THE INTERACTION OF STATISTICS AND GEOLOGY
-- FINITE DEFORMATIONS--

by

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ABSTRACT

The paper describes briefly the instances where the analysis of geological data has required the development of new statistical theory and methods. A new instance of this fruitful interaction of statistics and geology is then given. §2 develops the theory of finite deformations. Some of the classical and novel statistical problems which arise when objects embedded in a deformed rock are measured for strain estimation are discussed in §3.
1. INTRODUCTION

Sir Ronald Fisher (1953a) in a Presidential address to the Royal Statistical Society on the "Expansion of Statistics" used as his first example the statistical thinking of Lyell whose "Principles of Geology" is now 150 years old and whose publication is celebrated in this volume. While this is an example of statistics helping Geology, it did not lead to developments in Statistics. In this paper we wish to consider (with key references) some instances of mutually beneficial interactions and to describe some specific results of interest to structural geologists and statisticians.

In the same year Fisher published his famous paper on "Dispersion on a Sphere" (1953b). Its primary purpose was to provide statistical methods for the new data of palaeomagnetism but he also used it to illustrate his theory of Fiducial Inference. Though orientation data are not peculiar to Geology and Geophysics, it was these subjects which first demanded such statistical methods. This led to a new area of statistical theory and practice and to the improvement of data analysis in Geology. This story is now quite well known -- see e.g. the paper of Watson (1970) and the book by Mardia (1972). Watson's paper contains brief sections on orientation analysis in Palaeomagnetism, Sedimentology, Structural Geology and Petrofabrics. An update of this would discuss among other things the relation to Plate Tectonics and the use of orientation statistics to estimate the angular momentum vectors of
the plates and their finite displacements. (see e.g. Molnar et al)

The mutually beneficial interaction of Statistics and Geology and Mining in the description of the fabric of sediments and the dispersion of commercially valuable ores is also well known and particularly associated with Matheron and the Fontainebleau School.

Less well known perhaps is the enormous interaction in quantitative Seismology, mainly due to the towering figure of Sir Harold Jeffreys. In his book "The Earth" (1962-first published 1924) he remarks (p.395): "It is astonishing that experimenters will spend months in making a series of observations and grudge the day or so needed to present the results in an intelligible form". This led him to write two books "Scientific Inference" (1931) and "The Theory of Probability" (1939). The latter was the first large scale account of Statistics from a Bayesian point of view. Jeffrey's did not, as a classical scientist, espouse subjective priors. To obtain his priors he required that they be invariant under functional transformations of the parameter in question. This rule is the basis of some modern accounts of Bayesian methods e.g. Box and Tiao (1973).

But there is much more in the 1939 book that is of current interest to statisticians whatever their views on Inference. For example, he remarks that while different observers looking at a seismogram will usually agree to a second or so when a particular wave train arrived, occasionally there are discrepancies of 10 or so seconds. Thus the normal distribution for arrival times will not be followed. He models this both by a distribution with
heavier tails than normal and as a "contaminated" distribution. He points out that the maximum likelihood (m.l.) estimator \( \hat{\theta} \) for \( \theta \) in the density \( f(x-\theta) \) satisfies, with data \( x_1, \ldots, x_n \),
\[
\sum f'(x_i-\theta)/f(x_i-\theta) = 0.
\]
He writes
\[
\frac{f(x-\theta)}{(x-\theta)f(x-\theta)} = w(x-\theta)
\]
so that the m.l. equation can be written as
\[
\sum(x-\theta)w(x-\hat{\theta}) = 0,
\]
and that \( \hat{\theta} \) is thus a weighted mean of the observations. He goes on to regard the observations as a mixture of Gaussian and long-tailed distributions. These ideas are precisely those suggested much later by Tukey, Huber and others concerned with Robustness -- see e.g. Andrews et al. (1972), Mosteller and Tukey (1977).

Modern theory and data analytical methods in Quantitative Seismology may be best studied now in the two-volume work of Aki and Richards (1980). In an early paper however, Scheidegger (1964) suggested the method for estimating the fault plane movement along which caused the earthquake being analyzed. In this paper he introduced the probability density proportional to \( \exp(-\cos^2 \theta) \) which was independently suggested by Dimroth (1963) and Watson (1965) for other orientation problems. Scheidegger wrote other papers on this area with Fara with whom he also wrote the first paper on the stochastic description of sedimentary fabrics--Fara and Scheidegger (1961). However most seismological data analysis is either
generalized regression analysis or, more interestingly, very elaborate time series analysis. References to the latter topic may also be found Brillinger (1975) -- the review of the uses of spectral analysis in Geophysics by Tukey (1965) should be especially noted. Seismic methods for exploration raise many problems -- see e.g. the papers and books by Enders Robinson e.g. (1978).

The analysis of seismic signals may be pursued to investigate their source (e.g. earthquake or explosion) or to investigate the media they pass through from source to receivers. This theory is of course based on the theory of elastic deformations. Structural geologists also use the theory of elasticity to unravel the history of rock formations.

In the next section a brief account is given of a simple form of elastic deformation, homogeneous strain. In section three, some statistical problems suggested by homogeneous strain are described as another example of a fruitful interaction between Statistics and Geology.
2. HOMOGENEOUS STRAIN

While in seismology one usually deals with small reversible deformations, over long time periods rocks acquire large strains -- see e.g. Ramsey (1967). These might be the result of a sequence of linear deformations or homogeneous strains. In this section we summarize the description of such strains in p dimensions. In practice p = 2 or 3.

A physical deformation, if linear, is characterized by matrix $\mathbf{R}$ with whose determinant $|\mathbf{R}| > 0$. For the transformation must grow from $I$ and be $1 - 1$. Since its determinant cannot change sign and is initially positive, it must remain so. Any two points initially joined by a vector $\mathbf{x}_0$ of length $s_0$ are separated by $s$ after the deformation, where

$$\frac{s^2 - s_0^2}{s_0^2} = \frac{\mathbf{x}_0 \cdot (\mathbf{R}^T \mathbf{R} - I) \mathbf{x}_0}{\mathbf{x}_0 \cdot \mathbf{x}_0}$$

When the deformation is small, the left hand side of (1) is approximately $2(s - s_0)/s_0$. Hence the strain tensor or matrix $\mathbf{E}$ is defined by

$$\mathbf{E} = \frac{1}{2}(\mathbf{R}^T \mathbf{R} - I)$$

If the eigen vectors and values of $\mathbf{E}$ are $\mathbf{x}_1$ and $\eta_1$ respectively ($i = 1, \ldots, p$), the $\eta_1$ are called the extensions since they equal $(s - s_0)s_0$ when $\mathbf{x}_0$ is in the direction $\mathbf{x}_1$. The $\eta_1$ may be negative if there is compression in the direction $\mathbf{x}_1$, positive if there is tension and $\eta_1 > -1/2$. 
In spaces of odd dimension, since $|k| > 0$, $k$ must have at least one positive eigenvalue and to each positive eigenvalue corresponds an invariant direction. There are, however, $p$ mutually orthogonal directions which remain so after deformation and it is easy to verify that these are defined by the eigenvectors $e_i$ of $k$, the principal strain axes. Deformation corresponds to a rotation of these axes and extensions along them.

A strain $k$ is said to be pure if and only if it leaves invariant $p$ orthogonal directions $e_1, \ldots, e_p$, say. Thus these vectors must be right eigenvectors of $k$ with non-zero roots, $\alpha_1, \ldots, \alpha_p$, say. Writing $k = [e_1, \ldots, e_p]$, $k(\alpha) = \text{diag}(\alpha_1, \ldots, \alpha_p)$, we have the symmetric form for $k$

$$k = k^T k$$

In this case,

$$\xi = \frac{1}{2}(k^T k^2)^{\frac{1}{2}}$$

The general deformation $k$ may now be decomposed into a rotation $k_1$, $|k_1| = 1$, followed by a pure strain $e_1$, or a pure strain $\xi_2$ followed by a rotation $k_2$, $|k_2| = 1$. These are just the polar decompositions of $k$. Since $k = e_1 k_1 = k_2 \xi_2$, $k^T k = \xi_2^2 = 2\xi + \lambda_p$ so that a suitable choice for $\xi_2$ is

$$\xi_2 = k^T k^2$$

(5)
where \( s_1 = \sqrt{2n_1 + 1} \). Then \( R_2 \) is given by

\[
R_2 = R_{\xi_2} S_2^{-1}
\]

(6)

The other factorization uses the eigenvectors of \( R R' = S_1^2 \).

Deformations are often described in terms of their effects on a quadric surface, \( \xi' Q \xi = c^2 \) centered at \( \xi \). It will be moved and become the surface

\[
\xi'(R R'^{-1} R')^{-1} \xi = c^2
\]

Thus the image of a sphere, called the strain ellipsoid, is

\[
\xi'(R R')^{-1} \xi = c^2
\]

(7)

and the ellipsoid that has a spherical image, called the reciprocal strain ellipsoid, is

\[
\xi R' R \xi = c^2
\]

(8)

The principal axes of (7) and (8) are those of \( S_1 \) and \( S_2 \) respectively.

If the strain is small, \( B = I + A \), \( A \) small, so that, approximately,

\[
\xi = 1/2 (A + A')
\]

(9)

It is customary, when dealing with small strains, to write the displacement \( A \xi = Bx - x \) of a point \( x \) as
\[ A\chi = \frac{A - A'}{2} \chi + \frac{A + A'}{2} \chi, \]
\[ = \tilde{\chi} \chi + \epsilon \chi, \quad (10) \]

where the skew-symmetric matrix \( \tilde{\chi} \) describes the rotation and \( \epsilon \) the pure strain, which are now additive. Thus, approximately,
\[ R_1 = R_2 = \tilde{\chi} + \mathbb{I}_p, \quad S_1 = S_2 = \epsilon + \mathbb{I}_p, \quad (11) \]
3. STATISTICAL PROBLEMS WITH HOMOGENEOUS STRAINS

Strain must usually in Geology be determined by the deformation of objects embedded in the rock. It is e.g. rarely possible to use devices like strain gauges. Further the rock is opaque so we are usually restricted to data obtainable from the surface of plane sections cut through rock samples. We must of course know something of the original shape and distribution of the objects.

Point-like objects distributed at random (by a Poisson process) with unknown mean density \( \lambda \) per unit volume in the rock would be useless. For the points in any region go with it under the transformation \( \mathbf{R} \) while the volume of the region increases by the factor \( |\mathbf{R}| \) so the transformed field of points is again Poisson but with density \( \lambda / |\mathbf{R}| \). If \( \lambda \) were known \( |\mathbf{R}| \) could of course be found. \( |\mathbf{R}| \) is called the dilatation of the strain. To get more information about \( \mathbf{R} \), the points distribution must have more structure, as will be seen below. But interesting mathematical problems remain in the study of affine transformations of stationary point processes, more general than the Poisson process.

If we could measure the initial positions \( \mathbf{x}_i \) at \( n \) points and then measure the final positions \( \mathbf{R}\mathbf{x}_i \), \( \mathbf{R} \) may be estimated when e.g. the measurement errors in both cases are independently Gaussian with mean vectors zero and covariance matrices \( \sigma^2 I_p \) -- see Gleser and Watson (1973). Unfortunately though this might
be used in glaciology, it is not of use with ancient rocks. This problem is a generalization of the "errors in variables" problem in a situation where it admits a clean solution. The simple form (p=1) of this problem may be found in textbooks (see e.g. Theil (1971)) on Econometrics: $y = \beta \xi + f$, $x = \xi + e$ where the errors of measurement $e$ and $f$ of $x$ and $y$ are independent Gaussians with means zero and variances $\sigma_x^2$ and $\sigma_y^2$. If $\sigma_x^2$ and $\sigma_y^2$ and $\xi$ are arbitrary and unknown, there is no satisfactory solution basically because each new observation introduces a new unknown $\xi$. But if $\sigma_x = \sigma_y$, there is a satisfactory solution.

Useful information about the strain matrix may however be obtained from points with unknown initial positions but arranged in special patterns e.g.

(i) lines of known initial length
(ii) angles of known size
(iii) spherical or nearly spherical bodies.

As an example of (i), consider a crystal of tourmaline embedded in a rock which is then stretched in the direction of this long narrow crystal. The crystal will break into a number of pieces if the strain is large enough. The initial length is the sum of the pieces. The final length is the distance from the beginning of the first fragment to the end of the last. An example of (ii) would be a brachiopod whose shape is roughly like a semi-circle before deformation. The radius perpendicular to the base is, after deformation, inclined at a measurable angle to the base.
It is estimated that 70% of all strain studies are of type (iii). Oolites (concretory structures) are a common source of data. They are initially roughly spherical so their final shape will be (roughly) the strain ellipsoid. Cutting plane sections through solids and studying the statistics of the intersections with the embedded bodies leads to well known problems. The theory of such methods usually assumes purely random planes—however structural geologists usually make cuts related to the roughly known strain axes which changes the methods.

Statistical methods for these problems were outlined in Watson (1968) and will appear in Watson (1981). Many papers have appeared in the interim—see e.g. the discussion organized by Ramsey and Wood (1976) and the references therein. One paper—Owens (1973)—is particularly interesting and a sequel to March (1932). It discusses the modification under strain of an angular density distribution.

Let \( f_0(\xi) \) denote the density of lines with direction \( \xi \), \( \xi \xi = 1 \) in the solid before deformation. Then \( f_0(\xi)\delta\omega_0 \) is proportional to the number of lines in the cone about \( \xi \) with solid angle \( \delta\omega_0 \). After deformation, the axis of this cone will be parallel to \( R\xi \) and its volume will be \( |R| \) times its previous value \( \delta\omega_0/3 \). If the new cone has solid angle \( \delta\omega_1 \), its length is \( |R\xi| \), and so its volume is \( |R\xi|^3\delta\omega_1/3 \). Hence

\[
\frac{|R|\delta\omega_0}{3} = \frac{|R\xi|^3\delta\omega_1}{3}
\]
or

\[ \delta \omega_0 = \frac{||R \mathbf{e}||^3}{|R|} \delta \omega_1 \]  

(12)

The new density \( f_1 \) of line directions is then determined by the fact that the number of lines in each cone are equal i.e., by

\[ f_1(\mathbf{B} \mathbf{e} / ||R \mathbf{e}||) \delta \omega_1 = f_0(\mathbf{e}) \delta \omega_0 \]  

(13)

Using (2.12),

\[ f_1(\mathbf{B} \mathbf{e} / ||R \mathbf{e}||) = f_0(\mathbf{e}) ||R \mathbf{e}||^3 / |R| \]  

(14)

as obtained by Owens in different notation. Hence putting

\[ \mathbb{R} = \mathbf{R} \mathbf{e} / ||R \mathbf{e}||, \quad \mathbf{L} = \mathbf{R}^{-1} \mathbf{e} / ||B \mathbf{e}||, \]

(14) may be rewritten as

\[ f_1(\mathbb{R}) = f_0(\mathbf{R}^{-1} \mathbf{e} / ||R \mathbf{e}||) / ||R|| ||R^{-1} \mathbf{e}|| \]  

(15)

A full discussion of this method of modifying spherical distributions will be given in Watson (1981). Note however that if \( f_0(\mathbf{e}) = f_0(-\mathbf{e}) \), the same is true of \( f_1 \) and that if \( B \) is a rotation (14) reduces to \( f_1(B \mathbf{e}) = f_0(\mathbf{e}) \). These are both necessary checks. Furthermore if \( f_0 = (4\pi)^{-1} \), the uniform distribution, in (15), the non-obvious formula

\[ \int ||B^{-1} \mathbf{e}||^{-3} d\mathbf{e} = |B| \]

(16)

\[ ||\mathbf{L}|| = 1 \]

is a consequence of the integral of \( f_1(\mathbf{m}) \) being unity.
Much of the profit that statisticians may derive from the study of homogeneous strain comes from the physical intuition it associates with linear transformations. To those interested in orientation or directional statistics it may seem awkward because unit vectors before strain usually do not have unit length afterwards. However many directional distributions are often best thought of as distributions of vectors $\mathbf{y}$, conditional upon $\|\mathbf{y}\|=1$ or marginally i.e. after integrating out their length and retaining only their direction. For example, the Arnold-Fisher-von Mises distribution with density proportional to $\exp k'\mathbf{y}$ where $k > 0$, $\|\mathbf{y}\| = \|\mathbf{y}\|=1$ can be obtained exactly as the marginal distribution of $\mathbf{y} = R\mathbf{y}$, a Gaussian vector with mean $\mathbf{y}$, covariance matrix $\sigma^2 R$, when $R$ is fixed. But it may be obtained to a very good approximation as the marginal distribution of $\mathbf{y} = R\mathbf{y}$ -- the distribution actually obtained is the angular Gaussian. For mathematical and numerical comparisons see Watson (1980a,b).

As a matter of history it is interesting to note that Arnold's Thesis (1941) was motivated by the dissatisfaction of J.F. Bell with the then available methods for analyzing data on the preferred direction of the optical axes of crystals in rocks. Prof. Bell subsequently had a distinguished career at Johns Hopkins in Mechanics. Geology has certainly benefitted from the development of these methods. Thus this is an example of the fruitful interaction of Statistics and Geology.
REFERENCES


The paper describes briefly the instances where the analysis of geological data has required the development of new statistical theory and methods. A new instance of this fruitful interaction of statistics and geology is then given. It develops the theory of finite deformations. Some of the classical and novel statistical problems which arise when objects embedded in a deformed rock are measured for strain estimation are discussed.