The geologyGeometry library for R

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Abstract

The `geologyGeometry` library for R is designed to aid geologists in the analysis of five geometric data types: rays, lines, rotations, orientations, and ellipsoids. The core tools focus on plotting, describing mean and dispersion, inference about population means (confidence/credible regions and hypothesis tests), and regression. The library is accompanied by dozens of detailed tutorials, which use dozens of natural and synthetic data sets. This document summarizes these data types, tools, and tutorials. It also describes the installation procedure and version history. An appendix summarizes some of the mathematics of ellipsoids.

Keywords: directional statistics, orientation statistics, ellipsoid statistics

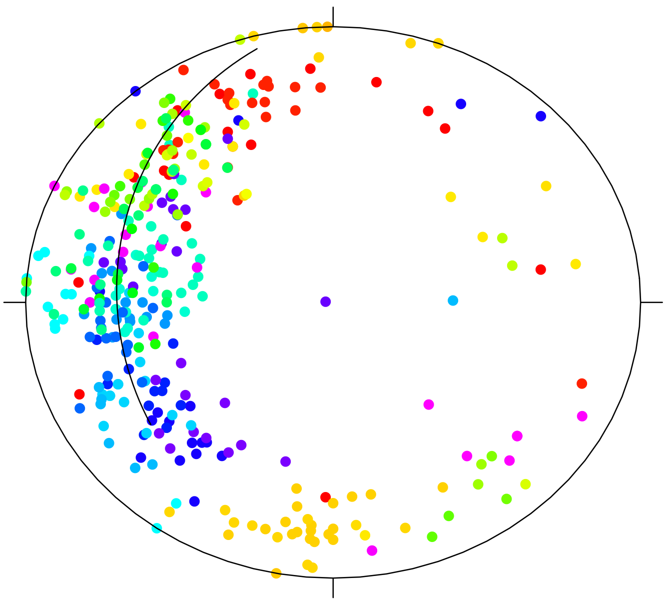

Figure 1: Geodesic regression of 348 dike poles from Cyprus (Scott et al., 2013). The poles are colored by northing, from south (red) to north (magenta). The superimposed best-fit curve represents a dike pole rotating steadily with respect to northing. See the line tutorial `4geodesicRegression.R`.

1. Tasks and tools

This library offers tools for several basic statistical tasks: plotting, describing the mean and dispersion of a data set, inference about the population mean, regression, clustering, sampling from distributions, testing uniformity, maximum likelihood estimation, etc. We explain a few of them in greater detail now.

The library offers several common kinds of geologic plots: equal-area hemispherical plots, Kamb contouring, Rose plots, etc. The user can export such plots as PDFs for use in publication. However, this library does not attempt to compete on those features with other programs such as *Stereonet* by Allmendinger and Cardozo or *Orient* by Vollmer. Rather, the library focuses on other plots that are much less common in geology: equal-angle rotation plots, equal-volume rotation plots, log-ellipsoid vector plots, etc. Many of these plots are three-dimensional and in color. They are intended primarily for interactive exploration of data, rather than publication figures. However, the user can customize them for publication and capture them as raster images.

For each data type we offer at least one way to quantify the location of a data set (the sample mean) and the dispersion of the data (standard deviation, variance, etc.). As the tutorials explain, these notions of mean are mathematically well-behaved and thus form a reliable foundation for more advanced techniques such as bootstrapping.

Loosely speaking, inference is the process of extrapolating from a data set to the larger population that it represents. Confidence intervals and hypothesis tests are two basic kinds of inference. For each data type we offer at least one way to perform inferences about the population mean. Sometimes we also offer techniques for comparing two data sets. Some of the methods are asymptotic, while others are simulation-based (bootstrapping, Markov chain Monte Carlo).

Similarly, for each data type we offer at least one kind of regression, which can be used to quantify how one aspect of the data depend on another aspect (a scalar variable, whose values are known with certainty). Some methods boil down to linear least squares. In other cases, we use permutation tests to assess the significance of results.

We have not created a graphical user interface (GUI) for these tools. Currently the user must interact with the

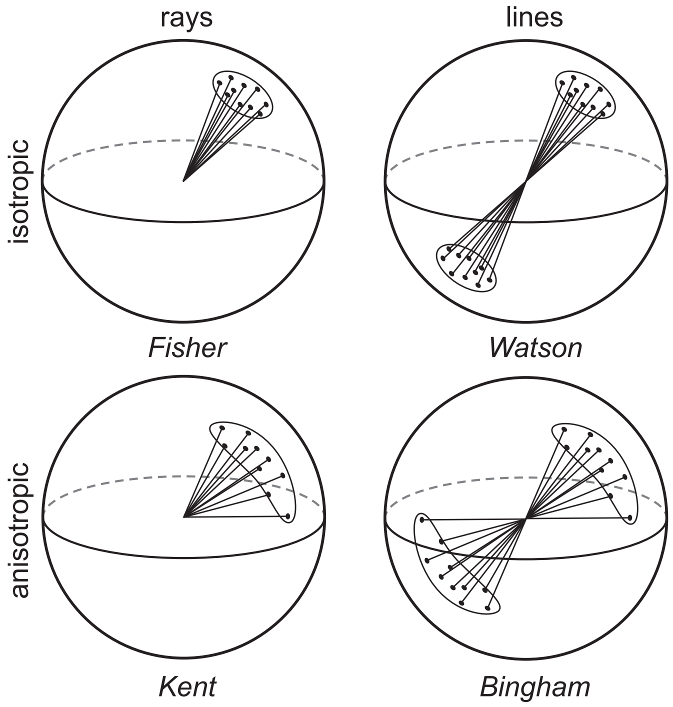

Figure 2: Four of the most popular analogues of the normal distribution for directions. The Fisher and Kent distributions are for rays. The Watson and Bingham distributions are for lines. The Fisher and Watson distributions are isotropic about their means. The Kent and Bingham distributions are anisotropic.

library by typing R commands. However, we believe that many geologists can get work done by mimicking the relevant tutorials. And those who are motivated can learn the basics of R in a few hours of study. Several of our tutorials teach general R concepts and skills.

2. Five geometric data types

This library deals with five big categories of geometric data: rays, lines, rotations, orientations, and ellipsoids. A noteworthy concept is the number of degrees of freedom (which equals the dimension of the underlying sample space).

2.1. Rays and lines

Directions come in two flavors: lines and rays. A ray is a line with a preferred direction along that line. Examples of line-like data include a lineation, a pole to a foliation or fault plane, the direction of the long axis of an ellipsoid, etc. Examples of ray-like data include a paleomagnetic direction, a vorticity vector describing the sense of slip on a fault, etc. A pole to a bedding plane is ray-like if the younging direction is known or line-like if it is unknown.

Directions in 3D have two degrees of freedom. This is a fancy way of saying that two numbers are needed to describe them. For example, a lineation might be described using trend and plunge. A foliation might be described using the trend and plunge of its pole or the strike and dip of its plane. However you record them, there are two non-redundant numbers describing the direction.

The standard textbook for this material is Mardia and Jupp (2000). It might be more statistical than a geologist would like, but at least many of the examples come from the geosciences.

Structural geologists use some directional statistics frequently: equal-angle and equal-area hemispherical plots, Kamb contouring of density, Bingham statistics for lines, etc. However, there are also many missed opportunities in the structural geology literature. Whenever your paper makes a statement such as “The faults on this side of the syncline are differently oriented than the faults on the other side of the syncline” or “Foliations steepen with proximity to the shear zone”, you should try to support those claims with statistical argumentation.

2.2. Rotations and orientations

An orientation is a complete description of how an object is oriented in 3D. It is more than just a direction. For example, if we know the direction of the long axis of an ellipsoid, then we still do not know how its other axes are oriented. Its short axis might point in any direction perpendicular to the long axis. That direction could be specified using a single angle. Once it is specified, the direction of the intermediate axis is determined. So we see that three numbers, not two, are needed to specify the orientation of an ellipsoid. Similarly, a foliation-lineation pair is specified by three numbers, such as the strike and dip of the foliation plane and the rake of the lineation within that plane. Orientations have three degrees of freedom.

Other than ellipsoids and foliation-lineation pairs, many geologic data types have orientations: cylindrical folds, principal stress directions, earthquake focal mechanisms, faults with known slip direction, crystallographic axes, etc. Statistical tools for analyzing these orientations have been developed and applied in numerous fields over the past four decades. However, structural geologists have been slow to adopt them.

Orientations are described as symmetric sets of rotations, in much the same way that a line is described as a symmetric set of two rays. Although rotations have some direct utility in geology — for example, in describing the relative motions of tectonic plates — we mainly use them as the foundation for orientations.

Orientation statistics is connected to directional statistics through a non-obvious mathematical trick (treating rotations as unit quaternions). Consequently the Mardia and Jupp (2000) textbook includes some material on orientations in its later chapters. However, that book’s treatment is too scant to address the myriad geological applications of this theory. We recommend our survey paper (Davis and Titus, 2017).

2.3. Ellipsoids

Structural geology uses many kinds of ellipsoids: finite strain, anisotropy of magnetic susceptibility (AMS), shape

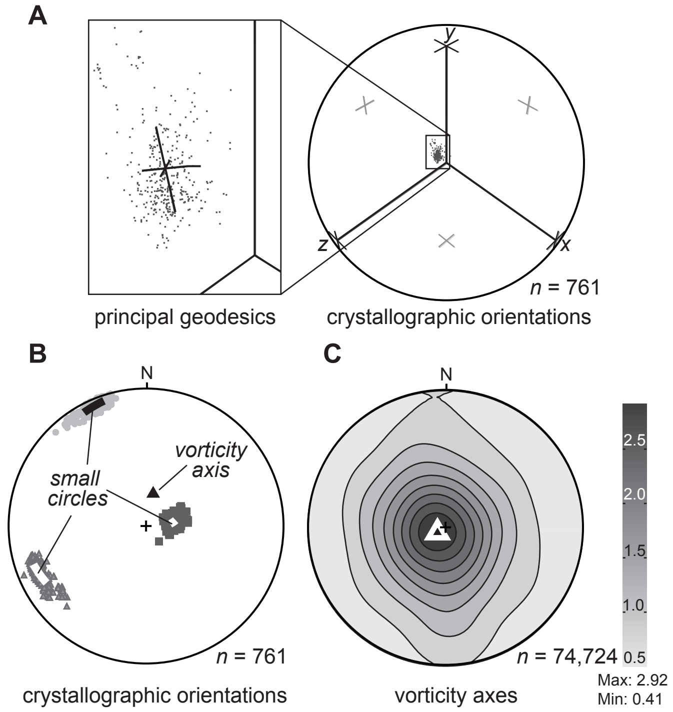

Figure 3: Inferring vorticity of deformation from dispersion of crystallographic orientations. See the miscellaneous tutorial `oriCVA.R`. A. Equal-volume plot of 761 quartz orientations from a single grain, with their principal geodesics (Strine and Wojtal, 2004; Michels et al., 2015). B. Equal-area lower-hemispherical plot of the same data set, with the inferred vorticity vector and small circles about that vector fitting the dispersed axes. C. Adapted from Michels et al. (2015). Density contours (multiples of uniform density, de la Vallée Poussin kernel) of vorticity vectors inferred from 74,724 such grains.

preferred orientation (SPO), individual clasts within a host rock, etc. Like orientation statistics, ellipsoid statistics has been used only rarely in structural geology, even as it has been developed and applied in related fields such as rock magnetism.

Triaxial ellipsoids have six degrees of freedom: three for orientation and three for magnitude. Frequently ellipsoids are normalized, and this normalization removes one degree of freedom from size and shape, leaving five degrees of freedom. The orientational degrees of freedom are poorly behaved for spheroids and near-spheroids, and calculating with the size-shape degrees of freedom is complicated. Hence statistics with ellipsoids is difficult.

Fortunately, there is a way to recast ellipsoids as five- (if normalized) or six-dimensional (if not) vectors, where statistical computations are quite convenient. So in practice we convert our ellipsoids over to these vectors, compute on those, and then convert our results back into a more understandable format. See Appendix A for some of the mathematical details.

3. Documentation

In the future, we plan to distribute this R library as an official R package through the Comprehensive R Archive Network (`http://cran.r-project.org/`). Documentation will then be provided in the standard R package format. In this release we instead rely on the following kinds of documentation. First there are three umbrella documents:

- This `readme.pdf` document gives an overview of the library's goals, features, and installation procedure.
- The enclosed text file `reference.txt` is a function-by-function reference for all parts of the library that are intended for use by end-users. It is compiled automatically from the R source code.
- See the enclosed text file `LICENSE.txt` for licensing information (Apache License 2.0).

Second, we offer dozens of concrete, friendly tutorials, organized into nine categories:

- The scalar tutorials are intended to provide an introduction to or review of "ordinary" statistics. However, we haven't written them yet. Stay tuned.
- The five core sets of tutorials — for rays, lines, rotations, orientations, and ellipsoids — explore techniques specific to those five data types. When we teach short courses for geologists, we begin with the line tutorials. We give scant attention to the rotation tutorials, because their main purpose is to lay a foundation for the orientation tutorials.
- The C tutorials require the C part of our library, which some users will find difficult to install. We like these tutorials, but they are few and not essential.
- The miscellaneous tutorials expand on the five core tutorial sets. Usually they go beyond the four basic tasks of plotting, describing mean and dispersion, inference, and regression.
- The R tutorials have little to do with geology or our library. Rather, they are a gentle introduction to the R programming language. Have the earlier tutorials left you wondering what `lapply` means? Then these tutorials are for you. After reading these brief tutorials, you might look for some larger R guides, such as `https://www.cran.r-project.org/doc/manuals/R-intro.pdf`.

4. Brief version history

2019/08/08: The convention for transforming between log-ellipsoid tensors and log-ellipsoid vectors has been changed. Files stored using the old convention need to be rebuilt. Functions using the `FRB` library have been removed. Bug fixes.

2018/01/04: Bug fixes in the library. Many new tutorials. All tutorials reorganized.

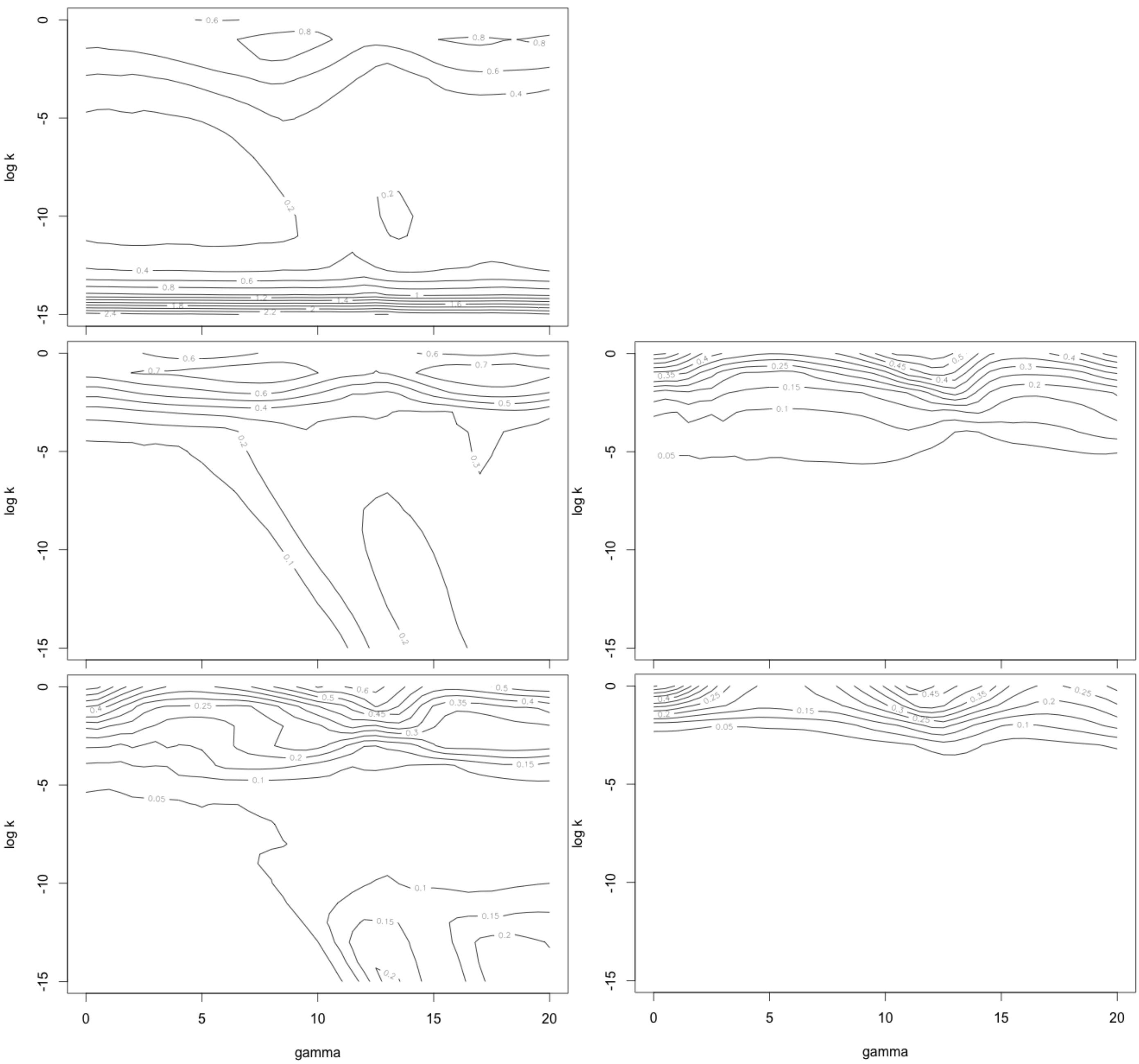

Figure 4: Development of fabric from deformable orthopyroxene clasts under monoclinic transpression. See miscellaneous tutorial `ellDeformableFabric.R`. The five plots show the five measures of ellipsoid dispersion (eigenvalues of the log-ellipsoid vector covariance) after varying amounts of deformation. The first column shows the first three measures; the second column shows the last two.

2017/06/20: Removed two-sample inference for orientations. Fixed and added ellipsoid functions.

2016/07/30: Bug fixes in the tutorials, in preparation for the Structural Geology and Tectonics Forum 2016.

2016/04/26: Added some more directional statistics. Now requires the `Directional` and `pracma` packages. Sourcing `library/all.R` now loads all of the dependencies.

2016/04/10: Essentially version 1.0. Some incompatibility with the earlier versions. Exercises are now called tutorials. Includes C library, C tutorials, R tutorials, and more bonus tutorials. More documentation.

2015/10/31: Preliminary version supporting our GSA 2015 short course. Exercises for directions, orientations, ellipsoids, and bonus. Poor documentation.

2015/01: Preliminary versions supporting a seminar for structural geology students at the University of Wisconsin-Madison.

2014/11: Began porting Mathematica code to R.

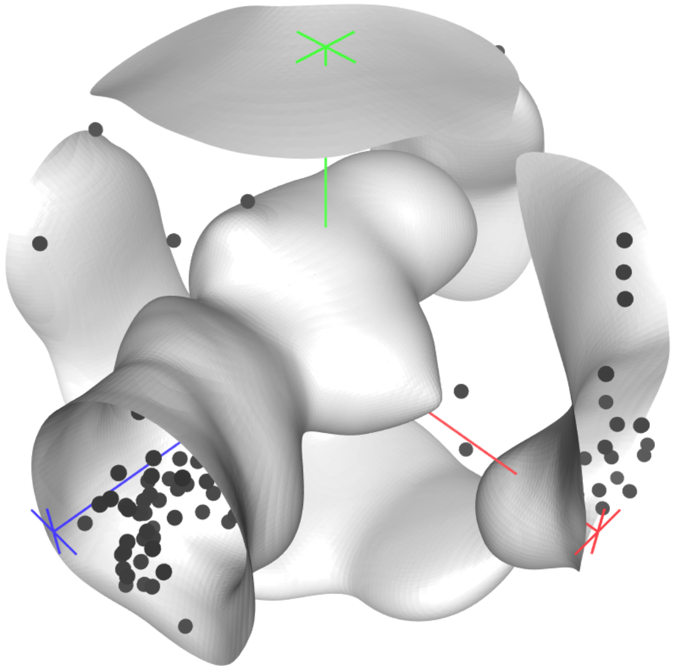

Figure 5: 3σ Kamb density level surface for a set of 168 slickenside orientations from California (Woodring et al., 1940). See the C tutorial `oriKambPlots.R`.

5. Installation

This section describes four steps for installing the R interpreter, some useful add-ons, and this R code library.

5.1. R itself

R is a statistical software system that is rapidly gaining popularity in academia and industry. The software is made by volunteers and published at no cost to the user. The software primarily uses a text interface rather than a graphical one. Nevertheless, we have tried to make common geology tasks easy and non-intimidating. Download and install R from `http://www.r-project.org/`.

5.2. XQuartz (macOS only)

The Windows version of R uses the standard Windows graphics system. The Linux version of R uses the X-Windows system, which is present on almost all Linux systems. The macOS version of R also uses X-Windows, which is not installed as part of macOS, but which must be installed separately.

So, if you are using a macOS computer and you have not already installed X-Windows, then visit `http://xquartz.macosforge.org/`, download the XQuartz package, and run the installer.

5.3. RStudio

When you use R, you often have many windows open at once: the R interpreter for running R commands, a text editor for writing programs, one or more windows for viewing plots, a file manager for opening files, a web browser for viewing help files, etc. Your screen gets cluttered quickly.

The RStudio application solves this problem by providing an integrated user interface for all of these tasks. I recommend it to all R users, but it will be especially useful in our short course, for providing a consistent user interface across multiple operating systems.

So download and install the free desktop version of RStudio from `https://www.rstudio.com/`.

5.4. Seven R packages

Hundreds of add-on packages are available for R, and the software provides a simple mechanism for downloading and installing them. We need a handful of them for these tutorials. Here is the procedure for installation.

1. Launch RStudio.
2. RStudio shows you a large window consisting of several "panes". Probably the Console pane is in the lower left corner of the window. It shows `>` as a command prompt. Copy and paste (or retype) the following line of code into the Console pane, and then press Return to execute it.
   ```
   install.packages("rgl")
   ```
   This command should cause a flurry of activity. If you see warnings about how some package was built with an earlier version of R, then ignore them. If an error occurs, then e-mail us the exact text of the error (and which package caused it), and perhaps we can help.
3. Similarly, install the following packages. (They do not have to be done in any particular order.)
   ```
   install.packages("fields")
   install.packages("MASS")
   install.packages("ICSNP")
   install.packages("expm")
   install.packages("Directional")
   install.packages("pracma")
   ```

5.5. This R code library

Most users have this `readme.pdf` document in a `geologyGeometry` directory with the rest of our library: subdirectories `data`, `library`, etc. If you have this document but not the rest of the library, then download the library from `http://www.joshuadavis.us/`.

Put this `geologyGeometry` directory somewhere accessible on your computer. You should probably not alter any of its contents, but feel free to add your own subdirectories to organize your own data and code.

5.6. The C parts of this library

This part of the installation is not essential. Windows users cannot do it. Linux/Unix users and Mac OS X users can do it easily, if they have C compilers installed.

There are many computer programming languages in the world, which fill various application niches. Roughly

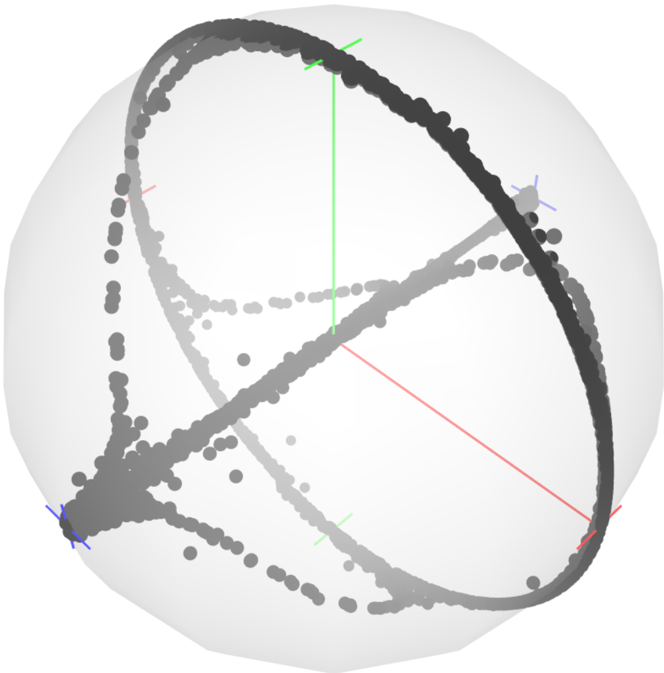

Figure 6: Equal-volume plot of the orientations of 1,000 rigid ellipsoidal inclusions after intense monoclinic transpression. See the miscellaneous tutorial `oriRigidFabric.R`.

speaking, higher-level languages, such as R, enable rapid development of programs that run slowly, while lower-level languages, such as C, require slow development of programs that run quickly. (The running speed difference is often around a factor of 100.) A common development strategy is to write a program in a higher-level language, determine which parts of the program require more speed, and then tactically rewrite those parts in a lower-level language. For this reason, R provides a facility for invoking C code from R, in a way that is mostly invisible to the user. So we have coded a few performance-sensitive parts of our library in C.

Installing the C parts of our library requires extra knowledge and work. The first step depends on your operating system:

- On Windows, you are probably not able to install the C parts at all right now. Sorry. The problem is that they depend on POSIX functions that are not easily installed on Windows. But don't be overly disappointed. You can still use over 90% of our library and tutorials. And the situation might improve in a future release of our library.

- On macOS, you need to have a C compiler installed. The simplest way to get one is to download Xcode from the Mac App Store. (Warning: It's big.) Once the compiler is installed, you need to launch the Terminal application, which gives you access to a command-line shell. You need to know some basic shell commands: `pwd` to print the working directory, `cd` to change the working directory, etc.

- On Linux, BSD, or any other Unix-alike, you almost certainly have C compilers installed and know how to use a command-line shell.

The second step is to compile the shared libraries. This must be done only once (per library version, per machine). You don't need to do this every time you start R. In the command-line shell, navigate to the `libraryC` directory, and enter these commands one-by-one:

```
R CMD SHLIB rotationsForR.c
R CMD SHLIB orientationsForR.c
```

The third step is to load the C parts into R's memory. This must be done every time you start R. The simplest way is to enter this command into R (from the appropriate working directory):

```
source("libraryC/all.R")
```

I have tested this procedure only on macOS. Please let me know if you run into problems.

While using C code from R, there is one other thing to know: It is not easy for R to stop C code while it is running. Pressing the Stop button in RStudio may not immediately stop the program. Eventually an interface may appear, giving you the option of killing R entirely. So activate a C routine only if you're sure that you want to.

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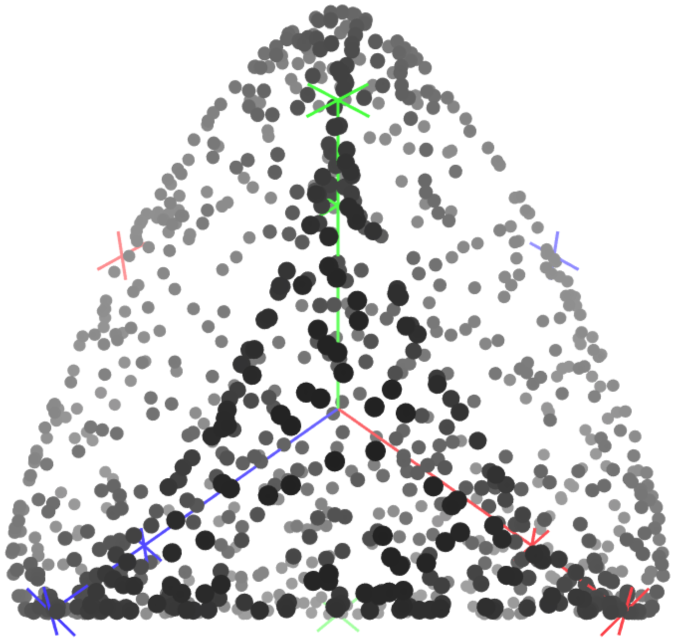

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Appendix A. Ellipsoids

There are six degrees of freedom in an ellipsoid. Intuitively, three are wrapped up in the ellipsoid's orientation and three are wrapped up in its size and shape. The specific manner in which these degrees of freedom are recorded has a significant effect on the ease of computations and theoretical derivations.

Appendix A.1. Orientation

There are various ways to define the orientation of an ellipsoid with three numbers. For example, one can specify the strike and dip of the plane containing the long and intermediate axes, and the rake of the long axis in that plane. Or one can specify a rotation matrix $\mathbf{Q}$ that rotates the ellipsoid into to some reference orientation. Although $\mathbf{Q}$ contains nine numbers, there are actually only three degrees of freedom, such as three Euler angles or the three non-redundant entries in an anti-symmetric matrix that exponentiates to $\mathbf{Q}$. Similarly, one can specify the orientation of an ellipsoid by specifying each of its semi-axis directions, perhaps using trend and plunge (six numbers total) or Cartesian coordinates (nine). In either of those systems there are redundancies; the actual number of degrees of freedom is three.

The treatment of ellipsoid orientations is greatly complicated when spheroids are present. A *spheroid* is an ellipsoid in which two of the axes have equal length. The orientation of a spheroid has only two degrees of freedom, such as the trend and plunge of the other axis. In other words, the three degrees of freedom are not well-defined. For ellipsoids that are nearly spheroidal, numerical calculations with orientations tend to be unreliable. In the deformable ellipsoid theory of Eshelby (1957); Bilby et al. (1975), spheroids must be handled as a special case (Jiang, 2007; Davis et al., 2013).

For a data set in which each ellipsoid is clearly triaxial, the orientations of the ellipsoids can be analyzed using orientation statistics. For a data set consisting of spheroids, the orientations can be analyzed using three-dimensional directional statistics of axial data (e.g., Mardia and Jupp, 2000). For a data set consisting of a mixture of triaxial ellipsoids and near-spheroids, neither of these approaches is ideal. We should use techniques that simultaneously account for orientation and size-shape. Such techniques are the major theme of this short course.

Appendix A.2. Magnitude (size and shape)

Similarly, the size and shape of an ellipsoid can be defined using three numbers in various ways. For example, one can specify the lengths a_1, a_2, a_3 of the three semi-axes, which are analogous to radii. As we shall see, geologists are often more interested in the (natural) logarithms of the semi-axis lengths. So let $\ell_i = \log a_i$.

The volume $V = \frac{4\pi}{3} a_1 a_2 a_3$ amounts to one degree of freedom. Frequently, but not always, volume is geologically irrelevant, so we normalize our ellipsoids to have the same volume as the unit sphere, meaning $a_1 a_2 a_3 = 1$ or equivalently $\ell_1 + \ell_2 + \ell_3 = 0$. The remaining two degrees of freedom describe shape, for which geologists use various conventions.

The *octahedral shear strain*

$$E_s = \sqrt{\frac{(\ell_1 - \ell_2)^2 + (\ell_2 - \ell_3)^2 + (\ell_3 - \ell_1)^2}{3}}$$

is 0 for spheres and positive for other ellipsoids. Its name derives from the situation in which a sphere is deformed to an ellipsoid by a homogeneous deformation. If the deformation is coaxial, then E_s measures the amount of work performed by the deformation (Nádai, 1963). However, E_s functions as an abstract measure of ellipsoid shape for ellipsoids of any provenance or meaning. In the normalized case it simplifies to $E_s = \sqrt{\ell_1^2 + \ell_2^2 + \ell_3^2}$.

Jelinek (1981) defined

$$P_j = \exp \sqrt{2((\ell_1 - \ell)^2 + (\ell_2 - \ell)^2 + (\ell_3 - \ell)^2)},$$

where $\ell = \frac{1}{3}(\ell_1 + \ell_2 + \ell_3)$. This P_j is tantamount to E_s, in that one can be easily transformed into the other via the relationship $P_j = \exp(\sqrt{2}E_s)$.

Assuming that the semi-axis lengths a_i are sorted so that $a_1 \geq a_2 \geq a_3$ or equivalently $\ell_1 \geq \ell_2 \geq \ell_3$, *Lode's parameter* is

$$\nu = \frac{2\ell_2 - \ell_1 - \ell_3}{\ell_1 - \ell_3}.$$

Lode's parameter is undefined for spheres and satisfies $-1 \leq \nu \leq 1$ for other ellipsoids. The cases $\nu = -1, 0, 1$ correspond to prolate spheroids, plane-strain ellipsoids, and oblate spheroids, respectively. Like octahedral shear strain, the term *plane-strain* derives from the study of deformation. Plane-strain homogeneous deformations produce finite strain ellipsoids that are plane-strain in the sense used here.

Again assuming $a_1 \geq a_2 \geq a_3$, *Flinn's* k is defined as

$$k = \frac{a_1/a_2 - 1}{a_2/a_3 - 1}.$$

Hrouda (1982) summarizes various other measures of ellipsoid shape, assuming $a_1 \leq a_2 \leq a_3$: $P = (a_1/a_3)^{-2}$ (different from the P_j of Jelinek (1981)), $L = (a_1/a_2)^{-2}$, $F = (a_2/a_3)^{-2}$, $T = 2(\ell_2 - \ell_3)/(\ell_1 - \ell_3) - 1$, etc.

We have expressed all of these measures of ellipsoid size-shape in terms of the three ℓ_i or the three a_i, but there is no theoretical sense in which the ℓ_i or a_i are primary. Except for a few redundancies such as E_s and P_j, any three measures of ellipsoid size-shape can be viewed as primary, with the other measures derivable from them. For example, suppose that we are given a volume V, octahedral shear strain E_s, and Lode's parameter ν. Combining the definitions of V and ν above yields $\ell_1 = \alpha + \beta\ell_3$ and $\ell_2 = \gamma + \delta\ell_3$, where

$$\begin{aligned} \alpha &= \frac{2}{\nu + 3}\log\left(\frac{3V}{4\pi}\right), \\ \beta &= \frac{\nu - 3}{\nu + 3}, \\ \gamma &= \left(1 - \frac{2}{\nu + 3}\right)\log\left(\frac{3V}{4\pi}\right), \\ \delta &= -1 - \frac{\nu - 3}{\nu + 3}. \end{aligned}$$

Then the definition of E_s amounts to $a\ell_3^2 + b\ell_3 + c = 0$, where

$$\begin{aligned} a &= 2 - 2\beta + 2\beta^2 - 2\delta - 2\beta\delta + 2\delta^2, \\ b &= -2\alpha + 4\alpha\beta - 2\gamma - 2\beta\gamma - 2\alpha\delta + 4\gamma\delta, \\ c &= 2\alpha^2 - 2\alpha\gamma + 2\gamma^2 - 3E_s^2. \end{aligned}$$

This quadratic equation can be solved for ℓ_3. Each value for ℓ_3 implies values for ℓ_1 and ℓ_2. The inequality $\ell_1 \geq \ell_2 \geq \ell_3$ can then be used to select the correct final solution for ℓ_1, ℓ_2, ℓ_3.

Appendix A.3. Ellipsoid tensors

Any ellipsoid can be described as an *ellipsoid tensor* $\mathbf{E}$ (e.g., Flinn, 1979), also called a *shape matrix* (Shimamoto and Ikeda, 1976) or *inverse shape matrix* (Wheeler, 1986; Robin, 2002). The ellipsoid is the set of points $\mathbf{x} = [x_1\ x_2\ x_3]^\top$ such that $\mathbf{x}^\top\mathbf{E}\mathbf{x} = 1$. The tensor is symmetric and positive-definite, and diagonalizes as $\mathbf{E} = \mathbf{Q}^\top\tilde{\mathbf{E}}\mathbf{Q}$, where $\mathbf{Q}$ is a rotation matrix,

$$\tilde{\mathbf{E}} = \begin{bmatrix} a_1^{-2} & 0 & 0 \\ 0 & a_2^{-2} & 0 \\ 0 & 0 & a_3^{-2} \end{bmatrix},$$

and the $a_i > 0$. The rows of $\mathbf{Q}$ are unit vectors (in the same $\mathbf{x}$-coordinates) indicating the directions of the ellipsoid semi-axes in a right-handed manner, and the a_i are the semi-axis lengths as above. The unit sphere is $\mathbf{E} = \mathbf{I}$, the identity tensor.

As a symmetric 3×3 tensor, an ellipsoid tensor has six non-redundant entries, which correspond to the six degrees of freedom in an ellipsoid. However, the orientation and volume-shape are all mixed up in the ellipsoid tensor. For example, the first entry of $\mathbf{E}$ is

$$E_{11} = \frac{Q_{11}^2}{a_1^2} + \frac{Q_{21}^2}{a_2^2} + \frac{Q_{31}^2}{a_3^2}.$$

This mixing makes ellipsoid tensors a little difficult to interpret, but it's advantageous in the long run. Orientation and volume-shape have to be mixed up, if our tensors are going to behave well mathematically, because they are inherently mixed up in the case of spheroids. For a given spheroid, there are infinitely many valid $\mathbf{Q}$s, but there is one and only one $\mathbf{E}$.

The characteristic polynomial of $\mathbf{E}$ is

$$\det(\mathbf{E} - \lambda\mathbf{I}) = -\lambda^3 + (\operatorname{tr}\mathbf{E})\lambda^2 - I\!I_{\mathbf{E}}\lambda + \det\mathbf{E},$$

where $I\!I_{\mathbf{E}} = a_1^{-2}a_2^{-2} + a_2^{-2}a_3^{-2} + a_3^{-2}a_1^{-2}$. The determinant of $\mathbf{E}$ is tantamount to the volume:

$$V = \frac{4\pi}{3}(\det\mathbf{E})^{-1/2}.$$

The other two coefficients $\operatorname{tr}\mathbf{E}$ and $I\!I_{\mathbf{E}}$ parametrize the shape of the ellipsoid, but in a way that is difficult to relate to other parametrizations. We return to this idea in a later section.

Each ellipsoid is describable as one and only one positive-definite symmetric tensor, and each positive-definite symmetric tensor describes one and only one ellipsoid. Further, this one-to-one correspondence preserves "nearness": for example, two tensors that are slightly different correspond to two ellipsoids that are slightly different. Therefore, for the purposes of mathematical calculations, we define the space of ellipsoids to be the space of positive-definite symmetric tensors. It is a subspace of the nine-dimensional space of all 3×3 tensors. It is six-dimensional, because there are six degrees of freedom.

Unfortunately, the space of ellipsoids is not a vector space. For example, it doesn't contain the zero tensor $\mathbf{0}$. You should think of the space of ellipsoids as curved. The lack of a vector space structure greatly inconveniences our calculations.

Appendix A.4. Log-ellipsoid tensors

A *log-ellipsoid tensor* $\mathbf{L}$ is the matrix logarithm of an ellipsoid tensor $\mathbf{E}$. The logarithm of a matrix is not simply the entry-by-entry logarithm of the matrix's entries, but it is easy to compute for ellipsoid tensors. If $\mathbf{E} = \mathbf{Q}^\top \tilde{\mathbf{E}} \mathbf{Q}$ as above, then $\mathbf{L} = \log \mathbf{E} = \mathbf{Q}^\top (\log \tilde{\mathbf{E}}) \mathbf{Q}$, where

$$\log \tilde{\mathbf{E}} = \begin{bmatrix} -2\ell_1 & 0 & 0 \\ 0 & -2\ell_2 & 0 \\ 0 & 0 & -2\ell_3 \end{bmatrix}$$

and $\ell_i = \log a_i$ as above. The unit sphere is $\mathbf{L} = \mathbf{0}$. As was true for $\mathbf{E}$, the ellipsoid's six degrees of freedom are all mixed up in $\mathbf{L}$. For example, the first entry in $\mathbf{L}$ is

$$L_{11} = -2(Q_{11}^2 \ell_1 + Q_{21}^2 \ell_2 + Q_{31}^2 \ell_3).$$

The characteristic polynomial of $\mathbf{L}$ is

$$\det(\mathbf{L} - \lambda \mathbf{I}) = -\lambda^3 + (\operatorname{tr} \mathbf{L})\lambda^2 - I\!I_{\mathbf{L}} \lambda + \det \mathbf{L},$$

where $I\!I_{\mathbf{L}} = 4(\ell_1\ell_2 + \ell_2\ell_3 + \ell_3\ell_1)$. The three nontrivial coefficients of this polynomial parametrize volume and shape in a meaningful way. First, because $\exp \operatorname{tr} \mathbf{M} = \det \exp \mathbf{M}$ for any tensor $\mathbf{M}$, the trace of $\mathbf{L}$ is tantamount to volume:

$$V = \frac{4\pi}{3} (e^{\operatorname{tr} \mathbf{L}})^{-1/2}.$$

A normalized ellipsoid is one where $\operatorname{tr} \mathbf{L} = 0$. Second, for normalized ellipsoids, a little algebra shows that $I\!I_{\mathbf{L}}$ is tantamount to E_s:

$$E_s = \sqrt{-\frac{1}{2} I\!I_{\mathbf{L}}}.$$

Finally, $\det \mathbf{L}$ contains information similar to Lode's parameter ν. To see so, assume that the ellipsoid is normalized and not a sphere, and order the semi-axes in decreasing order, so that $\ell_1 \geq \ell_2 \geq \ell_3$. Then $\det \mathbf{L} = -8\ell_1\ell_2\ell_3$ has the same sign as ℓ_2 does. For oblate, plane-strain, and prolate ellipsoids, $\det \mathbf{L}$ is positive, zero, and negative, respectively, much like ν. However, there is no simple formula for converting between $\det \mathbf{L}$ and ν (without involving the other degrees of freedom). For example, oblate spheroids have $\det \mathbf{L} = 16\ell_1^3$, but they all have $\nu = 1$. By the way, prolate spheroids have $\det \mathbf{L} = 16\ell_3^3$. So $\det \mathbf{L}$ can take on any real value.

Mathematicians like symmetry, both for aesthetic reasons (it's pretty) and for practical reasons (it often helps us simplify complicated calculations). In this case, symmetry suggests that geologists should abandon Lode's parameter in favor of some version of $\det \mathbf{L}$. (And Flinn's k is right out.)

Recall that ellipsoids correspond to positive-definite symmetric tensors. Similarly, log-ellipsoids correspond to symmetric tensors (that are not necessarily positive-definite). What's new here is that symmetric tensors form a vector space, so computations on them are comparatively easy. We now make the vector space structure more explicit.

Appendix A.5. Log-ellipsoid vectors

We can arrange the six non-redundant entries of a log-ellipsoid tensor $\mathbf{L}$ into a vector

$$\mathbf{l} = \begin{bmatrix} \sqrt{2} L_{12} \\ \sqrt{2} L_{13} \\ \sqrt{2} L_{23} \\ L_{11} \\ L_{22} \\ L_{33} \end{bmatrix}.$$

The $\sqrt{2}$ coefficients are chosen so that the dot product on vectors corresponds to the Frobenius inner product on tensors: If $\mathbf{L}_1$ and $\mathbf{L}_2$ are two log-ellipsoid tensors with vectors $\mathbf{l}_1$ and $\mathbf{l}_2$, then

$$\mathbf{l}_1 \cdot \mathbf{l}_2 = \operatorname{tr}(\mathbf{L}_1^\top \mathbf{L}_2).$$

That is, the conversion from log-ellipsoid tensors to vectors does not distort the geometry of the space of log-ellipsoid tensors.

For normalized ellipsoids, $\mathbf{L}$ contains only five non-redundant entries, because $L_{33} = -L_{11} - L_{22}$ for example. In this case we convert $\mathbf{L}$ to a vector $\mathbf{l}$ by

$$\mathbf{l} = \begin{bmatrix} \sqrt{2} L_{12} \\ \sqrt{2} L_{13} \\ \sqrt{2} L_{23} \\ \sqrt{\frac{3}{2}} (L_{22} + L_{11}) \\ \sqrt{\frac{1}{2}} (L_{22} - L_{11}) \end{bmatrix}.$$

Again the weightings are chosen so that the dot product corresponds to the Frobenius inner product.

In the end, ellipsoids are in smooth one-to-one correspondence with log-ellipsoid vectors, which form a vector space, which is a highly convenient setting for statistical calculations. So all of our complicated calculations operate on these vectors.

Appendix A.6. Ellipses in two dimensions

Most of the preceding discussion carries over to ellipses in two dimensions with minor modification. There are three degrees of freedom: orientation, area, and shape. The orientation can be analyzed using two-dimensional directional statistics (also called circular statistics) of axial data. The orientation is ill-defined for ellipses that are close to circular. The area and shape are functions of the two semi-axis lengths a_1, a_2 or their logarithms ℓ_1, ℓ_2. The area $A = \pi a_1 a_2$ is analogous to ellipsoid volume. The shape can be expressed as an *aspect ratio* a_1/a_2 or a_2/a_1, as a *shape factor*

$$B = \frac{a_1^2 - a_2^2}{a_1^2 + a_2^2}$$

(Bretherton, 1962), etc.

We can repackage an ellipse into an *ellipse tensor*

$$\mathbf{E} = \mathbf{Q}^\top \begin{bmatrix} a_1^{-2} & 0 \\ 0 & a_2^{-2} \end{bmatrix} \mathbf{Q}$$

or a *log-ellipse tensor*

$$\mathbf{L} = \log \mathbf{E} = \mathbf{Q}^\top \begin{bmatrix} -2\ell_1 & 0 \\ 0 & -2\ell_2 \end{bmatrix} \mathbf{Q},$$

where the rows of $\mathbf{Q}$ are the semi-axis directions. Rotations are dramatically simpler in two dimensions than in three dimensions, so that

$$\mathbf{Q} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix},$$

where θ is the heading of the first semi-axis, measured from the x-axis clockwise (toward the $-y$-axis). This angle θ is the one degree of freedom in orientation. The characteristic polynomial of $\mathbf{L}$ is

$$\det(\mathbf{L} - \lambda\mathbf{I}) = \lambda^2 - (\operatorname{tr}\mathbf{L})\lambda + \det\mathbf{L}.$$

The coefficient $\operatorname{tr}\mathbf{L}$ is tantamount to area. Normalization means $\operatorname{tr}\mathbf{L} = 0$ (or $\det\mathbf{E} = 1$). The coefficient $\det\mathbf{L} = 4\ell_1\ell_2$ is tantamount to shape.

Unnormalized log-ellipse tensors $\mathbf{L}$ can be converted to three-dimensional vectors $\mathbf{l}$ by

$$\mathbf{l} = \begin{bmatrix} \sqrt{2}L_{12} \\ L_{11} \\ L_{22} \end{bmatrix}.$$

Normalized $\mathbf{L}$ can be converted to two-dimensional

$$\mathbf{l} = \begin{bmatrix} \sqrt{2}L_{12} \\ \sqrt{2}L_{11} \end{bmatrix}.$$

In both cases the chosen weightings preserve the Frobenius inner product.