

Estimates of Parameters of Grain-Size Distribution from Weight Frequencies¹

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When grains of a sediment sample are separated by sieving into a number of size classes, the weight of the grains belonging to a particular size-class is called the weight frequency of that class. That the weight frequencies cannot be used as simple frequencies for the calculation of the mean and standard deviation of size of grains is well known. A method is developed in this paper for estimating these two as well as a third parameter, named shape parameter, by minimizing a quadratic form that arises naturally as an analogue of the χ^2 statistic. Two fully worked out numerical examples, with simulated data, are presented to illustrate the method. A computer program in FORTRAN language is also appended. Comparative study shows that the quicker conventional method used by geologists may produce reasonably good estimates of standard deviation when the sample size is large, but the estimates of mean may show large deviations.

KEY WORDS: weight frequency, shape, grain size, computer application.

INTRODUCTION

The method commonly followed by geologists for obtaining frequency distributions of grain sizes of sediment samples is to separate the grains into a number of size classes using sieves of different sizes and to obtain the bulk weight of the particles retained on each sieve separately. In such a method of analysis, the total weight of the grains in any particular sieve class is called the weight frequency of that class (Krumbein; Krumbein and Pettijohn, 1938). Counting the number of grains within each sieve class, being extremely tedious, is always avoided. The problem, therefore, is to determine the mean and the standard deviation of the size of the grains when the number of grains in each sieve class is unknown.

It has been customary for geologists to treat weight frequency as number frequency and to determine the mean, standard deviation, skewness, and kurtosis of the distribution in the usual way, from the various percentile values obtained from graph plots (e.g., the Folk and Ward, 1957, method often used by

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geologists). McCammon (1962) and Folk (1966) have discussed the relative efficiencies of the various percentile measures commonly used by geologists for this purpose. In a recent paper Swan, Clague, and Luternauer (1978) examined, through a simulation approach, the effectiveness of Folk and Ward graphic measures as descriptors of grain-size distributions.

That the weight frequencies cannot be used as simple frequencies for the calculation of the mean and the standard deviation of the size of grains has been pointed out by a number of authors (see Sahu, 1964 for a review of the early work). Sahu (1965) gave a method for estimating these two parameters, assuming that the weight W of a grain is strictly proportional to the cube of its size S ; $W \propto S^3$ and that the distribution of size is log-normal.

It should be noted, however, that the size of a grain as determined by sieving is not a simple geometric characteristic of a grain, except when the grain has a regular geometric shape, such as a perfect cube or a sphere. Again, the grains belonging to a particular size class may differ among themselves in density as well as in shape. It is therefore more realistic to assume a statistical rather than a deterministic relationship between the weights and sizes of grains.

Both from theoretical and empirical considerations the log-normal distribution has long been accepted as a standard model for the size distribution of homogeneous samples of grains. In this paper, it is assumed that the joint distribution of the size S and weight W of grains is bivariate log-normal. It follows as a consequence that the average weight \bar{W} of grains of a fixed size S is proportional to S^ν ; $\bar{W} \propto S^\nu$ which is a statistical relationship more realistic than the deterministic relationship $W \propto S^3$ assumed by Sahu. Here ν is the coefficient of linear regression of $\log W$ on $\log S$. For perfectly spherical grains of uniform density $\nu = 3$. If $\nu < 3$, it implies that the average weight of a grain is less than that of a spherical grain of the same size, and if $\nu > 3$ it is the other way around. The parameter ν is thus a general indicator of the shape of grains when they are of uniform density. We call ν the shape parameter.

It should be noted that the simple model used here assumes the shape parameter ν to be constant; this would be unrealistic in situations where ν might vary considerably with the size or density of grains.

Starting from the assumed bivariate log-normality of the joint distribution of the size and weight of grain, the asymptotic joint distribution of the weight frequencies in given size classes is worked out in this paper. This asymptotic distribution turns out to be multivariate normal and an explicit expression is obtained for the quadratic form associated with it. Apart from a multiplicative factor, this quadratic form is analogous to the χ^2 statistic and involves the mean μ and the standard deviation σ of the natural logarithm (base e) of the size of grains and the shape parameter ν . These three parameters are estimated by minimizing the quadratic form. The minimization is carried out by an iterative procedure which involves heavy computations. Numerical examples worked out on a

computer, together with programs written in FORTRAN IV language, are presented in this paper.

The number of grains in the sediment sample, and the mean and the standard deviation of the weight of grains are nuisance parameters which cannot be estimated by the proposed method. Nor is it possible to assess the sampling errors of the estimates since the sample size (the total number of grains, n) is unknown.

THE STATISTICAL SET-UP

We use the expression "sieve of dimension C " to describe a sieve with square holes in which the side of each square is of length C . In the present context, the size of a grain is the dimension of the finest sieve through which it can just pass. It is assumed that the grains that pass through a sieve of dimension C are all of size less than or equal to C .

We consider a set-up in which n grains of total weight w are separated into m size-classes, using $(m - 1)$ sieves of dimensions C_1, C_2, \dots, C_{m-1} where $C_1 < C_2 < \dots < C_{m-1}$. Let w_1 denote the total weight of the finest grains that pass through the first sieve of dimension C_1 ; w_m the weight of the coarsest grains that fail to pass through the last sieve of dimension C_{m-1} ; and for $j = 2, 3, \dots, (m - 1)$ let w_j denote the weight of the grains that pass through the j th sieve of dimension C_j but not through the $(j - 1)$ th sieve of dimension C_{j-1} . We thus have $w = w_1 + w_2 + \dots + w_m$ and the relative weight frequency of the j th size class is calculated as

$$p_j = w_j/w, \quad \text{for } j = 1, \dots, m \quad (1)$$

Inference regarding the parameters of particle-size distribution will be based on these relative weight frequencies and we work out their asymptotic joint distribution, as n tends to infinity, starting from certain assumptions regarding the joint distribution of particle size and weight. We note here that $p_1 + \dots + p_m \equiv 1$ and consequently their joint distribution is singular. For purposes of statistical inference any one of the m relative weight frequencies can be omitted without any loss of information, since the value of the omitted variable can be determined without error as the complement of the sum of the retained $(m - 1, \text{ variables})$. Without loss of generality, we base our inference procedure on (p_1, \dots, p_{m-1}) but express it later in a symmetric form involving each of p_1, \dots, p_m .

Let us denote the size and the weight of the i th grain by S_i and W_i , respectively, and observe that the total weight of all grains belonging to the j th size class can be written as

$$w_j = \sum_{i=1}^n t_j(S_i, W_i) \quad \text{for } j = 1, \dots, m \quad (2)$$

where $t_j(S, W) = W$ if $C_{j-1} < S \leq C_j$ and $= 0$ otherwise. Here $C_0 = 0$ and $C_m = +\infty$.

To work out the first- and second-order moments of w_j s, we need the first- and second-order moments of the t_j s. We calculate these on the assumption that the two-dimensional random variables $(\log_e S_i, \log_e W_i)$ for $i = 1, \dots, n$ are independent and follow a common bivariate normal distribution with the following parameters

$$\begin{aligned} E(\log_e S_i) &= \mu, & V(\log_e S_i) &= \sigma^2 \\ E(\log_e W_i) &= \mu_w, & V(\log_e W_i) &= \sigma_w^2, \text{ and} \\ \text{Cov}(\log_e S_i, \log_e W_i) &= \nu\sigma^2 \end{aligned} \tag{3}$$

We now need the following

Lemma. If (x, y) follows the standardized bivariate normal distribution with zero expectations, unit variances, and correlation-coefficient ρ and

$$z = \exp(ay) \quad \text{if } a < x \leq b \quad \text{and } = 0 \text{ otherwise} \tag{4}$$

where a, b, c are given constants, then

$$E(z) = \exp\left(\frac{1}{2} a^2\right) \{\Phi(c - a\rho) - \Phi(b - a\rho)\}, \quad \text{where} \tag{5}$$

$$\Phi(t) = \int_{-\infty}^t (2\pi)^{-1/2} \exp\left(-\frac{1}{2} t^2\right) dt \tag{6}$$

is the standardized normal probability integral. This can be proved by direct evaluation of the double integral

$$\begin{aligned} E(z) &= \int_b^c \left[\int_{-\infty}^{\infty} e^{ay} (2\pi)^{-1} (1 - \rho^2)^{-1/2} \right. \\ &\quad \left. \cdot \exp\left\{-\frac{1}{2} (x^2 - 2\rho xy + y^2)/(1 - \rho^2)\right\} dy \right] dx \end{aligned}$$

We now note that $x = (\log_e S_i - \mu)/\sigma, y = (\log_e W_i - \mu_w)/\sigma_w$ follow a standardized bivariate normal distribution with correlation-coefficient $\rho = \nu\sigma/\sigma_w$. The random variable $t_j \equiv t_j(S_i, W_i)$ can be written as

$$t_j = \exp(\mu_w + \sigma_w y) \quad \text{if } c_{j-1}^* < x \leq c_j^* \quad \text{and } = 0 \text{ otherwise}$$

where $c_j^* = (\log_e C_j - \mu)/\sigma$. The above lemma then gives

$$E(t_j^r) = \exp(r\mu_w + \frac{1}{2} r^2 \sigma_w^2) \{\Phi(c_j^* - r\nu\sigma) - \Phi(c_{j-1}^* - r\nu\sigma)\} \tag{7}$$

for $r = 1, 2$.

Let us now write

$$\begin{aligned}
 c_j &= \log_e C_j \\
 \lambda_1 &= \exp(\mu_w + \frac{1}{2} \sigma_w^2) \\
 \lambda_2 &= \exp(2\mu_w + 2\sigma_w^2) \\
 \pi_{t_1} &= \Phi(A_t + A_3 c_1) \\
 \pi_{t_j} &= \Phi(A_t + A_3 c_j) - \Phi(A_t + A_3 c_{j-1})
 \end{aligned}
 \tag{8}$$

for $j = 2, \dots, m - 1$, and

$$\pi_{tm} = 1 - \Phi(A_t + A_3 c_{m-1})$$

for $t = 1, 2$ where

$$A_1 = -[(\mu/\sigma) + \nu\sigma], \quad A_2 = -[(\mu/\sigma) + 2\nu\sigma] \quad \text{and} \quad A_3 = 1/\sigma \tag{9}$$

Then eq. (7) gives

$$\begin{aligned}
 E(t_j) &= \lambda_1 \pi_{1j} \\
 V(t_j) &= \lambda_2 \pi_{2j} - \lambda_1^2 \pi_{1j}^2, \quad \text{and} \\
 \text{Cov}(t_j, t_k) &= -E(t_j) \cdot E(t_k) = -\lambda_1^2 \pi_{1j} \pi_{1k}
 \end{aligned}
 \tag{10}$$

for $j \neq k = 1, \dots, m$.

We now note that the w_j s are sums of independently and identically distributed random variables $t_j(S_i, W_i)$ for $i = 1, \dots, n$. From the multivariate extension of the central limit theorem (see Varadarajan, 1958) we then conclude that, asymptotically as n tends to ∞ , the m -dimensional random-vector

$$\{n^{1/2} (w_j/n - \lambda_1 \pi_{1j}) : j = 1, \dots, m\}$$

follows the m -dimensional normal distribution with an expectation-vector of zero and a dispersion matrix whose elements are given by (10).

We now make use of the following theorem stated by Rao (1974)

Let T_n be a k -dimensional statistic (T_{1n}, \dots, T_{kn}) such that the asymptotic distribution of $\sqrt{n} (T_{1n} - \theta_1), \dots, \sqrt{n} (T_{kn} - \theta_k)$ is k -variate normal with means zero and dispersion-matrix $\Sigma = ((\sigma_{ij}))$. Let g_1, \dots, g_q be q functions of k variables and each g_i be totally differentiable. Then the asymptotic distribution of

$$\sqrt{n} u_{in} = \sqrt{n} [g_i(T_{1n}, \dots, T_{kn}) - g_i(\theta_1, \dots, \theta_k)], \quad i = 1, \dots, q$$

is q -variate normal with zero means and dispersion-matrix $G\Sigma G'$ where $G = ((\partial g_i / \partial \theta_j))$. The rank of the distribution is $R(G\Sigma G')$

Here $R(\cdot)$ denotes the rank of the concerned matrix. In our case, $k = q = m$, $T_{1i} = w_i/n$, $\theta_j = \lambda_1 \pi_{1j}$, $\sigma_{ij} = \lambda_2 \pi_{2i} \delta_{ij} - \lambda_1^2 \pi_{1i} \pi_{1j}$, $g_i(\theta_1, \dots, \theta_m) = \theta_i(\theta_1 + \dots + \theta_m)^{-1}$, for $i, j = 1, \dots, m$, where δ_{ij} is Kronecker's delta, $\delta_{ii} = 1$, $\delta_{ij} = 0$, for $i \neq j$. Thus $g_i(T_{1n}, \dots, T_{mn}) = p_i$ and $g_i(\theta_1, \dots, \theta_m) = \pi_{1i}$ for $i = 1, \dots, m$ since $\sum_{j=1}^m \pi_{tj} = 1$ for $t = 1, 2$. Also $\partial g_i / \partial \theta_k = (\delta_{ik} - \pi_{1i}) \lambda_1^{-1}$. Thus the asymptotic distribution of $n^{1/2}(p_1 - \pi_{11}), \dots, n^{1/2}(p_m - \pi_{1m})$ is m -variate normal with zero means and dispersion matrix $\Lambda = ((\lambda_{ij})) = G \Sigma G'$. Direct computation gives

$$\begin{aligned} \lambda_{ij} &= \sum_{k,l=1}^m (\partial g_i / \partial \theta_k)(\partial g_j / \partial \theta_l) \sigma_{kl} \\ &= \sum_{k,l=1}^m \lambda_1^{-2} (\delta_{ik} - \pi_{1i})(\delta_{jl} - \pi_{1j}) (\lambda_2 \pi_{2k} \delta_{kl} - \lambda_1^2 \pi_{1k} \pi_{1l}) \\ &= \lambda^2 \{(\pi_{2i} - \pi_{1i})(\pi_{2j} - \pi_{1j}) + \pi_{2i}(\delta_{ij} - \pi_{2j})\} \end{aligned} \tag{11}$$

for $j = 1, \dots, m$, where $\lambda^2 = \lambda_2 \lambda_1^{-2} = \exp(\sigma_w^2)$.

The rank of the $m \times m$ dispersion matrix Λ can be shown to be $(m - 1)$ and the distribution is thus singular. We therefore omit the last variable and consider the asymptotic distribution of $n^{1/2}(p_1 - \pi_{11}), \dots, n^{1/2}(p_{m-1} - \pi_{1,m-1})$ which is $(m - 1)$ dimensional nonsingular normal with means zero and dispersion matrix $((\lambda_{ij}))$ for $i, j = 1, \dots, (m - 1)$. The quadratic form associated with this distribution is

$$Q = n \sum_{i,j=1}^{m-1} \lambda^{ij} (p_i - \pi_{1i})(p_j - \pi_{1j}) \tag{12}$$

where the elements of $((\lambda^{ij})) = ((\lambda_{ij}))^{-1}$ are derived below.

Let us write x_j for the j th element in the t th column of the inverse matrix $x_j = \lambda^{jt}$, $j = 1, \dots, (m - 1)$ which by definition satisfy the equations

$$\sum_{j=1}^{m-1} \lambda_{ij} x_j = \delta_{it}, t = 1, \dots, (m - 1) \tag{13}$$

By substituting the values of λ_{ij} 's from (11) in (13), we get

$$\lambda^2 [(\pi_{2i} - \pi_{1i})D - \pi_{2i}P + \pi_{2i}x_j] = \delta_{it} \tag{14}$$

where

$$D = \sum_{j=1}^{m-1} (\pi_{2j} - \pi_{1j}) x_j \quad \text{and} \quad P = \sum_{j=1}^{m-1} \pi_{2j} x_j$$

Adding eq. (14) over $i = 1, \dots, (m - 1)$, and remembering that

$$\sum_{i=1}^{m-1} (\pi_{2i} - \pi_{1i}) = \pi_{1m} - \pi_{2m}, \quad \sum_{i=1}^{m-1} \pi_{2i} = 1 - \pi_{2m}$$

we get

$$\lambda^2 \{(\pi_{1m} - \pi_{2m})D + \pi_{2m}P\} = 1 \tag{15}$$

Again, multiplying both sides of (14) by $(\pi_{2i} - \pi_{1i})/\pi_{2i}$ and adding over $i = 1, \dots, (m - 1)$ we get after some simplification

$$\lambda^2 \{[S_0 - [(\pi_{2m} - \pi_{1m})]^2/\pi_{2m}\}D + (\pi_{2m} - \pi_{1m})P = 1 - (\pi_{1t}/\pi_{2t}) \tag{16}$$

where

$$S_0 = \sum_{i=1}^m \pi_{1i}^2/\pi_{2i} \tag{17}$$

Solving eqs. (15) and (16) for D and P , we get

$$D = [(\pi_{1m}/\pi_{2m}) - (\pi_{1t}/\pi_{2t})]/(\lambda^2 S_0)$$

$$P = (1/\lambda^2 \pi_{2m}) + [1 - (\pi_{1m}/\pi_{2m})]D$$

Finally, substituting the values of D and P in (14), we get

$$\lambda^{it} = x_i = \lambda^{-2} [(\delta_{it}/\pi_{2i}) + (1/\pi_{2m}) - (\epsilon_i \epsilon_t/S_0)], \quad \text{where}$$

$$\epsilon_i = (\pi_{1i}/\pi_{2i}) - (\pi_{1m}/\pi_{2m}) \tag{18}$$

Let us write $d_i = p_i - \pi_{1i}$, so that the quadratic form defined by (12) may be written as

$$Q = n\lambda^{-2} \sum_{i,j=1}^{m-1} \left(\frac{\delta_{ij}}{\pi_{2i}} + \frac{1}{\pi_{2m}} - \frac{\epsilon_i \epsilon_j}{S_0} \right) d_i d_j$$

$$= n\lambda^{-2} \left\{ \sum_{i=1}^{m-1} \frac{d_i^2}{\pi_{2i}} + \frac{1}{\pi_{2m}} \left(\sum_{i=1}^{m-1} d_i \right)^2 - \left[\left(\sum_{i=1}^{m-1} \epsilon_i d_i \right)^2 \right] / S_0 \right\}$$

But

$$\sum_{i=1}^{m-1} d_i = -d_m, \quad \text{and} \quad \sum_{i=1}^{m-1} \epsilon_i d_i = \sum_{i=1}^{m-1} \frac{\pi_{1i}}{\pi_{2i}} d_i - \frac{\pi_{1m}}{\pi_{2m}} \sum_{i=1}^{m-1} d_i = \sum_{i=1}^m \frac{\pi_{1i}}{\pi_{2i}} d_i.$$

Consequently,

$$Q = n\lambda^{-2} (S_2 - S_1^2/S_0) \tag{19}$$

where

$$S_2 = \sum_{i=1}^m \frac{(p_i - \pi_{1i})^2}{\pi_{2i}}, \quad \text{and} \quad S_1 = \sum_{i=1}^m \frac{\pi_{1i}}{\pi_{2i}} (p_i - \pi_{1i}) \quad (20)$$

and S_0 is defined by (17).

THE MINIMUM Q^* METHOD OF ESTIMATION

The quadratic form

$$Q^* = n^{-1} \lambda^2 Q = S_2 - S_1^2/S_0 \quad (21)$$

is seen to play a role analogous to that of a χ^2 statistic. It is a function of the observed weight frequencies and the three parameters A_1, A_2 , and A_3 , and consequently μ, σ , and ν since

$$\mu = A_3(2A_2 - A_1)$$

$$\sigma = 1/A_3$$

$$\nu = A_3(A_1 - A_2) \quad (22)$$

In a sense Q^* can be looked upon as a measure of deviation of the observed weight frequencies from the assumed statistical set-up: the larger the value of Q^* , the greater is the discrepancy between the model and the observations.

We propose to estimate the parameters A_1, A_2 , and A_3 and consequently μ, σ , and ν by minimizing the quadratic form Q^* with respect to A_1, A_2 , and A_3 . The estimates so obtained will be denoted by A_1^*, A_2^* , and A_3^* , respectively, and called minimum Q^* estimates. Statistical properties of these estimates are being investigated. For the present these estimates are offered on the heuristic ground that they provide the best agreement with the observed values in the sense of minimizing Q^* .

Since analytical methods for minimization do not lead in this case to neat expressions, essentially numerical iterative procedures are proposed in this paper which are minor variants of well-known techniques.

In the first stage, starting from a given initial point (A_1, A_2, A_3) one would like to reach another point $(A_1 - h_1, A_2 - h_2, A_3 - h_3)$ at a fixed distance h from the initial point; $h^2 = h_1^2 + h_2^2 + h_3^2$, such that the reduction $\Delta = Q^*(A_1, A_2, A_3) - Q^*(A_1 - h_1, A_2 - h_2, A_3 - h_3)$ is the maximum. This gives $h_i = r \delta_i$, $i = 1, 2, 3$ where δ_i is the partial derivative of Q^* with respect to A_i at the initial point that can be evaluated analytically, or, in this particular case, more conveniently estimated by the corresponding partial divided difference. Here $r^2 = h^2/(\delta_1^2 + \delta_2^2 + \delta_3^2)$, but since h is in any case arbitrary, one can take r itself as arbitrary and try to choose a suitably large value of r by trial and error. The procedure can then be repeated to move from the second point to the third and so on.

This is the so-called method of steepest descent, known otherwise as the gradient method or the linear method since only first-order partial derivatives are used.

Note that in each cycle of the above procedure the reduction in the value of Q^* is approximately $\Delta = \sum h_i \delta_i = r \sum \delta_i^2$, so that when the first-order partial derivatives become small in absolute value, the reduction falls off. It is at this stage that a second procedure involving the replacement of Q^* by a second-degree polynomial approximation is needed. There are various ways of obtaining a second-degree polynomial approximation. When first- and second-order partial derivatives can be obtained analytically and evaluated, one can use a Taylor series expansion retaining partial derivatives up to the second order. One could alternatively use a second-degree interpolation polynomial by using partial divided differences instead of partial derivatives. A third alternative is to obtain a second degree curve which best fits the function at a certain number of points in the sense of least squares. The least-squares approach is frequently used by statisticians for empirically determined functions subject to errors of observation and was first recommended by Box and Wilson (1951).

To obtain initial approximations for A_1, A_2 , and A_3 we write $P_j = \sum_{i=1}^i p_i$ for $j = 1, \dots, m - 1$ and note that P_j is an asymptotically unbiased estimate of $\Phi(A_1 + A_3 c_j)$. Writing $Y_j = \Phi^{-1}(P_j)$ we expect a linear relationship $Y_j \sim A_1 + A_3 c_j$ between Y_j and c_j . Let $t = [m/3]$, $\bar{Y}_1 = \sum_{j=1}^t Y_j/t$, $\bar{c}_1 = \sum_{j=1}^t c_j/t$; $\bar{Y}_2 = \sum_{j=1}^t Y_{m-j}/t$ and $\bar{c}_2 = \sum_{j=1}^t c_{m-j}/t$, so that $\bar{Y}_1 \sim A_1 + A_3 \bar{c}_1$ and $\bar{Y}_2 \sim A_1 + A_3 \bar{c}_2$ from which one gets to start

$$A_1 = (\bar{c}_2 \bar{Y}_1 - \bar{c}_1 \bar{Y}_2) / (\bar{c}_2 - \bar{c}_1)$$

$$A_3 = (\bar{Y}_2 - \bar{Y}_1) / (\bar{c}_2 - \bar{c}_1)$$

and taking $\nu = 3$ initially

$$A_2 = A_1 - 3/A_3$$

Using an arbitrary small value for h , say $h = 0.01$ one then estimates the partial derivative with respect to A_1 , namely $\delta_1 = [Q^*(A_1, A_2, A_3) - Q^*(A_1 - h, A_2, A_3)]/h$ and in a similar manner the other two partial derivatives δ_2 and δ_3 . Next choosing an arbitrary value for r , say $r = 0.0001$, one can compute the decrement $\Delta = Q^*(A_1, A_2, A_3) - Q^*(A_1 - r\delta_1, A_2 - r\delta_2, A_3 - r\delta_3)$ and check if it is positive. If it is positive, one can successively double the value of r until the largest decrement is obtained. If the decrement is negative, one tries $r/2$ in place of r and proceeds in the same way as before. With the value of r so determined, one computes $A'_i = A_i - r\delta_i, i = 1, 2, 3$ and (A'_1, A'_2, A'_3) is taken as the starting point for the next cycle of steepest descent calculations.

At the end of each cycle of such calculations, the decrement $\Delta = Q^*(A_1, A_2, A_3) - Q^*(A_1 - r\delta_1, A_2 - r\delta_2, A_3 - r\delta_3)$ is calculated. If this decrement is smaller than a preassigned quantity Δ_0 , steepest descent calculations are termi-

nated and one proceeds to the next stage of calculation of fitting second-degree polynomials. At this stage, 27 different values of Q^* are computed at the points (A'_1, A'_2, A'_3) where each A'_i takes successively the three values $A_i - h$, A_i and $A_i + h$ where h is some small chosen quantity. A second-degree polynomial

$$Q^* = \beta_0 + \sum_{i=1}^3 \beta_i A_i + \sum_{i=1}^3 \sum_{j=1}^3 \beta_{ij} A_i A_j$$

is fitted to these 27 points by the method of least squares. The value of (A_1, A_2, A_3) at which this second-degree polynomial is minimum is determined in the usual manner by equating the first-order partial derivatives to zero giving

$$(A_1, A_2, A_3) = -\frac{1}{2} (\beta_1, \beta_2, \beta_3) ((\beta_{ij}))^{-1}$$

One then checks if at this new point Q^* has indeed a smaller value and repeats the procedure if necessary.

A computer program in FORTRAN IV language for the minimum Q^* method of estimation is presented in the Appendix.

ILLUSTRATIVE EXAMPLES

In order to examine whether the minimum Q^* method provides good estimates of the three parameters μ , σ , and ν , the method was tried on two sets of simulated data. For the purpose of illustration simulated samples were preferred to actual sieve data because in the latter case the parameters would be unknown, and the assumed model also may not hold. The closeness of agreement of the estimates with the actual parameters indicate the usefulness of the method.

Two sets of simulated samples were generated in the following way. 1000 random pairs (S, W) were drawn from bivariate log-normal populations with the following parameters

$$\begin{aligned} \mu &= E(\log_e S) = 1.00, & \sigma^2 &= V(\log_e S) = 0.25 \quad \text{or} \quad \sigma = 0.50 \\ \mu_w &= E(\log_e W) = 0.50, & \sigma_w^2 &= V(\log_e W) = 2.25 \quad \text{or} \quad \sigma_w = 1.50 \end{aligned}$$

and the coefficient of correlation ρ between $\log_e S$ and $\log_e W$ as 0.95 in the first set and 0.50 in the second set, so that the shape parameters $\nu = \sigma_w/\sigma$ were different in the two sets, $\nu = 2.85$ in the first set and $\nu = 1.50$ in the second set.

The 1000 observations were divided into $m = 9$ size-classes in terms of the class limits $C_1 = 2.97$, $C_2 = 3.78$, $C_3 = 4.39$, $C_4 = 5.10$, $C_5 = 5.93$, $C_6 = 6.69$, $C_7 = 7.54$, and $C_8 = 9.03$. The total of W in each of these size classes was calculated and expressed as percentages of the grand total of W for all 1000 observations. These observed weight frequencies for the two sets of data, together with the expected frequencies, calculated after estimating the parameters, are shown in Table I.

The class limit and observed weight frequencies were inputs for the computer programs given in the Appendix which produced the following estimates:

Table 1. Observed and Expected Weight Frequencies in Two Sets of Simulated Data

Size class (1)	Weight frequencies (%)			
	set I		set II	
	observed (2.1)	expected (2.2)	observed (3.1)	expected (3.2)
less than 2.97	10.94	10.73	30.34	29.88
2.97-3.78	11.68	11.90	16.76	22.09
3.78-4.39	10.28	10.19	11.08	7.90
4.39-5.10	10.80	11.68	13.90	10.97
5.10-5.93	11.09	12.17	6.92	9.34
5.93-6.69	11.25	9.35	8.21	5.97
6.69-7.54	11.04	8.45	5.69	4.61
7.54-9.03	9.58	10.29	4.70	4.64
above 9.03	13.36	15.24	2.40	4.60

Table 2. Estimates of $A_1, A_2,$ and $A_3,$ and the Value of Q^* After Some Cycles of Iteration for Both Sets of Simulated Data

Set (1)	Iteration no. (2)	A_1 (3)	A_2 (4)	A_3 (5)	Q^* (6)	
1			steepest descent method			
	0	-3.567	-4.976	2.129	0.0336	
	1	-3.546	-4.968	2.137	0.0317	
	6	-3.511	-4.930	2.103	0.0280	
	10	-3.494	-4.909	2.088	0.0267	
	25	-3.473	-4.854	2.055	0.0238	
	48	-3.474	-4.621	2.046	0.0190	
	70	-3.468	-4.554	2.041	0.0180	
				least-square second-degree polynomial fit method		
	71	-3.468	-4.544	2.051	0.0180	
	79	-3.467	-4.553	2.042	0.0180	
	2			steepest descent method		
		0	-3.004	-4.343	2.240	0.0575
		1	-2.955	-4.329	2.281	0.0480
5		-2.910	-4.269	2.236	0.0437	
10		-2.848	-4.186	2.184	0.0392	
24		-2.761	-4.018	2.071	0.0308	
48		-2.688	-3.783	2.006	0.0268	
58		-2.708	-3.716	1.987	0.0258	
83		-2.701	-3.700	1.994	0.0254	
				least-square second-degree polynomial fit method		
84		-2.701	-3.700	1.994	0.0254	
90		-2.701	-3.699	1.994	0.0254	

Table 3. Values of μ , σ , ν and Their Estimates Obtained by Three Different Methods for Two Sets of Simulated Data

Set (1)	Parameter (2)	Actual values (3)	Estimates		
			Folk and Ward (4)	Sahu (5)	Min. Q^* (6)
1	μ	1.00	1.85	1.69	1.17
	σ	0.50	0.50	0.41	0.49
	ν	2.85	<i>a</i>	<i>a</i>	2.22
2	μ	1.00	1.49	1.37	0.85
	σ	0.50	0.49	0.44	0.50
	ν	1.50	<i>a</i>	<i>a</i>	1.99

^aCannot be estimated by these methods.

$\mu = 1.166$, $\sigma = 0.490$, $\nu = 2.217$ for the first set and $\mu = 0.850$, $\sigma = 0.501$, and $\nu = 1.992$ for the second set with the final values $Q^* = 0.0180$ and 0.0254 attained after about 80 cycles of the iterative calculations, as shown in Table 2.

For purposes of comparison, estimates for μ and σ were also obtained by using the quick methods given by (i) Folk and Ward (1957), and (ii) Sahu (1965), shown in Table 3.

It is seen from these examples that in both cases the minimum Q^* method provides closer estimates for μ (the mean of logarithmic size) than the other two methods. The estimates for σ obtained by these methods are all quite close to the actual value and to each other. This is understandable because the estimates of σ do not depend on the shape parameter ν , and the sample size is quite large. While the minimum Q^* method provides an estimate of the shape parameter, the other two methods can not be used for this purpose. Columns (2.2) and (3.2) of Table 1 show that the expected distributions of weight frequencies calculated after estimating the parameters by the minimum Q^* method agree reasonably well with the observed distributions given in columns (2.1) and (3.1), respectively.

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APPENDIX

The list of programs, including functions and subroutines for methods described in the text, is given here. The table below gives a short description of each routine.

Table 4. Short Description of Routines Used

Name (1)	Description (2)
PROBIT	This is a FUNCTION which computes for any S , $0 < S < 1$ the ordinate X such that $\int_{-\infty}^X \phi(t) dt = S, \quad \text{where} \quad \phi(t) = (2\pi)^{-1/2} e^{-t^2/2}$ <p>S is the argument of the FUNCTION.</p>
PRBTHN	This is a FUNCTION which gives an approximate value of X for any S , $0 < S < 1$, using Hasting's approximation where X is same as is described above. For Hasting's approximation see Hastings, Hayward, and Wong (1955).
STNORP	This function computes the probability that a standard normal variate is less than or equal to X , for any finite X .
CALCQ	This is a SUBROUTINE which computes Q^* , given weight frequencies (P), class limits in \log_e -scale (C), and parameters A_1 , A_2 , and A_3 . These are supplied to the subroutine through COMMON areas.
CONT	This SUBROUTINE finds initial estimates for A_1 , A_2 , and A_3 .

Table 4. Continued

Name (1)	Description (2)
MINQ1	This SUBROUTINE tries to optimize Q^* using steepest-descent method. Inputs to this subroutine are through COMMON areas. This terminates if either the number of iterations exceeds the number specified in INT1 or if no further improvement is possible by this method.
MINQ2	This SUBROUTINE optimizes Q^* by using the method of second-degree polynomial fit by the least-squares method. Here also iteration ceases when it either exceeds the number specified through INT2 or if no further improvement is possible.
MAIN	This is the main program which reads input cards and calls subroutines in the required order.

FUNCTION PROBIT(S)

C GIVEN S, EVALUATES X FOR WHICH NORMAL DISTRIBUTION FUNCTION
C EQUALS S.

DIMENSION P(51),A(3),C(51)

COMMON P,A,C,Q,M,INT1,INT2,N

IF(S-S*S)12,12,1

1 J=1

H=0.0005

XX=PRBTHN(S)

2 PP=STNORP(XX)

IF(ABS(PP-S)- 0.00001)11,3,3

3 GOTO(4,8,8),J

4 J=2

IF(PP-S)6,6,5

5 H=-H

6 XO=XX

PO=PP

GO TO (7,7,10),J

7 XX=XO+H

GO TO 2

8 IF((PO-S)*PP-(PO-S)*S)9,6,6

9 J=3

X1=XX

P1=PP

10 XX=XO+(X1-XO)*(S-PO)/(P1-PO)

GO TO 2

11 PROBIT=XX

RETURN

12 WRITE(6,13)

13 FORMAT(1H1/2X,6HERROR1)

STOP

END

FUNCTION STNORP(X)

C GIVEN X, COMPUTES THE STANDARD NORMAL FUNCTION.

DIMENSION P(51),A(3),C(51)

COMMON P,A,C,Q,M,INT1,INT2,N

```

SIGN=1.0
IF(X-7.0)2,11,11
2 IF(X+7.0)15,15,3
3 IF(X)4,5,6
4 Y=-0.5
SIGN=-1.0
X=-X
GO TO 19
6 Y=.5
19 T=X
AN=1.
Y1=X
9 Y2=Y1*X*X/(2.*AN+1.)
IF(ABS(Y2)-0.1E-7)7,7,8
8 T=T+Y2
AN=AN+1.
Y1=Y2
GOTO9
7 Y=Y+T*EXP ((-.5)*X*X)/2.506628275
Y=ABS (Y)
GOTO13
11 Y=1.
GOTO13
5 Y=.5
GOTO13
15 Y=0.
13 STNORP=Y
X=SIGN*X
RETURN
END

FUNCTION PRBTHN(S)
C HASTINGS APPROXIMATION TO NORMAL PROBIT
DIMENSION P(51),A(3),C(51)
COMMON P,A,C,Q,M,INT1,INT2,N
IF(S-S*S)7,7,1
1 IF(S-0.5)3,2,4
2 Y=0.0
GO TO 6
3 SIGN=-1.0
E=-2.0*ALOG(S)
GO TO 5
4 SIGN=1.0
E=-2.0*ALOG(1.0-S)
5 E=SQRT(E)
Y=SIGN*(E-((0.010328*E+0.802853)*E+2.515517)/(((0.001308*E+
10.189269)*E+1.432788)*E+1.0))
6 PRBTHN=Y
RETURN
7 WRITE(6,8)
8 FORMAT(5X,6HERROR2)
STOP
END

SUBROUTINE CALCQ
C THIS COMPUTES THE VALUE OF Q* GIVEN PARAMETERS AND OBSERVATIONS.
DIMENSION P(51),C(51),A(3),PHI(2,51)

```

```

COMMON P,A,C,Q,M,INT1,INT2,N
DO 4 I=1,2
  B1=0.
DO 3 J=1,N
  T=A(I)+A(3)*C(J)
  B2=STNORP(T)
  PHI(I,J)=B2-B1
3 B1=B2
4 PHI(I,M)=1.-B1
  S0=0.
  S1=0.
  S2=0.
DO 5 J=1,M
  S0=S0+(PHI(1,J)**2)/PHI(2,J)
  S1=S1+(P(J)-PHI(1,J))*PHI(1,J)/PHI(2,J)
5 S2=S2+((P(J)-PHI(1,J))**2)/PHI(2,J)
  Q=S2-(S1*S1/S0)
  RETURN
END
SUBROUTINE CONT
C   THIS IS THE FIRST PROGRAM - FOR FINDING INITIAL ESTIMATES. HERE
C   M= NUMBER OF SIEVE-CLASSES,
C   C-ARRAY STORES SIEVE-SIZES, AND
C   P-ARRAY STORES WEIGHT FREQUENCIES AS PROPORTIONS.
DIMENSION P(51),C(51), A(3),Y(51)
COMMON P,A,C,Q,M,INT1,INT2,N
L=N/3
T=0.
DO 45 I=1,N
  T=T+P(I)
45 Y(I)=PROBIT(T)
  Y1=0.0
  Y2=0.0
  C1=0.0
  C2=0.0
DO 55 I=1,L
  Y1=Y1+Y(I)
  J=M-I
  C1=C1+C(I)
  Y2=Y2+Y(J)
55 C2=C2+C(I)
  T=L
  A(1)=(Y1*C2-Y2*C1)/((C2-C1)*T)
  A(3)=(Y2-Y1)/(C2-C1)
  A(2)=A(1)-3./A(3)
  WRITE (6,46)((I,A(I)),I=1,3)
46 FORMAT(1H0/5X,17HINITIAL ESTIMATES/4X,18(1H-))/(3X,2HA(,11,2H)=,
1E16.9))
  RETURN
END

SUBROUTINE MINQ1
C   THIS IS THE SECOND PROGRAM WHICH USES STEEPEST DESCENT METHOD,
C   AS DISCUSSED IN THE TEXT, TO OPTIMIZE Q*.
DIMENSION A(3),P(51),C(51),QT(3),AL(3),B(3),CT(3)
COMMON P,A,C,Q,M,INT1,INT2,N
DO 1 I=1,3

```



```

1 AL(I)=A(I)
  CALL CALCQ
  ICTR=0
  QV=Q
  R=0.0001
  EPS=.01
90 Q0=QV
  ICTR=ICTR+1
  IF((INT1.GT.0).AND.(ICTR.GT.INT1))GO TO 15
  IT=0
  DO 11 I=1,3
  B(I)=AL(I)
  CT(I)=AL(I)
11 A(I)=B(I)
C  COMPUTES PARTIAL DERIVATIVES BY FIRST DIFFERENCES.
  CALL CALCQ
  QD=Q
  DO 5 I=1,3
  DO 6 J=1,3
6  A(J)=B(I)
  A(I)=A(I)+EPS
  CALL CALCQ
5  QT(I)=(Q-QD)/EPS
C  COMPUTES EXPECTED CHANGE IN THE VALUE
  T=0.
16 DO 7 I=1,3
  B(I)=R*QT(I)
  A(I)=A(I)-B(I)
7  T=T+B(I)*B(I)
  IF(((QV+T)-QV).EQ. 0) GO TO 15
C  A(3) SHOULD BE POSITIVE ALWAYS
  IF (A(3)) 37,37,69
37 R=R/2.
  GO TO 31
69 CALL CALCQ
  Q1=Q
  IF (IT) 20,20,21
20 IF (Q1-Q0) 10,10,12
10 Q0=Q1
  DO 14 I=1,3
  CT(I)=A(I)
14 A(I)=AL(I)
  R=2.*R
  GO TO 16
12 R=R*3./4.
  IT=1
  DO 19 I=1,3
19 A(I)=AL(I)
  GO TO 16
21 IF (Q1-Q0) 30,30,35
30 DO 32 I=1,3
32 AL(I)=A(I)
  QV=Q1
  GO TO 90
35 R=R*2./3.
31 DO 33 I=1,3
33 AL(I)=CT(I)

```

```

QV=Q0
GO TO 90
15 WRITE (6,201)((AL(I),I=1,3),QV)
201 FORMAT(5X,14HEND OF METHOD1/5X,3(E16.9,5X),2HQ=,E16.9)
RETURN
END

```

```

SUBROUTINE MINQ2
C THIS IS THE THIRD PROGRAM WHICH USES SECOND DEGREE LEAST SQUARE
C POLYNOMIAL FIT METHOD. TO OPTIMIZE Q*.
DIMENSION P(51),C(51),A(3),QT(3),AL(3),B(3),CT(3),X(27,3),Y(27)
COMMON P,A,C,Q,M,INT1,INT2,N
EPS=.01
ICTR=0
DO 81 I=1,3
81 AL(I)=A(I)
CALL CALCQ
90 ICTR=ICTR+1
IF((INT2 .GT. 0) .AND. (ICTR .GT. INT2)) GO TO 91
JK=1
DO 6 I=1,3
6 B(I)=AL(I)
C COMPUTES VALUES AT 27 POINTS
DO 4 I=1,3
DO 4 J=1,3
DO 4 K=1,3
DO 5 L=1,3
5 A(L)=B(L)
X(JK,1)=(I-2)*EPS
X(JK,2)=(J-2)*EPS
X(JK,3)=(K-2)*EPS
DO 8 L=1,3
8 A(L)=A(L)+X(JK,L)
CALL CALCQ
Y(JK)=Q-Q0
4 JK=JK+1
C LEAST SQUARE FIT OF A SECOND DEGREE POLYNOMIAL
DO 198 I=1,3
A(I)=0.
B(I)=0.
198 QT(I)=0.
DO 15 I=1,27
DO 16 J=1,3
16 CT(J)=Y(I)*X(I,J)
DO 17 J=1,3
A(J)=A(J)+CT(J)
B(J)=B(J)+CT(J)*X(I,J)
IF( J-3) 17,18,18
17 QT(J)=QT(J)+CT(J)*X(I,J+1)
18 QT(3)=QT(3)+CT(3)*X(I,1)
15 CONTINUE
T=2.*(B(1)+B(2)+B(3))/7.
QQ=EPS*EPS
Q1=QQ*QQ
DO 20 I=1,3
A(I)=A(I)/(18.*QQ)
B(I)=(B(I)-T)/(6.*Q1)

```

$Q_0 = Q$ →

```

20 QT(I)=QT(I)/(12.*Q1)
   A11=4.*B(2)*B(3)-QT(2)*QT(2)
   A12=- (2.*B(3)*QT(1)-QT(2)*QT(3))
   A13=QT(1)*QT(2)-2.*B(2)*QT(3)
   A22=4.*B(1)*B(3)-QT(3)*QT(3)
   A23=- (2.*B(1)*QT(2)-QT(1)*QT(3))
   A33=4.*B(1)*B(2)-QT(1)*QT(1)
   DT=2.*A11*B(1)+A12*QT(1)+A13*QT(3)
   B(1)=- (A11*A(1)+A12*A(2)+A13*A(3))
   B(2)=- (A12*A(1)+A22*A(2)+A23*A(3))
   B(3)=- (A13*A(1)+A23*A(2)+A33*A(3))
   DO 30 I=1,3
   B(I)=B(I)/DT
   A(I)=AL(I)+B(I)
30 AL(I)=A(I)
   CALL CALCQ
   IF(Q0-Q)91,91,90
91 WRITE(6,201)(AL(I),I=1,3),Q
201 FORMAT(5X,14HEND OF METHOD2/5X,3(E16.9,5X),2HQ=,E16.9)
   RETURN
   END

```

```

C THIS IS THE MAIN PROGRAM. IT READS ONE PUNCHED CARD GIVING NUMBER
C OF SIEVE-CLASSES(M), NUMBER OF ITERATIONS AFTERWHICH THE THIRD
C PROGRAM WILL BE INITIATED(INT1) AND NUMBER OF ITERATIONS
C AFTERWHICH THE THIRD PROGRAM WILL STOP. IT ALSO REQUIRES OTHER
C INPUT CARDS GIVING CLASS-LIMITS OF SIEVE-CLASSES(C) AND WEIGHT-
C FREQUENCIES EXPRESSED AS PROPORTIONS(P). FORMATS OF INPUT CARDS
C ARE GIVEN IN STATEMENT NUMBERS 1, 2 AND 3, - WHICH MAY BE CHANGED.
C IF REQUIRED.
C IF INT1 IS ZERO, THIRD PROGRAM WILL BE INITIATED ONLY WHEN NO
C FURTHER IMPROVEMENT IS POSSIBLE BY THE SECOND PROGRAM. THIRD
C PROGRAM COMES TO THE END IF EITHER NUMBER OF ITERATIONS EXCEEDS
C THE NUMBER SPECIFIED BY INT2 OR IF NO FURTHER IMPROVEMENT TAKES
C PLACE BY THIS METHOD.
C DIMENSION A(3),P(51),C(51),QT(3),AL(3),B(3),CT(3)
COMMON P,A,C,Q,M,INT1,INT2,N
READ (5,1)M,INT1,INT2
1 FORMAT(312)
N=M-1
READ (5,2)(C(I),I=1,N)
2 FORMAT(16F5.3)
READ (5,3)(P(I),I=1,M)
3 FORMAT(16F5.5)
WRITE (6,99)((C(I),P(I)),I=1,N)
99 FORMAT(5X,E16.9,5X,E16.9/)
DO 100 I=1,N
100 C(I)=ALOG(C(I))
   CALL CONT
   CALL MINQ1
   CALL MINQ2
   STOP
   END

```