

The fold test: an eigen analysis approach

L. Tauxe ^{a,1}, G.S. Watson ^b

^a *Scripps Institution of Oceanography, La Jolla, CA 92093-0220, USA*

^b *Department of Mathematics, Princeton University, Princeton, N.J., USA*

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Abstract

We combine eigen analysis and parameter estimation techniques for a newly constituted, more versatile fold test. The method is automatic, requiring no assumptions about the polarity or distribution of data, and gives confidence limits on the degree of unfolding required to produce the tightest grouping of data. We illustrate the method using several published data sets that show the tightest data groupings before, after and during correction for bedding tilt. The latter case is usually ascribed to acquisition of remanence during folding, but we show that this behavior can also arise from undetected multiple rotations. In our simulation, the beds undergo rotation about a vertical axis as well as a horizontal one, a case likely to occur in nature. These data, when rotated back to horizontal around what would be the observed strike, exhibit a peak in concentration at about 60% unfolding, very like the behavior of many published data sets. Thus, the origin of remanence in many such cases may not be syn-folding at all, but the behavior may purely be the result of an artifact of structural complications.

1. Introduction

Paleomagnetic analysis of rocks seeks to determine the direction of the ancient geomagnetic field. One of the key components in such studies is to determine the coordinate system for which the direction is valid. If a rock has moved from its original position, was it magnetized in the original, in the present or in some other position? Moreover, is simple rotation about strike an appropriate method for restoring the beds to their original positions? Graham [1] first suggested several so-called ‘field tests’ to provide a means for

assessing these questions. In the ‘fold test’, the directions of magnetization of a deformed rock unit are assumed to be most parallel in the orientation in which the magnetization was acquired. Thus, if a rock has retained an original magnetization through a subsequent folding or tilting event, the magnetic directions will cluster most tightly after they have been rotated back to their original positions.

Graham lived in a world with no adequate statistical framework for dealing with directional data; this was first introduced by Fisher [2]. McElhinny [3] proposed calculating the concentration of the data (using Fisher’s concentration parameter, κ) before and after correction for bedding tilt and comparing the ratio of the two to values for significance listed in statistical ‘F’ tables. The test can be done on the back of an

¹ Present address: Fort Hoofddijk Paleomagnetic Laboratory, The University of Utrecht, Budapestlaan 17, 3584 CD Utrecht, The Netherlands. e-mail: ltauxe@geof.ruu.nl. [RvdV]

envelope and was immediately embraced by the paleomagnetic community; indeed it is still in frequent use.

As many have noted previously [e.g., 4], the fold test appears at first glance to be simple, but it is not. The principal problem is that paleomagnetic vectors are never perfectly parallel. The scattered nature of the data means that a statistical test is necessary to determine if clustering is 'significantly' better in one orientation or another. Also, the geomagnetic field, itself, has two preferred states (normal and reversed) and is not perfectly dipolar [5]. Observed directions are thus not only scattered and but are often of two polarities. Furthermore, the magnetic vectors may be complicated sums of several components, an aspect we will ignore in this paper. The final problem is that structural attitudes are also imperfectly known. Not only are the bedding orientations themselves often difficult to measure accurately, but detection of complications, such as plunging folds, and multiple phases of tilting, are also very difficult to detect, requiring extensive field work. Finally, it is nearly impossible to detect rotation about the vertical axis on the basis

of field relations alone, as it results in no visible effect on the attitude of the beds themselves.

There are several fundamental problems with the fold test as defined by McElhinny [3]. As noted by McFadden and Jones [6], the test is invalid because the two estimates of κ are not independent but are related through the bedding attitude. Second, as noted by McCabe et al. [7], among others, the fact that complete unfolding yields a 'significantly' more concentrated distribution, does not mean that unfolded directions are necessarily the correct ones. The tightest distribution may well be somewhere between the present geographic coordinates and complete unfolding, suggesting that neither pre-folding nor post-folding coordinate systems are appropriate.

Several new tests have been proposed to compensate for the perceived difficulties [4,6,8–10]. All of these tests rely on the assumption that the directional data are Fisher distributed (that is spherically symmetric and of single polarity), or that they can be subdivided into subsets that are Fisher distributed. As pointed out by Tauxe et al. [11], however, data used in a fold test are usually not Fisher distributed. The calculation of κ as-

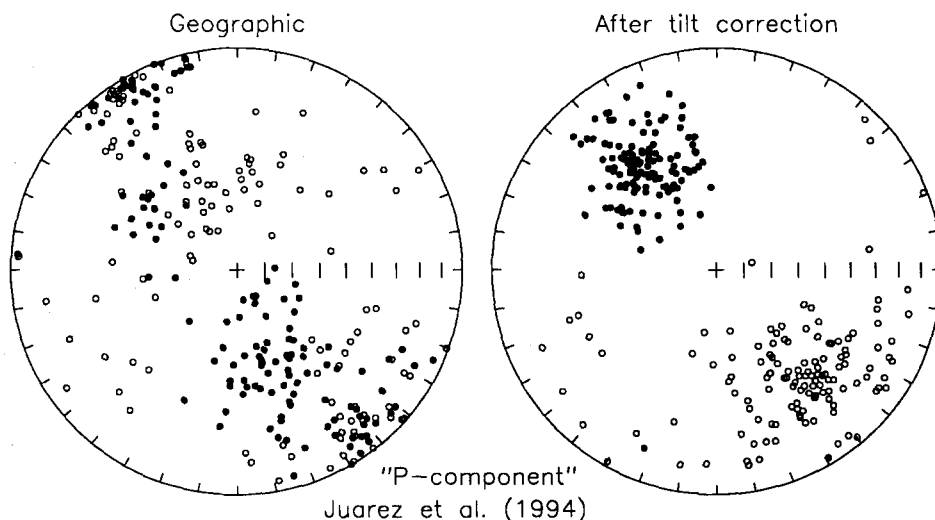


Fig. 1. Paleomagnetic data of Juarez et al. [12]. Data are characteristic directions of individual specimens plotted on an equal area projection. Solid symbols = lower hemisphere; open symbols = upper hemisphere. 'Geographic' are directions in the present reference system and 'tilt corrected' data have been rotated about the strike. Only after correction for bedding tilt can polarity be discerned and, even then, there are intermediate points whose polarity is ambiguous. The calculation of the Fisher concentration parameter is tedious at best under such circumstances.

sumes only one polarity is present, whereas real data are often of two polarities. The directions may be distorted during rotation from an originally symmetric distribution into something that is not. At times the distortion is so severe that polarity becomes ambiguous and one must actually assume a positive (or negative) fold test in order to identify the polarities and take the antipodes of the reversed sites correctly.

Consider the data of Juarez et al. [12] shown in Fig. 1. These data are specimen directions, each with a tectonic correction. The samples were taken for magnetostratigraphic purposes and one specimen constitutes one site. In geographic coordinates (and even in some cases after correction for tilt), the polarity is ambiguous and the calculation of κ necessitates using the tilt-corrected data to identify normal and reversed samples. None of the proposed fold tests handle such data well because they begin with the assumption that the data are Fisher distributed, which requires single polarity data.

Tauxe et al. [11] proposed a different approach based on the orientation matrix. Given n unit vectors with direction cosines x , y , z , the orientation matrix was defined by Scheidegger [13] as:

$$\mathbf{T} = \frac{1}{n} \begin{pmatrix} \sum x_i^2 & \sum x_i y_i & \sum x_i z_i \\ \sum x_i y_i & \sum y_i^2 & \sum y_i z_i \\ \sum x_i z_i & \sum y_i z_i & \sum z_i^2 \end{pmatrix}$$

Note that the polarity of the unit vectors does not matter. The orientation matrix is somewhat similar to the moment of inertia matrix if unit mass is assigned to each data point on the surface of a sphere. The two matrices yield the same eigenvectors when diagonalized, but the axis of least moment of inertia yields the largest eigenvalue in the orientation matrix. This eigenvector, γ_1 , tends to be parallel to the unit vectors. When these are closely bunched, unimodal or antipodal, γ_1 will estimate the axis of the vectors and the associated eigenvalue, τ_1 , will be much larger than the other two. Because \mathbf{T} is normalized by n , the eigenvalues sum to unity. If the data are drawn from a Fisher distribution, γ_1 is a very good estimate of the Fisherian mean and τ_1 plays

a role similar to the resultant vector, R , in Fisher statistics, but tends towards 1 instead of n . If the data points lie on or near a great circle, the smallest eigenvalue, τ_3 , will be close to 0 and the associated eigenvector estimates the normal to the great circle. The advantage of using the eigenparameters of the orientation matrix instead of the equivalent Fisherian parameters is that the data need not be of single polarity nor need they be spherically symmetric.

Watson and Enkin [10] describe a method for estimating the degree of unfolding that maximizes κ . Because of the complications in the practical application involved with the calculation of κ , we follow [11] in maximizing τ_1 . A FORTRAN program implementing the fold test described here is available from L. Tauxe on request. The method is automatic, requiring no data editing and unlike [11] gives confidence limits on the degree of unfolding required to produce the tightest grouping of data. We illustrate the method using several published data sets. We also demonstrate the power of the method to raise the suspicion that a given tilt correction may not take into proper account undetected structural complications. Finally, we show that our test performs as well as that of Watson and Enkin [10], yielding identical confidence bounds when used on strictly Fisherian data sets, but allows application to the more typical case of non-Fisherian data sets.

2. The simple bootstrap

In the fold test, one could just calculate the eigenvalues τ_i of \mathbf{T} as a function of the degree of unfolding and seek the maximum in τ_1 (or the minima in τ_2 and τ_3). This was essentially the fold test proposed by [11]. However, the τ_i suffer the same degree of statistical variability as κ and we need a more powerful test than just a difference in values of τ . As pointed out by [10], the problem is really one of parameter estimation. In the following we will take a bootstrap approach to estimating the variability in the τ_i . Our bootstrap comes in two flavors: the simple bootstrap and the parametric bootstrap.

The ability to discover the statistical behavior of a given parameter without resorting to restrictive parametric models was greatly enhanced by the availability of fast computers. By repeated calculations, one can 'pull oneself up by one's

bootstraps' to determine, for example, 95% confidence bounds on a given parameter [see, for example, 14]. The so-called statistical 'bootstrap' has found its way into paleomagnetism in a variety of papers [e.g., 4,8,11,15–18].

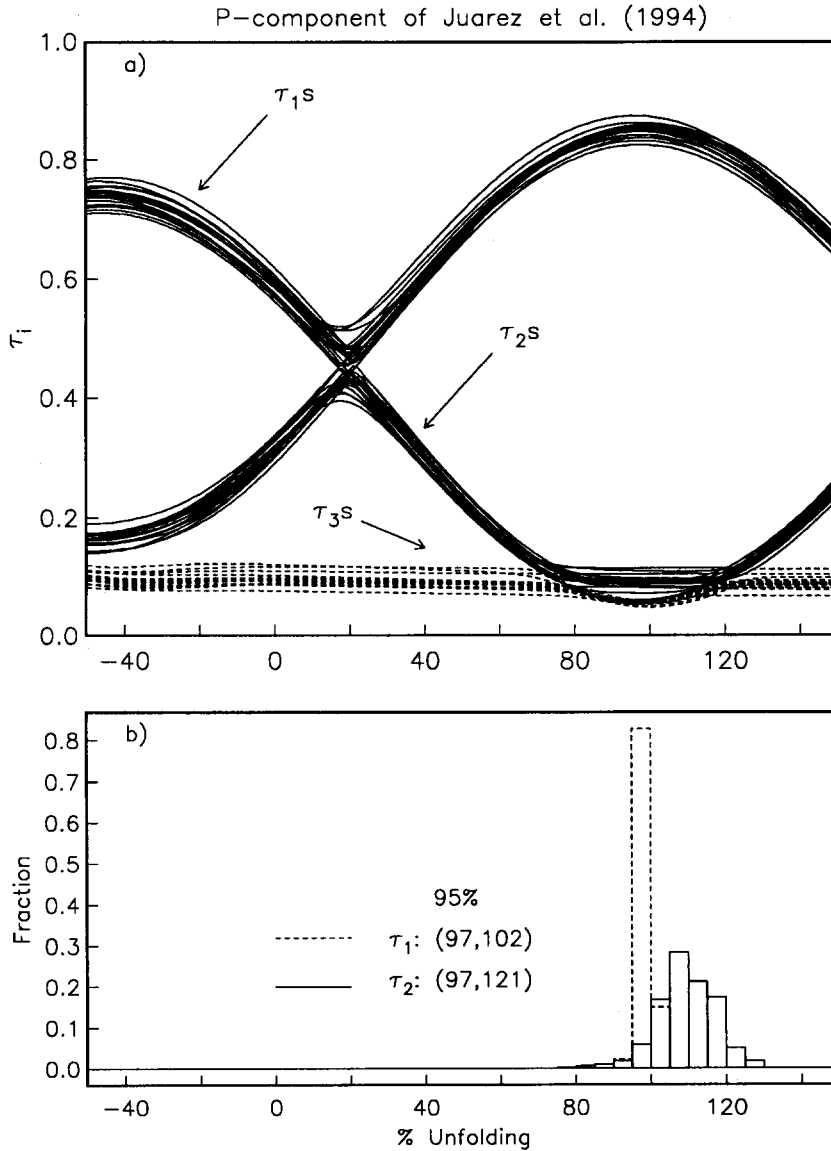


Fig. 2. (a) Eigenvalues of the orientation matrix for 20 para-data sets of the data shown in Fig. 1, as they undergo incremental rotation. The maximum in τ_1 and the minima in τ_2 and τ_3 occur when the sample directions are most parallel, in this case near 100% unfolding. (b) Histogram of the locations of the maxima in τ_1 and the minima in τ_2 for 500 para-data sets of the data shown in Fig. 1. Complete unfolding lies within the 95% confidence limits, suggesting a pre-folding remanence with a high degree of confidence.

In the application of the bootstrap to the fold test, we will proceed as follows. A ‘para-data set’ (technically known as a pseudosample) is created by randomly drawing n data points (with replacement) from the original data set. Each para-data set is the same size as the original data set and each data point may occur any number of times in a given para-data set. Each para-data set is

then rotated using the given strike and dip. The rotation is done incrementally from -50% to 150% unfolding. The eigenparameters for the orientation matrix of each para-data set are calculated at each unfolding step. Examples of the behavior of the τ_i for 20 such para-data sets are shown in Fig. 2a. Please note that, for a strictly Fisherian distribution, τ_2 and τ_3 should be very

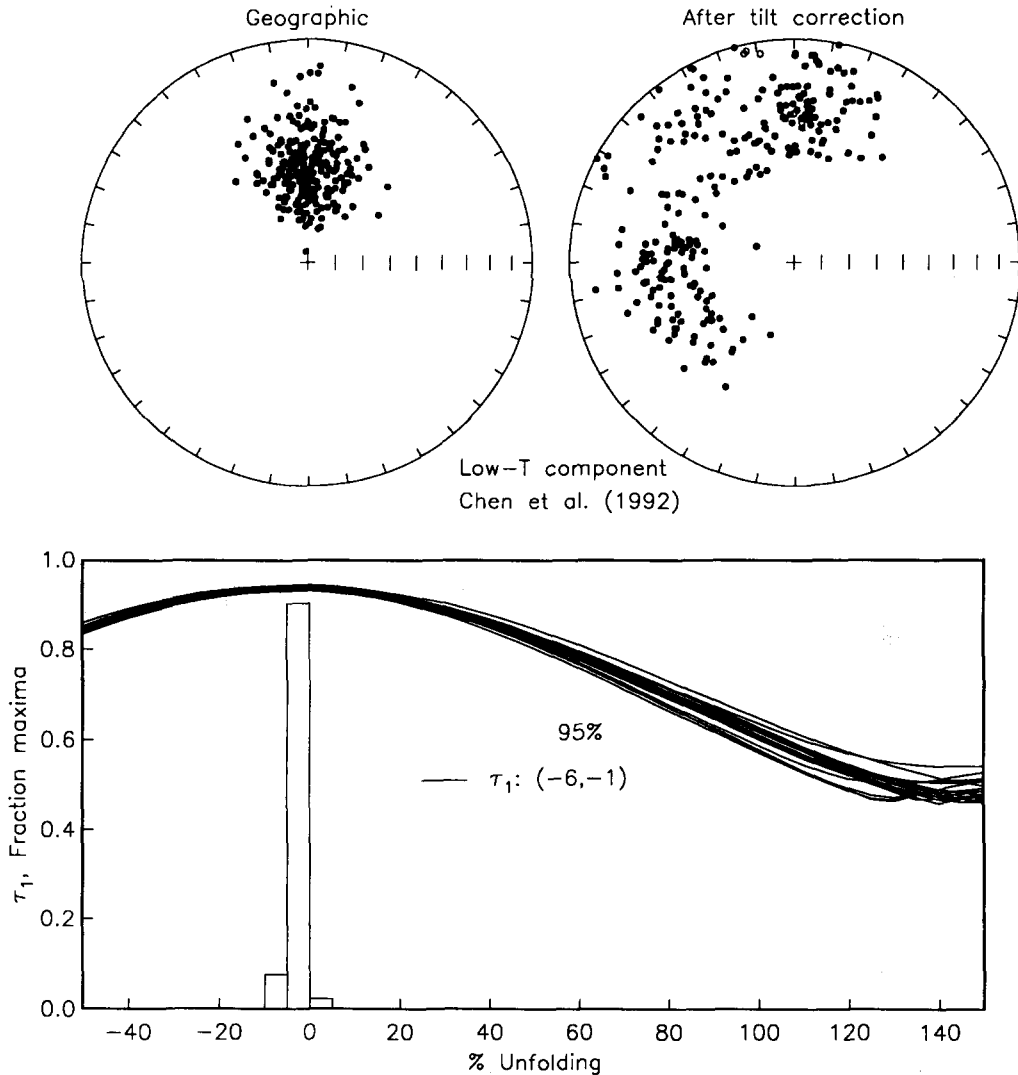


Fig. 3. The ‘low temperature’ component of Chen et al. [19]. After tilt correction, the data lie in a girdle distribution and are not Fisher distributed. Shown are graphs of τ_1 from 20 para-data sets, created by the simple bootstrap described in the text, as well as histograms of locations of the maxima in τ_1 .

nearly equal; this is only the case near 100% unfolding and the data are, indeed, in a girdle distribution at about 20% unfolding.

In Fig. 2b we plot a histogram of the positions of the maxima in τ_1 and the minima in τ_2 for 500 para-data sets of the data shown in Fig. 1. One could use any of the three eigenvalues, but the example shown here is typical, in that τ_1 is the

most sensitive, and in later examples we will consider only τ_1 . The tightest grouping of data occurs between 97% and 102% unfolding in 95% of the para-data sets, suggesting that the 'tilt correction' yields the most clustered data and the remanence is likely to be pre-folding.

An example of remanence acquired after folding was recently published by Chen et al. [19].

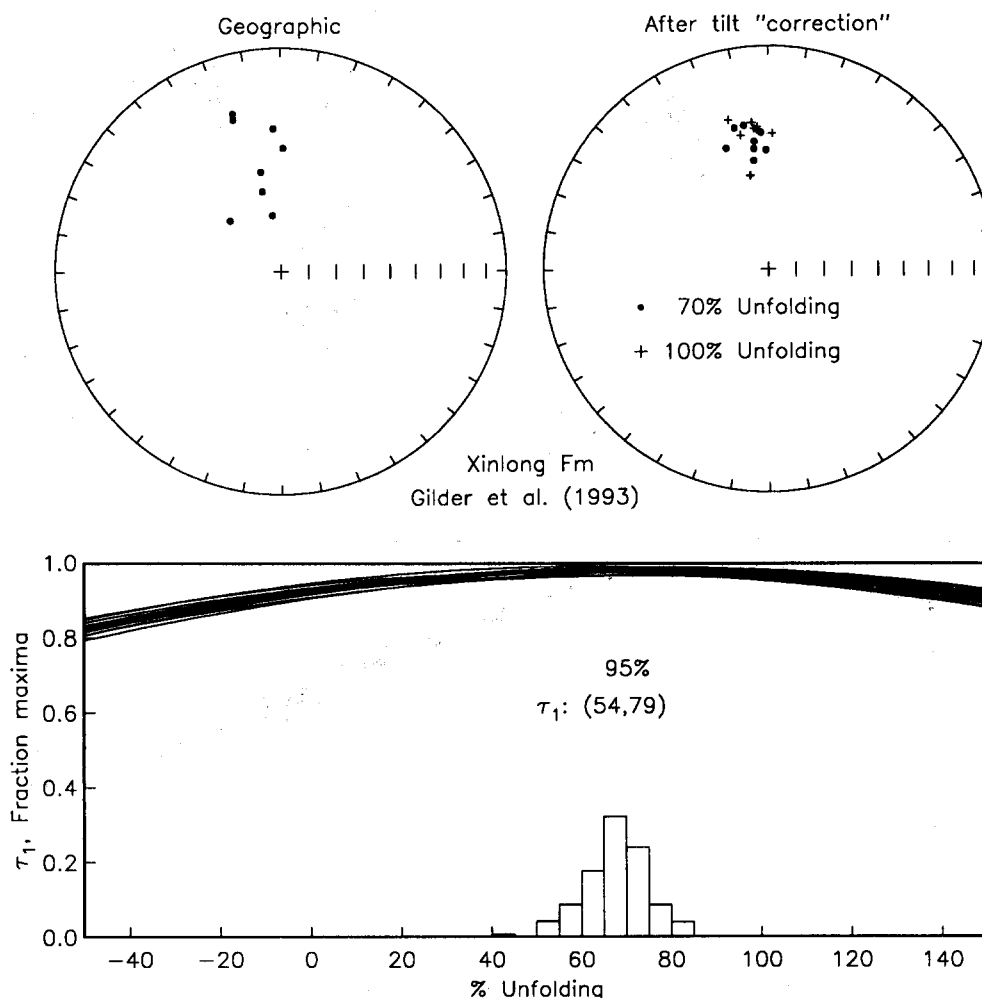


Fig. 4. Top: directional data of Gilder et al. [21] from the Xinlong Formation. Data are the site means of characteristic components. Data are shown in geographic coordinates and after 70% unfolding (tightest grouping) and 100% unfolding. Below are τ_1 s from 20 para-data sets and histograms of the positions of 500 maxima (τ_1). Both geographic and 100% unfolded coordinate systems are excluded at the 95% confidence level, suggesting either a complex magnetization, complex folding regime or a syn-folding remanence acquisition.

Their ‘low-temperature component’ is shown in geographic and tilt corrected coordinates in Fig. 3. While the data are of uniformly normal polarity, the data in neither coordinate system is Fisher distributed using the M_u/M_e test [see 20]. We show results of the simple bootstrap fold test below and the data are clearly most tightly grouped in near-geographic coordinates.

The procedure just outlined is a simple bootstrap and is suitable for cases in which there are a

large number of data (more than ~ 25 data points) and no other information is available. The data from [12] are characteristic directions from individual specimens taken for magnetostratigraphic purposes. There are no ‘site’ means, but there are 268 data directions with associated bedding attitudes and the simple bootstrap works well. In most tectonic studies there are fewer data (sometimes as few as seven), but each data point is the average of several specimens. In such

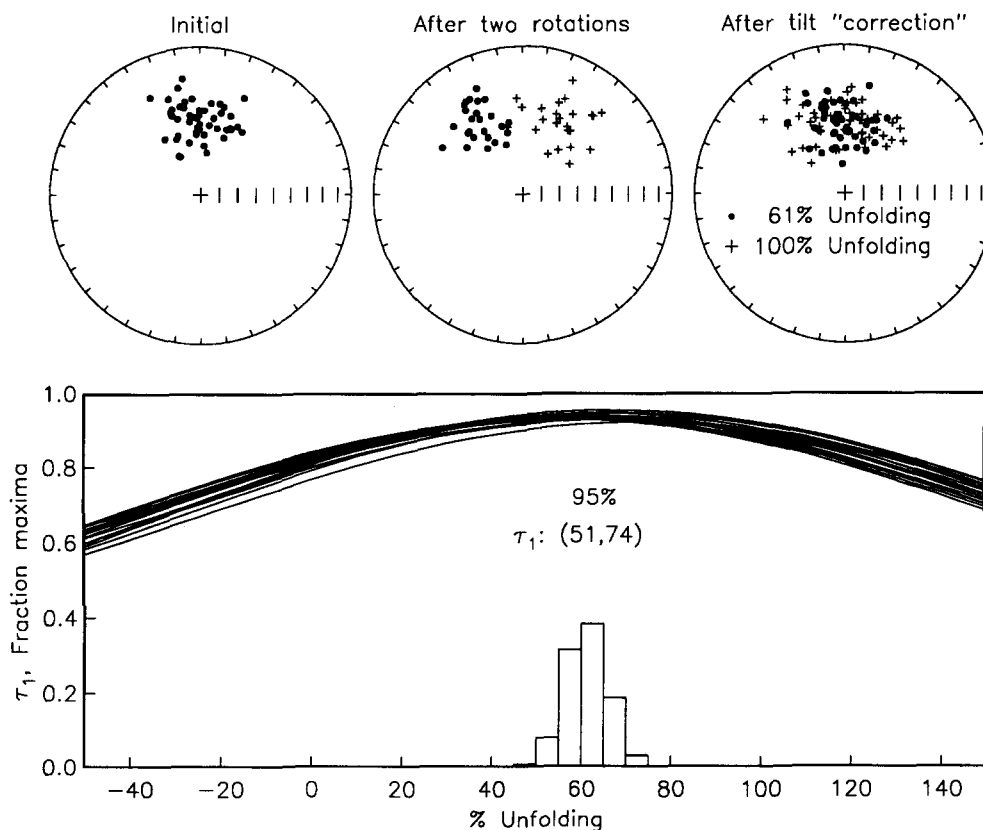


Fig. 5. The ‘initial’ figure shows synthetic data set drawn from a Fisher distribution with $\kappa = 30$. The data were split into two groups (shown as dots and plus signs) and each subjected to two rotations. The dots were rotated first by 20° about a vertical axis, then 45° to the west about a North/South horizontal axis. The plus signs were rotated first by -20° about a vertical axis, then 45° to the east about the horizontal axis. The tilt correction only accounted for the latter (observable) rotation and the fold test was performed as described in the text. As in Fig. 4, both geographic and 100% unfolded coordinate systems are excluded at the 95% confidence level. Note that use of a partially corrected data set, despite the fact that it represents the tightest concentration of data, is ill advised because, in this case, the initial distribution is not recovered, owing to the lack of correction for the vertical axis rotation.

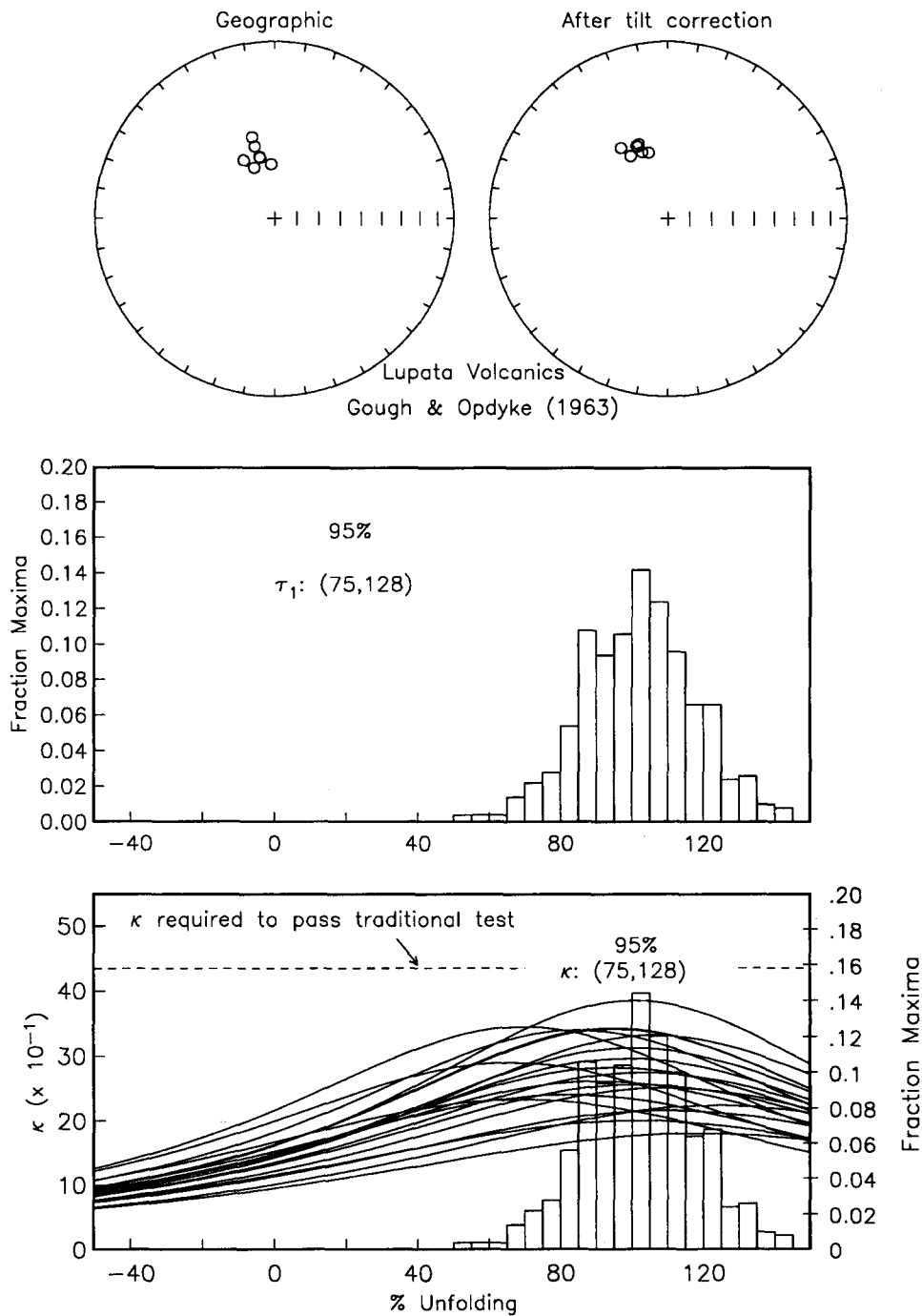


Fig. 6. Directional data of the Lupata Volcanics from Gough and Opdyke [22], plotted in geographic and tilt corrected coordinates. Shown below are the results of the parametric bootstrap using τ_1 and κ . All are compatible with a pre-folding remanence. Also shown is the κ required for a positive traditional fold test, never achieved by any para-data set.

cases the simple bootstrap does not work well, but a slightly modified version does: the parametric bootstrap.

3. The parametric bootstrap

It is reasonable to assume that paleomagnetic data are Fisher distributed at the site level, because multiple samples were taken to average out orientation noise, assess the stability and reproducibility of the magnetization, and so on. Indeed, if the data are not Fisher distributed at the level of the site, they are generally not used in further analysis. Thus, we often have more information available to us than in the cases illustrated above. Watson and Enkin [10] suggested creating para-data sets from a set of sites each calculated from n_s specimens yielding a Fisher concentration parameter, κ_s , in the following way. Using the methods outlined by Fisher et al. [20], a direction can be drawn from a Fisher distribution having the same κ and mean direction as a given site. To generate a simulated site mean for the para-data set, then, we draw n_s directions from the equivalent Fisher distribution and calculate the new site mean. This is done for each site and the para-data set is treated as described in the section on the simple bootstrap. For the purpose of the parametric bootstrap, therefore, it is helpful when authors publish their data sets including not only site mean directions and bedding attitudes but also κ_s and n_s for each site. We note that this is the current trend in the paleomagnetic literature.

Results of a parametric bootstrap are shown in Fig. 4. The data are the characteristic components of the Xinlong Formation [21]. We have used their preferred data set (excluding L138 and including L107). These data were said to have passed a fold test at the 99% level of confidence and yet it fails ours at the 99% level of confidence. The remanence achieves its tightest grouping at about 70% unfolding.

The meaning of a fold test in which the tightest grouping is achieved in neither geographic nor tilt corrected coordinates in terms of remanence acquisition is not straightforward. It is possible

that the remanence was acquired during folding and such data are usually interpreted as an indication of 'syn-folding remanence' [see, e.g., 7]. However, two phases of folding (or one that is not a simple rotation about strike), incorrectly 'unfolded' can also behave as the data shown in Fig. 4. To illustrate this, we have taken a simulated data set, drawn from a Fisher distribution having a κ of 30 and a mean direction of North, dipping 45° (shown in Fig. 5 as 'initial'). The data were then split into two 'limbs' and subjected to two rotations; one $\pm 20^\circ$ about the vertical axis and one $\pm 45^\circ$ about a N–S horizontal axis. These rotated directions are shown in Fig. 5 as 'after two rotations'. The only observable effect in the field would be the latter, so we performed a 'fold test' undoing only the second rotation. The 'tilt corrected' data are shown at the top right at both peak concentration (61%) and at 100% unfolding.

The maximum in τ_1 occurs at about 61%, excluding 0 and 100% unfolding as the appropriate coordinate systems at the 95% level of confidence. However, 61% unfolding does not yield precisely the initial distribution because of the failure to account for the vertical axis rotation. This simulation produces results quite similar to those in Fig. 4 and prove that a peak in concentration between 0 and 100% unfolding does not necessarily mean a syn-folding remanence. Nonetheless, it does mean that, either because of incorrect structural information or complications in the remanence itself, the '100% corrected' data are not valid for paleomagnetic purposes and justifiably fail our fold test. Of course, it would be dangerous to use the mean direction from even the partially corrected data for paleomagnetic purposes.

Finally, it is worthwhile to make the point that if, in the unusual case, the data are, indeed, Fisher distributed throughout the fold test, nothing is lost by using the Fisher assumption. To illustrate this, we compare the results of the parametric bootstrap using τ_1 maxima with that of Watson and Enkin [10], who use the κ maxima. We compare the methods on the data from the Lupata volcanics of Gough and Opdyke [22] as these were the data used by McElhinny [3] to introduce the fold test. In Fig. 6 we show the data

in geographic and tilt corrected coordinates; note that there is a very slight tightening of the distribution on unfolding. Below are the parametric bootstrap results using τ_1 and κ . Both suggest a pre-folding remanence (the 95% confidence limits include 100% unfolding), the κ and τ_1 tests give identical confidence limits. Also shown is the κ required to pass the traditional fold test [3], and we see that none of the example para-data sets reach that level, yet we have a weakly positive fold test.

4. Summary and conclusions

In this paper we develop a newly constituted fold test. The test involves eigen analysis of the data set. The variability along the principal axis (estimated by the largest eigenvalue, τ_1 , of the orientation matrix) is an estimate of the degree to which the directions are parallel and, when calculated as a function of the degree of unfolding, this identifies the point at which the tightest grouping of directions is achieved. Confidence limits can be derived in two ways. For data sets with n larger than about 25 directions, a simple bootstrap works well. Para-data sets are created by randomly drawing (with replacement) n directions from the original data set. Each para-data set is then rotated incrementally from -50% to 150% of the measured dip, and the eigenparameters are calculated at each increment. The degree of unfolding yielding a maximum in τ_1 is noted. Many (some 500) para-data sets are created and the 95% confidence limits are the degrees of unfolding producing 95% of these maxima. In cases with few data points, a parametric bootstrap can be used in which sites are assumed to be Fisher distributed and para-data sets are created by generating new site means by drawing the same number of directions from a Fisher distribution with the same κ and mean direction. These para-data sets are treated exactly as in the simple bootstrap. We illustrate the technique on a variety of data sets and find that it works as well or better than other published methods, yet is much easier to use because no data editing is required.

We also show by simulation that data sets exhibiting a peak in concentration between 0 and 100% unfolding do not necessarily arise from 'syn-folding' remanence acquisition. This behavior can also be the result of incorrectly accounting for structures more complicated than simple rotation about strike.

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