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The least-squares line and plane and the analysis of palaeomagnetic data

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Summary. The classic, multivariate technique of principal component analysis can be used to find and estimate the directions of lines and planes of best least-squares fit along the demagnetization path of a palaeomagnetic specimen, thereby replacing vector subtraction, remagnetization circles and difference vector paths with one procedure. Eigenvalues from the analysis are the variance of the data along each principal axis, and provide a relative measure of collinearity or coplanarity which may be used to define a general palaeomagnetic precision index. Demagnetization planes found with principal component analysis may be used in place of difference vector paths for locating Hoffman–Day directions, avoiding unnecessary vector subtraction and intensity truncation steps. Two methods are discussed for jointly estimating an average remanence direction from demagnetization lines and planes.

1 Introduction

The Earth's magnetic field continually changes in polarity, direction, and intensity when viewed through geologic time. After its formation, a rock is exposed to a variety of changing magnetic fields. If at certain times during this history, it is subjected to physical or chemical conditions which alter its mineralogy or magnetic properties, it may completely or partially gain a new magnetic remanence. Typically, this new remanence will form a discrete component parallel to the local geomagnetic field direction and add vectorially to any of the original remanence remaining in the rock. Although it is desirable in most palaeomagnetic studies to find the direction of all these various components, techniques currently in use do not exploit all of the available data (especially intensity). Ideally, analytical methods at both the specimen and sample levels should be based on as much of the original magnetic information as possible, with minimal assumptions. To accomplish this goal, it is necessary to first apply the classic multivariate technique of principal component analysis to collinear and coplanar points along a specimen's demagnetization path. Principal component analysis provides estimates of relative collinearity or coplanarity of the data, as well as directions of best least-squares fit. Next, if groups of lines and planes of specimens from different samples respectively yield clusters (bipolar with mixed N and R data) and girdles of directions on a stereonet which indicate a common magnetic component, all of the directions should be combined into a joint estimate for the average remanence. Techniques for both of these are discussed and developed in Sections 2 to 6, and applied to palaeomagnetic examples in Section 7.

Although principal component analysis is based partly on least-squares minimization, it should not be confused with the exponential least-squares modelling technique of Stupavsky & Symons (1978). Their technique presumes a log-normal grain size-coercivity distribution in space and requires systematic af demagnetization data; when applicable, their exponential models may have greater ability to resolve superimposed components. Many sedimentary rocks, however, do not respond well to af demagnetization, and the magnetic grain-size distributions of freshwater and marine sediments may for example be disturbed by a discrete, single domain spike of biogenic magnetite (Frankel, Blakemore & Wolfe 1979; Kirschvink & Lowenstam 1979). Techniques discussed in this paper are generally applicable to all remagnetization data regardless of demagnetization procedure, magnetic mineralogy, type of remanence or grain-size distribution.

2 Separation of magnetic components

Directions of magnetic components within a rock may be separated by progressively destroying in small increments the natural remanence through heating, af demagnetization, chemical leaching or other demagnetizing procedures; these experiments attempt in part to reverse in the laboratory the mechanisms by which the remanence was gained in nature. The orientation and intensity of the magnetism measured after an incremental demagnetization experiment constitutes a magnetic vector, the 'tip' of which forms a point in magnetic three-space; the set of all such points produced during progressive demagnetization defines the demagnetization path for the specimen. Conversely, a point in magnetic three-space represents a vector pointing from the origin to it. Ordered points along these paths conceptually fall into three geometric groups: lines, planes and three-dimensional curves. A series of points which are collinear usually indicate the progressive removal of one magnetic component; the direction of the line containing them is, of course, parallel to the discrete magnetic vector that was removed. Coplanar points are likewise found when two discrete magnetic components are simultaneously removed in differing ratios; this plane is best described by its pole (perpendicular direction). It should be emphasized that the direction found for a line on a demagnetization path is an estimate of where the remanence *is*, while a pole to a demagnetization plane is an estimate of where the remanence *is not*. Both are of use in palaeomagnetic studies as will be discussed in Sections 5 and 6. The third category, a three-dimensional curve, is produced by the simultaneous, progressive removal of more than two discrete magnetic components. These three geometrical groups may be encountered individually, or together in any order along the demagnetization path of a palaeomagnetic specimen, and it is important in nearly all such studies to recognize the lines and planes within the data and estimate their direction.

Many techniques have been proposed and are currently used in palaeomagnetic studies to locate and estimate the direction of collinear and coplanar points along a demagnetization path. The most popular include the best demagnetization step, stable end point, orthogonal projection, vector subtraction, remagnetization circles and difference vector paths (for example Collinson, Creer & Runcorn 1967; Zijderveld 1967; Khramov 1958; Halls 1976, 1978; Hoffman & Day 1978). The success of these palaeomagnetic techniques is generally unquestioned; they often yield reasonably accurate estimates of the desired magnetic directions. However, all of these techniques either use only one or two of the data points (such as vector subtraction) or exclude a major part such as the intensity (remagnetization circles and difference vector paths). The classic multivariate technique of principal component analysis (Pearson 1901; Hotelling 1933) was developed to handle this type of data without such unnecessary exclusion, but it has not been used in progressive demagnetization studies. Because recent technological developments have substantially reduced the effort required to progressively demagnetize and measure a rock specimen (Molyneux 1971; Goree & Fuller 1976), large amounts of data are rapidly becoming available. It therefore seems timely to replace the graphical and vector-subtraction techniques currently in use with the analytic rigor of principal component analysis. For lines and planes, this method provides directions of best least-squares fit to the data as well as a measure of their collinearity or coplanarity.

3 Principal component analysis

Principal component analysis is simply a linear transformation of the orthogonal coordinate axes to a new orthogonal reference frame that corresponds to the geometry of the data set. The origin in the new system corresponds to the 'centre of mass', while the new axes are positioned by least-squares to best fit the data. Each axis in the new reference system has associated with it a measure of the variance (σ^2) about the mean in that particular direction; two of the axes are positioned to correspond to the maximum and minimum direction of variance, while the other (in the three-dimensional case) is intermediate. Through the use of Lagrange multipliers, it can be shown that the principal axes parallel the eigenvectors of the matrix of sums of squares and products,

$$H = \begin{bmatrix} \Sigma(x_i - \bar{x})^2 & \Sigma(x_i - \bar{x})(y_i - \bar{y})^2 & \Sigma(x_i - \bar{x})(z_i - \bar{z}) \\ \Sigma(x_i - \bar{x})(y_i - \bar{y}) & \Sigma(y_i - \bar{y})^2 & \Sigma(y_i - \bar{y})(z_i - \bar{z}) \\ \Sigma(x_i - \bar{x})(z_i - \bar{z}) & \Sigma(y_i - \bar{y})(z_i - \bar{z}) & \Sigma(z_i - \bar{z})^2 \end{bmatrix} \tag{1}$$

where $P_i = [x_i, y_i, z_i]$, $i = 1, N$ are the N data points in the old coordinate system and $U = [\bar{x}, \bar{y}, \bar{z}]$ is the position of the origin for the new system. Eigenvalues ($\lambda_{\text{max}}, \lambda_{\text{int}}, \lambda_{\text{min}}$) associated with each eigenvector are the variance of the data along the new axes. If the points all lie precisely along a line, for example, all of the variance is parallel to it. One principal component completely represents the data, and the dimensionality of the total system may be reduced. In this case two eigenvalues will be zero while the third is large, one eigenvector will parallel the line and the other two will be at arbitrary right angles to it. Similarly, there is no variance perpendicular to a plane which contains all of the data; the pole to this plane is the eigenvector associated with the zero variance.

This mathematical procedure is equivalent to finding the lines and planes of best least-squares fit as derived by Schomaker *et al.* (1958) and Blow (1960). If the data are treated as point masses, the mathematics are equivalent to finding the principal axes of inertia about the point U. Note that if U is taken as some point other than the centre of mass, the lines and planes will still be constrained to pass through it while at the same time minimizing the sum of squared deviations. Matrix H is also equivalent to Watson's (1960) matrix of sums of squares and products if each data point, P_i, is truncated to unit distance from the origin and the point U is taken as $[0, 0, 0]$. In this form H serves as the basis for Dimroth–Watson and Bingham spherical statistics (Watson 1960, 1965, 1966; Dimroth 1963; Bingham 1964, 1974). Most computing centres have standard software programs for computing eigenvectors and eigenvalues from symmetric matrices, the IBM Scientific Subroutine Package (SSP) routine EIGEN is one such program.

4 Application to palaeomagnetics

4.1 LOCATION OF LINES AND PLANES

Groups of points which belong to lines and planes along a demagnetization path have been recognized in most palaeomagnetic studies using graphical techniques. Lines are recognized

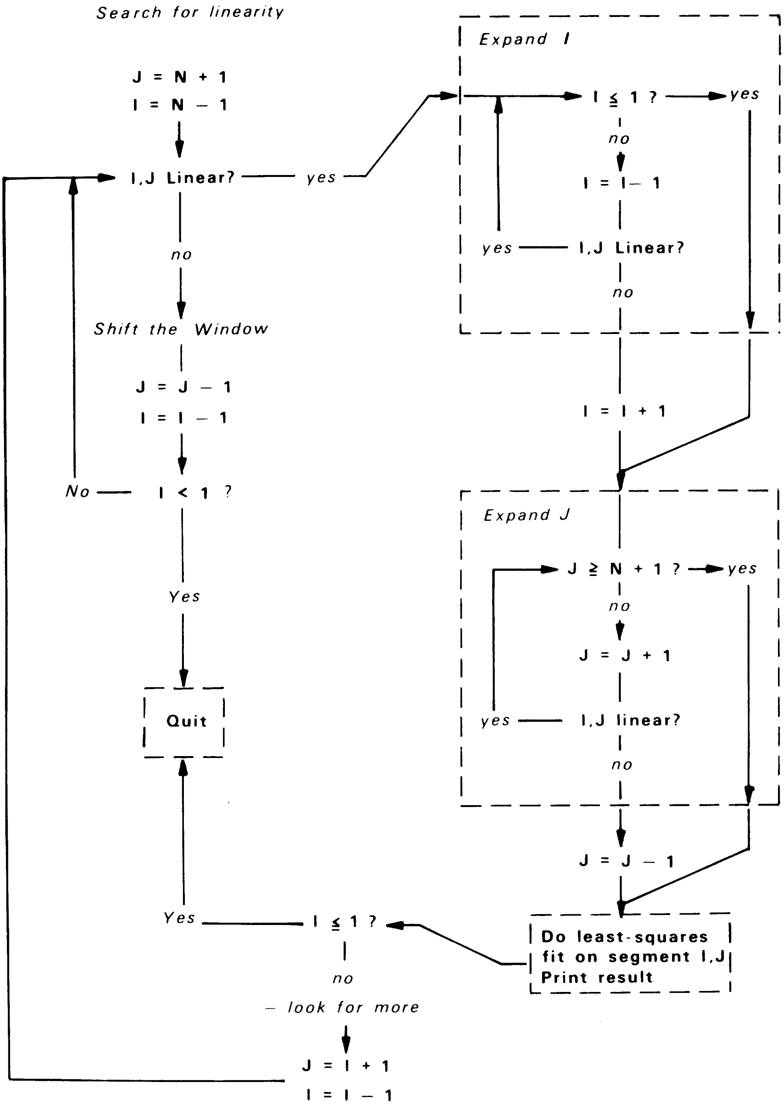

Figure 1. A flow chart for locating collinear and coplanar pieces of the demagnetization path. The N data points are numbered sequentially starting with the NRM, and a search begins by setting the J index on the origin (0, 0, 0) and the index I on the N-1th point. These three points in the first window between I and J are checked for linearity. If they do not fall on a line, the window is moved further down the demagnetization path and again tested. When three collinear points are found, neighbouring points are added until the boundaries of the straight segment are located. The window is then repositioned and the search process repeated until no further linearity remains. The 'I, J linear?' test is positive if the MAD for the points I to J is less than a given value. Data points which lie on a plane may be found by starting with a similar four-point search window.