ACTA STEREOL 1983; 2/1· 39-45
PAPER

# A COMPARATIVE STUDY OF METHODS OF UNFOLDING SIZE DISTRIBUTIONS

Alan G. Flook

Unilever Research, Colworth Laboratory,
Colworth House,
Sharnbrook, Bedfordshire, Gt. Britain

## ABSTRACT

Practical experiments had indicated that errors obtained when unfolding particle size distributions from chord data were much greater than might be expected from reading the current stereological literature. Idealised experimental procedures were modelled in a computer program. The results confirm that, even with 'error-free measurements', the distortions in the frequency distributions produced would rule-out this method for most practical purposes.

A similar computer simulation was used to compare the results with those obtained from the Schwartz-Saltykov method.

## INTRODUCTION

In the fields of biological and materials science it is often necessary to determine the size distribution of 'particles' embedded in an opaque matrix where measurements can only be made on the profiles obtained by sectioning the material. Many analytical procedures have been developed to reconstruct the size distributions of spherical particles from distributions of chord, diameter or area measurements of the profiles revealed by these thin sections. It is often unnecessary to know how well these unfolded distributions represent the true size distribution since the results are used for comparison with others obtained by the same procedure. We have recently needed to compare size distributions of different types of material where their diverse physical nature has necessitated the use of a variety of sampling and measuring techniques. Early results indicated a need for a better understanding of the analytical procedures used. The two methods chosen for the initial study were the chord method due to Spektor and the diameter method due to Schwartz and Saltykov.

## THEORY

The theoretical basis of each technique is well documented in the literature (See Underwood, 1968 for example) but it is not immediately clear, from the way in which the equations are derived, why the chord method should give such a simple procedure for analysis compared with the diameter method. For this reason an alternative derivation of the Spektor equation was sought. This derivation follows a similar line of reasoning to that used in the Schwartz-Saltykov method. The distribution of chord sizes is assumed to be continuous whereas the distribution of the particle sizes is considered to be discrete.

Let $n$ be the number of size classes,

$\Delta$ the interval between classes,

$N_V(j)$ the number density of spheres of diameter $j\Delta$,

$N_L(i,j)$ the intercept number density of intercepts of length between $(i-1)\Delta$ and $i\Delta$ originating from spheres of diameter $j\Delta$,

and $N_L(i)$ the intercept number density of all intercepts of length between $(i-1)\Delta$ and $i\Delta$.

Consider a sample volume formed by a cube with sides of unit length. From simple geometric considerations the probability of a sphere of diameter $j\Delta$ having an intercept of length $l \geq i\Delta$ is given by:-

$$\frac{\pi\Delta^2}{4}(j^2 - i^2) \qquad (1)$$

For the same sphere the probability of an intercept of length between $(i-1)\Delta$ and $i\Delta$ is:-

$$\frac{\pi\Delta^2}{4}\left((j^2-i^2)-(j^2-(i-1)^2)\right) = \frac{\pi\Delta^2}{4}(2i-1) \quad (2)$$

Therefore $N_L(i,j) = \frac{\pi\Delta^2}{4}(2i-1)N_V(j)$ (3)

It should be noted that this expression is independent of the sphere diameter $j\Delta$. In other words, the probability of a sphere giving an intercept of length lying between any two limits is independent of the size of the sphere (provided, of course that $j \geq i$).

The total number of intercepts between $(i-1)\Delta$ and $i\Delta$ is given by:-

$$N_L(i) = \sum_{j=i}^{n} N_V(i,j) = \frac{1}{\alpha_i}\sum_{j=i}^{n} N_V(j)$$

or $$\alpha_i N_L(i) = \sum_{j=i}^{n} N_V(j) \quad (4)$$

where $$\alpha_i = \frac{4}{\pi\Delta^2(2i-1)}$$

By subtracting the intercept number densities of two adjacent classes and rearranging we get Spektor's equation

$$N_V(i) = \frac{4}{\pi\Delta^2}\left(\frac{N_L(i)}{(2i-1)} - \frac{N_L(i+1)}{(2i+1)}\right) \quad (5)$$

## EXPERIMENTAL

Experimental measurements must always be subject to error and thus may violate many of the assumptions made in the analysis. For example the theory assumes that the sample is obtained from an infinitely thin section through truly spherical particles, and that the method of measurement has infinite resolution so as to be able to measure the smallest intersecting chord or diameter. The magnitude of these experimental errors will depend on the type of sample and the experimental conditions used and this will cause difficulties in comparing the efficiency of the methods. To eliminate these sources of error entirely, a computer program was written to simulate the experimental sampling procedure. The program accepts any distribution of spheres and places them at random in a three dimensional matrix. Each sphere is tested for intersection with a fixed plane. If the plane is intersected the diameter of the circle of intersection is recorded and a further test is made to determine whether this section intersects a fixed line in the same plane and, if so, calculate and record the length of the intersecting chord. In this way simultaneous distributions of chord and section data are found for a known distribution of spheres.

The test 'sample' for this first study was a series of spheres forming a discrete distribution with class frequencies chosen to approximate a normal distribution having a mean diameter of 8 units and a standard deviation of 1.77 units. Each 'experiment' was terminated after approximately 1000 chord or area intersections were recorded. The 'experiment' was repeated 25 times for each method.

RESULTS

The results are shown in figure 1. All distribution statistics were calculated by setting negative frequencies to zero. Table 1 shows the results after unfolding the pooled data sets, i.e. 26,458 chord and 24,909 diameter measurements.

TABLE 1

| J | Expected % frequency | Spektor diameter method | Schwartz-Saltykov method |
|---|---|---|---|
| 1 | .01 | 12.5 | -0.5 |
| 2 | .07 | -3.5 | 0.7 |
| 3 | .42 | -1.1 | 1.8 |
| 4 | 1.74 | 3.8 | 2.0 |
| 5 | 5.35 | 4.7 | 6.0 |
| 6 | 11.90 | 8.2 | 10.3 |
| 7 | 19.23 | 17.6 | 19.3 |
| 8 | 22.56 | 19.3 | 21.5 |
| 9 | 19.23 | 17.0 | 18.9 |
| 10 | 11.90 | 10.5 | 12.5 |
| 11 | 5.35 | 4.6 | 4.8 |
| 12 | 1.74 | 1.4 | 1.6 |
| 13 | 0.42 | 0.4 | 0.5 |
| 14 | 0.07 | 0.0 | 0.1 |
| 15 | 0.01 | 0.0 | 0.0 |
| mean | 8.0 | 7.09 | 7.89 |
| std. dev. | 1.77 | 2.87 | 1.93 |

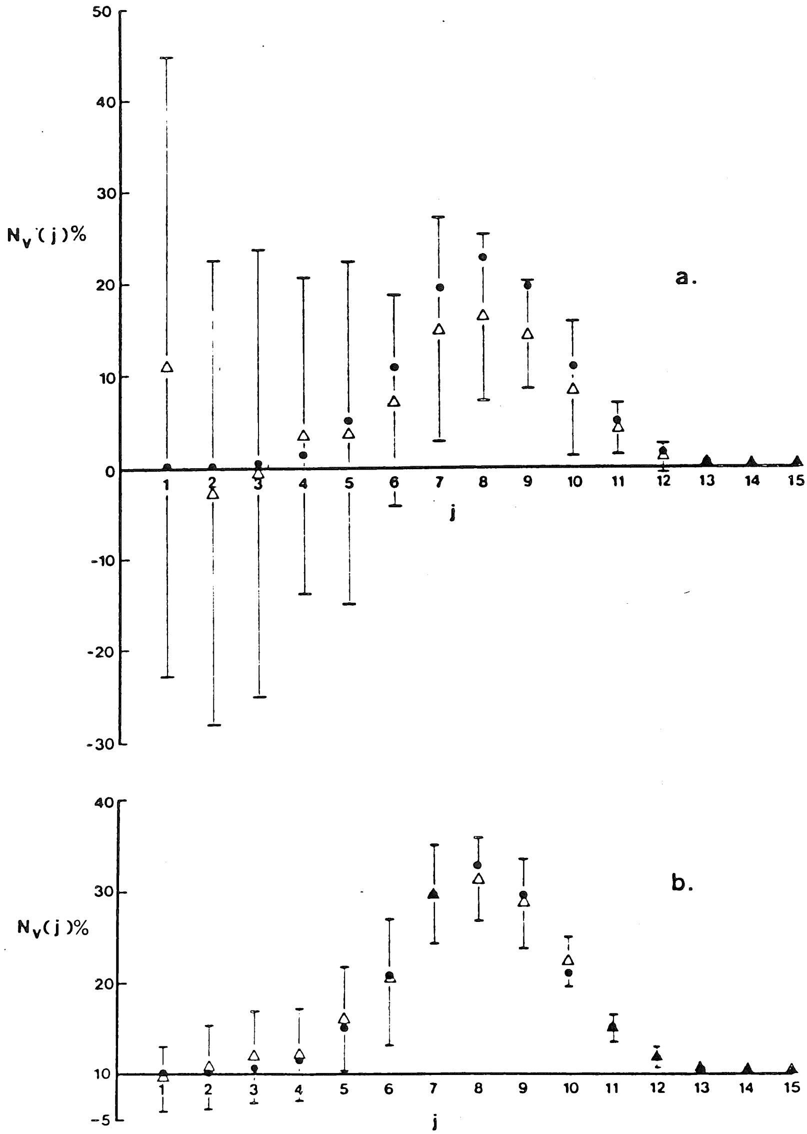


Figure 1. Plots showing the scatter of the size distributions resulting from a) the Spektor and b) the Schwartz-Saltykov methods. The solid circles represent the expected frequencies, the triangles represent the mean of 25 separate 'experiments' and the vertical bars indicate the 95% confidence intervals.

## CONCLUSIONS

The simplicity of the Spektor equation is a consequence of the remarkable property of spheres shown in equation 3 which, although making calculation easier, also implies that random chord sampling is an inefficient method prone to inaccuracy.

The diameter method gave results in closer agreement with the original distribution than the chord method. It must be concluded from this study that the accuracy of the chord method is much more sensitive to errors due to under-sampling than the diameter method which should be the preferred method of analysis.

Although the results from the pooled data show that the Spektor method will converge towards the expected distribution, the quantity of experimental data required would rule-out its use for most practical purposes.

## REFERENCES

Underwood, EE. In: Quantitative Microscopy, edited by DeHoff RT and Rhines FN. McGraw-Hill Book Company, New York. 1968; 162-168 and 181-188.