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Error Analysis for the Stereological Estimation of Sphere Size Distribution: Abel Type Integral Equation

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Computational errors are analyzed for existing schemes and their variants of estimating the sphere size distribution from the observed size distribution of cross sections. First, possible methods are classified according to their discrete approximation schemes of the basic integral equation, and the condition numbers of the coefficient matrices are examined. Then, asymptotic forms of error are derived. It is shown that the main source of error is the singularity of the basic integral equation of Abel type and that the magnitude of the error largely depends on the treatment of the singularity. Numerical examples are also given.

1. INTRODUCTION

Estimating the size distribution of particles in a material from an observed size distribution of their cross sections on a cutting plane randomly placed in the material is an important problem in material science, geology, biology and medical science. This problem has been studied by a number of people as an application of so called "integral geometry" or "stereology" [1–12]. Especially, the case of spherical particle has been extensively studied. This is partly because spheres make the theory simple, and partly because particles are spherical or nearly spherical in many important problems.

Procedures of solving this problem have been separately proposed in many different fields, often independently and repeatedly. In fact, there is so much research on this subject, scattered over a wide range of areas, that a complete review is almost impossible. (See, for example, the lists of literature in the recent articles of Cruz-Orive [13–15] and Coleman [15, 16].) However, almost all this research aimed to obtain superior procedures by heuristic approaches, and accuracy has been tested only by numerical experiments using actual or synthetic data. There has

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not been a rigorous analysis of the degree of accuracy for these schemes. It is true from a practical point of view that it suffices to know only one most recommended scheme. However, a scheme which shows high accuracy for some data of some problem is not necessarily good for other data of other problems. It is necessary, therefore, to understand the "error mechanism," in other words, to classify possible sources of error and to estimate the behavior of each error source separately.

The purpose of this paper is not to try to devise a new scheme. Rather, we will try to understand the mechanism which produces computational errors for existing schemes. First, we classify possible schemes into several classes. There exist a number of schemes which are mutually equivalent. It has been customary to classify the schemes according to their derivation techniques and many names have been given to them—finite difference methods, product integration methods, statistical methods, to name a few. However, as long as we are interested in the error mechanism of a given scheme, it is not essential to know how the scheme was originally devised. There exists an exact analytical formula (an integral equation of Abel type), and in principle the problem can be solved analytically. Hence, all the existing numerical schemes are approximations of the analytical solution in some sense or other. Therefore, we have only to know in what "sense" a given scheme is an approximation to the analytical solution.

All existing procedures divide the range of possible particle sizes into, say, n intervals and give a set of linear equations to compute. As the number n approaches infinity, the results of all the procedures must converge to the analytical one. However, the speed of convergence differs from procedure to procedure, and hence it provides a measure of precision inherent to each procedure. In this paper, we concentrate on this "computational" viewpoint. We do not consider other sources of error like the sampling error, which is also very important in practice. Of course, those who use this type of procedure are interested in the "overall" accuracy. However, if, for instance, we use a scheme very accurate in computation but obtain inaccurate results, we are sure that the error sources should be spotted elsewhere. Thus, in order to specify the error sources accurately, we must divide the overall procedure into several stages and analyze them separately.

2. Basic Equations of Stereological Estimation

Let us first consider the basic equations. They are well known and have been discussed again and again by many authors. Here, therefore, we do not give detailed and sophisticated arguments of derivation. Actually, the basic principle is very simple and is as follows. Suppose spheres of various sizes are distributed in the space, and let $F(R)$ be the radius distribution density, i.e., $F(R)\,dR$ is the number, per unit volume, of those spheres whose radii are between R and $R+dR$. Place a plane in the space. Then, we get a radius distribution density of cross sections, and let it be $f(r)$, i.e., $f(r)\,dr$ is the number, per unit area of the plane, of those cross sections whose radii are between r and $r+dr$. Suppose the spheres are distributed randomly

and homogeneously, and the cutting plane is infinite. Also assume that the distribution is sufficiently sparse so that overlapping of particles is negligible. The probability that a sphere of radius R is cut by the plane equals the probability that the center of that sphere falls within distance R from the plane. Since there are $F(R)\,dR$ such spheres per unit volume, that probability equals $2RF(R)\,dR$ per unit area of the plane. The probability that a sphere of radius R yields a cross section of radius between r and $r+dr$ on the condition that the sphere intersects the plane is $|2dx|/2R = |d(\sqrt{R^2-r^2})|/R = r\,dr/R\sqrt{R^2-r^2}$, as is shown in Fig. 1. Multiplying this by $2RF(R)\,dR$, and integrating it over possible values of R, we obtain

$$f(r) = 2r\int_r^{R_{\max}} \frac{F(R)\,dR}{\sqrt{R^2-r^2}}, \tag{2.1}$$

$R_{\max}$ being a maximum possible radius (cf. [2, 4–6, 8]). Of course, Eq. (2.1) is the "expected value" of $f(r)$. However, the assumption of random distribution and an infinite cutting plane assures the "law of large number," and hence it can be regarded as the actual distribution density. The same is true if we place a finite cutting plane at random independently a great number of times and take the average over these trials. In this case, the distribution should not necessarily be homogeneous. Equation (2.1) has a realistic meaning in this sense.

On the other hand, we are sometimes interested in observing not a cutting surface, but a thin layer of finite thickess, especially when optical microscopes are used. If we observe the distribution of cross sections by projection through the layer, we always overestimate them. This is kown as the "Holmes effect" or the "overprojection effect." If the center of a sphere is inside the layer, its exact radius is observed. If t is the thickness of the layer, there are $tF(r)\,dr$ such spheres of radius between r and $r+dr$ per unit area of the layer. If the center of a sphere is outside the layer, the cross section on the side of the particle center is observed, and the relation between

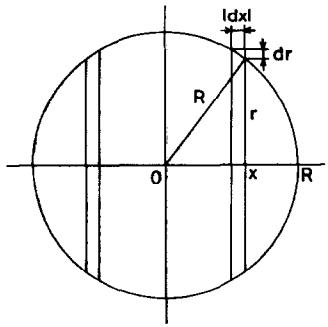

FIG. 1. The relationship between the position of a cutting plane and the radius of the cross section.

its size and the sphere size is the same as in the case of a cutting plane (cf. [18–20, 15, 16]). Hence, instead of Eq. (2.1) we obtain

$$f(r) = tF(r) + 2r \int_r^{R_{\max}} \frac{F(R)\, dR}{\sqrt{R^2 - r^2}}. \tag{2.2}$$

If we examine the above reasoning carefully, we can easily see that the same formulation also holds in the case of distributed circles on a plane cut by randomly placed line. In this case, $F(R)$ is interpreted as the distribution density of the radius per unit area and $f(r)$ the distribution density of the "half length" of the cross section per unit length of the probe line. It turns out that the formulation is also similar in the case of distributed circular disks in the space cut by a randomly placed plane. Let $F(R)$ be the distribution density of the radius of circular disks, i.e., $F(R)\, dR$ is the number, per unit volume, of those disks whose radii are between R and $R + dR$. Similarly, let $f(r)$ be the distribution density of the half length of the cross section on the cutting plane. Note that the intersection line of a given direction on a circular disk is uniformly distributed along the direction normal to it whatever the orientations of the circular disk and the cutting plane may be. Hence, we obtain, instead of Eq. (2.2), the following equation (cf. [2, 21]):

$$f(r) = tF(r) + \frac{\pi}{2} r \int_r^{R_{\max}} \frac{F(R)\, dR}{\sqrt{R^2 - r^2}}. \tag{2.3}$$

There are several other assumptions sometimes relevant. One is the effect of "resolution threshold," which means that cross sections smaller than a certain size are not visible. Another is the effect of the "capping angle," which means that spherical caps in a thin layer subtending angles smaller than a certain angle are not visible. If these assumptions are adopted, the range of r and R and the domain of integration in Eqs. (2.1) and (2.2) are modified. (See Cruz-Orive [15] for details.) However, as we will see later, the computational error mainly comes from the treatment of the singularity $R = r$ of the integration. Hence, the error mechanism does not change if we assume the resolution threshold or the capping angle. For this reason, we do not consider these effects here.

As has been seen, we consider, in this paper, distributions in the space and on the plane in terms of "per unit volume" and "per unit area", respectively. Namely, $\int_0^{R_{\max}} F(R)\, dR$ is the "number of particles per unit volume" and $\int_0^{R_{\max}} f(r)\, dr$ is the "number of cross sections per unit area," and we do not normalize them to 1. This is most natural when we are considering geometrical distributions in the space or on the plane, for our interest is in the "amount" of distribution, not the "probability." Moreover, we can obtain linear relations between observed data and quantities of interest. If we normalized them, the relations would become fractional. Since the expected value of a ratio is not equal to the ratio of expected values, the computational error would enter nonlinearly, and we could not easily understand its effect. For this reason, we treat our schemes in terms of Eq. (2.1) or (2.2). This is

one of the viewpoints different from other papers on this subject. In the following analyses, we assume that $F(R)$ (and hence $f(r)$) is smooth and bounded.

3. General Framework of Numerical Schemes

In actual numerical computations, the integration in Eq. (2.1) or (2.2) must be replaced by some kind of summation, and different ways of discrete approximation yield different forms of computational schemes. In any case, we divide the interval $[0, R_{\max}]$ into n subintervals and approximate the integration by some form of summation involving values at fixed n points. Thus, if we are to seek an accurate result, we must choose a large number n. However, it is sometimes not possible to make n large. Usually, we can observe only a finite number of cross sections in any experiment. The radius distribution density $f(r)$ must be estimated from the histogram, but, as is well known, the estimation is unreliable if the class intervals are too small. Thus, the choice of n is limited. This difficulty can be avoided if we consider, instead of the "density" $f(r)$, the (cumulative) "distribution function" $\phi(r)$, i.e., the number, per unit area, of cross sections of radii equal to or smaller than r. It is obtained without regard to class intervals.

In physics and engineering, chemical engineering in particular, distributions are treated in the cumulative sense, because measurement and analysis become easier. Various types of scales have been devised so that a given family of distribution functions may become straight lines when plotted according to them, and the values of involved parameters are immediately read out. As a matter of fact, the probability distribution is defined in terms of the distribution function in the theory of probability, because it alone is a "function" in the usual sense. (Densities are "distributions" in the sense of Schwartz [22, 23].) In order to obtain the density profile from a given distribution function, one must differentiate it. If a given distribution function is an experimentally observed one, there arises considerable difficulty in differentiation, and many techniques have been devised for that. Most of them employ "smoothing" of the observed distribution function by one way or another and differentiating the result either analytically or numerically. These include fitting by spline functions and application of low-pass digital filters. Recently, Anderssen and Jakeman [24] and Anderssen [25] proposed what they called "spectral differentiation," taking into account the power spectrum of the noise (see also Anderssen and Bloomfield [26, 27]).

What we should note here is that the process of differentiation provides a source of error different from the approximation of integration and that these two error sources are completely different in their behavior. Hence, they must be studied separately. Anderssen and Jakeman [24] and Anderssen [25] studied the overall accuracy and concluded that division of the interval $[0, R_{\max}]$ into too many subintervals for numerical computation would result in poor accuracy. However, as will be shown later, the accuracy improves as the number of division increases if we treat distribution functions. This forces us to conclude that the inaccuracy observed

by Anderssen *et al.* is due to the differentiation process. In this paper, we divide the process into three stages; (i) estimation of the distribution function of cross sections, i.e., the sampling technique; (ii) computation of the particle size distribution from the distribution of cross sections; and, if desired, (iii) conversion to the density, i.e., numerical differentiation. These three stages involve errors of different characters. In this paper, we concentrate on stage (ii) of numerical computation, assuming that a "good" distribution function of cross sections is obtained, say, by averaging a sufficiently large number of data or applying an appropriate smoothing technique.

Integration of Eq. (2.2) yields

$$\phi(r) = t\Phi(r) + 2\bar{R}N - 2\int_r^{R_{\max}} \sqrt{R^2 - r^2}\, d\Phi(R), \tag{3.1}$$

where $\Phi(R)$ is the distribution function of the sphere size, i.e., the number, per unit volume, of spheres of radii equal to or smaller than R. Here, N is the "numerical density," i.e., the number of spheres per unit volume and $\bar{R}$ is the "mean radius" given respectively by

$$N = \Phi(R_{\max}) = \int_0^{R_{\max}} F(R)\, dR, \tag{3.2}$$

$$\bar{R} = \frac{1}{N}\int_0^{R_{\max}} RF(R)\, dR. \tag{3.3}$$

In general, there are two types of approximations which convert this integral equation into discrete equations. One is to replace the integral of Eq. (3.1) by summation of some kind, resulting in a set of linear equations of the form

$$\phi(a_i) = \sum_{j=1}^{n} A_{ij}\Phi(a_j), \tag{3.4}$$

where a_i's are prescribed radius values and A_{ij} is a constant matrix. If its inverse matrix B_{ij} is computed beforehand, the radius distribution of particles is readily computed from the radius distribution of cross sections by

$$\Phi(a_i) = \sum_{j=1}^{n} B_{ij}\phi(a_j). \tag{3.5}$$

The other way is to invert Eq. (3.1) analytically to express $\Phi(R)$ in terms of $\phi(r)$ and then to replace the integral by summation of some kind, resulting in a formula of the form of Eq. (3.5). This is easily done when $t = 0$. In this paper, we call formulae of the former type "implicit formulae" and those of the latter type "explicit formulae."

4. Classification of Implicit Formulae

Consider implicit formulae first. Choose n points $0=a_0<a_1<\cdots<a_n=R_{\max}$ in the interval $[0, R_{\max}]$, and put $\phi_i=\phi(a_i)$, $\Phi_i=\Phi(a_i)$. According to Eq. (3.1), we obtain

$$\phi_i=t\Phi_i+2N\bar{R}-2\sum_{j=i+1}^{n}\int_{a_{j-1}}^{a_j}\sqrt{R^2-a_i^2}\,d\Phi(R), \tag{4.1}$$

for $i=0,\ldots, n$. If we adopt approximation

$$\begin{aligned}\int_{a_{j-1}}^{a_j}\sqrt{R^2-a_i^2}\,d\Phi(R)&\sim\sqrt{a_j^2-a_i^2}\int_{a_{j-1}}^{a_j}d\Phi(R)\\&=\sqrt{a_j^2-a_i^2}\,(\Phi_j-\Phi_{j-1}),\end{aligned} \tag{4.2}$$

we obtain a formula

$$\phi_i=t\Phi_i+2N\bar{R}+2\sum_{j=i}^{n}(\sqrt{a_{j+1}^2-a_i^2}-\sqrt{a_j^2-a_i^2})\,\Phi_j, \tag{4.3}$$

for $i=0,\ldots, n$. Throughout this paper, we adopt the following convention: If the argument of a square root is either negative or undefined, the square root assumes 0. If a summation does not have sense, like $\sum_{j=n}^{n-1}$, the sum also assumes 0.

If $t=0$, Eq. (4.3) coincides with one of the earliest formulae of this problem developed by Scheil [28], Schwartz [29] and Saltykov [30]. However, they all wrote the formula in terms of the frequency of each class to suit hand calculations. An expression in terms of frequencies is obtained by rewriting Eq. (4.3) in terms of $f_i=\phi_i-\phi_{i-1}$ and $F_i=\Phi_i-\Phi_{i-1}$. Then, the equation becomes

$$f_i=2\sum_{j=0}^{n}(\sqrt{a_j^2-a_{i-1}^2}-\sqrt{a_j^2-a_i^2})\,F_j,\qquad i=1,\ldots, n, \tag{4.4}$$

which is a familiar form. However, as was stated earlier, we prefer to use Eq. (4.3). Equation (4.3) is rewritten in the form of Eq. (3.4) by noting that $\phi_0=\Phi_0=0$ and hence $1N\bar{R}=-2\sum_{j=1}^{n}(\sqrt{a_{j+1}^2}-\sqrt{a_j^2})\,\Phi_j$. We call this Method 1. If we resolve the matrix A_{ij} into $t\delta_{ij}+A'_{ij}$, where δ_{ij} is the Kronecker delta, we obtain the following expression for A'_{ij}.

Method 1.

$$A'_{ij}=\begin{cases}2[-(a_{j+1}-a_j)+\sqrt{a_{j+1}^2-a_i^2}-\sqrt{a_j^2-a_i^2}], & j<n\\ 2[a_n-\sqrt{a_n^2-a_i^2}], & j=n.\end{cases} \tag{4.5}$$

In Eq. (4.2), the square root is evaluated at the right end of the interval

$[a_{j-1}, a_j]$. If, instead, we use the mean of the values at both ends, we can expect a more accurate approximation. Namely, if we use approximation

$$\int_{a_{j-1}}^{a_j} \sqrt{R^2-a_i^2}\, d\Phi(R) \sim \frac{1}{2}\left(\sqrt{a_{j-1}^2-a_i^2}+\sqrt{a_j^2-a_i^2}\right)\int_{a_{j-1}}^{a_j} d\Phi(R), \tag{4.6}$$

and determine $2\bar{N}R$ from $\phi_0=\Phi_0=0$, we obtain the following:

Method 2.

$$A'_{ij}=\begin{cases} -(a_{j+1}-a_{j-1})+\sqrt{a_{j+1}^2-a_i^2}-\sqrt{a_{j-1}^2-a_i^2}, & j<n \\ a_n+a_{n-1}-\sqrt{a_{n-1}^2-a_i^2}-\sqrt{a_n^2-a_i^2}, & j=n. \end{cases} \tag{4.7}$$

Instead of using the mean of the values at both ends, we can also use the value at the midpoint, i.e.,

$$\int_{a_{j-1}}^{a_j} \sqrt{R^2-a_i^2}\, d\Phi(R) \sim \sqrt{a_{j-1/2}^2-a_i^2}\int_{a_{j-1}}^{a_j} d\Phi(R), \tag{4.8}$$

where $a_{j-1/2}=(a_{j-1}+a_j)/2$. This scheme corresponds to the approaches of Wicksell [31], Goldsmith [18] and others. Again, $2\bar{N}R$ is determined from $\phi_0=\Phi_0=0$. The coefficient matrix becomes:

Method 3.

$$A'_{ij}=\begin{cases} 2[-(a_{j+1/2}-a_{j-1/2})+\sqrt{a_{j+1/2}^2-a_i^2}-\sqrt{a_{j-1/2}^2-a_i^2}], & j<n \\ 2[a_{n-1/2}-\sqrt{a_{n-1/2}^2-a_i^2}], & j=n, \end{cases} \tag{4.9}$$

where $a_{j+1/2}=(a_j+a_{j+1})/2$.

All the above methods approximate $\sqrt{R^2-a_i^2}$ by a constant in each subinterval. However, it has a singularity at $R=a_i$, and the derivatives of all ranks become infinity there. In other words, it is "strongly curved" in its neighborhood. Hence, replacing it by a constant in each subinterval is a very poor approximation. Since we are considering a smooth distribution, we can expect a higher precision approximation if we approximate $\Phi(R)$ by a linear function in each subinterval and execute the integration analytically. Namely, if we put $d\Phi(R)\sim(\Phi_j-\Phi_{j-1})\, dR/h_{j-1}$ in the interval $[a_{j-1}, a_j]$, where $h_j=a_{j+1}-a_j$, we obtain

$$\int_{a_{j-1}}^{a_j} \sqrt{R^2-a_i^2}\, d\Phi(R) \sim \frac{1}{h_{j-1}}(\Phi_j-\Phi_{j-1})\int_{a_{j-1}}^{a_j} \sqrt{R^2-a_i^2}\, dR, \tag{4.10}$$

and $\phi_0=\Phi_0=0$ determines $2\bar{N}R$. This leads to Method 4, which is mathematically equivalent to those described by Bach [32], Cruz-Orive [15] and others:

Method 4.

$$A'_{ij}=\begin{cases} -(a_{j+1}-a_{j-1}), & j<i\leqslant n \\ -(a_{i+1}-a_{i-1})+\dfrac{1}{h_i}(\alpha_{i,i+1}-\alpha_{ii}), & i=j<n \\ -(a_{j+1}-a_{j-1})+\dfrac{1}{h_j}\alpha_{i,j+1}-\dfrac{h_{j-1}+h_j}{h_{j-1}h_j}\alpha_{ij}+\dfrac{1}{h_{j-1}}\alpha_{i,j-1}, & i<j<n \\ a_{n-1}+a_n-\dfrac{1}{h_{n-1}}(\alpha_{in}-\alpha_{i,n-1}), & i<j=n \\ a_{n-1}+a_n, & i=j=n, \end{cases} \tag{4.11}$$

where we have put

$$\alpha_{ij}=a_j\sqrt{a_j^2-a_i^2}-a_i^2\log(a_j+\sqrt{a_j^2-a_i^2}). \tag{4.12}$$

(If one is uneasy about the dimensionality, replace $\log(\cdot)$ by $\log[(\cdot)/a]$, where a is a constant whose dimension is length. The result would be the same.)

5. Classification of Explicit Formulae

A small change of variables reduces Eq. (2.1) to an integral equation of Abel type, and it can be inverted analytically (cf. [2, 33]). The final form of $\Phi(R)$ becomes

$$\Phi(R)=N-\frac{1}{\pi}\int_R^{R_{\max}}\frac{d\phi(r)}{\sqrt{r^2-R^2}}. \tag{5.1}$$

Inversion of Eq. (2.2) for $t>0$ is also possible (cf. [18, 19]). However, since it does not turn out a simple form suitable for numerical computation, we consider here only Eq. (5.1). Choosing $0=a_0<a_1<\cdots<a_n=R_{\max}$, we have

$$\Phi_i=N-\frac{1}{\pi}\sum_{j=i+1}^{n}\int_{a_{j-1}}^{a_j}\frac{d\phi(r)}{\sqrt{r^2-a_i^2}}. \tag{5.2}$$

Here again, various kinds of approximation are just as possible as in the case of implicit formulae. Corresponding to Method 1 is approximation

$$\int_{a_{j-1}}^{a_j}\frac{d\phi(r)}{\sqrt{r^2-a_i^2}}\sim\frac{1}{\sqrt{a_j^2-a_i^2}}\int_{a_{j-1}}^{a_j}d\phi(r). \tag{5.3}$$

As before, N is determined from the condition $\Phi_0=0$, which yields the following:

Method 5.

$$B_{ij}=\begin{cases} -\dfrac{1}{\pi}\left(\dfrac{1}{a_{j+1}}-\dfrac{1}{a_j}\right), & j<i\leqslant n \\ \dfrac{1}{\pi}\left[-\left(\dfrac{1}{a_{i+1}}-\dfrac{1}{a_i}\right)+\dfrac{1}{\sqrt{a_{i+1}^2-a_i^2}}\right], & j=i<n \\ \dfrac{1}{\pi}\left[-\left(\dfrac{1}{a_{j+1}}-\dfrac{1}{a_i}\right)+\dfrac{1}{\sqrt{a_{j+1}^2-a_i^2}}-\dfrac{1}{\sqrt{a_j^2-a_i^2}}\right], & i<j<n \\ \dfrac{1}{\pi}\left[\dfrac{1}{a_n}-\dfrac{1}{\sqrt{a_n^2-a_i^2}}\right], & i<j=n \\ \dfrac{1}{\pi}\dfrac{1}{a_n}, & i=j=n. \end{cases} \tag{5.4}$$

Corresponding to Method 2 is approximation $1/\sqrt{r^2-a_i^2}\sim(1/\sqrt{a_{j-1}^2-a_i^2}+1/\sqrt{a_j^2-a_i^2})/2$. However, this cannot be applied, since $1/\sqrt{r^2-a_i^2}$ has a singularity at $r=a_i$ and hence becomes infinity there. This can be avoided by adopting, in correspondence with Method 3, approximation

$$\int_{a_{j-1}}^{a_j}\frac{d\phi(r)}{\sqrt{r^2-a_i^2}}\sim\frac{1}{\sqrt{a_{j-1/2}^2-a_i^2}}\int_{a_{j-1}}^{a_j}d\phi(r). \tag{5.5}$$

Again, N is determined from $\Phi_0=0$, which yields the following:

Method 6.

$$B_{ij}=\begin{cases} -\dfrac{1}{\pi}\left(\dfrac{1}{a_{j+1/2}}-\dfrac{1}{a_{j-1/2}}\right), & j<i\leqslant n \\ \dfrac{1}{\pi}\left[-\left(\dfrac{1}{a_{i+1/2}}-\dfrac{1}{a_{i-1/2}}\right)+\dfrac{1}{\sqrt{a_{i+1/2}^2-a_i^2}}\right], & j=i<n \\ \dfrac{1}{\pi}\left[-\left(\dfrac{1}{a_{j+1/2}}-\dfrac{1}{a_{j-1/2}}\right)+\dfrac{1}{\sqrt{a_{j+1/2}^2-a_i^2}}-\dfrac{1}{\sqrt{a_{j-1/2}^2-a_i^2}}\right], & i<j<n \\ \dfrac{1}{\pi}\left[\dfrac{1}{a_{n-1/2}}-\dfrac{1}{\sqrt{a_{n-1/2}^2-a_i^2}}\right], & i<j=n \\ \dfrac{1}{\pi}\dfrac{1}{a_{n-1/2}}, & i=j=n. \end{cases} \tag{5.6}$$

Corresponding to Method 4 is approximating the distribution function $\phi(r)$ by a linear function in each subinterval. Put $d\phi(r)\sim(\phi_j-\phi_{j-1})\,dr/h_{j-1}$ in the interval

$[a_{j-1}, a_j]$. This approximation was also used by Anderssen and Jakeman [24] and Anderssen [25]. In our case, we have

$$\int_{a_{j-1}}^{a_j} \frac{d\phi(r)}{\sqrt{r^2-a_i^2}} \sim \frac{1}{h_{j-1}} (\phi_j - \phi_{j-1}) \int_{a_{j-1}}^{a_j} \frac{dr}{\sqrt{r^2-a_i^2}}. \tag{5.7}$$

The numerical density N is determined from $\Phi_0 = 0$. Here, special care is necessary. The integral in the right-hand side of Eq. (5.7) does not converge for $j=1$ when $i=0$. However, the integral of Eq. (5.1) is convergent even when $R=0$, because $f(r)=O(r)$ near $r=0$ (cf. Eq. (2.1)). If we approximate $\phi(r)$ near $r=0$ by a quadratic function

$$\phi(r) \sim \left(\frac{r}{h_0}\right)^2 \phi_1, \tag{5.8}$$

we obtain the following:

Method 7.

$$B_{ij} = \begin{cases} \frac{1}{\pi}\left[\frac{2}{h_0} - \frac{1}{h_1}(\log a_2 - \log a_1) + \frac{1}{h_1}(\beta_{12} - \beta_{11})\right], & i=j=1 \\ \frac{1}{\pi}\left[\frac{2}{h_0} - \frac{1}{h_1}(\log a_2 - \log a_1)\right], & 1=j<i \\ \frac{1}{\pi}\left[-\left(\frac{1}{h_j}\log a_{j+1} - \frac{h_{j-1}+h_j}{h_{j-1}h_j}\log a_j + \frac{1}{h_{j-1}}\log a_{j-1}\right)\right], & 1<j<i \\ \frac{1}{\pi}\left[-\left(\frac{1}{h_i}\log a_{i+1} - \frac{h_{i-1}+h_i}{h_{i-1}h_i}\log a_i + \frac{1}{h_{i-1}}\log a_{i-1}\right)\right. & \\ \quad \left. + \frac{1}{h_i}(\beta_{i,i+1} - \beta_{ii})\right], & i=j<n \\ \frac{1}{\pi}\left[-\left(\frac{1}{h_j}\log a_{j+1} - \frac{h_{j-1}+h_j}{h_{j-1}h_j}\log a_j + \frac{1}{h_{j-1}}\log a_{j-1}\right)\right. & \\ \quad \left. + \frac{1}{h_j}\beta_{i,j+1} - \frac{h_{j-1}+h_j}{h_{j-1}h_j}\beta_{ij} + \frac{1}{h_{j-1}}\beta_{i,j-1}\right], & i<j<n \\ \frac{1}{\pi}\left[\frac{1}{h_{n-1}}(\log a_n - \log a_{n-1}) - \frac{1}{h_{n-1}}(\beta_{in} - \beta_{i,n-1})\right], & i<j=n \\ \frac{1}{\pi}\frac{1}{h_{n-1}}(\log a_n - \log a_{n-1}), & i=j=n, \end{cases} \tag{5.9}$$

where

$$\beta_{ij} = \log(a_j + \sqrt{a_j^2 - a_i^2}). \tag{5.10}$$

(Again, all $\log(\cdot)$ can be replaced by $\log[(\cdot)/a]$, where a is a constant whose dimension is length.)

6. The Condition Number of the Scheme

We have shown that all the computational schemes studied so far have, irrespective of the derivation techniques, the same form

$$\boldsymbol{\phi} = \mathbf{A}\boldsymbol{\Phi}, \qquad \boldsymbol{\Phi} = \mathbf{B}\boldsymbol{\phi}, \tag{6.1}$$

where $\boldsymbol{\phi}$ is the input vector whose ith component is ϕ_i, $\boldsymbol{\Phi}$ is the output vector whose ith component is Φ_i, and $\mathbf{B} = \mathbf{A}^{-1}$. Hence, once these matrices are computed, all the necessary computation for given data is just a matrix multiplication, and no difference exists in computation speed. Now, if the input vector $\boldsymbol{\phi}$ contains errors, the output vector $\boldsymbol{\Phi}$ has corresponding errors. It is very difficult to describe the amount of the output error in general terms because it depends on the form of the input data $\boldsymbol{\phi}$. Still, there is an input independent index which describes a "bound," not the exact amount, of errors. It is called the "condition number" of a matrix and is widely used as a rough index of error sensitivity in numerical analysis (cf. [34]). Let $\|\mathbf{x}\|_p$ denote the "L^p norm" of a vector $\mathbf{x}$ and $\|\mathbf{A}\|_p$ its "adjoint norm" of a matrix $\mathbf{A}$, i.e.,

$$\|\mathbf{A}\|_p = \sup_{\mathbf{x} \neq 0} \|\mathbf{A}\mathbf{x}\|_p / \|\mathbf{x}\|_p. \tag{6.2}$$

Hence, we always have $\|\mathbf{A}\mathbf{x}\|_p \leqslant \|\mathbf{A}\|_p \|\mathbf{x}\|_p$. Here, we consider only the case $p = 1, \infty$:

$$p = 1: \qquad \|\mathbf{x}\|_1 = \sum_{i=1}^{n} |x_i|, \qquad \|\mathbf{A}\|_1 = \max_j \sum_{i=1}^{n} |A_{ij}| \tag{6.3}$$

$$p = \infty: \qquad \|\mathbf{x}\|_\infty = \max_i |x_i|, \qquad \|\mathbf{A}\|_\infty = \max_i \sum_{j=1}^{n} |A_{ij}|. \tag{6.4}$$

In functional analysis, the L^2 norm is most frequently used because it is easy to treat analytically. For example, variations are expressed in linear forms. However, the L^1 and L^∞ norms are most convenient in numerical analysis, because they have simple intuitive meanings, i.e., the "maximum" and the "average," respectively, while no such simple meaning is associated with the L^2 norm. Moreover, the adjoint L^1 and L^∞ norms of Eqs. (6.3) and (6.4) are readily computed from a given matrix, whereas numerical computation of the adjoint L^2 norm involves eigenvalues, which are difficult to compute accurately, especially when the dimension is large.

Let $\boldsymbol{\phi}$ be an ideal input value and $\boldsymbol{\Phi}$ the associated ideal output value. If $\boldsymbol{\phi} + \Delta\boldsymbol{\phi}$ is the actual input, the output becomes $\boldsymbol{\Phi} + \Delta\boldsymbol{\Phi}$, where $\Delta\boldsymbol{\Phi} = \mathbf{B}\Delta\boldsymbol{\phi}$. Hence,

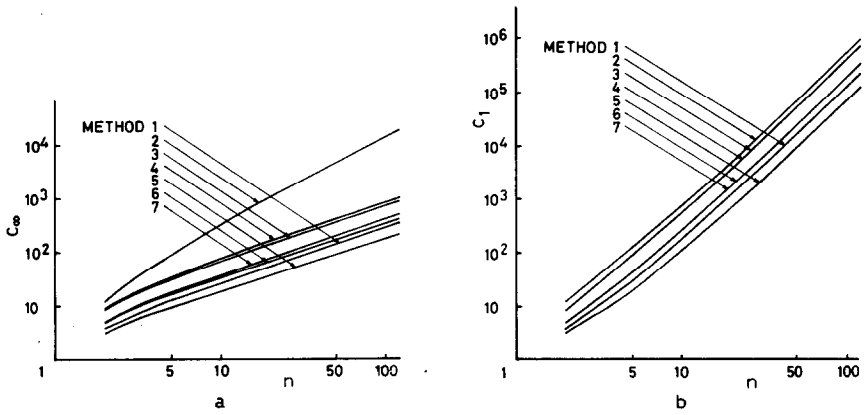

FIG. 2. Condition numbers of Methods 1–7; (a) c_∞ and (b) c_1

$\|\Delta\mathbf{\Phi}\|_p \leqslant \|\mathbf{B}\|_p \|\Delta\boldsymbol{\phi}\|_p$. Since $\|\boldsymbol{\phi}\|_p = \|\mathbf{A}\mathbf{\Phi}\|_p \leqslant \|\mathbf{A}\|_p \|\mathbf{\Phi}\|_p$, the relative errors of the input and the output are related by

$$\|\Delta\mathbf{\Phi}\|_p/\|\mathbf{\Phi}\|_p \leqslant c_p \|\Delta\boldsymbol{\phi}\|_p/\|\boldsymbol{\phi}\|_p, \tag{6.5}$$

where c_p is the condition number defined by

$$c_p = \|\mathbf{A}\|_p \|\mathbf{B}\|_p. \tag{6.6}$$

From this, we can conclude that if the condition number is very large, the scheme might be vulnerable to input errors. Figures 2a and b plot the condition numbers c_1 and c_∞ of Methods 1–7. As is seen, the condition number is approximately proportional to a certain power of n. As will be shown later, Methods 4 and 7 give a high order of accuracy, but their condition numbers are not small compared with other methods. In contrast, Methods 1 and 5, which turn out to be of poor accuracy, have smaller condition numbers than the rest. Thus, we must realize that methods of high accuracy may be very sensitive to input errors, though the amount of error depends on a particular form of the input data. The correlation between the condition numbers and actual errors is studied later for a synthetic model.

7. ERRORS OF THE IMPLICIT FORMULAE

We now consider the errors due to the discrete approximations we used and derive their asymptotic forms for large n. Since we are not necessarily demanding that the partition $0 = a_0 < a_1 < \cdots < a_n = R_{\max}$ be equidistant over the interval $[0, R_{\max}]$, we must first define the way in which the partition points are increased. Let $m(R)$ be the "partition point density" defined in such a way that $\lim_{n\to\infty}$ (the number of partition points in $[a, b]$)$/n = \int_a^b m(R)\,dR$. By definition,

$\int_0^{R_{\max}} m(R)\,dR = 1$. We consider only those partitions for which $m(R)$ is defined as a smooth positive function over $[0, R_{\max}]$. Furthermore, we assume that the partition for finite n is done in such a way that

$$h_i = 1/nm(a_i) + O(1/n^2), \tag{7.1}$$

where $h_i = a_{i+1} - a_i$ is the length of the ith subinterval.

Next, we define "residuals" $\Delta_1\phi_i$, $\Delta_0\phi$ and $\Delta\phi_i$ respectively by

$$-2\int_{a_i}^{R_{\max}} \sqrt{R^2 - r_i^2}\,d\Phi(R) = (\text{approximate form}) + \Delta_1\phi_i, \tag{7.2}$$

$$2\bar{R}N = (\text{approximation form}) + \Delta_0\phi, \tag{7.3}$$

$$\phi_i = (\text{approximate form}) + \Delta\phi_i. \tag{7.4}$$

Hence, $\Delta\phi_i = \Delta_0\phi + \Delta_1\phi_i$. Then, we obtain the following asymptotic forms:

Method 1.

$$\Delta_1\phi_i = \frac{1}{n}\int_{a_i}^{a_n} \frac{RF(R)}{\sqrt{R^2 - a_i^2}} \frac{dR}{m(R)} + O\left(\frac{1}{n\sqrt{n}}\right), \tag{7.5}$$

$$\Delta_0\phi = -\frac{1}{n}\int_0^{a_n} F(R)\frac{dR}{m(R)} + O\left(\frac{1}{n^2}\right), \tag{7.6}$$

$$\Delta\phi_i = \frac{1}{n}\left[\int_{a_i}^{a_n} \frac{RF(R)}{\sqrt{R^2 - a_i^2}} \frac{dR}{m(R)} - \int_0^{a_n} F(R)\frac{dR}{m(R)}\right] + O\left(\frac{1}{n\sqrt{n}}\right). \tag{7.7}$$

This result is obtained by expanding $\sqrt{R^2 - a_i^2}$ into a Taylor series at $R = a_j$ in each subinterval $[a_{j-1}, a_j]$ and by approximating the summation of the remainders by an integration. In doing it, special care is necessary to take into account the singularity at $R = a_i$. The integrals in these equations appear because the approximation (4.2) of Method 1 replaces $\sqrt{R^2 - a_i^2}$ in each subinterval by its value at the right end. The integral in Eq. (7.5) is convergent but is a singular integral. Hence the terms $O(1/n\sqrt{n})$ appears:

Method 2.

$$\Delta_1\phi_i = \frac{C_2\sqrt{a_i}\,F(a_i)}{m(a_i)^{3/2}n^{3/2}} + O\left(\frac{1}{n^2}\right), \tag{7.8}$$

$$\Delta_0\phi = \frac{1}{6n^2}\int_0^{a_n} F'(R)\frac{dR}{m(R)^2} + O\left(\frac{1}{n^3}\right), \tag{7.9}$$

$$\Delta\phi_i = \frac{C_2\sqrt{a_i}\,F(a_i)}{m(a_i)^{3/2}n^{3/2}} + O\left(\frac{1}{n^2}\right), \tag{7.10}$$

where C_2 is a constant. This result is obtained by applying the Lagrange interpolation formula in each subinterval $[a_{j-1}, a_j]$ and by considering the sum of the remainders. It turns out that the errors near the singular point $R=a_i$ are predominant over the rest. It is difficult to determine the exact value of the constant C_2. However, its approximation is obtained by replacing the sum by a divergent integral and by evaluating its asymptotic behavior, and we obtain $C_2 \sim -5\sqrt{2}/12$.

Method 3.

$$\Delta_1\phi_i = \frac{C_3\sqrt{a_i}\,F(a_i)}{m(a_i)^{3/2}n^{3/2}} + O\left(\frac{1}{n^2}\right), \tag{7.11}$$

$$\Delta_0\phi = \frac{1}{6n^2}\int_0^{a_n} F'(R)\frac{dR}{m(R)^2} + O\left(\frac{1}{n^3}\right), \tag{7.12}$$

$$\Delta\phi_i = \frac{C_3\sqrt{a_i}\,F(a_i)}{m(a_i)^{3/2}n^{3/2}} + O\left(\frac{1}{n^2}\right). \tag{7.13}$$

Thus, the form is the same as Method 2 except for the constant C_3. This result is also obtained by expanding $\sqrt{R^2-a_i^2}$ at $R=(a_{j-1}+a_j)/2$ in each subinterval $[a_{j-1}, a_j]$ and by considering the sum of the remainders. Again, it turns out that the errors near $R=a_i$ are predominant. An approximate value of C_3 is obtained similarly, and we have $C_3 \sim (48-31\sqrt{2})/24$.

Method 4.

$$\Delta_1\phi = -\frac{1}{6n^2}\int_{a_i}^{a_n} \frac{RF'(R)}{\sqrt{R^2-a_i^2}}\frac{dR}{m(R)^2} + O\left(\frac{1}{n^2\sqrt{n}}\right), \tag{7.14}$$

$$\Delta_0\phi = \frac{1}{6n^2}\int_0^{a_n} F'(R)\frac{dR}{m(R)^2} + O\left(\frac{1}{n^3}\right), \tag{7.15}$$

$$\Delta\phi_i = -\frac{1}{6n^2}\left[\int_{a_i}^{a_n} \frac{RF'(R)}{\sqrt{R^2-a_i^2}}\frac{dR}{m(R)^2} - \int_0^{a_n} F'(R)\frac{dR}{m(R)^2}\right] + O\left(\frac{1}{n^2\sqrt{n}}\right). \tag{7.16}$$

Since this method approximates $\Phi(R)$ by a piecewise linear function, the error term is estimated by applying the Lagrange interpolation formula to $\Phi(R)$ of Eq. (3.1) in each subinterval $[a_{j-1}, a_j]$ and by approximating the sum of the remainders by an integral. The integral in Eq. (7.14) is convergent but is a singular integral. Hence, the term $O(1/n^2\sqrt{n})$ appears.

Let $\Delta\boldsymbol{\phi}$ be a vector whose ith component is $\Delta\phi_i$. Since $\boldsymbol{\phi} = \mathbf{A}\boldsymbol{\Phi} + \Delta\boldsymbol{\phi}$, we have $\boldsymbol{\Phi} = \mathbf{B}\boldsymbol{\phi} - \mathbf{B}\Delta\boldsymbol{\phi}$. Hence, the error involved in the solution $\mathbf{B}\boldsymbol{\phi}$ is given by

$$\Delta\Phi_i = -\sum_{j=1}^{n} B_{ij}\Delta\phi_j. \tag{7.17}$$

Since $B_{ij} = O(1/n)$, the order of error is about the same as that of $\Delta\phi$, and we can roughly say that the order of error is $1/n$ for Method 1, $1/n\sqrt{n}$ for both Method 2 and Method 3, and $1/n^2$ for Method 4. However, the amount of the error is also affected by the form of $\Phi(R)$, as has been shown.

8. Errors of the Explicit Formulae

Define the error terms $\Delta_1\Phi_i$, $\Delta_0\Phi$ and $\Delta\Phi_i$ by

$$-\frac{1}{\pi}\int_{a_i}^{a_n}\frac{d\Phi(r)}{\sqrt{r^2-a_i^2}} = (\text{approximate form}) + \Delta_1\Phi_i, \tag{8.1}$$

$$N = (\text{approximation form}) + \Delta_0\Phi, \tag{8.2}$$

$$\Phi_i = (\text{approximate form}) + \Delta\Phi_i, \tag{8.3}$$

respectively. Hence $\Delta\Phi_i = \Delta_1\Phi_i + \Delta_0\Phi$.

Method 5.

$$\Delta_1\Phi_i = \frac{C_5 f(a_i)}{\sqrt{a_i}\sqrt{m(a_i)}\sqrt{n}} + O\left(\frac{1}{n}\right), \tag{8.4}$$

$$\Delta_0\Phi = \frac{C_5' f'(0)}{m(0)}\frac{\log n}{n} + O\left(\frac{1}{n}\right), \tag{8.5}$$

$$\Delta\Phi_i = \frac{C_5 f(a_i)}{\sqrt{a_i}\sqrt{m(a_i)}\sqrt{n}} + \frac{C_5' f'(0)}{m(0)}\frac{\log n}{n} + O\left(\frac{1}{n}\right). \tag{8.6}$$

This result is obtained by expanding $1/\sqrt{r^2-a^2}$ into a Taylor series at $r = a_j$ in each subinterval $[a_{j-1}, a_j]$ and by considering the sum of the remainders. Since both Eqs. (8.5) and (8.6) have the term $O(1/n)$, we obtain Eq. (8.6). It follows that the errors near $r = 0$ and $r = a_i$ are predominant, though the approximation (5.3) of Method 5 replaces $1/\sqrt{r^2-a_i^2}$ in each subinterval by its value at the right end. Approximate values of C_5 and C_5' are obtained as before, and we have $C_5 \sim -3\sqrt{2}/4\pi$ and $C_5' \sim 1/2\pi$.

Method 6.

$$\Delta_1\Phi_i = \frac{C_6 f(a_i)}{\sqrt{a_i}\sqrt{m(a_i)}\sqrt{n}} + O\left(\frac{1}{n\sqrt{n}}\right), \tag{8.7}$$

$$\Delta_0\Phi = \frac{C_6' f''(0)}{m(0)^2}\frac{\log n}{n^2} + O\left(\frac{1}{n^2}\right), \tag{8.8}$$

$$\Delta\Phi_i = \frac{C_6 f(a_i)}{\sqrt{a_i}\sqrt{m(a_i)}\sqrt{n}} + O\left(\frac{1}{n\sqrt{n}}\right). \tag{8.9}$$

This result is obtained by expanding $1/\sqrt{r^2-a_i^2}$ at $r=(a_{j-1}+a_j)/2$ in each subinterval $[a_{j-1}, a_j]$ and by considering the sum of the remainders. It turns out that the errors near $r=a_i$ are predominant. Approximate values of C_6 and C_6' are obtained as before, and we have $C_6 \sim -(97\sqrt{2}-96)/96\pi$ and $C_6' \sim -1/24\pi$.

Method 7.

$$\Delta_1 \Phi_i = \frac{C_7 f'(a_i)}{\sqrt{a_i} m(a_i)^{3/2} n^{3/2}} + O\left(\frac{1}{n^2}\right), \tag{8.10}$$

$$\Delta_0 \Phi = \frac{C_7' f'(0)}{m(0)\, n} + O\left(\frac{1}{n^2}\right), \tag{8.11}$$

$$\Delta \Phi_i = \frac{C_7' f'(0)}{m(0) n} + \frac{C_7 f'(a_i)}{\sqrt{a_i} m(a_i)^{3/2} n^{3/2}} + O\left(\frac{1}{n^2}\right). \tag{8.12}$$

This result is obtained by applying the Lagrange interpolation formula to $\phi(r)$ in each subinterval $[a_{j-1}, a_j]$ and by considering the sum of the remainders. It turns out that $\Delta_1 \Phi_i$ is dominated by the errors near $r=a_i$ and $\Delta_0 \Phi$ by the errors near $r=0$. Since both Eqs. (8.10) and (8.11) have the term $O(1/n^2)$, we obtain Eq. (8.12). Approximate values of the C_7 and C_7' are obtained as before, and we have $C_7 \sim 5\sqrt{2}/24\pi$ and $C_7' \sim -1/12\pi$.

Thus, the order of error is lower for the explicit formulae than for the corresponding implicit formulae. This is because the degree of singularity of the explicit integral equation (5.1) is higher than that of the corresponding implicit equation (3.1) and hence the same scheme of approximation yields larger errors for the explicit formulae. Of course, the amount of the error also depends on the particular form of $\phi(r)$.

9. Numerical Examples and Concluding Remarks

As an example, let $R_{\max}$ be 1 and the numerical denity N be 1, and consider the distribution density

$$F(R) = 30R^2(R-1)^2. \tag{9.1}$$

The mean radius $\bar{R}$ is 1/2. The distribution function is given by

$$\Phi(R) = R^3(6R^2 - 15R + 10). \tag{9.2}$$

Consider the case of $t=0$. The corresponding distribution function of cross sections is determined by Eq. (3.1) and is given by

$$\phi(r) = 1 - \frac{1}{4}(49r^4 - 8r^2 + 4)\sqrt{1-r^2} + \frac{15}{4} r^4 (r^2+2) \log \frac{1+\sqrt{1-r^2}}{r}. \tag{9.3}$$

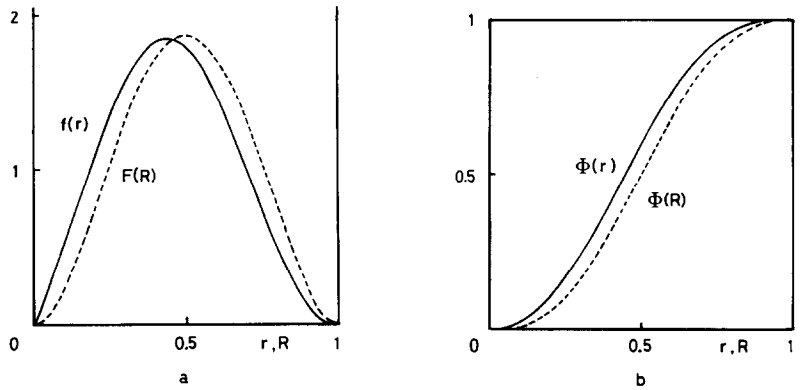

FIG. 3. A sphere size distribution and the corresponding size distribution of cross sections; (a) distribution densities and (b) distribution functions.

Its distribution density is given by

$$f(r) = -\frac{5}{2} r(23r^2 - 2)\sqrt{1-r^2} + \frac{15}{2} r^3(3r^2 + 4) \log \frac{1+\sqrt{1-r^2}}{r}. \tag{9.4}$$

Equations (9.1)–(9.4) are plotted in Fig. 3. Let Eq. (9.3) be the input to reconstruct Eq. (9.2). For simplicity, we adopt equipartition of radius ($a_i = i/n$). Hence, $m(R) = 1$. We adopt $\|\Delta\Phi\|_\infty = \max_i |\Delta\Phi_i|$ (maximum error) and $\|\Delta\Phi\|_1/n = \sum_{i=1}^n |\Delta\Phi_i|/n$ (average error) as measures of the error magnitude. They are plotted in Fig. 4, which shows that the orders of convergence are in good accordance with our estimates. Fig. 5 shows the error distributions (solid) for Methods 5–7 with $n = 30$, 60, 120 and their estimates (dashed), i.e., Eqs. (8.6), (8.9) and (8.12) with terms of $O(\cdot)$ neglected. As is seen, our estimate is fairly good. Note that the error is zero at $R = 0$ because we used the relation $\Phi_0 = 0$ in constructing the schemes. We could easily guess that primitive schemes like Methods 1 and 5 may turn out poor

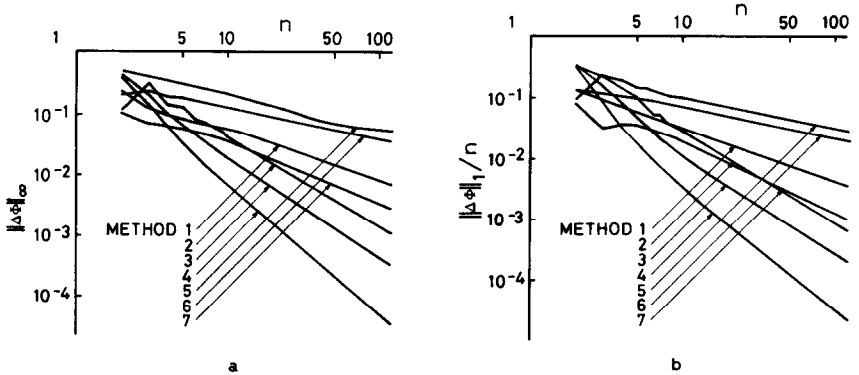

FIG. 4. Errors of Methods 1–7 for the distribution of Fig. 3; (a) $\|\Delta\Phi\|_\infty$ and (b) $\|\Delta\Phi\|_1/n$.

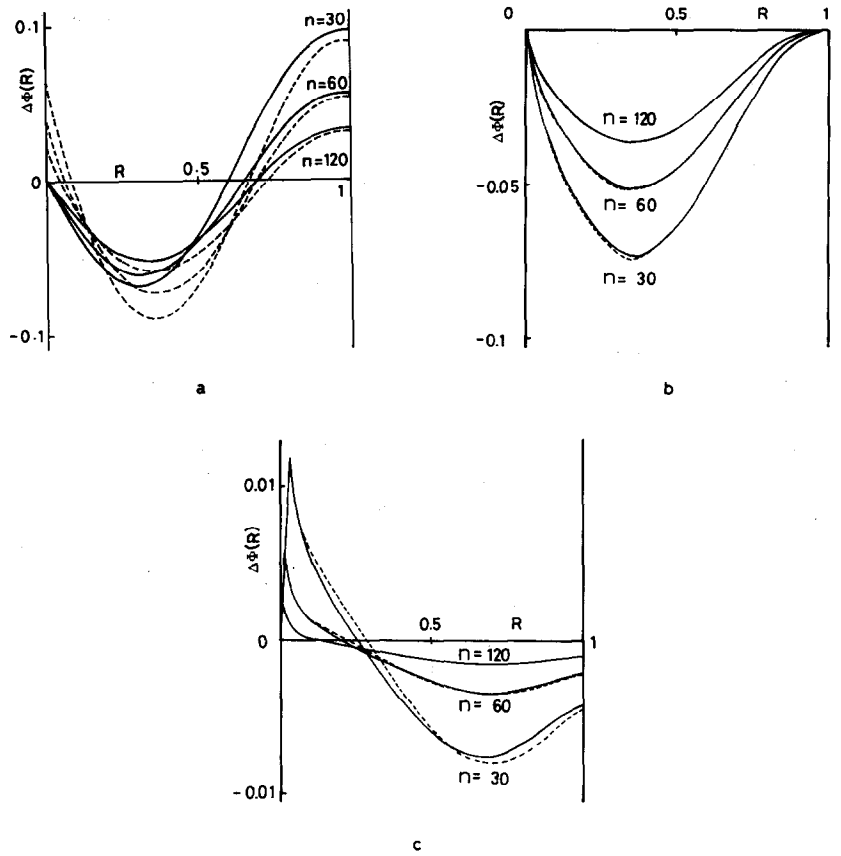

FIG. 5. Distributions of actual errors (solid) and estimations (dashed) for the distribution of Fig. 3 with $n = 30, 60, 120$; (a) Method 5, (b) Method 6 and (c) Method 7.

accuracy, but we cannot guess to what extent they are poor and to what extent elaborate ones like Methods 4 and 7 are superior unless the error behavior is analyzed.

As is expected, implicit formulae, especially Method 4, exhibit high accuracy for this example. Therefore, they are expected to be of practical value, though the conclusion is not decisive and we must be careful about the possible input error sensitivity. This may appear to be in contradiction to the claim of Anderssen and Jakeman [20] and Anderssen [21], who reject implicit formulae. The basic difference between their approach and ours lies in the fact that theirs involves differentiation processes, i.e., the use of densities, and overall accuracy is examined with the input noise taken into account, while ours concentrates on the computational aspect in terms of distribution functions.

Next, consider the input error sensitivity for this input. Adopting a simple model, we suppose that the particle distribution is subject to a stochastic Poisson process.

Since all the quantities involved are linear in observed number of particles, the variance of an input value is proportional to its expectation value. Hence, if ϕ_i is interpreted as the expactation value, the variance is $k\phi_i$, where k is a constant depending on the sampling method, e.g., the area of the probe plane and the number of trials over which the average is taken. Suppose, for simplicity, ϕ_i is obtained by independent trials for each i. (This is rather an artificial hypothesis, for ϕ_i's are always correlated.) The variance of Φ_i is $k\sum_{j=1}^{n} B_{ij}^2\phi_j$ and its standard deviation is its square root. Put $\sigma_i = \sqrt{\phi_i}$ and $\Sigma_i = \sqrt{\sum_{j=1}^{n} B_{ij}^2\phi_j}$. Figure 6 plots $\|\Sigma\|_\infty/\|\sigma\|_\infty$ and $\|\Sigma\|_1/\|\sigma\|_1$. We can see a clear correlation between this result and the condition numbers (cf. Fig. 2).

As we have seen, implicit formulae are in general expected to be computationally superior to explicit formulae. However, aside from the fact that no matrix inversion is necessary, explicit formulae have the advantage that the asymptotic error can be estimated in terms of the observed size distribution of cross sections. In other words, though the error may be larger, we can estimate its behavior. The fact is utilized for various purposes. For example, we can make a correction by using the asymptotic estimate. The error behavior of Method 7 after this correction is shown in Fig. 7, where $f'(0)$ and $f'(a_i)$ in Eq. (8.12) are estimated by the four and three point difference formulae, respectively, over $\phi_0, \phi_1, \ldots, \phi_n$. This may seem in contradiction to our previous statement that accurate numerical differentiation is difficult, but here differentiation need not be accurate. Even if errors of order $1/n$ for $f'(0)$ and of order $1/\sqrt{n}$ for $f'(a_i)$ are involved, they are absorbed in the term $O(1/n^2)$ of Eq. (8.12). In our case, the error order of differentiation is $1/n^2$ for both $f'(0)$ and $f'(a_i)$ and small errors need not be worried about. We can see that the correction of Method 7 is about as good as Method 4.

Another thing we can make use of out of this study is the Richardson-type "acceleration." Consider the correction of Method 7, and put its output to be

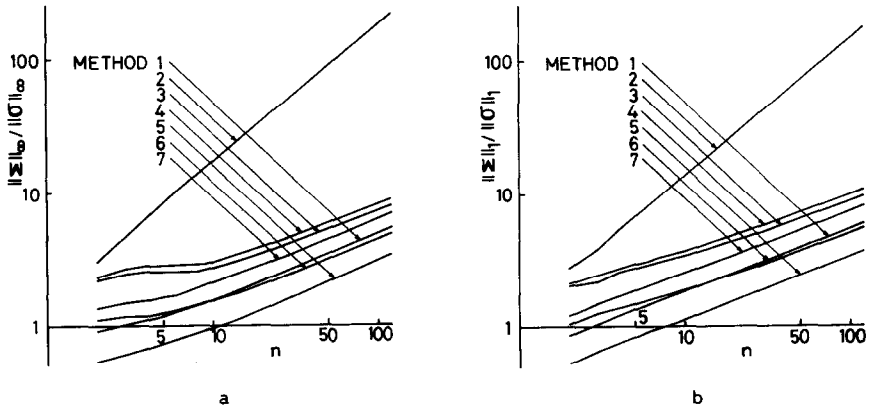

FIG. 6. Input error sensitivity for the input of Fig. 3 based on a Poisson model; (a) $\|\Sigma\|_\infty/\|\sigma\|_\infty$ and (b) $\|\Sigma\|_1/\|\sigma\|_1$.

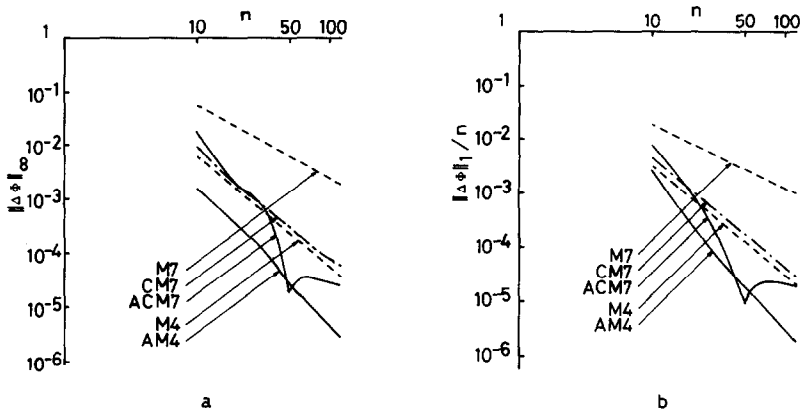

FIG. 7. Errors of Method 4 (M4), acceleration of Method 4 (AM4), Method 7 (M7), correction of Method 7 (CM7) and acceleration of corrected Method 7 (ACM7); (a) $\|\Delta\Phi\|_\infty$ and (b) $\|\Delta\Phi\|_1/n$.

$\Phi_n(a_i)$ when the number of partition is n. Since the order of the remaining error is about $1/n^2$, we can improve accuracy by

$$\tilde{\Phi}_n(R) = \frac{1}{3}(4\Phi_n(R) - \Phi_{n/2}(R)) \tag{9.5}$$

for $R = a_i$ with even i when n is even. The same idea applies to Method 4 as well, since it has also errors of order about $1/n^2$. Figure 7 shows the error behavior after the acceleration, indicating a considerable improvement. (The norms are taken only for even-indexed components.) Thus, our study of the error mechanism not only makes us explain observed error behaviors but also gives us various techniques to improve accuracy. It is true that, in practice, computational accuracy is not the only concern. Also important is the sampling error, which seriously affects the estimation even if we have a "perfect scheme" which exactly converts the basic equation (e.g., see Watson [35]). However, if an accurate scheme is available, it can accurately single out other error sources. Since integral equations of Abel type are frequently encountered in various problems in physics, our analysis is also applicable to many problems other than stereology where similar numerical computation is involved.

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