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ERROR ESTIMATION IN STEREOLOGICAL DETERMINATION OF PARTICLE SIZE DISTRIBUTION

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ABSTRACT

Stereological determination of particle size distribution normally amounts to solving a Volterra's integral equation of the first kind. Computationally speaking, this integral equation must be discretized and converted into a set of n algebraic equations in n unknowns. As the value of n increases the accuracy of estimation also increases. Here is proposed a technique of replacing the distribution density f(r) obtained from randomly intersecting planes with comulative distribution density $\phi(r)$. Here $\phi(r)$ is the number of cross-sections with radii equal to or smaller than r per unit area. Similarly $\Phi(R)$ is defined as the number of spheres with radii equal to or smaller than R per unit volume. The integral equation is thus reduced to an Abel's type. Finally, the error involved in discrete approximation with large n is obtained and the best formula to minimize the error is derived.

1. INTRODUCTION

Recently Kanatani and Ishikawa (1983) have reported some applicable results on error analysis for the stereological estimation of sphere size distribution. The purpose of this paper is to extend their results to rotund particles with random geometrical variations.

A standard stereological technique will be employed here, namely that, the size distribution of randomly distributed particles in a material matrix will be estimated from an observed size distribution of their cross-sections on a randomly intersecting plane thru the material matrix. For some recent results in connection with the present problem refer to Shahinpoor (1983), Shahinpoor and Shahrpass (1983), and Shahinpoor and Minis (1983). Classically, these problems have been extensively treated as the Wicksel problem (Wicksel, 1925, 1926).

2. GOVERNING INTEGRAL EQUATIONS

Consider a material matrix dispersed with rotund particles whose mean local radius is R such that R+R' is the actual radius of individual particles where R' is the fluctuation associated with the mean radii R. Let P(R) be the radius distribution density. Thus, P(R)dR is the number of particles whose mean radii are between R and R+dR per unit volume. Now let a flat plane randomly interset the material matrix, i.e., a plane is placed in the material matrix. Now, a radius distribution density p(r) of the rotund particle cross-sections are obtained such that r is the local mean radius of individual templates such that r+r' is the actual size of templates with r' a random fluctuation field associated with r. Note that p(r) dr is the number of those templates whose mean radii are between r and r+dr, per unit area of the intersecting plane. We assume that the particles are distributed randomly and homogeneously and the intersecting plane is of infinite extent. Note that the probability for a particle of mean radius R to R+dR to be intersected by the plane is the same as the probability that the center of volume of such a particle falls within the distance R from the plane. The two-dimensional distribution p(r) can generally be obtained through the distribution of line transects as shown in Fig. 1.

Note that there are P(R)dR such particles per unit volume and therefore that probability equals 2RP(R)dR per unit area in the plane. The probability that a particle of mean radius between R and R+dR create a template with a mean radius between r and r+dr, provided the plane has intersected the particle, is simply equal to |dx|/R, where x is the distance from the plane to the center of volume. Thus, the probability distribution p(r) is obtained by multiplying |dx|/R by 2RP(R)dR and integrating over all possible values of R, i.e.,

$$p(r) = \int_r^{R_M} \left(\frac{|dx|}{R}\right) 2RP(R)dR \ , \tag{2.1}$$

which can be simplified to the following Volterra type integral equation of the 1st kind:

$$p(r) = 2r \int_r^{R_M} P(R)[R^2-r^2]^{-\frac{1}{2}}dR \ , \tag{2.2}$$

where R_M is the maximum possible mean radius such that $p(R_M)=0$. Equation (2.2) can be inverted by techniques employed by Wicksel (1925,1926). Here we choose to deviate from the classical Wicksel problem by reverting to cumulative distributions.

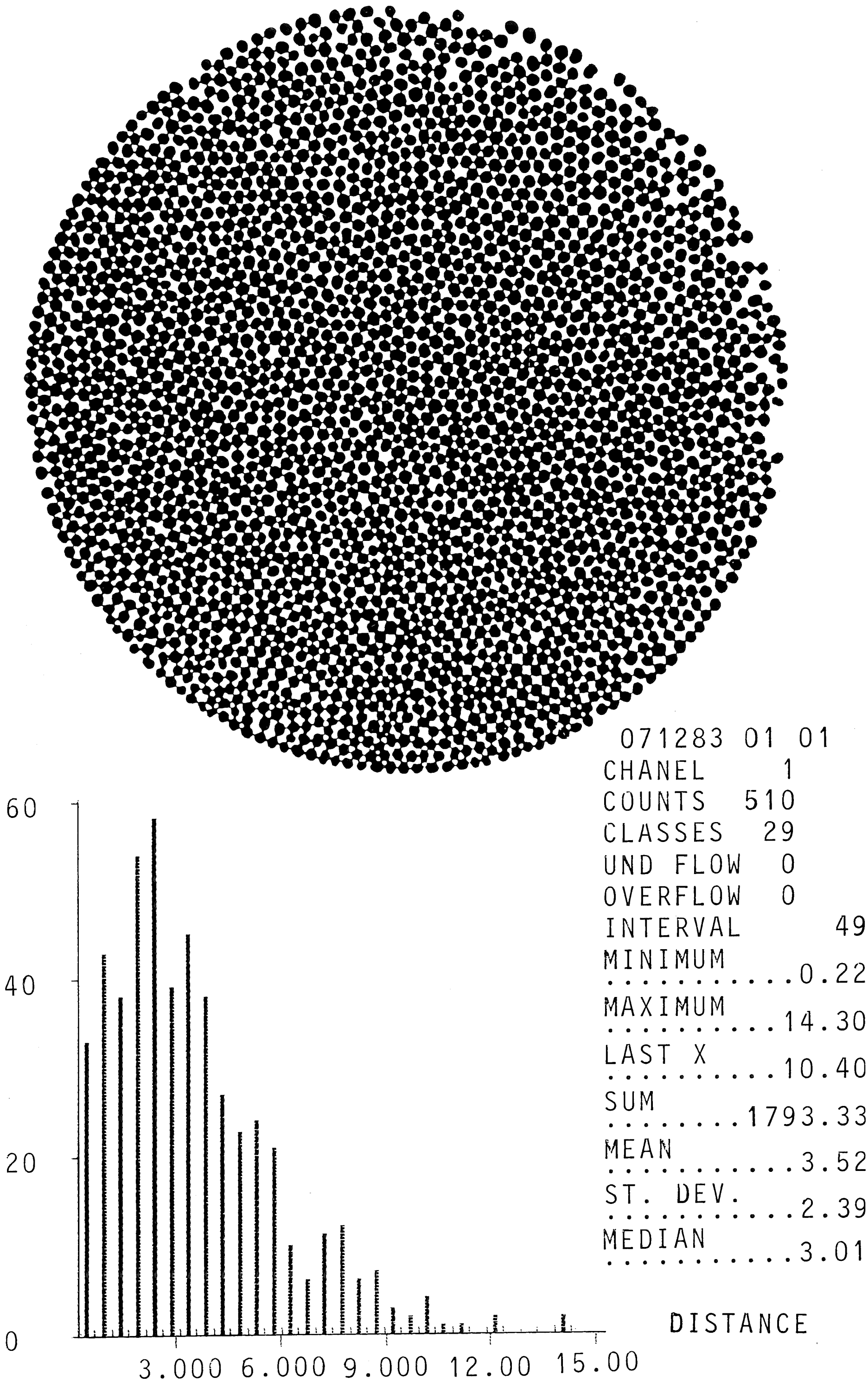

Fig. 1. A Typical Distribution of Line Transects for Green Peas

Since the actual measurements are finite thus one has to resort to discrete numerical techniques in order to evaluate P(R). One way to circumvent the difficulty is to define a cumulative distribution density $\phi(r)$ and its 3-D counterpart $\Phi(R)$, such that: $\phi(r)=\int_o^r p(r)dr$, (2.3), where $\phi(r)$ is the number of templates with mean radii equal to or smaller than r per unit area. Thus, from equations (2.2) and (2.3) one obtains.

$$\phi(r) = 2\bar{R}N-2\int_r^{R_M} P(R)[R^2-r^2]^{-\frac{1}{2}}dR, \qquad (2.4)$$

where N is the number of particles per unit volume, and $\bar{R}$ is the "mean radius" of all particles, such that,

$$N = \int_o^{R_M} P(R)dR \ , \quad (2.5) \qquad \bar{R} = \frac{1}{N}\int_o^{R_M} RP(R)dR \ . \qquad (2.6)$$

Integrating equation (2.4) by parts we obtain the following Abel's type integral equation:

$$\phi(r) = 2N[\bar{R}-(R_M^2-r^2)^{\frac{1}{2}}]+2\int_r^{R_M} R\Phi(R)[R^2-r^2]^{-\frac{1}{2}}dR \ , \qquad (2.7)$$

where $\Phi(R)$ is the cumulative distribution function, i.e., the number of particles with mean radii equal to or smaller than R per unit volume. For a description of such Abel's type integral equations and their numerical solutions please refer to the classical works of Jakeman and Anderson (1974), (1975). Again our technique differs from theirs due to the fact that we employ the cumulative distributions in our computational algorithm which follows.

3. DISCRETIZATION AND ERROR ESTIMATION

Equation (2.7) can be discretized and reduced to a set of n algebraic equations of the form $\phi(r_i)=A_{ij}\Phi(R_j)$, i,j=1,2,..., n, (3.1). Where A_{ij}'s are constant coefficients, and the Einstein's summation convention's is applied to repeated indices.

Equation (3.1) can be inverted to yield: $\Phi(R_i)=B_{ij}\phi(r_j)$, (3.2). Let us first invert equation (2.2) to an Abel's type integral equation and then apply the discretization. Changing the variables in equation (2.2) from r to $s=\pi r^2$ and from R to $S=\pi R^2$, this equation is reduced to

$$p(s) = \pi^{-\frac{1}{2}}\int_s^{S_M} P(S)(S-s)^{-\frac{1}{2}}dS \ , \qquad (3.3)$$

where $S_M=\pi R_M^2$. Multiplying (3.3) by $(s-\alpha)^{-\frac{1}{2}}$ and integrating from α to ∞ yields the following inverse equation

$$\Phi(R) = N-\pi^{-1} \int_R^{R_M} p(r)(r^2-R^2)^{-\frac{1}{2}}dr \ . \tag{3.4}$$

Discretizing (3.6) we obtain

$$\Phi(R_j) = N-\pi^{-1} \sum_{j=i+1}^{n} \int_{r_{j-1}}^{r_j} p(r)(r^2-r_i^2)^{-\frac{1}{2}}dr \ , \tag{3.5}$$

provided that $o=r_o<r_1<r_2<\ldots<r_n=R_M$. Equation (3.5) is finally reduced to

$$\Phi(R_j) = N-\pi^{-1} \sum_{j=i+1}^{n} (r_j^2-r_i^2)^{-\frac{1}{2}}\phi(r_j) \ . \tag{3.6}$$

Thus the problem is reduced to the matrix equation (3.2) such that $\Phi(r_o)=\Phi(o)=o$ determines the value N. In deriving equation (3.6) we have used the following approximation:

$$\int_{r_{j-1}}^{r_j} (r^2-r_i^2)^{-\frac{1}{2}} p(r)dr \approx (r_j^2-r_i^2)^{-\frac{1}{2}} \int_{r_{j-1}}^{r_j} p(r)dr$$

$$\approx (r_j^2-r_i^2)^{-\frac{1}{2}} \phi(r_j) \ . \tag{3.7}$$

5. ERROR ESTIMATION

Considering equation (3.2) again one notes that the output vector $\Phi(R_i)$ pertaining to the cumulative particle mean size distribution is obtained by multiplying the matrix B_{ij} by the input vector $\phi(r_j)$ which is obtained from experimental observations. The experimental observation contains errors from a number of different sources. These sources could be purely observational or purely computational. At any rate let the input stereological error on particle size distribution be denoted by $\Delta\phi(r_j)$ such that equation (3.2) may be rewritten in the form: $\phi(R_i)+\Delta\Phi(R_i)=B_{ij}[\phi(r_j)+\Delta\phi(r_j)]$, (4.1); where clearly: $\Delta\Phi(R_i)=B_{ij}\Delta\phi(r_j)$, (4.2); is the error contained in the final cumulative particle size distribution. In other words how much is the error magnified or diminished in the final result and how susceptible is the numerical scheme to input errors. As discussed by Wilkinson (1963), this susceptibility is determined by what is called the "condition number." This condition number is defined as C such that

$$C_m = ||A_{ij}||_m ||B_{ij}||_m \ , \tag{4.3}$$

where $||\underset{\approx}{A}||_m$ is the "L^m adjoint norm" of a matrix $\underset{\approx}{A}$. If the condition number is very large, the susceptibility is large and the scheme is not expected to yield accurate results.

Now consider equation (3.6) and note that: $\Delta\Phi(R_j)=\Delta\Phi_o + \Delta\Phi_1(R_j)$, (4.6); where $\Delta\Phi_o$ is the error on computing $\bar{N}$ and $\Delta\Phi_1(R_j)$ is the error in computing the summation for a given $\Delta\Phi(R_j)$. Neglecting $\Delta\Phi_o$ we obtain:

$$\Delta\Phi(R_i) = -\pi^{-1} \sum_{j=i+1}^{n} (r_j^2 - r_i^2)^{-\frac{1}{2}} \Delta\Phi(r_j) \quad . \tag{4.7}$$

Therefore, for a given error introduced in the measurement of $\phi(r)$ one can compute the output error on the particle size distribution by equation (4.7).

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