Using Fourier Transform Analysis to extract information from the shapes of folded layers.

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Abstract

Objective methods of fold shape analysis are necessary to better understand the behavior of folds and the folding process. I examined two methods of analysis, and used a method based on the Fourier Transform to show that the method based on the Fourier Series was insufficient for identifying shape characteristics of aperiodic natural fold trains. I also showed that the Fourier Transform method accessed information that was inaccessible using the Fourier Series method.
Introduction

Differences in fold shape have long attracted the interest of geologists, in part because of the wide variety of shapes that natural folds assume. While all folds share superficial shape similarities, differences often arise under closer scrutiny. Geologists seek to understand these differences by recognizing several characteristic features of folded layers. We can identify four points that provide a foundation on which to build methods of analysis (Fig. 1). The fold crest (c) is the highest point on the fold, and the trough (t) is the lowest. These points move along the fold surface as it is rotated because we choose their location with respect to an external frame of reference. For this reason, we call them \textit{variant} points. The other two points will not move, however, as we choose their location by measuring values of curvature along the fold's length, which do not change under rotation. The hinge (h) is the point of maximum curvature, while the inflection point (i) is the point at which the curvature changes from concave up to concave down. Both are \textit{invariant} points.

Geologists have made many attempts to quantify the shape characteristics of folds, in an effort to ease statistical studies and to provide an unambiguous language for discussing fold geometry. The methods they propose to accomplish this, however, vary according to the shape attributes of the fold on which they focus. One method focuses on thickness/dip relations, and in this way distinguishes between similar and parallel folds. Parallel folds are those that exhibit constant layer thickness measured perpendicular to bedding. In contrast, similar folds exhibit constant layer thickness measured parallel to the axial surface (Fig. 2). Ramsay (1967) proposed a more detailed method based on the orientation of dip isogons within the fold (fig. 3). Under this scheme, folds would be placed into one of five groups. We place those that possess convergent dip isogons in class 1, and make further distinctions based on the distribution of layer thickness. Folds that exhibit parallel dip isogons occupy class 2 (all class 2 folds are similar folds), and class 3 folds are those with divergent dip isogons. More detailed still is the method Hudleston (1973a) proposed, which focuses on three parameters related to limb thickness, dip, and angles between isogons and tangents to bedding. The most mathematically rigorous method, however, is that of Harmonic, or Fourier, analysis.

Within the field of physics, Fourier analysis has enjoyed widespread acceptance as a useful mathematical technique for examining complex waveforms. It is used in signal processing applications to determine the frequency content of "noisy" signals (Stearns & Hush, 1990; Broch, 1990), in experimental physics to identify the onset of turbulence in fluids (Gollub & Swinney, 1975), and in theoretical physics to study the nature of
dynamical systems (Crutchfield et al, 1980). Despite its success in physics, there has been relatively little use of Fourier analysis in geology (outside the area of geophysics, e.g. Barber, 1966).

During the sixties, structural geologists began to recognize the potential value of this type of mathematical analysis (see Norris, 1963). Chapple (1968), Stabler (1968), and others, for example, developed methods of fold analysis and classification based on the Fourier Series. Hudleston (1973a, 1973b) used this new method to the greatest extent in his studies of arbitrary fold shapes, and of natural folds in the Monar region of Scotland. The problem with this method, however, is that it requires folds to be perfectly periodic, an unrealistic requirement for natural folds. Thus, in order to carry out his analysis, Hudleston (1973a, 1973b) had to break the folds up into quarter wavelength segments, which he could then conceptually make periodic. In this way, Hudleston was not so much analyzing the shape of natural folds as he was analyzing the shape of periodic simplifications of natural folds.

In this study, I introduce a new method of analysis based on a close relative of the Fourier Series, the Fourier Transform. I show that this method is better suited to the analysis of natural folds, and that it provides more detailed information on the shape content of fold trains than does the Fourier Series. I also enumerate some ways in which the Fourier Transform provides information that we cannot get using a method based on the Fourier Series.

Mathematical considerations

The Fourier Series

Fourier theory states that one can approximate almost any curve by means of a series expansion. Because the Fourier Series is unfamiliar, it is useful to "derive" it from a more common series expansion. A Taylor expansion serves this purpose well. One can use the Tayor series to approximate an irregular curve by a sum of polynomials given by:

\[ F(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3 + \cdots = \sum_{n=0}^{\infty} \alpha_n \cdot x^n \]  

which is a power series in \( x \) (Simmons, 1985). Replacing \( x \) with \( \beta \sin(\gamma) \) (Broch, 1990) and substituting using the identities
yields:

\[
\sin^2(\gamma) = \frac{1}{2} - \frac{1}{2} \cos(2\gamma)
\]

\[
\sin^3(\gamma) = \frac{3}{4} \sin(\gamma) - \frac{1}{4} \sin(3\gamma)
\]

\text{etc.}

This series is called the \textit{Fourier Series} (FS). While eq. 2 is a valid expression, the FS is more commonly written in terms of time, where \( \gamma = \omega_0 t \) so that the series looks like

\[
F(t) = \sum_{n=0}^{\infty} A_n \cos(n\omega_0 t) + \sum_{n=0}^{\infty} B_n \sin(n\omega_0 t)
\]

(3)

where \( t \) is the time variable, and \( \omega_0 \) is the frequency of the fundamental wave. The coefficients \( A \) and \( B \) are called the Fourier Coefficients, and are unique to each waveform. This uniqueness provides a simple method of curve classification based on these coefficients, as we will see later in this paper.

In addition to being expressed as a trigonometric function, the FS is sometimes written as a complex exponential function of the form:

\[
F(t) = \sum_{n=-\infty}^{\infty} c_n e^{i2\pi n\omega_0 t}
\]

(4)

where

\[
c_n = \frac{1}{T} \int_{-T/2}^{T/2} F(t) e^{-i2\pi n\omega_0 t} dt, \quad n = 0, \pm 1, \pm 2, \ldots
\]

(5)

As the first sentence in this section implies, not every curve will have a Fourier Series expansion. In order to insure that a FS for the curve can be found, the curve must meet the following conditions:

1) the curve must be periodic with period \( T \)
2) the curve must be bounded
3) in any one period, the curve must have at most a finite number of discontinuities and a finite number of maxima and minima.

These conditions are called the Dirichlet conditions, and they impose some cumbersome constraints on the types of folds we can analyze.

These conditions show an important property of the FS: it can approximate only periodic curves. This is clear when one examines eq. (3). The variable \( n \) is always an integer, so the sine and cosine terms always repeat at integer multiples of \( \omega_0 \), (i.e. \( \sin(2\omega_0) \), \( \sin(3\omega_0) \), \( \sin(4\omega_0) \), etc. This fact becomes important when we identify the third coefficient within a plot of the Fourier Transform.)

The requirement of periodicity is often problematic when analyzing naturally occurring curves or time sequences, as they are rarely exactly periodic. In cases where a curve is not periodic, but varies randomly (containing frequencies not at integer multiples of some fundamental frequency), frequency analysis is still possible. All that happens mathematically is that the sum in the FS becomes an integral, and we call the resulting "series" a Fourier Transform.

The Fourier Transform

The main difference between a FS and a Fourier Transform (FT) is that the FT is a continuous function of time and is defined for the interval \(-\infty\) to \(\infty\) instead of just \(-T/2\) to \(T/2\). The FT itself is given by:

\[
H(\omega) = \int_{-\infty}^{\infty} F(t)e^{-i\omega t} \, dt \quad (6)
\]

where

\[
F(t) = \int_{-\infty}^{\infty} H(\omega)e^{i\omega t} \, d\omega \quad (7)
\]

In both of these equations, \( H(\omega) \) is a continuous function of time, so that it requires sinusoids of all frequencies for its expansion (Richards, 1991). In cases where the curve is periodic, the FT yields the same information as the FS (Richards (1991) provides a non-rigorous proof of this), indicating a clear connection between the two techniques.
Figure 1  Showing four kinds of points used as references when describing a folded layer. The crest (c) is the highest point on the fold, and the trough (t) is the lowest. We place the hinge at the point of maximum curvature, and the inflection point where the curvature changes sign.
Figure 2  a) parallel folds exhibit constant layer thickness measured perpendicular to bedding. b) similar folds, however, exhibit constant thickness measured parallel to the axial surface.
Figure 3  Classification of single layer folds based on the orientations of dip isogons.
(From Suppe, 1985)
The true utility of this method of analysis, however, is that curves need not meet the first Dirichlet condition. We may analyze almost any continuous curve, which means that we do not have to find folds that "fit" our method of analysis. Instead, we can analyze all folds (subject to some additional constraints that I will discuss later), and analyze their entire length at once, rather than breaking them up into periodic segments.

Clearly, the FT has its liabilities, the most prominent being that the integral goes from \(-\infty\) to \(\infty\), a condition rarely met by time sequences, and never met by natural folds. The result is that one rarely calculates the FS or FT when working with real-world data. Instead, one calculates a kind of "series" related to both of them, but also different from both, called the *Discrete Fourier Transform* (DFT).

**The Discrete Fourier Transform**

The DFT is given by:

\[
H_n = \frac{1}{N} \sum_{k=0}^{N-1} h_k e^{-2\pi i nk/N}
\]  

(8)

While the DFT is only an approximation of the continuous FT, it is an exact transformation of the N sampled data points (Richards, 1991). Like the FT, it is also exactly invertible (Stearns & Hush, 1990), allowing us to recover the original curve from the resulting data, a feat not possible with the FS as applied by Hudleston (1973a & 1973b).

The output of both the FT and DFT is a graph in frequency space called a spectrum (not to be confused with a power spectrum, which is the square of the FT or DFT). In the case of the FT, the graph is an unbroken curve representing a continuous function, and in that of the DFT, the graph is a sequence of separate values representing a function. Table 1 summarizes the relationship between the FS, FT, and DFT.

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<tr>
<th></th>
<th><strong>Input</strong></th>
<th><strong>Output</strong></th>
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<tbody>
<tr>
<td>Fourier Series</td>
<td>a function</td>
<td>a sequence of numbers</td>
</tr>
<tr>
<td>Fourier Transform</td>
<td>a function</td>
<td>another function</td>
</tr>
<tr>
<td>Discrete Fourier Transform</td>
<td>a sequence of numbers</td>
<td>a sequence of numbers</td>
</tr>
<tr>
<td></td>
<td>representing a function</td>
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Table 1 summarizing the relationships between the three methods of Fourier analysis.
One negative attribute of the DFT is that certain errors can occur if the curve is not sampled correctly. A minor one for our purposes, quantization error, occurs when the computer one is using to carry out the calculations receives numbers representing a curve from an analog-to-digital converter. The numbers will be integers, so that the largest signal will be associated with a large integer, and the smallest with a small integer. Most often, though, the closest small integer is not exactly correct for a linear correspondence. This is quantization error (see Broch, 1990; Stearns & Hush, 1990; Richards, 1991). A more crucial error, however, is aliasing.

When one samples a curve, there is an upper limit to the frequencies that can be transferred to the data set. Fig. 4 (taken from Blackman & Tukey, 1958) shows a sine wave that is sampled at six points along its length. Clearly, the sample interval is insufficient to describe the overall shape of the sine curve, but more importantly, the data set produced by this interval is indistinguishable from that which would be produced by sampling the lower frequency curve indicated by the dotted line. In this way, our results are not only imprecise, but grossly incorrect. One can avoid this error, however, by choosing an appropriately small sample interval, an interval where the sampling frequency is at least twice the highest frequency in the curve \( f_s > 2f_{\text{max}} \).

In this study, I will calculate both the FS and the DFT of data representing fold segments. For simplicity’s sake I usually talk of calculating the FT, but the reader should be aware that almost always I am actually calculating the DFT.

Analysis of Fold Shapes

Analyzing fold shape for its own sake may be interesting, but it is easier to complete such a time consuming process when the results lead to a better understanding of the process of fold formation. The ultimate aim, then, of all fold analyses is to use a fold’s shape to infer the processes behind its formation. For example, we can conceive three primary folding mechanisms: buckling, bending, and passive amplification. We can also envision that each of these will carry with it some diagnostic fold shape. The expectation, then, is that by objectively measuring the shape of a fold, we can infer the particular process behind its formation. The following is an attempt to determine which method of analysis (FS or FT) most objectively, and completely, portrays the information contained in a folded layer.

With any scientific study involving preliminary observations, it is customary to restrict the observed system to as few degrees of freedom as possible. Huang & Turcotte
Figure 4 Sampling of sinusoidal waves, illustrating the origin of aliasing. The dashed curve indicates the wave that will effectively be sampled due to the insufficiently large sampling interval.
(1990), for instance, studied complex fault systems by constructing experiments consisting of single or multiple blocks allowed to move only in one direction along a horizontal plane. In that study, and in others, the experimenters were able to control (somewhat) the behavior of their system, and as such, were able to identify the factors that most affect its behavior. In this spirit, I sought to limit the folds I examined to only those in isolated single layers. This approach is useful for a number of reasons, among them the possibility that the spectra for such a layer will have a spectrum that is characteristic of one or more folding mechanisms. For example, spectra that indicate that both the top and bottom of a folded layer have exactly the same shape will indicate that the fold formed by a passive amplification mechanism. Folds that have a chevron to kink geometry may be associated with a bending mechanism, and buckle folds should develop a dominant wavelength (indicated by peak on the spectrum of the fold). The single layer approach is also useful because it allows easier comparison with theoretical analyses. The theory for single layer folding is much more developed than the theory for multiple layer folding.

Many works, such as introductory structure texts, provide good illustrations of fold profiles (Ramsay & Huber, 1987; and Weiss, 1972 also provide such illustrations). The folds used in this study, however, came from Hudleston (1973b). I chose the folds I did because they were isolated single layers, they provided good resolution, and they had already been analyzed (albeit by a method based on the Fourier Series). Working from these folds allowed me to test the reproducibility of Hudleston's analysis, as well as giving me an opportunity to test the quality of my own FT analysis.

Figure 5 shows the two sets of folds that I used for my analysis, as well as their quarter-wavelength divisions. Fig. 5a is a ptygmatic vein in a pelitic rock, and Fig. 5b shows portions of folds in a package of layered granulites. Both of these sets are relatively small, consistent with my attempt to reduce the number of factors taking part in the development of the folds. By using small folds, I hoped to limit the effect that body forces (such as gravity) had on the fold's shape. Small-scale structures also tend to provide longer fold trains within a single exposure than do larger structures.

Because this study centered around the applications of functional analysis to that of fold shape, I needed to impose a fundamental constraint on the folds that I used. I had to be able to define the fold as a continuous and everywhere differentiable function in order for either the FT or FS methods to work (Stearns & Hush, 1990). This does not imply that I actually needed a mathematical equation for the fold, but simply that the fold must behave geometrically like a function. Simmons (1985) and other texts detail what constitutes a function, but we can reduce our definition to include only two criteria: 1)
when placed in a Cartesian coordinate system, the fold must have only one sampled value for a given value along the horizontal axis, and 2) it must not have any breaks (see Fig 6). Again, natural folds do not often meet this criterion. We can, however, generalize the requirement and state that the fold, if it cannot be defined as a function, must simply be able to be broken up into segments that can.

After determining which folds would be suitable for my analysis, I converted them into a sequence of numbers that could be manipulated by computer. I did this using a digitizing program called Sigma Scan that allowed me to sample the folds at various equally-spaced intervals. (The samples needed to be taken at equal intervals because of the way in which the FT was ultimately calculated) Before I could digitize the fold, however, Sigma Scan required that I place it in a coordinate system that it could use as a reference. In each case, I chose a system that would allow the fold to meet my first criterion for a function, despite the fact that the system was admittedly non-unique for some folds (Fig. 7). (I remind the reader that the DFT is ultimately invertable, so that I can reproduce the original fold shape, regardless of its orientation.) Because I traced the folds by hand, and because I traced the resulting image once more using Sigma Scan’s plotter, there was likely a good deal of fine-scale error in the final product (Fig. 15). For this reason, I chose a sampling interval that would provide approximately 125 data points for a segment roughly 20 centimeters long, although I could have achieved much better resolution. By doing so, I was able to produce enough data points to reduce the effects of aliasing ($f_s > 2f_{max}$), without generating so many points that I illuminated shape characteristics that were not present in the original fold.

**Traditional Harmonic Analysis**

Before calculating the FT of the entire train, I first employed the more conventional method of harmonic analysis based on the FS. I calculated the first few FS coefficients using the method outlined in Hudleston (1973a), who maintains that an important requirement in harmonic analysis is that an unambiguous frame of reference be chosen. To this end, he submits that a coordinate system based on the quarter-wavelength segment between adjacent hinge and inflection points (also called invariant points) is most appropriate (Hudleston, 1973a). Their placement, however, is not always easy (especially as the fold segment becomes more circular). The difficulty in placing the invariant points must be overcome, however, as the values of the resulting coefficients are very sensitive to their placement.
One may position the invariant points using a method that involves calculating the values of the first and second derivatives along the length of the fold. Under this scheme, the hinge points are placed where the first derivative is zero, and the inflection points where the second derivative changes sign. This method only works if the fold is perfectly sinusoidal, so that the value of the first derivative at any hinge point will be zero (Fig. 8). If the fold is not perfectly sinusoidal, the slope of the tangent at the hinge point may not be zero, and the method fails (Fig. 8b).

With these difficulties in mind, I chose to use a different method that focused on the value of the curvature along the curve, rather than on the value of the first and second derivatives. Under this scheme, the curvature is given by:

\[ k = \frac{d^2y/dx^2}{[1+(dy/dx)^2]^{3/2}} \]  

(9)

I calculated the actual values of \( \frac{dy}{dx} \) and \( \frac{d^2y}{d^2x} \) by fitting a second-degree polynomial to sequential triplets of points along the digitized curve using a program called Cricket Graph III. Once I found a polynomial, I substituted the value of the central point into the appropriate equation for \( \frac{dy}{dx} \) and \( \frac{d^2y}{d^2x} \) to find the value of \( k \). I then placed the inflection points where \( k = 0 \), and the hinge points where \( k \) was at a maximum.

With the hinge and inflection points in hand, I was able to establish an appropriate "quarter-wavelength" coordinate system by which I could calculate the FS coefficients. I carried the calculations out in a manner consistent with Hudleston's technique by using the equations produced by Stabler (1968) to find the first three sine-series coefficients. The equations are based on three sampled values (Fig. 9) taken at equally spaced intervals, and are given by:

\[ b_1 = (y_1 + \sqrt{3}y_2 + y_3)/3 \]
\[ b_3 = (2y_1 - y_3)/3 \]
\[ b_5 = (y_1 - \sqrt{3}y_2 + y_3)/3 \]  

(10)

I used the resulting values of \( b_1 \) and \( b_3 \) for the rest of the study.
Figure 5 The folds that I used for my analysis. a) is a ptygmatic vein in a pelitic rock, and b) is a package of layered granulites.
Figure 6  a) this curve may not be defined as a function (using cartesian coordinates) because it has more than one value of $y$ for a given value of $x$, indicated by the vertical line. b) This curve may be defined as a function.
Figure 7  a) this coordinate system does not allow the curve to be defined as a function b) Showing the same curve in a coordinate system that will allow it to be defined as a function.
a. if the curve is sinusoidal, the value of the first derivative at a hinge point will always be zero. b) if, however, the curve is not sinusoidal, the value of the first derivative at the hinge point will not always be zero.

Figure 8 a) if the curve is sinusoidal, the value of the first derivative at a hinge point will always be zero. b) if, however, the curve is not sinusoidal, the value of the first derivative at the hinge point will not always be zero.
Results of the Harmonic Analysis

I pointed out earlier that the FS coefficients are the components of the series that are unique to a given curve, and are useful in classifying fold shape. They also traditionally constitute the most important part of Fourier analysis (see Hudleston, 1973a & 1973b). Each of the coefficients represents a portion of the shape information contained in the entire series, with the lower order harmonics holding most of the information (this is the case for most naturally occurring folds). For this reason, it is most appropriate to focus on the first few coefficients when comparing shape information between folds. Plots of the third harmonic coefficient b3 against the first b1 are particularly useful in representing fold information, as are plots of log bn against log n (Hudleston, 1973a).

Figures 10 and 11 (taken from Hudleston, 1973a) illustrate some of the above representations for a few idealized fold types. Figure 10 shows a generalized plot of b1 vs. b3; Fig. 11 shows "spectral graphs" for box folds, sine waves, and chevron folds. The spectral graphs are simply plots of log bn vs. log n, which are useful because they allow us to view the shape content of a fold, not just in spatial terms (to which we are accustomed), but in terms of the extent to which the fold is, or is not, sinusoidal. The plots are also convenient because they allow us quantitatively to assign qualitative names to fold segments. Although this may seem pointless, it provides a way to link Fourier analysis to well-worn methods, such as the Ramsay classification (see Suppe, 1989 or any other introductory text in structural geology), and makes it easier to speak of the folds in more general terms.

Using the method outlined above, I calculated the first three FS coefficients. Figure 12 shows the resulting b1 vs. b3 plots for the ptygmatic vein; Fig. 13 shows the corresponding plots for the folds in the granulites. Both plots are similar to those obtained by Hudleston (1973b), suggesting an appropriate degree of repeatability in his analysis. They also show some degree of clustering about a small area, which suggests that each quarter-wavelength segment contains some information about the entire fold train, although it is not clear how much, or in what way, the quarter wavelengths relate to the train.

Comparing these figures with Fig. 10, it is clear that the plots of b1 vs. b3 span three different shape fields, from sine waves to semi-ellipses. This spread indicates, in contrast to the "clustering", that the individual values of b1/b3 convey different information. Table 2 summarizes the data contained in Figs. 12 and 13.
Figure 9 showing a portion of a curve being sampled at three equally-spaced points. These provide the values used to calculate the first three Fourier sine-series coefficients according to the Stabler (1968) equations.
Figure 10 a generalized plot of $b_1$ vs. $b_3$. Each field represents a different shape. (From Hudleston, 1973a).
Figure 11 spectral graphs for three idealized fold shapes. a) for a semi-circle, b) for a sine wave, and c) for a chevron fold. (From Hudleston, 1973a).
Figure 12  Plot of $b_1$ vs $b_3$ for the ptygmatic vein. Notice that the points cluster around one area, but they still spread across different shape fields according to Fig. 10.
Figure 13 Plot of $b_1$ vs. $b_3$ for the layered granulites.
Calculating the Fourier Transform

In the section on mathematical considerations, we learned that the FT was useful in a number of respects, but that two stood out. The first is that it enables us to take a curve in the space or time domain and view it in the frequency domain (making clear some shape characteristics we would not otherwise see). Secondly, it allows us to analyze virtually any fold, regardless of periodicity. These and other positive attributes suggest that the FT might be a powerful tool in analyzing the shape of naturally occurring folds, which have inherently questionable periodicity.

There are, however, three additional positive attributes that are more applicable to the present study, and provide a logical sequence with which to discuss the results of the FT analysis:

1) The FT allows us to recover the information supplied by the FS.
2) The FT allows us to assess the quality of the FS information.
3) The FT gives us information not contained in the FS.

These, plus the fact that the FT allows us to examine an entire fold train at once, further suggest that the FT is a much more powerful tool for analyzing natural folds than the FS.

Calculation of the FT

A number of data analysis programs such as Mathcad and Systat, as well as some more sophisticated spreadsheet programs like Microsoft Excel, calculate Fourier Transforms of data sets. I chose to calculate the FT of my sampled folds using Mathematica, a program for doing mathematics by computer. I chose it for the ease in which I could import the fold data, and for the flexibility to manipulate the output that the program gave me. (These manipulations took the form of changing the maximum and

<table>
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<th>Range of b1/b3</th>
<th>Average value of b1/b3</th>
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<td>ptygmatic vein, lower</td>
<td>5.08-20.26</td>
<td>10.95</td>
</tr>
<tr>
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<td>4.78-17.14</td>
<td>9.15</td>
</tr>
<tr>
<td>surface</td>
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Table 2 summarizing the data in Figs. 12 & 13
minimum values along the axes to improve resolution. I never changed the numerical
values of the FT.) Mathematica required that the imported data be only a list of sampled
values (i.e. "y-values"), which meant that I had to drop the x-values from the digitized list
of coordinates. This is why I sampled the fold at equally-spaced x-intervals.

When Mathematica processed the resulting list (minus the x-values), it assigned
each of the y-values an arbitrary value for x, so that the first y-value was given an x-value
of 1, the second an x-value of 2, and so on. Because the x-values were originally equal
distances apart, this process did not affect the shape of the fold.

The program calculated a DFT (eq. 8) of the data and plotted it in a graph of
transform value vs. frequency, called a spectrum (Fig. 14 provides an example of a
Mathematica worksheet). Although this plot resembles the familiar power spectrum, it is
important to note that it is not. The power spectrum, by definition, is again given by:

\[ H_p(\omega) = |H(\omega)|^2 \]  

(11)
or simply the square of the FT. Mistaking Mathematica's output for a power spectrum
would not alter one's interpretations of the fold's frequency, but it would drastically affect
the ratio of transform values at two different frequencies.

Recovery of FS information

Stearns & Hush (1990) and Richards (1991) give detailed examples showing that
the FT contains the same information provided by the FS. Moreover, Richards (1991)
shows that the FT of a periodic curve is a FS. Because they handle this topic so well, I
defer to these works for the formal proofs, and simply offer the following thought
experiment to justify my contention that the FT of a fold train contains the FS coefficients
of a smaller piece of the fold.

Consider a periodic curve (a sine wave, for simplicity's sake) like the one shown
in Fig. 15, and suppose that we identify a quarter-wavelength segment like the one
marked "A". This curve will have a FT spectrum comparable to the one in Fig. 15b, and
because the curve is assumed to be periodic, the FT value at \( \omega=1 \) will be equal to the
value of the FS coefficient \( b_1 \) (Richards, 1991). Now suppose that we fix the hinge and
inflection points surrounding "A", and deform the rest of the fold. As the fold becomes
more aperiodic, non-zero values for the FT begin to show up at frequencies other than 1.
Because "A" has not moved, however, the point on the spectrum that represented its
shape will still exist, also not having moved. At the end of the deformation sequence, we
are left with the more natural-looking fold shown in Fig. 15 c. The fold's FT has changed markedly, but the original value of b1 is still present.

Given that the FS coefficients are present in the FT spectrum, how do we find them? What follows below is an outline of the process.

Figure 5 shows the folded ptygmatic vein from Hudleston (1973b), and Fig. 16 shows the digitized plots for each of the surfaces. The jagged regions indicated by the circles are areas of "experimental noise", where my hand shook or the plotter did not move smoothly across the paper. Because these errors occurred as isolated incidents (as well as non-periodic), they will not show up on the FT plot as substantial shape contributions, rather, they will show up only as "noise" (signals of undetermined frequency, but with almost no power).

The result of the FT calculations for the two curves is shown in Fig. 17. In these plots, we can see that there are peaks in the value of the FT at certain frequencies for both curves. The four dominant peaks in Fig. 17a correspond to frequencies of 2, 4, 6, and 9, and the first four peaks in Fig. 17b correspond to frequencies of 1, 4, 7, and 10. One can easily read these values off of the x-axis, but what do they mean? Mathematica's convention is to use the length of the sampled curve (about 125 data points for both curves in Fig. 16) as an arbitrary unit length. A frequency of 4 means that the analyzed curve contains a sinusoidal component that repeats 4 times along the length of the sampled segment. Because \( \omega = 1/T \), we may also identify the period of the sinusoid (1/4 in the present case).

To make clearer this relationship between the peaks and their corresponding sinusoids, I superimposed the graphs of the first four sine waves onto each fold surface (Fig. 18). In Fig. 18a we see that the first peak represents a large scale wave of which our fold segment makes up approximately one wavelength. If I were to rotate this entire segment a few degrees clockwise or counterclockwise, the value of the first peak would change, indicating that the first peak is somehow responsible for the bulk orientation of the segment. It does not, however, seem to contain much information on the bulk shape of the segment. We see the same relationship in Fig. 18b, only in this case, the first peak represents a sinusoid of period 1.

When the segment rotates, the second peak does not move appreciably. This suggests that this peak represents a wave that is controlling a major portion of what is not changing during rotation: the bulk shape of the segment. Because of this implied control over bulk shape, I associated this peak in the value of the FT with the FS coefficient b1.
Figure 14 This is an example of a *Mathematica* worksheet.
Figure 15 If we start with the curve in a), we will generate a spectrum comparable to the one in b). As we deform the fold, holding the segment "A" constant, the spectrum will change, but it will always contain a portion of the original information to account for the shape of "A".
Figure 16 The digitized plots of the folds in Fig. 5. The circled regions denote areas of experimental error.
Figure 17 Results of the FT calculation for the curves in Fig. 15, indicating the location of the FS coefficients b1 and b3.
Figure 18 The first few harmonics of the FS expansion.
While this association seems reasonable, we may check its validity by locating the coefficient $b_3$ and seeing if we find values of $b_1/b_3$ similar to those in Table 2.

I located $b_3$ by using the equations for the FS. From eq. 3, the equations for the first three sine components are:

$$ \sin(\omega_0 t), \quad \sin(2\omega_0 t), \quad \text{and} \quad \sin(3\omega_0 t) $$

(12)

(Each of these would be preceded by the coefficients $b_1$, $b_2$, and $b_3$, respectively, but these provide only the amplitude of the waves, which is not important here.) The graphs of these equations are analogous to the component waves in Fig. 18, and eqs. 12 indicate that we can find their graphs if we know $\omega_0$. From the results of the FT, and according to my assumption from the previous paragraph, we know that $\omega_0$ (again, the frequency of the fundamental wave) is equal to 4 for both surfaces in the ptygmic vein. It is clear, then, that the $b_3$ wave must have a frequency of $3\omega_0$, or 12 (Fig. 17). The locations of $b_1$ and $b_3$ at $\omega=4$ and $\omega=12$ will be the same for both the upper and lower fold surfaces.

In the case of the lower surface, the FT values (and hence the associated FS coefficients) at these two frequencies are 9.6 and 0.8, respectively, meaning that $b_1/b_3=12$. The values of the FT for the upper surface are 10 and 1, respectively, so that $b_1/b_3=10$. Both of these $b_1/b_3$ values are well within the range of values in Table 2, and both are strikingly close to the average values given for each surface. Table 3 summarizes this information.

<table>
<thead>
<tr>
<th></th>
<th>Range of $b_1/b_3$</th>
<th>Average value of $b_1/b_3$</th>
<th>Value of $b_1/b_3$ given by the FT</th>
</tr>
</thead>
<tbody>
<tr>
<td>ptygmic vein, lower</td>
<td>5.08-20.26</td>
<td>10.95</td>
<td>12.0</td>
</tr>
<tr>
<td>surface</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>ptygmic vein, upper</td>
<td>4.78-17.14</td>
<td>9.15</td>
<td>10.0</td>
</tr>
<tr>
<td>surface</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3 showing a comparison for the values of $b_1/b_3$ found by using the FS and those found using the FT.

Quality assessment of the FS information

I have calculated both the first few FS coefficients, and the FT for the same group of folds, and I have illustrated how, in some respects, the FT yields the same information contained in the FS. The fact remains, however, that the FT calculation is based on the
entire length of the fold while the FS is based on only individual segments. As such, the FT must yield shape information not contained in the FS. What has not been clear up to now is just how much more information it contains. The FS appears to provide very reliable information on the shape of small segments of folds (Hudleston, 1973a &1973b; Stowe, 1987), but does it provide valuable information on the shape of the fold that the segment came from?

To answer this, I refer again to Fig. 17, this time focusing on where, within the FT spectrum, the values of b1 and b3 fall. The coefficient b1 occupies a powerful position (literally) in the low frequency portion of the spectrum, indicating that it contains much information about the shape of the fold. The coefficient b3, however, falls in an area of relatively low power, indicating that it contains little information on the shape of the fold. If we continue out along the frequency axis to find even higher order b-values, we find that each contains successively less shape information for the fold train. This indicates that plots such as those in Figs. 12 and 13, as well as those in Fig. 11, draw on information that is largely inconsequential with respect to the overall fold train. This fact is significant because people have used such higher order coefficients as part of their analysis of folds. Hudleston (1973b), for instance, used as many as 15 values of bn (n going from 1 to 15), in the spectral graphs that he used to illustrate similarities between various spatially contemporaneous folds. Likewise, Stowe (1988) used as many coefficients as he could reasonably calculate for his computer representations of fold profiles, on the premise that ignoring higher order coefficients reduced precision. It is interesting, then, that the FT data indicates that a plot of the first 15 b-values contains scarcely more information than does a plot of the first value alone.

This information suggests that, while a FS analysis based on the quarter-wavelength may be sufficient to recognize the shape characteristics of fold segments, it is inadequate for recognizing those of longer trains of folds. Thus, the answer to the question of whether or not the FS provides valuable information on the shape of the fold train appears to be no.

Information not contained in the FS

Humans, by nature, tend to learn best when the information they are required to process is visual. On this score, the FT's greatest asset is the graphical nature of its output. The Fourier spectrum allows us to view all of the various frequency contributions simultaneously, and it partitions them so that we can quickly discern which has the most influence over the fold's bulk shape. What exactly, though, does the FT give us that the
FS does not? The short answer is: perspective. It allows us to look beyond the quarter-wavelength segment to see what is "happening" in the rest of the fold. The longer answer, however, is: completeness of information. The fact is, one could obtain a FT-like representation of FS data, but only at great expense of time and energy. (It is also likely that one would still need to refer to the FT as a guide.) Even so, the end result must still be a loss of information.

Thus, the FT does offer information that the FS cannot give us. I divide this information into two areas:

1) Information on the dominant wavelength of the fold train
2) Information on the fold's behavior supplied by its power spectrum.

The concept of a dominant wavelength (Ld), while perhaps not the most familiar concept in structural geology, is well established (Biot, 1957; Ramberg, 1961; Price & Cosgrove, 1990). Prior to lateral compression, a layer will have any number of surface irregularities, each with a particular amplitude (height above the surface). As compression ensues, the irregularity with the greatest amplitude will be preferentially amplified. Those irregularities that lie a distance L from the largest will also be preferentially amplified. This distance L is given by:

\[
L_d = 2\pi \sqrt{\frac{\mu_1}{6\mu_2}}
\]  

and is the dominant wavelength, where \( \mu_1 \) is the viscosity of the layer and \( \mu_2 \) is the viscosity of the matrix. The FT method provides a direct and objective way to identify the existence, as well as the numerical value, of Ld.

We know that the horizontal axis of the FT spectrum has the units of frequency, and that \( \omega = 1/T \). This means that we can read the period T directly off the axis by finding the reciprocal of the frequency. "Period", a time sequence term, corresponds to the spatial term wavelength (Halliday & Resnick, 1988). It follows, then, that we may also read the wavelength directly off the axis. This becomes significant when coupled with the fact that the FT spectrum shows which frequency component dominates the fold train (by "dominate" I mean that it has the largest "y-value" on the FT spectrum). In effect, all we need to do is locate the peak corresponding to the dominant frequency, and read the wavelength off the axis. The value that we read will be (by definition) the wavelength of the dominant wave, and (by implication) the dominant wavelength.
The FT's contribution to understanding fold behavior may not be clear at first, because it appears that the FT is simply a more complete representation of the fold's information than is the FS. What is important, however, is that the FT provides the fold's power spectrum according to eq. 11. It is with this that we can gain insight into the behavior of folds.

Many works describe the significance and structure of power spectra (Stearns & Hush, 1990; Broch, 1990; Blackman & Tukey, 1958; Bloomfield, 1976). Blackman & Tukey (1958) is devoted only to power spectra. The reason for all this discussion is that power spectra are often as opaque as they are useful. The essence of the power spectrum, though, is that it describes the behavior of the system from which it is derived (Schroeder, 1991; Gollub & Baker, 1990). Behavior information is manifested in the arrangement (or absence) of the spectral peaks that make up the spectrum. If the system behaves periodically, there will be sharp, well-defined peaks at the various frequencies of oscillation. An example is a spectrum of air temperature records. Among the many oscillations in temperature, there will be a well-defined peak at a period of 24 hours, corresponding to the rising temperatures associated with the rising sun. If, on the other hand, the system behaves randomly, the power spectrum will exhibit a broad-band spectrum that lacks any systematic arrangement of well-defined peaks. Figure 19 shows an example of periodic system evolving into a chaotic one.

With regard to folding, the power spectrum gives us information on two fronts. The first (or static case) deals with information we gain by analyzing the power spectrum of an isolated folded layer. The second (or dynamic case) deals with information we gain by looking at the power spectra of sequential episodes of folding.

The static case

By applying spectral (FT) analysis to single folded layers, we gain shape information that is inaccessible by harmonic analysis. In particular, spectral analysis explicitly indicates what is the value of Ld. This is significant, as the the value of Ld plays an integral role in buckling theory, and thus in how well we understand rock behavior.
Figure 19  Time series plots and power spectra for the local fluid velocity in the Rayleigh-Benard convection experiment. (a)-(e) show the dynamical states as convection insensifies. Two distinct oscillations at frequencies $f_1$ and $f_2$ develop, phase lock, then finally lead to chaos in (d). (From Gollub & Baker, 1990)
A fundamental question of fold mechanics is whether rocks deform according to a linear, or non-linear flow law. Linearly viscous layers require shortening of at least 50% before finite amplitude folds develop, while non-linearly viscous layers may develop such folds at much smaller shortening values. Thus, a measure of layer non-linearity would be useful for determining the amount of shortening that takes place prior to buckling (especially in cases where strain indicators are not present, or were destroyed by the buckling process). Such a measure of linearity is the power-law exponent, n. Layers with n>1 have a greater buckling instability than those with n=1, and the buckling instability is sensitive to changes in n (Hudleston & Holst, 1984). Hudleston & Holst (1984) indicate that Ld is also sensitive to changes in n. It follows, then, that we will be able to chart the relative buckling instabilities of folded layers by analyzing their spectra.

Spectral analysis also allows us to calculate the viscosity ratio $\frac{\mu_1}{\mu_2}$ from eq. 13. This calculation will represent an improvement over the value that Hudleston & Holst (1984) obtained. In their analysis, Hudleston & Holst (1984) used as a value for Ld the value of the average wavelength L, and it is not clear that this will always be a valid assumption. An objective determination of Ld will also improve all the results Hudleston & Holst (1984) obtained in using L for Ld.

The dynamic case

The dynamic case addresses information we gain by applying spectral analysis to the spectra of sequential episodes of folding. Under this scheme, the FT method offers significant contributions to experimental fold studies.

We can calculate the power spectra of sequential "frames" of a folding experiment, allowing us to examine the behavior of the fold train as it evolves from an unperturbed layer to a true fold train. This is useful for re-examining previous experimental studies, as well as for gaining new insights into the nature of deformation processes. For instance, Price & Cosgrove (1990) observed that wavelength selection will occur during initial layer compaction. That is, there will be a certain wavelength (with a corresponding frequency) that will be amplified, preferentially to other wavelengths, as the percent compaction increases. Such an occurrence will be clearly indicated on the power spectrum by a distinct, well-defined peak at the period that corresponds to the selected wavelength. In this way, the FT method not only allows us to test the accuracy of
Price & Cosgrove's observations, but if such a wavelength selection does occur, this method also allows us to readily determine the value of the selected wavelength.

Studies also indicate that the folding process changes as folding progresses. The FT method can be useful for examining these changes. For example, Hudleston (1973b) shows that during initial compression, an isolated layer will behave in two ways: 1) it will deform as a result of a buckling mechanism, and 2) it will thicken as a result of homogenous flattening. These two events occur together up until limb-dips reach an angle of about twenty degrees, at which point the thickening of the layer ceases. This transition from one mode of deformation to another indicates that the whole deformation system is changing. Such changes are analogous to phase transitions, which the FT finds very effectively. (There have many books written on the nature of phase transitions, but at the most basic level, a phase transition represents a point at which a system stops behaving one way and starts behaving another way.) These transitions are manifested in the power spectrum as bifurcations (where frequencies other than multiples of the fundamental frequency show up as peaks on the spectrum). Figure 20 illustrates this. With this in mind, we should be able to identify the point at which occurrences such as Hudleston's buckling/flattening to buckling transition take place, as well as others that we don't presently know about.

Referring to Fig. 18, it is interesting to hypothesize what might happen if we continue to deform our isolated layer. Figure 18, again, illustrates a periodic to chaotic sequence. If in fact, bifurcations occur as we deform the layer (as evidence such as Hudleston's suggest), it would be interesting to see whether this process is followed by phase locking and broad-band spectra, indicating chaotic behavior. If so, it would suggest that, after a certain point, no single mechanism is more likely than another to dominate the folding process. This would clearly have extremely interesting implications.
Figure 20 In (a), only one frequency is observed, indicating periodic oscillation. In (b), a second frequency develops indicating a bifurcation. (From Stewart, 1989).
Discussion

My observations indicate that a method of fold analysis based on the FS will be insufficient to identify shape characteristics of an aperiodic natural fold train. While the determination of the first few Fourier coefficients may be useful for statistical studies (i.e. "n% of quarter-wavelengths in this fold population have values within..."), it is not useful for studies that focus on more general questions regarding fold geometry and fold behavior. The more appropriate method of analysis for these kinds of studies is one that utilizes all information contained in the fold, and does so in a way that does not require the examiner to change the fold to fit the method.

The results of my harmonic analysis were consistent with those obtained by previous researchers (i.e. Hudleston, 1973b). My analysis produced plots of \( b_1/b_3 \) that fell within the same shape fields as those that Hudleston used to make inferences on the shape characteristics of fold populations. When I compared these data to those I obtained using a method based on the FT, I found that the FS coefficients (and ratios thereof) contained little information on the general shape of the larger fold train. This suggests that studies such as Hudleston's (1973b) may be precise (meaning internally consistent) without being wholly accurate.

A method based on the FT allows us to examine a fold train "as is" so that we do not have to break it up into periodic segments that no longer resemble the original fold train. We may do so by simply digitizing the train, and loading the resulting data set into a program that will calculate its FT. The result will be a spectrum that illuminates the shape characteristics most important to the train. This process takes much less time than the FS method, and it contains only one step in which error could be introduced to the shape of the fold being analyzed (the step involving physically digitizing the fold), as opposed to numerous opportunities for error in the FS method.

Aside from the benefits of utility and compactness, the FT method provides information that we could not obtain any other way. It permits us to directly calculate the dominant wavelength, and gives us insight to the layer's power-law behavior. This method will also be useful for improving the results of experimental fold studies. These attributes indicate that the FT provides a more useful method for examining real-world fold data than does the FS.
References Cited


Hudleston, P.J. and Lan, L. Rheological controls on the shapes of single-layer folds.


Appendix

The purpose of this appendix is to aid future researchers in reproducing my results. For this reason, I have tried to make it as complete as possible. I do not, however, address topics that are covered in the text of the thesis (i.e. selecting an appropriate curve, selecting an appropriate coordinate system, etc.). I have also assumed that the digitizing and mathematics programs are on separate computers: the digitizing program being on a DOS machine, and the mathematics program being on a Macintosh.

The process for calculating the Fourier Transform (FT) of an arbitrary curve consists of three steps: 1) digitizing the curve, 2) translating the data set from a DOS to a Macintosh format, and 3) calculating the FT.

1) digitizing the curve

Sigma Scan's users manual provides sample sessions that are useful for learning how to use the program. For the purposes of reproducing my work, a session would be as follows:

• Bring the program up on the departmental PC (by typing "CD\SCAN" then "SCAN").
• Once loaded, calibrate the program for the session by choosing "CALIB" on the right-hand side of the screen. Having done this, a blue screen will appear and ask a series of questions. Your answers should be as follows: 1) Choose to use Cartesian coordinates by typing "C" followed by the return key. 2) For simplicity, name the axes x and y. 3) Choose continuous sampling for the y-values (sample interval of 0), and a sample interval of 0.1 for the x-values. 4) The program then asks for three reference points in the fold's coordinate space.
• After you answer the last question, the program will return to the original screen and ask you to give it the three reference points. With these points established, you may then trace the fold. Do so by typing the escape key and dragging the plotter over the length of the fold while holding down the button.
• Once you have traced the fold, press the escape key again to return to the menu screen. Choose "DATA" from the menu. This will bring up a spreadsheet-like screen that contains the x and y values for the fold. The x-values should all occur at equally-spaced intervals. Since the intervals are equal, the x-values become arbitrary reference points (reference point #1, 2, 3, etc.). This allows us to get rid of them, because Mathematica will assign equally arbitrary sequential reference points to each
y-value when we import the fold data. Erase the x-values by choosing "DEL BLK" from the menu and following the on screen instructions.

- The last step is to save the data to disk. One should be able to save the data directly to a floppy disk, but I always had to save it on the hard disk and copy it to a floppy. The *Sigma Scan* manual discusses how to save the data.

2) translating the data

Unless the department acquires *Software Bridge*, the easiest way to translate the data from DOS to Mac is to go to the consultant's office and have them do it. Because the data is simply in ASCII format, one should be able to use any number of translation programs, but for some reason *Mathematica* will only import data that is in ASCII MAC format. So take the floppy to the consultant and ask them to convert it from ASCII to ASCII MAC. One word of caution: the consultant may tell you that the data could as easily be saved as an *MS Word* file, since that is also an ASCII file. For some reason, however, I have never successfully imported a *Word* file into *Mathematica*, so stick with *Software Bridge*.

3) calculating the FT

Before carrying out any calculations in *Mathematica*, it would be useful to read some of the manual to become familiar with the program. It is an easy program to work with as long as you know what kind of input it expects (for instance, ReadList does not mean the same thing as Readlist). What follows is an example of how to calculate the FT of the fold data set.

- After you double-click the *Mathematica* icon, the program will present you with a worksheet that is blank except for "In[1]" in the upper left hand corner. Figure 14 shows the process of calculating the FT (minus the In/Out prompts and any non-graphical output), I will simply elaborate here.

- You begin by importing the fold data. The command that does this is: "ReadList["filename", Number]" followed by Shift-Return. Because this is the first command you have given *Mathematica*, it will take a little while for the program to set itself up, so do not be surprised if it takes longer than you think to import the file. A few seconds after you type in the command, *Mathematica* will display a window saying that it could not find the file. You then need to use the "Open..." command in the File menu to show the program where file is. (This is the only time you should
need to do this. *Mathematica* "learns" from its mistakes, so that the next time you import a file, it will first check in the place where it found the last file.) Once *Mathematica* finds the file, it will acknowledge the fact by outputting the list of y-values.

- The list of y-values is rather unwieldy, so it is useful to assign it a name. The appropriate command is "a=%1", meaning: assign the name "a" to the output of line 1. The program will do this and output the list once again.
- The command to calculate the FT of the data set is: "ListPlot[Abs[Fourier[a]], PlotJoined->True, PlotRange->All]". This gives you a plot of the absolute value of the FT. The resulting plot is actually a set of points, and using the Plot Joined command connects the points. "PlotRange->All" gives you the entire frequency spectrum of the plot, but as Figure 14 shows, you can adjust the plot range to give a more detailed view of the spectrum.