector n, it can be expressed as a "spherical harmonics expansion." In Cartesian tensor notation, this become as follows (Kanatani: 1984a):

$$f(\mathrm{n}) = \frac{c}{4\pi}\,[1 + D_{ij}n_in_j + D_{ijkl}n_in_jn_kn_l + \ldots], \tag{7}$$

where we adopt the Einstein summation convention over repeated indices. Terms of odd degrees do not appear because $f(\mathrm{n})$ is "symmetric" with respect to the origin, i.e., $f(\mathrm{n}) = f(-\mathrm{n})$. Here, $c = \int f(\mathrm{n})\mathrm{d}\Omega(\mathrm{n})$ (the "total density") and D_{ij}, D_{ijkl}, ... are "deviator tensors," i.e., contraction of any two indices yields 0. These tensors were called the "fabric tensors" of the distribution. This expansion is the same as the "multiple moment expansion" of an electric potential in electromagnetics. Since spherical harmonics of each degree form a basis of an irreducible representation of the three-dimensional rotation group SO(3), this expansion corresponds to resolution to spaces of irreducible representation of SO(3) (cf. Kanatani: 1984a).

Suppose a cutting plane of unit normal m is placed randomly in the material, and let $N(\mathrm{m})$ be the number of intersections with line tissues per unit area of the cutting plane (Fig. 1(c)). Then, the expectation value of $N(\mathrm{m})$ is shown to be related to the distribution density $f(\mathrm{n})$ of line tissues in the form

$$N(\mathrm{m}) = \int |\mathrm{m}\cdot\mathrm{n}| f(\mathrm{n})\,d\Omega(\mathrm{n}). \tag{8}$$

This relation was first suggested by Hilliard (1967) and was called the "Buffon transform" by Kanatani (1984b). Suppose a probe line of orientation m is placed randomly in the material, and let $N(\mathrm{m})$ be the number of intersections with surfaces per unit length of the probe line (Fig. 1(e)). Then, the expectation value of $N(\mathrm{m})$ is also shown to be related to the distribution density $f(\mathrm{n})$ of surfaces by the Buffon transform of (8) (cf. Kanatani: 1984b). Suppose a cutting plane of unit normal m is placed randomly in the material, and let $N(\mathrm{m})$ be the length of intersections with surfaces per unit area of the cutting plane (Fig. 1(b)). Then, the expectation value of $N(\mathrm{m})$ is shown to be related to the distribution density $f(\mathrm{n})$ of surfaces in the form

$$N(\mathrm{m}) = \int |\mathrm{m}\times\mathrm{n}| f(\mathrm{n})\,d\Omega(\mathrm{n}), \tag{9}$$

which was also called the "Buffon transform" by Kanatani (1984b).

Thus, estimation of the distribution density $f(\mathrm{n})$ is reduced to inversion of the Buffon transform of (8) or (9). Let the right-hand side of (8) or (9) be written as $Bf(\mathrm{m})$ and the operator B be termed the "Buffon operator." Let the rotation operator R be defined by $Rf(\mathrm{m}) = f(R^{-1}\mathrm{m})$. Then, the Buffon operator B "commutes" with the rotation operator R and hence is an "invariant" operator, i.e., $BRf(\mathrm{m}) = RBf(\mathrm{m})$ or $B = R^{-1}BR$. Hence, the spherical harmonics generate "eigenspaces" of the operator B, and the inversion of (8) or (9) is computed if observed $N(\mathrm{m})$ is also expanded into a spherial harmonics expansion

$$N(\mathrm{m}) = \frac{C}{4\pi}\left[1 + F_{ij}m_i m_j + F_{ijkl}m_i m_j m_k m_l + \ldots\right]. \tag{10}$$

Then, c, D_{ij}, D_{ijkl}, ... are given as follows (Kanatani: 1984b):

$$D_{i_1 i_2 \cdots i_n} = \lambda_n F_{i_1 i_2 \cdots i_n}, \tag{11}$$

For (8), $c = C/2\pi$, $\lambda_n = (-1)^{n/2-1}2^{n-1}(n-1)(n+2)/\binom{n}{n/2}$ (12)

For (9), $c = C/\pi^2$, $\lambda_n = -2^{2n-1}(n-1)/\binom{n}{n/2}^2$ (13)

Now, the problem is finally reduced to estimating the expansion (10) from a finite number of observed data $N(\mathrm{m}^{(1)})$, $N(\mathrm{m}^{(2)})$, ..., $N(\mathrm{m}^{(N)})$. A most straightforward method is the "Monte Carlo method," choosing $\mathrm{m}^{(1)}$, $\mathrm{m}^{(2)}$, ..., $\mathrm{m}^{(N)}$ randomly on the unit sphere defined by m (Kanatani: 1984b). To do so, however, we must prepare a large number of material samples all of which are supposed to have the same statistical characteristics and cut them from various different orientations. This is often difficult to perform in practice. On the other hand, if the anisotropy is weak and the distribution is nearly isotropic, higher order terms of (7) or (10) can be neglected. Then, there exist methods using only three types of surfaces, say planes parallel to the xy-, the yz- and the zx-planes, and errors involved in this approximation are also estimated (Kanatani: 1985b).

The above principle leads to a variety of applications in many different fields. This method can be used for characterization of particles in powder technology. For example, the orientation of maximum alignment of the needle-like particles

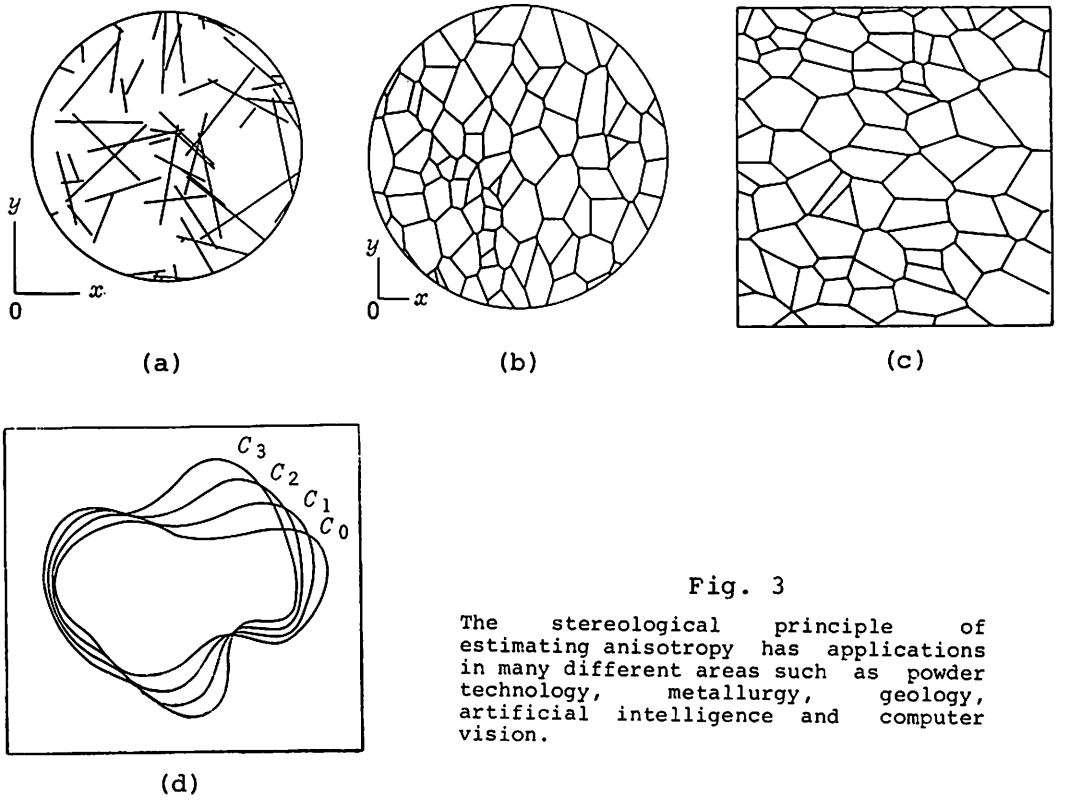

Fig. 3

The stereological principle of estimating anisotropy has applications in many different areas such as powder technology, metallurgy, geology, artificial intelligence and computer vision.

of Fig. 3(a) is estimated to be 125° from the x-axis (Kanatani: 1985c). In geology, the internal crack distribution in a rock can also be estimated from observations of its surfaces (Kanatani: 1985a). Applying this principle, we can also measure the strain of a material by observing the structural anisotropy if the internal structure is assumed to be isotropic in the original state. For example, the orientations of maximum extension and compression of the material shown in Fig. 3(b) are estimated to be 2° and 92° from the x-axis respectively and the shearing strain to be 0.18 in the xy-plane (Kanatani: 1984b). The same principle is also used in computer vision and artificial intelligence to reconstruct three dimensional information from two dimensional camera images. For example, Fig. 3(c) is estimated to be a plane with isotropic texture slanted by 49° (Kanatani: 1984c). We can also compute the three-dimensional motion of a moving plane which is seen as Fig. 3(d) (Kanatani 1984d).

CONCLUDING REMARKS

Stereology is an interdisciplinary area, and the same principle can be used in many different areas for many different purposes. Hence, results in a particular area could bring about new applications in other areas. However, this is possible only if the results are described in precise mathematical terms. So far, researches in a particular area seem to have been aiming only at researchers in that area, and the same principle has been rediscovered many times separately in different areas.

The present article is intended to give a unified mathematical viewpoint that should be shared by all the areas concerned. A basic philosophy described here is (I) first formulating the problem exactly in purely mathematical terms and (II) then devising necessary experimental means that are easy to perform. We have also shown the importance of mathematical techniques such as numerical analysis, tensor analysis and group theory. Further advances can be expected if the viewpoint stated in this article is applied and coupled with various other mathematical techniques.

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翻訳要旨

ステレオロジーによる推定の数学的原理について

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ステレオロジーによる推定の代表的な場合をとりあげ、数学的原理の面から分類し、相互関係、基本となる考え方を示した。最初に種々の幾何学的対象が物質中に分布している場合の、対象の平均密度の推定法を概観し、次に対象の寸法の分布の推定の代表的な例として、種々の球状粒子の半径分布の推定を考えた。球の半径の分布と物質の切断面上に現われる粒子断面の半径分布とは積分方程式によって関係づけられており、その方程式を解析的に解くこともできる。したがって、原理的な問題は解決している。そこで、実際の有限個のデータから数値的に行う計算法を考えるには、それが厳密な積分方程式をどのような意味で、どの程度よく近似しているかを考慮する必要がある。これが数値解析の基本的な考え方である。これをKanatani and Ishikawa(1985)に基づいて説明し、陽公式、陰公式、誤差の漸近評価、等にもふれ、密度関数ではなく（累積）分布関数を用いる理由、分布を規格化しない理由についても述べた。

次に物質中に分布する内部組織による異方性の推定法を論じた。基本的な考え方は（I）まず測定法とは無関係に、数学的に明確に分布の異方性を定義し、求めるべきパラメータを定式化し、（II）次にそのパラメータの測定法を考える、直接的な測定が不可能なときは近似的な推定法を考える、という順序である。この方法により、Kanatani(1984b)に基づいて、分布密度、ファブリックテンソルを定義し、測定データとの関係を与えるBuffon変換が回転群と可換な不変な作用であることから、球面調和関数による展開を用いて解が定まることを示し、それをテンソル方程式で表わした。そして、この考え方が、粉体工学、金属工学、地質学、人工知能、コンピュータービジョン、等の多くの分野に応用できることを、例をあげて説明した。

ステレオロジーは境界領域に属する学問であるから、個別の分野だけで考えるのではなく、一般的、普遍的な形で数学的に定式化して初めて、いろいろな分野での応用が可能になる。本文で述べたように、理論的に一貫した考え方に立ち、数値解析やテンソル解析のようなさまざまの数学的手法を組み合わせれば、ステレオロジーの適用範囲とその有効性がますます増大すると思われる。

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