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Three-dimensional strain analysis using Mathematica

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ABSTRACT

A suite of geological computer programs written in Mathematica is currently available both within the online repository for the Journal of Structural Geology as well as on the first author's website (http://www.sonoma.edu/users/m/mookerje/ProgramPage.htm). The majority of these programs focus on three-dimensional strain analysis (e.g., determining best-fit strain ellipsoids, plotting elliptical data on either a Flinn or Hsu diagram, and determining error bounds for three-dimensional strain data). This program suite also includes a ternary diagram plotting program, a rose diagram program, an equal area and equal angle projections program, and an instructional program for creating two-dimensional strain path animations. The bulk of this paper focuses on a new method for determining a best-fit ellipsoid from arbitrarily oriented sectional ellipses and methods for determining appropriate error bounds for strain parameters and orientation data. This best-fit ellipsoid method utilizes a least-squares approach and minimizes the error associated with the two-dimensional data-ellipse matrix elements with the corresponding matrix elements from sectional ellipses through a general ellipsoid. Furthermore, a kernel density estimator is utilized to yield reliable error margins for the strain parameters, octahedral shear strain, Flinn's *k*-value, and Lode's ratio. By assuming a gamma distribution for the simulated principal axes orientations, more realistic error bounds can be estimated for these axes orientations.

1. Introduction

Among its many applications, Mathematica is particularly useful for manipulating and graphically displaying data. While Mathematica is relatively user-friendly, building complex programs from scratch can be very time-consuming and is inefficient, considering that many Earth Science users are ultimately doing very similar types of analyses (for instance, see Haneberg's text, Computational Geosciences with Mathematica (Haneberg, 2004)). To this end, the first author has assembled a suite of seventeen Mathematica files that have applications for the earth sciences, with a particular emphasis on strain analysis (Table 1). This suite, as well as several sample data files, can be downloaded from the following website: http://www.sonoma.edu/users/m/mookerje/ProgramPage.htm. Eight of the programs deal specifically with the process of determining a best-fit ellipsoid from sectional data sets. These programs utilize new methods for defining a best-fit ellipsoid, and four of them utilize a novel approach for determining the error bounds of the fit data in terms of both the ellipsoid shape and its orientation. These methods are described in detail in Sections 3 and 4. The remaining nine programs are primarily graphical in nature.

For several decades, structural geologists have investigated three-dimensional strains and have illustrated how useful these techniques are for understanding the kinematics of deforming materials (e.g., Cloos, 1947; Flinn, 1962; Hossack, 1967; Gairola, 1977; Mitra, 1978; Wheeler, 1986; Dewey et al., 1998; Merschat et al., 2005; Galon et al., 2008; Mookerjee and Mitra, 2009; Thigpen et al., 2010). Additionally, many investigators have contributed to efforts for determining a best-fit ellipsoid from two-dimensional data. Initially, the methods were confined to three mutually perpendicular sections (Ramsay, 1967; Shimamoto and Ikeda, 1976; Oretel, 1978; Miller and Oertel, 1979), then three non-perpendicular section (Milton, 1980), and finally three or more non-perpendicular sections (Gendwill and Stauffer, 1981; Owens, 1984; Shao and Wang, 1984; Robin, 2002; Launeau and Robin, 2005). As with our proposed method, several investigators have employed some form of a least-squares approach (Oretel, 1978; Miller and Oertel, 1979; Shao and Wang, 1984). Robin (2002) provides an informative chronology for these contributions. Furthermore, Yonkee (2000) incorporated statistics into his best-fit ellipsoid program using a Monte Carlo simulation. Taking a similar, simulation-based approach, our method uses kernel density estimation to determine error bounds for the strain parameters,

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Table 1
List of programs in the geological programs for Mathematica suite.

List of programs
Best-fit ellipsoid
Best-fit ellipsoid with statistics
Best-fit ellipsoid for ImageJ
Best-fit ellipsoid-absolute
Best-fit ellipsoid-absolute for ImageJ
Best-fit ellipsoid with statistics for ImageJ
Best-fit ellipsoid with statistics-absolute
Best-fit ellipsoid with statistics-absolute for ImageJ
Flinn plot
Flinn plot with error regions
Hsu plot
Hsu plot with error regions
Equal area & angle projections
Rose diagram
Ternary diagram
Section data through an ellipsoid
2D pure versus simple shear

octahedral shear strain (ε_s), Flinn's *k*-value, and Lode's ratio (ν). While this approach is new to the application of strain analysis, it is used for other applications in the earth sciences (e.g., grain size distributions (Buscombe, 2008), special distribution of volcanism (Connor et al., 2008), storm frequencies (Joyner and Rohli, 2010), mass extinctions (Wang, 2003), etc.). We believe that adding these sorts of confidence estimations to strain analysis will help investigators make informed and reasonable geological interpretations while providing feedback about their data collection techniques, and help them to decide when more data is needed to constrain a structural problem. The methods proposed in this contribution build on these investigators' work, and our program suite is intended to fulfill most of the computational and graphical needs of the structural geologist community for three-dimensional strain analysis.

2. Why Mathematica?

The primary reason for using Mathematica is that it allows for the relatively easy modification of the programs to suit the users' specific needs. While the programs are designed to accommodate many different user preferences, more specific user requirements will exist. Fortunately, Mathematica provides a favorable environment for user customization, including a very useful help system, on-line support forums, and their Technical Support Group. Mathematica runs on most operating systems (e.g., Windows, Mac OS, and Linux). Additionally, Wolfram Research ensures that new versions of Mathematica that are functional with older Mathematica files/programs. Finally, Mathematica has superb graphical capabilities which produce interactive three-dimensional plots (e.g., ellipsoids) and create animations, both of which usefully convey complex ideas and geometric relationships.

3. Determining the best-fit ellipsoid

The term "best-fit" is often employed with little thought for what criterion makes something the "best." With regards to a best-fit ellipsoid, our initial preference was to define the best fit as the one that has the minimum difference between the set of "mean" axial ratios (Rf) and "mean" angular orientations (ϕ) from the initial data set and those of a general ellipsoid (e.g., see the Methods section of Strine and Wojtal (2004)). This outcome is achieved by calculating the equations for the Rf and the ϕ of a specific plane in terms the matrix elements of a symmetric 3×3 matrix. These equations are then subtracted from their corresponding "mean" Rfs and ϕs for the specific plane. Then, in a typical least-squares approach, the differences are squared and summed together, and this entire error function is minimized in terms of the six matrix elements. While this approach does yield reasonable results, we now believe that this method falls just short of generating the best fit because it treats the Rfs and the ϕs as independent parameters. If a two-dimensional strain marker is very nearly circular, its individual angular orientation is largely independent of the "mean" angular orientation. In contrast, the angular orientation of a strain marker with a relatively large aspect ratio should have a significantly greater effect on the "mean" angular orientation (e.g., Dunnet, 1969; Matthews et al., 1974; Shimamoto and Ikeda, 1976; Robin, 1977; Mulchrone et al., 2003; Choudhury and Mulchrone, 2006). Thus, simply using the vector and harmonic means as defined by Lisle (1985) neglects to account for this interdependence. A further weakness of the method proposed by Strine and Wojtal (2004) is that a quantitative judgment is required by the user on which parameter (Rf or ϕ) is weighted more heavily. This extra degree of freedom makes it difficult to call any solution the best fit.

Despite these imperfections in the Strine and Wojtal (2004) method, we appreciate the approach of minimizing the error between the input data and the fit solution. Furthermore, we suggest that any fitting method needs to be evaluated with this criterion in mind, i.e., a best-fit ellipsoid is the one that has the minimum difference between the input data and the fit solution. For this reason, the method that we propose involves the minimization of an error function, i.e., a function that represents that error associated with the difference between the input sectional data and any general ellipsoid. While this numerical approach may seem to employ brute force, particularly when compared to the more analytical solution of Robin (2002), we hope that our users will benefit from the transparency of our relatively simple procedure. We hope that demystifying this process will help investigators think more critically about the quality of their data and potentially make improvements and customizations to the software. During the testing of our method, we generated one hundred ellipsoids of random shape and orientation and calculated the sectional ellipses for three to six randomly oriented planes for each ellipsoid. This data set was used to compare the results of our program with those of Launeau and Robin (2005). The results were consistently similar in that the median angular difference between the two methods for the principal axes orientations is less than one degree, the median difference in octahedral shear strain was 0.004, and the median difference in Lode's ratio was 0.019. Therefore, we conclude that both methods are equally valid. We hope that users will find value in the customizability of our programs (e.g., adding a statistical analysis as described below) as well as the variety of graphical outputs.

3.1. Two-dimensional data

To begin fitting a three-dimensional ellipsoid to data, one first needs two-dimensional sectional data. Many methods exist for determining a two-dimensional "mean" ellipse (e.g., the Fry Method, Rf/ϕ, various Mohr circle methods, the Haughton–Breddin method of using fossils with bilateral symmetry, etc.). The resulting ellipses from any of these methods can be input into one of the best-fit ellipsoid programs (either manually or read in from a file). However, if an investigator has a data set of individual elliptical measurements (e.g., measurements from deformed quartz grains), then those data sets can be copied into the appropriate *.txt or *.xls file, and the program will read in this file and determine the "mean" elliptical shape for each of the sections automatically. The "mean"