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Computational Methods for the Determination of Roundness of Sedimentary Particles[1]

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A number of subjective and objective methods have been proposed to determine the roundness of rock particles, roundness being one of three properties describing the shape of a particle.

Methods that make use of the Fourier transform of the polar coordinates of particles' edge elements are proposed in this paper. Lowpass filters are used to smooth the profiles of rock particle, roundness is then determined from the differences between the original and smooth profiles. Further methods that are proposed make use of different measures of inequality to quantify the distribution of the energy among the transform coefficients of the profiles of rock particles. These values are then used to determine the roundness of the particles. Entropy and Emlen's modified entropy are the measures of inequality that are used. Different methods of determining the centre point of a particle and different methods to interpolate the edge elements are compared. The sensitivity of the methods to different resolutions is also investigated.

The results obtained with the proposed methods are comparable to those obtained with an existing Fourier transform based method, however it is shown that the proposed methods are computationally less demanding. It is also shown that the proposed methods are better than the existing method when the comparison is based on the correlation between the mean roundness of samples of particles and the actual roundness of the particles.

KEY WORDS: Fourier transform, entropy, Emlen's modified entropy, Kullback–Leibler distance.

INTRODUCTION

The shape of sedimentary particles is an important property in determining their transport history and behaviour in hydrodynamic systems (e.g. Krumbein, 1941a). It is therefore important to have an objective quantitative measure of particle shape with which the differences between the shapes of different populations can be identified. The shape of a particle is described by three independent properties

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(Barrett, 1980, p. 292):

- *Form* describes the extent to which a particle approaches a sphere in shape;
- *Roundness* is the extent to which a particle has been smoothed;
- *Surface texture* describes the markings on the surface of a particle.

Traditionally the determination of roundness has been either very subjective or very time consuming. Even with the objective methods that have been proposed some form of subjectivity still exist (Barrett, 1980, p. 302). Diepenbroek, Bartholomä and Ibbeken (1992), Ehrlich and Weinberg (1970) and Schwarcz and Shane (1969) have proposed methods to determine roundness based on the Fourier transform. In this paper alternative methods using the Fourier transform are proposed.

Roundness can be defined as the ratio between the mean radius of curvature of the corners of a particle and the radius of the largest inscribed circle thereof (Wadell, 1932, p. 448):

$$\frac{\frac{1}{N}\sum_{i=1}^{N} r_i}{R}$$

with r_i being the curvature of the i-th corner and R the radius of the largest inscribed circle. Corners are defined as the parts of the profile of a particle with a radius of curvature not greater than the radius of the largest inscribed circle of the profile.

Barrett (1980) did a comprehensive review of the quantitative measures proposed in the literature. Of these methods only the procedure proposed by Wadell measures mean roundness (Barrett, 1980, p. 301). Most of the quantitative methods proposed are still prone to some form of subjectivity, be it in locating the different axis, identifying corners or fitting arcs to the particle profile (Barrett, 1980, p. 302).

As an alternative to quantitative methods pebble comparison charts have been developed to aid in the determination of roundness (e.g. Krumbein, 1941b; Powers, 1953). The disadvantage of these charts is that the values obtained are more subjective than the quantitative methods. The Wadell roundness values have been determined for the profiles on Krumbein's chart, the preferred visual estimation chart as it has the largest number of roundness classes. (The profiles in Figure 1 are representative of the rest of the chart.) The argument for using the chart with the largest number of classes is that it is closest to a continuous measure. It is, however, required that adjacent classes be distinguishable (Barrett, 1980, p. 301).

The preprocessing of the data is discussed in the next section. This is followed by a brief introduction to Fourier transform based methods, the implementation of the method of Diepenbroek, Bartholomä and Ibbeken (1992) and the results obtained with their method. The proposed methods are then discussed followed by a comparison of the different preprocessing methods.

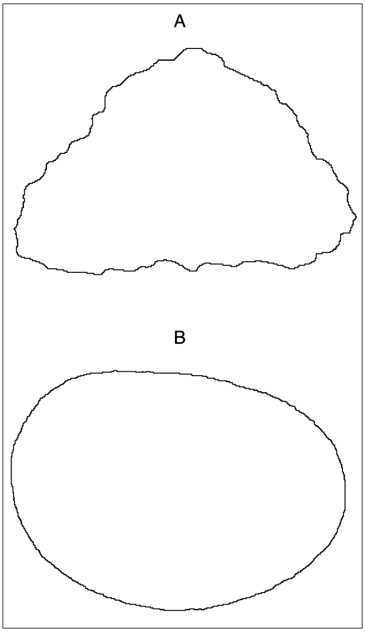

Figure 1. The profile of rock fragments with roundness values of (A) 0.1 and (B) 0.9. These profiles are representative of the profiles on the chart proposed by Krumbein (1941b).

PREPROCESSING OF DATA

All the methods proposed in this paper are based on the Fourier transform. The first step of these methods is to obtain the edge elements $(x(i), y(i)), i = 1, 2, 3, \ldots, M$, of the profile being measured. A centre point, (x_c, y_c), is determined and used to calculate the polar coordinates, $(\tilde{\rho}(i), \tilde{\theta}(i)), i = 1, 2, 3, \ldots, M$, of the edge elements. The centre point can either be calculated as the mean of the edge elements

$$x_m = \frac{1}{N}\sum_{i=1}^{N} x(i), \quad y_m = \frac{1}{N}\sum_{i=1}^{N} y(i) \tag{1}$$

or as the centre of gravity of the edge (Ehrlich and Weinberg, 1970; Clark, 1987, p. 261)

$$x_{cog} = -\frac{\sum_{i=1}^{N}[x^2(i) + x(i)x(i+1) + x^2(i+1)][y(i) - y(i+1)]}{3\sum_{i=1}^{N}(y(i) + y(i+1))(x(i) - x(i+1))}$$
$$y_{cog} = \frac{\sum_{i=1}^{N}[y^2(i) + y(i)y(i+1) + y^2(i+1)][x(i) - x(i+1)]}{3\sum_{i=1}^{N}(y(i) + y(i+1))(x(i) - x(i+1))}. \tag{2}$$

Full and Ehrlich (1982) suggested that a centre point be found that minimises the amplitude of the first Fourier transform coefficient, $F(1)$. This can be done either with an iterative technique or by minimising the derivative of $F(1)$.

The coordinates $(\rho(i), \theta(i))$, $i = 1, 2, 3, \ldots, N$, which are spaced at equal angular intervals, are then obtained by interpolation. Initially the linear interpolation

$$\rho = \frac{[\tilde{\rho}(i+1) - \tilde{\rho}(i)]\theta + \tilde{\rho}(i)\tilde{\theta}(i+1) - \tilde{\rho}(i+1)\tilde{\theta}(i)}{\tilde{\theta}(i+1) - \tilde{\theta}(i)} \tag{3}$$

was used where (ρ, θ) is the interpolated coordinate with θ lying between $\tilde{\theta}(i)$ and $\tilde{\theta}(i+1)$. Jarvis (1976, p. 1154) stated that the use of this linear interpolation is erroneous and that the trigonometric interpolation

$$\rho = \frac{\tilde{\rho}(i+1)\tilde{\rho}(i)\sin[\tilde{\theta}(i+1) - \tilde{\theta}(i)]}{\tilde{\rho}(i)\sin[\theta - \tilde{\theta}(i)] + \tilde{\rho}(i+1)\sin[\tilde{\theta}(i+1) - \theta]} \tag{4}$$

should rather be used. Clark (1987, p. 263) suggested the use of spline interpolation but found that the three methods' results do not indicate any clear superiority.

The Fourier transform of the radii, ρ, is then calculated and the roundness is determined from the Fourier transform coefficients, $F(u)$. Methods to determine the roundness from the Fourier transform coefficients have been proposed by Diepenbroek, Bartholomä and Ibbeken (1992), Ehrlich and Weinberg (1970) and Schwarcz and Shane (1969).

Procedure

The Krumbein chart was used to test the methods proposed in this paper. The chart was scanned at four different resolutions, thresholded and segmented to obtain the edge elements $(x(i), y(i))$, $i = 1, 2, 3, \ldots, M$ of the profiles. The mean lengths of the edges at each of the four resolutions were 749, 1499, 2286 and 4591 elements. The centre (x_c, y_c) of each profile was calculated using the mean of the edge elements (Eq. (1)), the centre of gravity of the edge (Eq. (2)) and the point that minimises the amplitude of the first Fourier coefficient, $F(1)$. It is furthermore proposed that the point that minimises the amplitude of the zeroth Fourier transform coefficient, $F(0)$, that is the mean radius, be used as centre point. These centres were then used to obtain the polar coordinates $(\tilde{\theta}(i), \tilde{\rho}(i))$ of the edge elements. The evenly spaced polar coordinates $(\theta(i), \rho(i))$ were then obtained using both linear (Eq. (3)) and trigonometric interpolation (Eq. (4)) (Fig. 2). Interpolation was done to give 512, 1024, 2048 and 4096 (the largest power of 2 less than the original resolution) coordinates for the four resolutions.

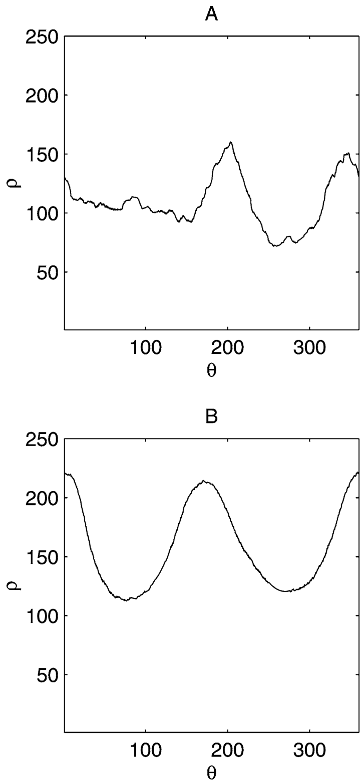

Figure 2. Polar coordinates of the rock fragments in Figure 1.

These data sets are referred to as OR (Original Resolution), ORL and ORT are used to distinguish between linear (Eq. (3)) and trigonometric interpolated (Eq. (4)) data sets (Table 1).

Furthermore, it is proposed that the edges of all four resolutions be downsampled to 512 edge elements. Downsampling was done with and without smoothing the $\tilde{\rho}$-values. Smoothing of the $\tilde{\rho}$-values was done using the Gaussian smoothing function

$$\bar{\rho}(i) = \frac{1}{T} \sum_{j \in W} \tilde{\rho}(j) e^{-(\tilde{\theta}(j)-\tilde{\theta}(i))^2/2\sigma^2}, i = 1, 2, \ldots, M \quad (5)$$

with

$$T = \sum_{j \in W} e^{-(\tilde{\theta}(j)-\tilde{\theta}(i))^2/2\sigma^2}.$$

Table 1. Abbreviations Used

Data sets	
DS	Downsampled without smoothing
DSG	Downsampled with smoothing
DSGL	Downsampled with smoothing, linear interpolated
DSGT	Downsampled with smoothing, trigonometric interpolated
DSL	Downsampled without smoothing, linear interpolated
DST	Downsampled without smoothing, trigonometric interpolated
GWM	Gaussian weighted mean
OR	Original resolution
ORL	Original resolution, linear interpolated
ORT	Original resolution, trigonometric interpolated
Methods	
BLPF	Butterworth lowpass filter
ILPF	Ideal lowpass filter
K–L	Kullback–Leibler distance

Note. Linear interpolation was done using (Eq. (3)) while trigonometric interpolation was done using (Eq. (4)). Downsampling was done to 512 edge elements. The Gaussian smoothing function (Eq. (5)) was used to smooth the data before it was downsampled. The Gaussian weighted mean data was obtained by using (Eq. (6)) to downsample the data to 512 edge elements.

The angular width, ω, of the smoothing function is

$$\omega = 2\lceil M/N \rceil \max(d\theta)$$

with M the number of edge elements, N the desired number of downsampled edge elements and $\max(d\theta)$ the maximum angular distance between two adjacent edge elements. Given the width, ω, of the smoothing function, the set W is defined as

$$W = \{j | \tilde{\theta}(i) - \omega/2 \leq \tilde{\theta}(j) \leq \tilde{\theta}(i) + \omega/2\}$$

while σ is defined as

$$\sigma = \frac{\omega}{5}.$$

This is an adequate relation between σ and ω as the smoothing function subtends 98.76% of the area under the Gaussian function (e.g. Trucco and Verri, 1998, p. 59).

The downsampled edge elements with polar coordinates, $(\rho(i), \theta(i)), i = 1, 2, \ldots, N$, were then obtained using (Eq. (3)) and (Eq. (4)) to interpolate between each pair of elements $(\bar{\rho}(j), \tilde{\theta}(j))$ and $(\bar{\rho}(j+1), \tilde{\theta}(j+1))$ that satisfies the relation $\tilde{\theta}(j) \leq \theta(i) \leq \tilde{\theta}(j+1)$. In the case of downsampling without smoothing

$\bar{\rho}(i) = \tilde{\rho}(i), i = 1, 2, \ldots, M$. These data sets are referred to as DS (downsampled without smoothing) and DSG (downsampled with smoothing). DSL and DSGL refers to linear interpolated (Eq. (3)) data sets while DST and DSGT refers to trigonometric interpolated (Eq. (4)) data sets (Table 1).

A further downsampling method proposed is the Gaussian weighted mean

$$\rho(i) = \frac{1}{T} \sum_{j \in W} \tilde{\rho}(j) e^{-(\tilde{\theta}(j)-\theta(i))^2/2\sigma^2}, \quad i = 1, 2, \ldots, N \tag{6}$$

where $(\rho(i), \theta(i)), i = 1, 2, \ldots, N$ are the N downsampled coordinates, T, ω and σ are as given above and

$$W = \{j | \theta(i) - \omega/2 \leq \tilde{\theta}(j) \leq \theta(i) + \omega/2\}.$$

These data sets are referred to as GWM (Gaussian weighted mean, Table 1).

The two interpolation methods (ORL and ORT) and five downsampling methods (DSL, DST, DSGL, DSGT and GWM) were used with the four centre determination methods giving 28 combinations. Each of these combinations was applied to the four resolutions resulting in 112 data sets on which the methods to determine roundness were tested. The results reported for the different methods and shown in the figures were obtained with the 2048 edge element ORL data set using the mean of the edge coordinates (Eq. (1)) as centre.

FOURIER TRANSFORM METHODS

Ehrlich and Weinberg (1970) proposed the use of the Fourier transform coefficients to determine a roughness coefficient,

$$P = \left[\frac{1}{2} \sum_{u=1}^{N-1} [R^2(u) + I^2(u)] \right]^{\frac{1}{2}}$$

where

$$F(u) = R(u) + jI(u).$$

They also proposed a modified roughness coefficient,

$$P_{kl} = \left[\frac{1}{2} \sum_{u=k}^{l} [R^2(u) + I^2(u)] \right]^{\frac{1}{2}}, \tag{7}$$

which is a function of a selected range of Fourier transform coefficients.

The method of Diepenbroek, Bartholomä and Ibbeken (1992) is based on the roughness coefficient (Eq. (7)) as it makes use of the sum of the amplitudes of the first 24 coefficients of the Fourier transform. To compensate for different size rock fragments the coefficients were divided by the zeroth coefficient. The ellipse which best approximates the profile of a rock fragment was obtained from the second Fourier coefficient. Subtracting the Fourier transform of this ellipse from that of the rock fragment made the method insensitive to sphericity. The removal of the effects of digitization or pixel noise, which was determined empirically as a function of the number of edge pixels, was also proposed.

The Diepenbroek method was implemented and the results obtained with this method were used as a reference against which the proposed methods could be compared. The method was tested using the first $N = 5, 6, \ldots, 60$ coefficients of the Fourier transform. The correlation between the calculated and actual roundness values, as a function of N, is shown in Figure 3. The first 23 coefficients of the Fourier transform gave the best results with a correlation of 0.95 (Table 2). The

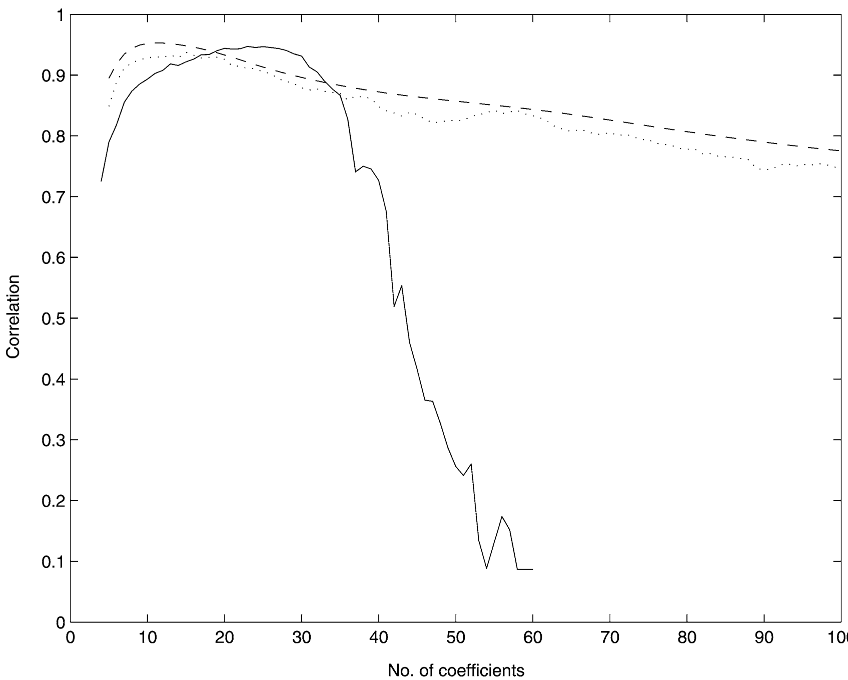

Figure 3. The correlation between the Diepenbroek (*solid line*), ILPF (*dotted line*) and BLPF (*dashed line*) roundness values and the actual roundness values as a function of the number of coefficients used.

Table 2. Summary of the Different Methods Used

Method	Corr.	Coef.	CoMR	e_{RMS}
BLPF	0.9531	11	0.9782	0.08198
Diepenbroek	0.9473	23	0.9731	0.1278
Emlen	0.9530	7	0.9873	0.08207
Entropy	0.9514	6	0.9908	0.08359
ILPF	0.9374	15	0.9778	0.09593
K–L	0.9269	4	0.991	0.1045

Note. These results were obtained with the 2048 edge element ORL data set using the mean of the edge elements (Eq. (1)) as centre. "Corr." is the correlation between the calculated and actual roundness values, "Coef." is the number of coefficients used, "CoMR" is the correlation between the mean roundness obtained for each class and the actual roundness and "e_{RMS}" is the root-mean-square error between the calculated and actual roundness values.

relationship between the Diepenbroek (with $N = 23$) and actual roundness values is shown in Figure 4.

In practice the mean roundness of a population of particles is used. Viewing each of the roundness classes as a population, the mean roundness was determined for each class. The correlation between the mean roundness values, as determined by the Diepenbroek method, and the actual roundness values was 0.97 (Table 2).

The motivation for using the mean of each roundness class is that the correlation of the individual roundness values is influenced by the spread of the values in each class while the spread of the values has no influence on the the correlation of the mean values.

These results were obtained with the 2048 edge element ORL data set using the mean of the edge elements (Eq. (1)) as centre. Similar results were obtained with the rest of the data sets. The correlation between the roundness values obtained with the different data sets were all above 0.98 (Table 3). The method is insensitive to resolution, centre point used and method of interpolation or downsampling (Table 3).

LOWPASS FILTER

Schwarcz and Shane (1969, p. 222) proposed that the difference between the lowpass filtered radii (ρ_f) and original radii (ρ) be used as a measure of roundness. They used the index of the cutoff coefficient, which resulted in an error of a specified size, as a roundness measure.

As an alternative it is proposed that the size of the error at a specified cutoff coefficient be used as roundness measure. This is done by attenuating the

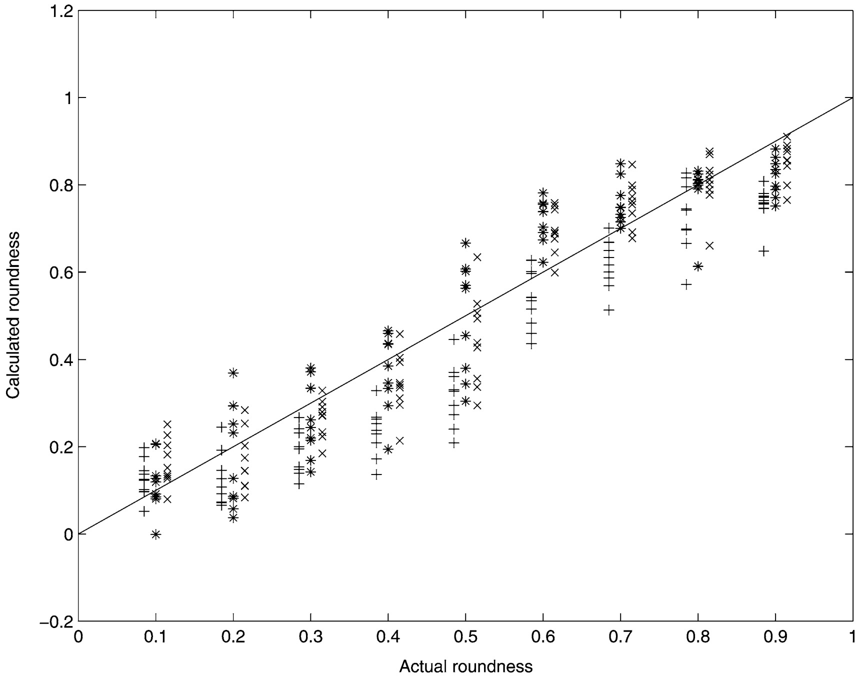

Figure 4. The relationship between the Diepenbroek (+), ILPF (∗) and BLPF (×) roundness values and the actual roundness values. The first 23 Fourier coefficients were used to calculate the Diepenbroek roundness values. An ideal lowpass filter (ILPF) with cutoff coefficient $N = 15$ and a Butterworth lowpass filter (BLPF) of order 2 and cutoff coefficient $N = 11$ were used to calculate the two sets of lowpass filtered roundness values.

Table 3. Summary of the Correlation Between Roundness Values Obtained with the Different Data Sets Using the Proposed Methods

	Resolution		Centre point		Downsampling		Filtering	
Method	Min	Max	Min	Max	Min	Max	Min	Max
BLPF	0.977	0.997	0.998	1.000	0.998	1.000	0.985	0.997
Diepenbroek	0.981	0.997	0.987	0.999	0.999	1.000	0.986	0.999
Emlen	0.954	0.998	0.989	0.999	0.991	1.000	0.957	0.990
Entropy	0.940	0.996	0.988	0.999	0.987	1.000	0.943	0.985
ILPF	0.949	0.989	0.978	0.999	0.999	1.000	0.950	0.995
K–L	0.928	0.996	0.981	0.999	0.929	1.000	0.930	0.997

Note. All pairs of data sets at different resolutions are compared in the columns headed “Resolution.” In the columns headed “Centre point” all pairs of data sets obtained with the different centre points are compared. The data set pairs (OR, DS) and (GWM, DSG) are compared in the “Downsampling” columns while the data set pairs (DS, DSG) and (DS, GWM) are compared in the “Filtering” columns.

high-frequency coefficients of the Fourier transform $F(u)$ using

$$G(u) = H(u)F(u)$$

where $H(u)$ is the filter transfer function. The inverse Fourier transform of $G(u)$ is the lowpass filtered radii ρ_f. The transfer function of the ideal lowpass filter (ILPF) with cutoff coefficient N is defined as

$$H_I(u) = \begin{cases} 1 & \text{if } u \leq N \\ 0 & \text{if } u > N \end{cases}$$

resulting in the N lowest order coefficients of the Fourier transform being kept unchanged and the rest set equal to zero.

An alternative to the ideal lowpass filter is to use the Butterworth lowpass filter (BLPF). The transfer function of the BLPF of order n, with cutoff coefficient N, is defined as

$$H_B(u) = \frac{1}{1 + [u/N]^{2n}}.$$

The difference between ρ_f and ρ represents the information in the high order coefficients which in turn represents the roughness, or deviation from roundness, of the rock fragment. This difference was determined using the mean absolute difference d_{m}, the maximum absolute difference $d_{\max}$ and the root-mean-square difference d_{RMS}. The least squares method was used to fit a function of the form

$$y = b_0 b_1^x,$$

where x is the difference and y is the actual roundness values, to the data. This was done for all the proposed methods.

The Fourier coefficients were used unchanged as well as normalised (divided by the zeroth coefficient). All the different combinations of filter (BLPF with $n = 1, 2, 3, \ldots, 10$ and ILPF), Fourier coefficients (normalised and unchanged) and difference measures (d_{m}, $d_{\max}$ and d_{RMS}) were tested.

Of the different variations, the BLPF of order 2 using normalised Fourier coefficients and the mean absolute difference gave the best results. The correlation between the calculated and the actual roundness values, as a function of N, is shown in Figure 3 while the relationship between the calculated and actual roundness values using $N = 11$ is shown in Figure 4. A correlation of 0.95 was obtained while the correlation between the mean roundness values and actual roundness values was 0.98 (Table 2). Similar results were obtained with all the data sets. The correlation between the roundness values obtained with the different data sets were all above 0.98 (Table 3).

Using the ILPF with $N = 15$, normalised Fourier coefficients and mean absolute difference resulted in a correlation of 0.94 while the correlation between the mean and actual roundness values was 0.98 (Figs. 3 and 4, Table 2). Similar results were obtained with all the data sets. The correlations between the roundness values obtained with the different data sets were all above 0.95 (Table 3).

Both methods showed a slight improvement in the correlation between the actual roundness values and the roundness values obtained as the resolution increased. However, using the DSG and GWM data sets gave slightly worse results than those obtained with the DS data sets. The lowpass filter methods is not sensitive to the centre point used or to the method of interpolation or downsampling (Table 3).

The results obtained using these variations of the method of Schwarcz and Shane (1969) agree well with the results obtained using the method of Diepenbroek, Bartholomä and Ibbeken (1992), however, these variations are much simpler. Furthermore, these methods are less sensitive to the number of Fourier coefficients that are used (Fig. 3).

MEASURES OF INEQUALITY

The Fourier transform produces a set of coefficients which are uncorrelated and have a large proportion of the total energy concentrated in a small number of coefficients. The transform coefficients of smooth data (such as the edge elements of a smooth particle) would tend to have a larger part of the total energy concentrated in a smaller number of coefficients than would be the case of less smooth data. It is therefore proposed that a measure which describes the energy distribution of the transform coefficients be used to determine roundness.

The following measures of inequality have been used as criteria in the selection of best mother wavelet (basic wavelet function), that is the mother wavelet that gives the best energy compaction for a given data set (Goel and Vidakovic, 1995, p. 7):

- Entropy (Shannon and Weaver, 1949, p. 21): The Shannon entropy, H, for a distribution, p, is given by

$$H(p) = -\sum_i p(i)\log(p(i)) \tag{8}$$

with

$$0\log(0) \stackrel{\text{def}}{=} 0.$$

- Emlen's modified entropy measure (Goel and Vidakovic, 1995, p. 7): This measure is related to the entropy measure and can be obtained by substituting $p(i)$ in (Eq. (8)) with $e^{-p(i)}$ resulting in

$$\phi_E(p) = \sum_i p(i)e^{-p(i)}.$$

If $p(i)$ in (Eq. (8)) is not normalised it should rather be substituted with $e^{\frac{-p(i)}{T}}$, where $T = \sum_i p(i)$ (Goel and Vidakovic, 1995, p. 7). This substitution results in

$$\phi_E(p) = \sum_i \frac{p(i)}{T} e^{\frac{-p(i)}{T}}.$$

Other measures of inequality exist, however it has been shown that the entropy and Emlen measures are the most successful at selecting the best mother wavelet (Goel and Vidakovic, 1995, p. 9; Drevin, 1999, p. 76). Entropy has also been used to determine cutoff coefficients with the Fourier transform (Drevin, 1999, p. 43; Drevin and Stoker, 2003).

A particle's form (sphericity) is described by its low order transform coefficients. For a method to be independent of sphericity it is therefore necessary that the low order coefficients be excluded from the determination of roundness. The measures of inequality were used to determine roundness values using Fourier transform coefficients with the $N = 1, 2, 3, \ldots, 100$ lowest order coefficients excluded. With both the Entropy and Emlen methods the $p(i)$ values were normalised using the sum of all the coefficients.

Both the entropy measure, with the 6 lowest order coefficients excluded, and the Emlen measure, with the 7 lowest order coefficients excluded, resulted in a correlation of 0.95 (Table 2, Fig. 6). The corresponding correlations between mean and actual roundness values in both cases were 0.99 (Table 2).

Similar results were obtained with all the data sets. The correlations between the roundness values obtained with the different data sets were all above 0.94 using the entropy measure and above 0.95 using the Emlen measure (Table 3). With both methods the correlation between the roundness values obtained and the actual roundness values improved slightly at the higher resolutions. However, using the DSG and GWM data sets gave results that were slightly worse than those obtained with the DS and OR data sets. These two methods are not sensitive to the centre point used or to the method of interpolation or downsampling (Table 3).

KULLBACK–LEIBLER DISTANCE

The Kullback–Leibler distance (Kullback and Leibler, 1951) between the distribution, p, of observed data and a model or predicted distribution, g, is given by

$$I(p, g) = \sum_i p(i) \log\left(\frac{p(i)}{g(i)}\right) \tag{9}$$

subject to the condition

$$\sum_i p(i) = \sum_i g(i) = 1.$$

The Kullback–Leibler distance is not symmetric, that is $I(p, g) \neq I(g, p)$. Adding $I(p, g)$ and $I(g, p)$ together gives

$$I_{\mathrm{m}}(f, g) = \sum_i p(i) \log\left(\frac{p(i)}{g(i)}\right) + \sum_i g(i) \log\left(\frac{g(i)}{p(i)}\right) \tag{10}$$

which is symmetric and therefore a metric distance (Brink and Pendock, 1996, p. 180).

The Kullback–Leibler distance between the profile and smoothed profile of a rock particle as a measure of the roundness of the particle is proposed. The distribution p is defined as the normalised cumulative distribution of the energy of the coefficients of the Fourier transform

$$p(i) = \frac{\sum_{j=0}^{i} E(j)}{\sum_{j=0}^{M} E(j)}$$

where $E(j)$ is the energy of the j'th Fourier coefficient and M is the number of coefficients. The model or smoothed profile is defined as the N low order Fourier coefficients of the particle with the distribution g defined as

$$g(i) = \frac{\sum_{j=0}^{i} E(j)}{\sum_{j=0}^{N} E(j)}$$

with $E(j) = 0$ for $j = N + 1, N + 2, N + 3, \ldots, M$.

The correlation between the Kullback–Leibler distance (for $N = 1, 2, 3, \ldots,$ 100) and the actual roundness values was calculated (Fig. 5) and it was found that

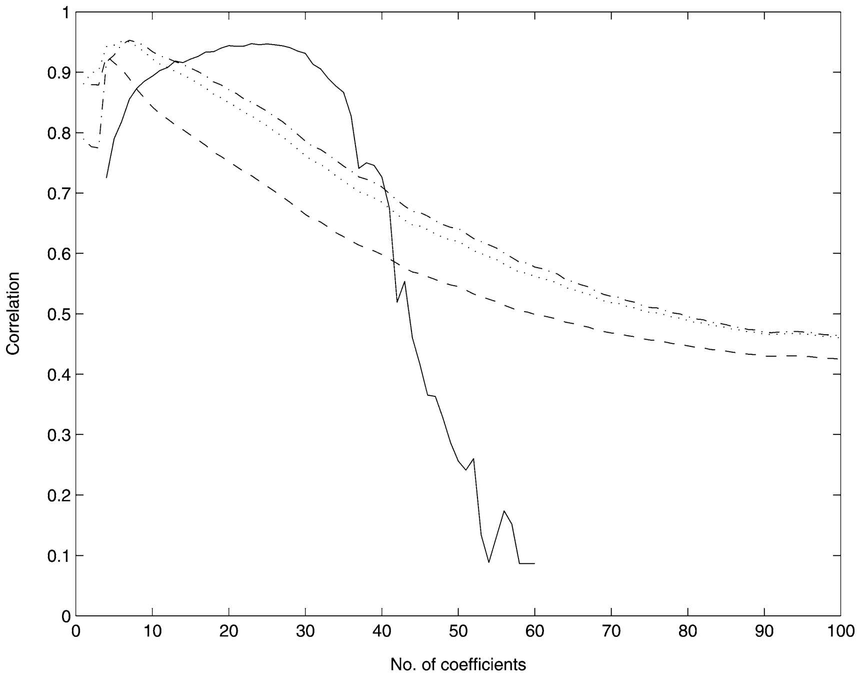

Figure 5. The correlation between the Diepenbroek (*solid line*), Entropy (*dotted line*), Emlen (*dash-dot line*) and K–L distance (*dashed line*) roundness values and the actual roundness values as a function of the number of coefficients.

using the 4 lowest order coefficients as model gave the best result with a correlation of 0.93 while the correlation between the mean and actual roundness values was 0.99. (Fig. 6 and method K–L in Table 2). It was further found that both the standard definition (Eq. (9)) and the symmetric definition (Eq. (10)) gave identical results.

The correlation between the actual roundness values and those obtained using the OR data sets decreased from 0.95 to 0.89 with increasing resolution while there was a slight improvement in correlation with increasing resolution for the DS data sets. However, the DSG and GWM data sets gave slightly worse results than those obtained with the DS and OR data sets. The method seems to be insensitive to the centre point used (Table 3).

COMPARISON OF PREPROCESSING METHODS

As stated previously, the different combinations of preprocessing steps resulted in 112 data sets. Roundness values for the profiles in these data sets were

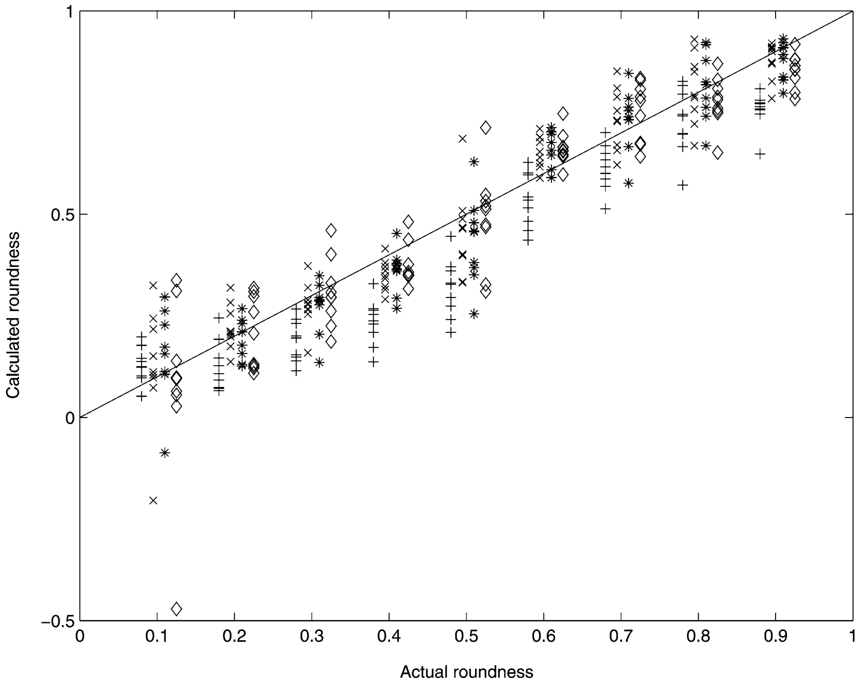

Figure 6. The relationship between the Diepenbroek (+), Entropy (×), Emlen (∗) and K–L distance (◇) roundness values and the actual roundness values. The 6 lowest order Fourier coefficients were excluded with the entropy method, the lowest 7 with the Emlen method while the 4 lowest order coefficients were used as model for the K–L distance method.

obtained using the proposed methods. The correlation between the roundness values obtained for the different data sets with the different methods are summarised in Table 3.

The correlation between all pairs of data sets at different resolutions were calculated while keeping the preprocessing parameters for each pair constant (heading "Resolution" in Table 3). The proposed methods are not that sensitive to resolution. Generally the correlation between the different resolutions was higher for the OR and DS data sets. The minimum correlation for the BLPF method using the OR and DS data sets as well as for the Emlen measure was 0.99 while it was 0.98 for the entropy measure. The ILPF method however did slightly better with the DSG and GWM data sets, giving a minimum correlation between resolutions of 0.96. The K–L method did best with the DS data sets, giving a minimum correlation between resolutions of 0.98.

The correlation between all pairs of data sets obtained with the different centre points were calculated while keeping the other preprocessing parameters constant (heading "Centre point" in Table 3). The choice of centre point is not critical, however one centre point must be used consistently as the choice of centre point has an influence on the number of coefficients and the regression parameters that have to be used.

To compare the downsampling and interpolation of the edge elements the correlations between the OR and DS data sets as well as between the GWM and DSG data sets were calculated while keeping the other preprocessing parameters constant (heading "Downsampling" in Table 3). There is very little difference between the roundness values obtained with the BLPF, Diepenbroek, Emlen and entropy methods. With the K–L method the GWM and DSG data sets gave close to identical results while the correlation between the OR and DS data sets improved with lower resolution.

To test the use of the Gaussian smoothing function the correlations between the DSG and DS data sets as well as between the GWM and DS data sets were calculated while keeping the other preprocessing parameters constant (heading "Filtering" in Table 3). Generally the use of the Gaussian filter had the least effect at the higher resolutions.

Both linear (Eq. (3)) and trigonometric (Eq. (4)) interpolation were used. The ORL and ORT data sets gave identical roundness values with all methods, as did the DSL and DST data sets and the DSGL and DSGT data sets. This result confirms the recommendation of Clark (1987, p. 263) that linear interpolation (Eq. (3)) be used as it is computationally the least expensive.

COMPUTATIONAL COMPLEXITY

All the methods were implemented in Matlab. To compare the computational complexity of the methods use was made of the FLOP (floating-point operation) counting function under Matlab Release 11 to time the methods using the OR data sets (Fig. 7). All the methods have a linear relation between execution time and the size of the data sets. The Diepenbroek method has the longest execution time, taking about 2.5 times as long as the lowpass filter methods and 5 to 7 times as long as the inequality (Entropy and Emlen) and K–L methods. The long execution time of the Diepenbroek method is due to the number of processing steps that have to be done. The methods proposed in this paper are much simpler and therefore have shorter execution times. It is necessary to do an inverse Fourier transform with the two lowpass methods resulting in longer execution times than for the K–L and inequality based methods for which no inverse Fourier transform is done. The ILPF method is slightly faster than the BLPF method due to the fact that with the BLPF method all the Fourier coefficients have to be multiplied with the filter transfer function while the high order coefficients are replaced by zeros with the ILPF method.

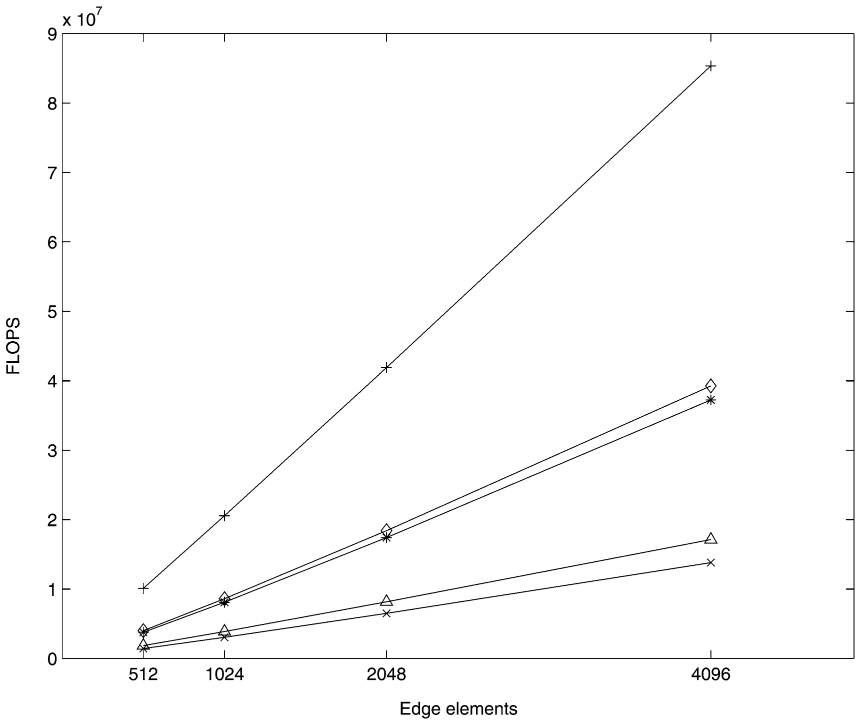

Figure 7. The execution times for the Diepenbroek method (+), Emlen (×), K–L (△), ILPF (*) and BLPF (◇) methods. The execution time for the entropy method lies between the execution times of the Emlen (×) and K–L (△) methods.

CONCLUSION

A number of computational methods that can be used to determine the roundness of rock particles have been proposed. Although the results obtained are generally comparable to those obtained with the method of Diepenbroek, Bartholomä and Ibbeken (1992), it was shown that the proposed methods are computationally less expensive.

Using linear (Eq. (3)) and trigonometric (Eq. (4)) interpolation gave identical results, as was stated by Clark (1987, p. 263).

The methods make use of the Fourier transform coefficients of the polar coordinates of the particles' edges. It was shown that the methods are insensitive to the centre point used to calculate the polar coordinates.

The methods were tested using different resolution images. It was found that the methods are more sensitive to differences in resolution than they are to the use of different centre points. However, most of the methods are less sensitive to resolution when the OR and DS data sets are used.

The significance of measuring the correlation of the mean values of the roundness classes can be seen when comparing the results of the Diepenbroek and K–L methods (Table 2, Fig. 6). While the correlation for the individual roundness values is higher for the Diepenbroek method than for the K–L method the opposite is true for the correlation of the mean roundness values. The spread of the roundness values in the roundness classes is generally the same or smaller for the Diepenbroek method (+) than for the K–L method (◇) (Fig. 6). However, the mean values for each class, obtained with the K–L method, is generally closer to the actual roundness values than is the case of the values obtained with the Diepenbroek method. If correlation of mean roundness is used to compare the different methods it follows that all the proposed methods are better than the Diepenbroek method with the K–L and entropy methods being far superior.

There is no difference between the results obtained with the methods where the high order coefficients are used (Emlen, entropy and K–L) and the methods where they are not used (Diepenbroek, BLPF and ILPF). Therefore, it does not seem that high frequency noise due to the scanning of the profiles has any influence on the results. It was however shown that methods fared worse when used on data sets that were smoothed with the Gaussian smoothing function. The use of a lowpass filter to remove spurious high-frequency noise does however need further investigation.

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