J Geophys (1984) 54:174-182

Journal of Geophysics

Estimate of confidence in paleomagnetic directions derived from mixed remagnetization circle and direct observational data

R.C. Bailey and H.C. Halls
Department of Geology, University of Toronto, Toronto, Ontario, Canada M5S 1A1

Abstract. A method is presented for obtaining the direction and confidence oval for a paleomagnetic component at a site given a number of independently oriented samples, some of which give an estimate of the remanence direction, while others yield only remagnetization circles. Such mixed remagnetization circle-remanence direction data frequently characterise paleomagnetic sites carrying two remanence components where the component of interest is small and less dispersed compared to a more easily removed one. The method described maximises the amount of usable data per site and thus leads to an improved site direction estimate.

Key words: Paleomagnetism - Remagnetization Circles - Mixed Circle and remanence direction data

Introduction

Paleomagnetic study of rocks carrying more than one component has developed considerably in recent years. A common occurrence in two-component systems is the preferential removal during stepwise demagnetization of the desired component. If only this component is initially demagnetized, then its direction is given by that of each incrementally removed vector, demagnetized up to that level at which the more resistant component begins to be destroyed. On orthogonal vector diagrams of the demagnetization path (Zijderveld, 1967) linear segments are produced over this demagnetization interval, and the orientation of the corresponding line in three-dimensional space gives the direction of the removed component (Kirschvink, 1980). If both components decay throughout the demagnetization treatment, the direction of the less resistant one cannot normally be found unless it has a lower dispersion than the other, in which case the method of intersecting remagnetization circles can be used (Halls, 1976, 1978). This method is based on the least squares fitting of great circles to data points on a sphere, a procedure that has been presented in the literature many times in various contexts. The error theory for this fitting procedure was originally discussed by Watson (1960, 1965) and applied to paleomagnetic data by Creer (1962) and then treated as a special case of Bingham distribution errors by Onstott (1980).

Since Halls' original paper on remagnetization circles, several papers have examined extensions to the method. In particular, McFadden (1977) and Kirschvink (1980) state the desirability of being able to combine remagnetization circle data with directional estimates of the component, so that a mean direction and confidence limits at the paleomagnetic site level can be obtained based on all available data. However, neither of the two solutions proposed is based rigorously on an underlying probability distribution for the dispersion of the required component.

The main purpose of this paper is to remedy this situation by bringing the analysis of the two types of data under a common theoretical framework.

Background

A requirement for the successful use of remagnetization circles on their own is that the component of interest has a much lower dispersion than that of the other component. The difference can be generated in a number of ways (Halls, 1978). One example for illustrative purposes is a conglomerate carrying volcanic pebbles which becomes partially overprinted. If the pebbles carry a primary magnetization inherited from the parent volcanic formation (the undesired component), then this component should be randomly directed within the pebble population, whereas the overprint (the desired component) should have a relatively uniform direction between pebbles (e.g. Palmer et al., 1981). When the pebble population is subject to stepwise AF or thermal demagnetization, the resultant remanence path for each pebble will be a great circle and these so-called remagnetization circles will converge to the overprint direction.

Now it may be possible to determine the overprint direction for individual pebbles from linear segments on vector diagrams if there is a recognizable demagnetization interval over which the secondary component only is being removed. In some cases, even where the component does not yield linear segments it may still be possible to recover its direction if it is one of three components and has an intermediate resistance (Hoffman and Day, 1978; Halls, 1979). Thus in our pebble population some samples yield the overprint direction

while others do not because of the failure of the foregoing methods arising from sample behaviour or instrumental limitations. We will refer to all directions derived from individual samples, regardless of the exact method used, as "direct observations". However, those samples failing to yield such data can still be used in the estimate of the component direction if they generate remagnetization circles. Such samples will thus be referred to as contributing "remagnetization circle" or "pole" data, where the pole is the normal to the remagnetization circle plane.

In the above example it is obvious that the best estimate of the overprint direction will be obtained by using *both* remagnetization circle and direct observational data, providing that each piece of data regardless of type comes from an independent sample. The method for combining these data sets is given below.

Procedure

Three sample remagnetization circles, shown in Fig. 1 A, converge to the direction E of the desired component. The intersection point of these circles thus exactly determines E. In practice the circles do not exactly intersect at a common point (Fig. 1 B) because the component E has some dispersion caused in part by measurement error and because the various samples may respresent slightly different times of component acquisition and the direction will vary due to secular variation. In Fig. 1 B the preferred method of estimating E is based on a least squares approach (Watson, 1965; Creer, 1962) in which E is chosen so that its mean square distance from the passing circles is a minimum (e.g. Jones et al., 1975; Halls, 1976; Kirschvink, 1980). As we show later, this method also estimates the most probable location of E, given certain plausible assumptions, and as such is optimal. The best estimate of E is shown in Fig. 1 B as the large open circle; the perpendicular distances whose mean square is being minimised are shown as dotted lines. The small open circles are the points of closest approach to E for each remagnetization circle; about these we will say something later. There are different ways of actually computing E: Jones et al. (1975) proceed iteratively by successive adjustments of the estimate of E until the desired minimum distance is located, while the method of Halls (1976), although not as graphically illuminating, obtains the same estimate in a single step. Another method (e.g. Khramov, 1958, 1971) is equivalent to the so-called beta-point method used in structural geology to find the orientation of cylindrical fold axes (e.g. Ramsay, 1967, p. 12). In this method, illustrated in Fig. 1 C, each intersection point of any two circles is taken to be an estimate of E. These points are then subjected to a normal paleomagnetic Fisher analysis as if they actually represent true remanence directions, which of course they do not. Since they do not, incorrect estimates of the remanence component and its reliability result.

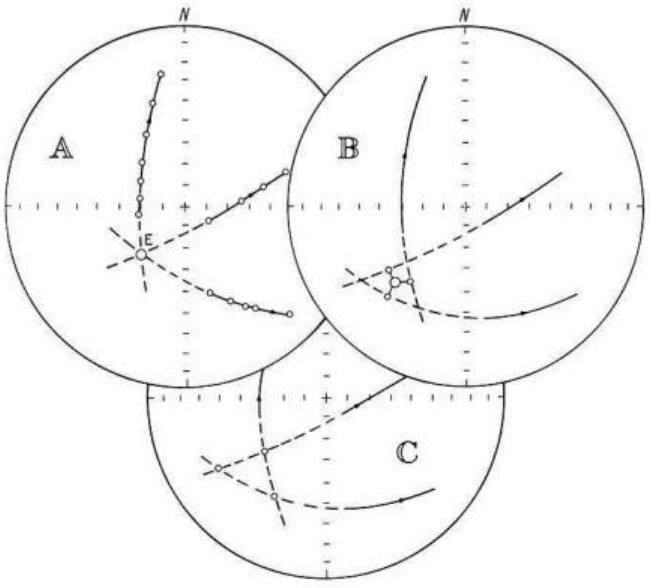

Fig. 1A–C. Convergence point of great circle intersections obtained from: **A** exact convergence of circles, **B** the mean of points of closest approach (Jones et al. 1975) and **C** from the mean of all points of intersection between pairs of circles

The results obtained in this paper contain two advances over previous work. First, we show for a single paleomagnetic site, how direct estimates and pole data may be combined to obtain a unified component estimate. McFadden (1977) suggests doing this by treating the points of closest approach to E of each great circle as equivalent to direct estimates of E, and applying a Fisherian analysis to the resulting fictitious and real direct estimates. That this cannot be rigorous is clear from the fact that it always gives a circle of confidence, even when the region of uncertainty is highly elliptical (as would be the case with nearly parallel great circles).

The second advance lies in the connection made between the pole distribution and underlying Fisher precision parameter of the components which gave rise to the poles. For the case where only remagnetization circle data exist, the error estimate provided by this paper reduces to that previously used by Watson (1965) and Onstott (1980). These estimates however are based on the a priori assumption of a girdle (e.g. axial Bingham) distribution. The parameters of this distribution relate only to the scatter of sample remagnetization circle poles about a great circle and not to the paleomagnetically significant scatter of the underlying remanence component as expressed by its Fisherian precision parameter, k, or angular standard deviation. The approach used here, however, permits an estimate of k as well as a calculation of the error in the estimated component direction. We shall also show why the least-squares method is appropriate for the problem and how direct observations can be included in the estimate of the mean component direction.

The probability distribution

The quantities which occur in the formulation of the problem by Watson and by Halls are shown in Fig. 2. E_i, $(i=1\rightarrow 3)$ are the directions of the desired component in each of three specimens. The solid great circles show the *measured* demagnetization paths which can be projected as dashed lines back to pass through the E_i. Since the E_i are dispersed around the mean E,

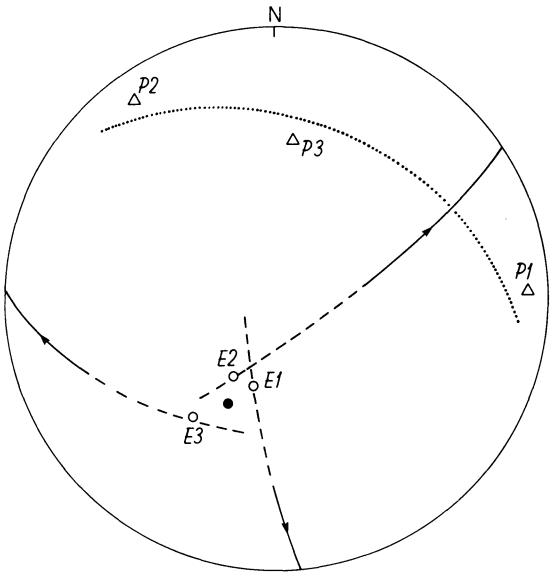

Fig. 2. Relations between three directions (E1, E2, E3), the measured demagnetization circle paths and the poles (P1, P2, P3) to these circles

the great circles do not converge to a common point. We will assume that the distribution of the E_i about E is given by Fisher's distribution. This is, of course exactly our assumption had it been possible to obtain the E_i directly, but all we are given are the three remagnetization circles. These circles are most conveniently described by their poles which are shown by the open triangles P_i $(i=1\rightarrow 3)$ in Fig. 2. If there was no dispersion in E, the poles would lie exactly on a great circle, which is shown as a dotted line in Fig. 2. Since there is dispersion and we do not know exactly where the great circle lies, we must find the most probable location of E given P_i. To solve this problem we need to know the probability distribution of a pole direction given E. We shall assume that the *only* reason that a pole does not lie perpendicular to E is the dispersion of the individual specimen directions E_i and that the error in determining pole positions from remagnetization circles is negligible by comparison.

The probability distribution, derived in the Appendix, is given by:

$$P(\phi)=\frac{kI_0(k\sin\phi)}{4\pi\sinh(k)}. \tag{1}$$

where $P(\phi)$ is the probability, per unit solid angle, that a pole direction makes an angle ϕ with E; I_0 is the modified Bessel function of the first kind of order zero and k is the precision parameter of the underlying Fisher distribution of the E_i. For large k, $P(\phi)$ peaks sharply near $\phi=90°$ and the expression simplifies to the more tractable form:

$$P(\phi)=\frac{\exp(k)k^{\frac{1}{2}}\exp(-\frac{1}{2}k\cos^2\phi)}{2\cdot(2\pi)^{\frac{3}{2}}\sinh(k)} \tag{2}$$

which is now similar to Watson's (1965) distribution. The main difference is that k here is the precision parameter of the underlying Fisher distribution; in Watson's formulation a different k (by a factor of 2) is used which is unrelated to any underlying component distribution. Watson's experience suggests that our expression will be accurate to better than a few percent if $k>10$.

Since a number of poles constitute the input data, we wish to estimate E as that direction which maximises the combined likelihood of our particular set of poles occurring. The joint probability density of our observations, given a supposed E, is the product of the probabilities for each pole, assuming they are independently obtained poles. Thus

$$P=P(\phi_1)\,P(\phi_2)\ldots P(\phi_N) \tag{3}$$

where N is the number of poles and $\phi_1\ldots\phi_N$ are the angles between each pole and E. If we also have direct observations of the desired remanence component, then these have a probability of occurring given by Fisher's distribution. If $F(\theta)$ is this distribution and θ is the angle between the direct component observation and E, then the joint probability of all observations is:

$$P=P(\phi_1)\,P(\phi_2)\ldots P(\phi_N)\,F(\theta_1)\,F(\theta_2)\ldots F(\theta_M), \tag{4}$$

where M is the number of direct observations.

Equations (3) and (4) assume that the same precision parameter k (which describes the inter-sample scatter of actual remanence directions for a given component) applies to all direct observations and to those component directions for which we have only poles. This assumption is reasonable for a site where samples have similar lithology, as there is no reason to believe that k for a primary component should depend upon the relative size of an overprint, although the converse may not always be true (e.g. Bailey and Hale, 1981). A further assumption inherent in Eq. (4) is that the scatter of poles along a great circle is random (see Appendix). This is equivalent to the assumption that the "undesired" components (as opposed to the desired component) in a suite of samples are randomly dispersed and uncorrelated with each other. There will be situations where this is not in fact true; for example, a set of samples all from the same site will often have similar "undesired" components. The extent to which this will introduce errors in the method of this paper is discussed later in the section on consistency tests. A test is there developed to check this assumption; should the assumption prove untrue, one should use only direct observational data.

A final assumption in Eq. (4) is that all individual pieces of data, whether belonging to either the direct or pole sets, are obtained from independent samples. Frequently an individual sample may yield both a direct estimate of the component direction *and* a remagnetization circle. Assuming that both are equally well determined, only the former quantity should be used, as it has fewer degrees of freedom.

If we now substitute the explicit expressions for the pole probability and Fisher distributions into the above formula, it becomes:

$$P=A\exp k\left(\sum_{j=1}^{M}\cos\theta_j-\frac{1}{2}\sum_{i=1}^{N}\cos^2\phi_i\right)^2 \tag{5}$$

where A is a normalising factor given by

$$A=\left[\frac{k}{4\pi\sinh(k)}\right]^M\left[\frac{k^{\frac{1}{2}}\exp(k)}{(8\pi)^{\frac{3}{2}}\sinh(k)}\right]^N. \tag{6}$$

Rewriting this expression for P in a more convenient form involving unit vectors rather than angles, we obtain:

$$P=A\exp\left\{k\left(\sum_{j=1}^{M}(\mathbf{d}_j\cdot\mathbf{t})-\frac{1}{2}\sum_{i=1}^{N}(\mathbf{p}_i\cdot\mathbf{t})^2\right)\right\}=A\exp(kB) \tag{7}$$

where $\mathbf{p}_i, \mathbf{d}_j$ are the unit vectors giving the direction of the i'th pole and j'th direct component observation respectively, and $\mathbf{t}$ is the true mean component direction that we are trying to find.

The maximum likelihood solution

The maximum likelihood solution for the true mean endpoint $\mathbf{t}$ is that value for which the joint probability of occurrence of the actual observations is a maximum. This will occur when the exponent B is a maximum. Thus we choose $\mathbf{t}$ to maximize B. It is convenient to rewrite B using

$$(\mathbf{d}\cdot\mathbf{t})=1-\tfrac{1}{2}|\mathbf{d}-\mathbf{t}|^2 \tag{8}$$

to give

$$B=M-\tfrac{1}{2}S \tag{9}$$

where

$$S=\sum_{j=1}^{M}|\mathbf{d}_j-\mathbf{t}|^2+\sum_{i=1}^{N}(\mathbf{p}_i\cdot\mathbf{t})^2. \tag{10}$$

Maximizing B is equivalent to minimizing S. S is the sum of the squared deviations from parallelism of the direct observations $\mathbf{d}_j$ and $\mathbf{t}$ and of the squared deviations from perpendicularity of the poles $\mathbf{p}_i$ and $\mathbf{t}$. Thus we have reduced the problem to the least-squares one suggested by Kirschvink (1980).

Where we have only direct observations $\mathbf{d}_j$ and no remagnetization circle poles, the problem reduces to the standard Fisher analysis of a set of directions. Where we have only remagnetization circle poles, $\mathbf{p}_i$ the problem reduces to that solved by McFadden and by Halls, for which the error theory given by Watson is applicable. As the above solutions are known, we shall not discuss these special cases individually at this point.

For convenience, let

$$\mathbf{r}=\sum_{j=1}^{M}\mathbf{d}_j \tag{11}$$

be the resultant of the direct observations. Let the matrix $\mathbf{H}$ be defined by

$$\mathbf{H}=\sum_{i=1}^{N}\mathbf{p}_i\mathbf{p}_i^T \tag{12}$$

where the superscript T denotes vector transposition. In terms of these introduced quantities, we can write B simply as

$$B=\mathbf{r}^T\mathbf{t}-\tfrac{1}{2}\mathbf{t}^T\mathbf{H}\mathbf{t}. \tag{13}$$

We wish to maximize B subject to the constraint that $\mathbf{t}$ be of unit length. This constraint ($\mathbf{t}^T\mathbf{t}=1$) prevents the occurrence of the useless solution $\mathbf{t}=\mathbf{0}$.

Using the method of Lagrange multipliers to incorporate this constraint, we therefore maximize

$$B+\tfrac{1}{2}\omega(\mathbf{t}^T\mathbf{t}-1) \tag{14}$$

where a Lagrange multiplier of $\frac{1}{2}\omega$ has been used for future convenience. Differentiating the above expression with respect to the three unknown components of $\mathbf{t}$ yields three equations which may be reassembled into the single matrix equation

$$\mathbf{H}\mathbf{t}-\omega\mathbf{t}=\mathbf{r}. \tag{15}$$

It is not simple to solve this for $\mathbf{t}$ directly using the original coordinate system in which the measurements were made. Rather, it is easier to work in a new system whose axes are the eigenvectors of the matrix $\mathbf{H}$. Let these eigenvectors be denoted by $\mathbf{e}_1$, $\mathbf{e}_2$, and $\mathbf{e}_3$, and the corresponding eigenvalues by (in order of increasing size) λ_1, λ_2, and λ_3. These quantities can be obtained straightforwardly by standard techniques. We will now express $\mathbf{t}$ and $\mathbf{r}$ in this new coordinate system as

$$\mathbf{t}=a_1\mathbf{e}_1+a_2\mathbf{e}_2+a_3\mathbf{e}_3 \tag{16}$$

and

$$\mathbf{r}=b_1\mathbf{e}_1+b_2\mathbf{e}_2+b_3\mathbf{e}_3. \tag{17}$$

The coefficients b_1, b_2, and b_3 can be calculated from

$$b_k=\mathbf{e}_k^T\mathbf{r}. \tag{18}$$

The coefficients a_1, a_2, and a_3 are now the unknowns for which we wish to solve.

Substitution of the above expansions into the equation for $\mathbf{t}$ and using the fact that

$$\mathbf{H}\mathbf{e}_k=\lambda_k\mathbf{e}_k \tag{19}$$

gives

$$\begin{aligned}&(\lambda_1-\omega)a_1\mathbf{e}_1+(\lambda_2-\omega)a_2\mathbf{e}_2+(\lambda_3-\omega)a_3\mathbf{e}_3\\&\quad=b_1\mathbf{e}_1+b_2\mathbf{e}_2+b_3\mathbf{e}_3.\end{aligned} \tag{20}$$

As the eigenvectors $\mathbf{e}_k$ are orthogonal, this is equivalent to the three equations

$$a_1=\frac{b_1}{\lambda_1-\omega},\qquad a_2=\frac{b_2}{\lambda_2-\omega},\qquad a_3=\frac{b_3}{\lambda_3-\omega}. \tag{21}$$

The multiplier ω is now determined as that value which satisfies the constraint that $\mathbf{t}$ has unit length, i.e. that

$$a_1^2+a_2^2+a_3^2=1. \tag{22}$$

Using the above expressions for the a's, the constraint becomes

$$\frac{b_1^2}{(\lambda_1-\omega)^2}+\frac{b_2^2}{(\lambda_2-\omega)^2}+\frac{b_3^2}{(\lambda_3-\omega)^2}-1=0. \tag{23}$$

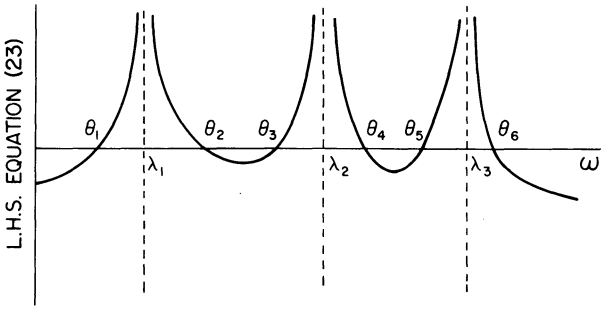

Fig. 3. Sketch of the left-hand side of Eq. (23), showing the six possible solutions (θ) of ω

This can be solved for ω and the resulting value used to determine the a's, from which $\mathbf{t}$ can be calculated. Equation (23) may have up to six solutions for ω, as shown by the sketch of the left-hand side in Fig. 3. A geometrical analysis shows that the minimum root is normally the one that minimizes B. This might not be the case with very bad (i.e. inconsistent) data. Goodness can be assessed using the precision parameter estimates below, consistency using the consistency tests below.

Using this value of ω, we can now solve for the a's and thus for the desired direction $\mathbf{t}$, using Eqs. (16) and (21). Note that this direction does not, in general, correspond to any eigenvector of $\mathbf{H}$, as was suggested by Kirschvink (1980), unless only pole data are being considered.

Estimate of the underlying precision parameter

A quantity which we shall shortly need and which is of interest in its own right is the precision parameter k of the underlying Fisher distribution of the desired component $\mathbf{t}$ over the various samples. To obtain this, we examine the joint probability distribution of poles and direct observations

$$P = A' \exp\left\{-\tfrac{1}{2}k\left[\sum_{j=1}^{M}|\mathbf{d}_j-\mathbf{t}|^2+\sum_{i=1}^{N}(\mathbf{p}_i\cdot\mathbf{t})^2\right]\right\} \tag{24}$$

where $A' = A\exp\{Mk\}$.

If we transform to a new coordinate system such that its 3-axis lies along $\mathbf{t}$, this distribution becomes

$$P = A' \exp\left\{-\tfrac{1}{2}k\left[\sum_{j=1}^{M}(d_{j1}^2+d_{j2}^2)+\sum_{i=1}^{N}p_{i3}^2\right]\right\} \tag{25}$$

where $(d_{j3}-t_3)^2$ has been dropped, since the vectors $\mathbf{d}_j$ are very close to $\mathbf{t}$ if k is not too small. Inspection of this new form reveals that each of the d_{j1}, d_{j2}, and p_{i3} are approximately normally distributed with zero mean (in this coordinate system) and standard deviation $k^{-\frac{1}{2}}$. Strictly the distribution is exactly normal as $k\to\infty$. Thus the quantity

$$kS = k\left\{\sum_{j=1}^{M}\left(d_{j1}^2+d_{j2}^2\right)+\sum_{i=1}^{N}p_{i3}^2\right\} \tag{26}$$

is by definition approximately distributed as a chi-square distribution with $2M+N$ degrees of freedom. Now the value $\hat{S}$ of S that is actually obtained is the result of minimizing $\hat{S}$ by varying two parameters (those needed to specify $\mathbf{t}$). Thus the actual value $k\hat{S}$ is distributed as a chi-square distribution with only $2M+N-2$ degrees of freedom. If we equate the actual value $k\hat{S}$ to its expectation value, we obtain

$$k\hat{S} = 2M+N-2 \tag{27}$$

and thus an unbiased estimator of k^{-1} is

$$\hat{k}^{-1} = \frac{\hat{S}}{2M+N-2}. \tag{28}$$

This is perhaps more easily computed in the form

$$\hat{k}^{-1} = \frac{2M-r+\omega}{2M+N-2} \tag{29}$$

where ω is the Lagrange multiplier found in estimating $\mathbf{t}$, as described earlier, and r is the magnitude of the resultant of unit vectors for direct observations.

Test of proposed directions

We will now formulate a test of the hypothesis that $\mathbf{t}$ equals a given direction, say $\mathbf{t}_1$, specified a priori and presumably not the same as our estimated direction $\hat{\mathbf{t}}$. Let the residual sum of squares for this direction be

$$S_1 = \sum_{j=1}^{M}|\mathbf{d}_j-\mathbf{t}_1|^2+\sum_{i=1}^{N}(\mathbf{p}_i\cdot\mathbf{t}_1)^2 \tag{30}$$

and let the residual sum of squares for the estimated direction $\hat{\mathbf{t}}$ be

$$S_0 = \sum_{j=1}^{M}|\mathbf{d}_j-\hat{\mathbf{t}}|^2+\sum_{i=1}^{N}(\mathbf{p}_i\cdot\hat{\mathbf{t}})^2. \tag{31}$$

Now kS_1 and kS_0 have chi-square distributions with $2M+N$ and $2M+N-2$ degrees of freedom respectively, as discussed previously. Thus the difference $k(S_1-S_0)$ is also chi-square with two degrees of freedom. The ratio

$$F = \frac{k(S_1-S_0)/2}{kS_0/(2M+N-2)} = \left(M+\frac{N}{2}-1\right)\left(\frac{S_1}{S_0}-1\right) \tag{32}$$

is then by definition distributed as an F distribution with 2 and $2M+N-2$ degrees of freedom. If the value we compute for F is larger than F_α, we must reject the hypothesis that $\mathbf{t}=\mathbf{t}_1$ at the $\alpha\%$ significance level.

Consistency of pole and direct data

One of the assumptions of the analysis of mixed data is that both poles and direct estimates are based on the same population of desired remanence components. It is therefore important to be able to test this assumption. This consistency test, however, has another purpose: in those sites where the undesired components of the pole samples are similar to each other, we must know the extent to which the pole data are biassing the estimated remanence direction towards the undesired component. In the extreme case where undesired com-

ponents are less dispersed than desired ones, the pole data will estimate a remanence direction close to the undesired component (i.e. where the actual remagnetization circles converge).

Since we cannot estimate the amount of such bias without a knowledge of the distribution of the undesired component, we prefer to adopt the conservative position that pole data should not be incorporated if there is *any* significant evidence of bias from the pole data. If the directions separately estimated from pole and direct data agree, then there is no evidence for such bias. In the special case where only one pole is used, there can be by definition no such bias, since a single pole does not constrain the remanence estimate at all along the great circle joining the desired and undesired components.

The consistency test actually tests two hypotheses:

(a) that the underlying precision parameters of the pole and direct data are not different;

(b) if test (a) is passed, that the underlying component directions of the pole and direct data are not different.

If both these tests are passed, the mixed analysis is validated.

We first outline test (a). Let $\hat{S}_p$ and $\hat{S}_d$ be the residual sums of squares obtained using only pole data and only direct data respectively. Then (as per the discussion of the precision parameter estimate) $k\hat{S}_p$ and $k\hat{S}_d$ have chi-square distributions with $N-2$ and $2M-2$ degrees of freedom respectively.[1] If the same k applies to both data sets, then $\dfrac{\hat{S}_p/(N-2)}{\hat{S}_d/(2M-2)}$ should be of the order unity. This ratio has an F distribution with $N-2$ and $2M-2$ degrees of freedom, and an F test may thus be performed to see if the value is improbably different from one. Should the calculated ratio be less than unity, it is customary to invert the ratio and reverse the degrees of freedom.

Turning now to test (b), we assume that the pole and direct data arise from the same remanence direction, and we formulate a statistic to test this. This test is essentially analogous to a one-way analysis of variance, in which we look for a significant difference between two methods of estimating the remanence direction. The error sum of squares within data types is $\hat{S}_w = \hat{S}_p + \hat{S}_d$, where $\hat{S}_p$ and $\hat{S}_d$ are defined above. The error sum of squares between data types is $\hat{S}_0 - \hat{S}_w$, where $\hat{S}_0$ is the residual sum of squares when both types of data are included as defined in Eq. (31).

Following the discussion of the precision parameter estimate, we deduce:

$$k\hat{S}_p \sim \chi^2_{N-2}$$

$$k\hat{S}_d \sim \chi^2_{2M-2}$$

and thus

$$k\hat{S}_w \sim \chi^2_{2M+N-4}$$

and also

$$k\hat{S}_0 \sim \chi^2_{2M+N-2}. \tag{33}$$

[1] They are clearly independent, being estimated from different data sets

The amount by which the error sum of squares increases when both data types are fitted by the same estimate is $\hat{S}_I = \hat{S}_0 - \hat{S}_w$, which has a χ^2_2 distribution.

We thus test the quantity

$$Q = \frac{\hat{S}_I/2}{\hat{S}_w/(2M+N-4)} \tag{34}$$

against an F distribution with 2 and $2M+N-4$ degrees of freedom. If Q is improbably large, we must reject the hypothesis that pole and direct data refer to the same remanence component.

Normally one would choose for this test a small significance level (e.g. 1%) and reject the hypothesis only if compelled to (e.g. with 99% confidence in the rejection). If, however, this test is used to see if there is any biassing by the undesired component, one is in the awkward position of wanting to accept the hypothesis, with no way of computing the probability of false acceptance (type II error). To avoid any possibility of bias, one should choose very large significance levels (e.g. 50%); this, however, leads to the rejection of perfectly good pole data a large portion (e.g. 50%) of the time. The choice of significance level is ultimately up to the user, but should be as large as possible consistent with reasonable utilization of pole data.

The ellipse of confidence for the direction estimate

The region of directions acceptable to all the data as determined by the F-test (32) for proposed directions is the confidence region. In other words, the region of 100-α% confidence is that in which the residual sum of squares S_1 for that direction satisfies

$$\left(M+\frac{N}{2}-1\right)\left(\frac{S_1}{S_0}-1\right) \leqq F_\alpha, \tag{35}$$

where F_α is the appropriate tabulated F statistic at the α% significance level. To make this useful, we have to express S_1 in terms of the actual direction $\mathbf{t}_1$ being considered:

$$S_1 = \sum_{j=1}^{M} |\mathbf{d}_j - \mathbf{t}_1|^2 + \sum_{i=1}^{N} (\mathbf{p}_i \cdot \mathbf{t}_1)^2. \tag{36}$$

We may consider the direction $\mathbf{t}_1$ as the estimate $\hat{\mathbf{t}}$ plus an error $\boldsymbol{\varepsilon}$. Substitution of this in the above equation and some manipulation yields

$$\boldsymbol{\varepsilon}^T(\mathbf{H}-\omega\mathbf{I})\boldsymbol{\varepsilon} \leqq C^2 \tag{37}$$

where

$$C^2 = \frac{S_0 F_\alpha}{M+\frac{N}{2}-1} \tag{38}$$

and ω is the Lagrange multiplier obtained earlier.

This is the equation describing the elliptical region of confidence of the error $\boldsymbol{\varepsilon}$ in the component direction derived using direct observations and poles from other samples. The major and minor axes of the error ellipse are in the directions $\mathbf{e}_2$ and $\mathbf{e}_3$, the two eigenvectors of

the matrix H corresponding to the largest and intermediate eigenvalues. The major and minor semiaxes have lengths (in radians) of

$$\frac{C}{(\lambda_2-\omega)^{\frac{1}{2}}} \quad \text{and} \quad \frac{C}{(\lambda_3-\omega)^{\frac{1}{2}}}. \tag{39}$$

These results are easily obtained by transforming to the coordinate system defined by the eigenvectors of **H**.

In the case of pole data alone, the Lagrange multiplier ω should be set equal to zero in the above semiaxis lengths, and the error ellipse is then the same as that provided by Watson's (1965) analysis of the pole of a girdle distribution.

A FORTRAN computer programme based on the foregoing theory is available from the authors by request.

Practical considerations of the method

In practice the demagnetization path for each sample in a site is plotted on a transparent overlay on a stereonet, and the overlay is then rotated to see if any portion of the path follows a meridional line on the stereonet and hence a great circle trajectory. Care is necessary in this procedure because usually sample paths are not entirely along great circles, indicating that at least three components are present. Sometimes where one component is easily erased compared to the other two, two great circle paths can be generated. Selection of the correct great circle depends on the component sought. If it is one of the two most resistant ones, the circle generated during the higher coercivity or unblocking temperature path is the one used. If the least-resistant component is of interest, then the lower coercivity/unblocking temperature circle is chosen. It is important in the former case that a great circle trend is only selected, providing there are no significant deviations from it at higher demagnetizing fields.

Once all the great circle trends are identified, remagnetization circles are then fitted to the points defining each path by least squares and circles accepted if the mean angular deviation (MAD) as defined by Kirschvink (1980) or the mean radius of the 95% error ellipse about the pole are less than or equal to 5°, for example.

When all accepted great circles are plotted on the same stereonet, it is usually apparent whether they are converging toward or passing in the vicinity of any stable end points or other direct observational data that may characterise a component (and which yield linear segments with MAD $\leqq 5°$). The two sets of data can then be combined using the foregoing analysis.

It is important to check that great circle convergence is not the product of two nearly antiparallel components; otherwise the least-squares intersection point of the circles is a function of *both* component directions.

Application of the method

A problem frequently encountered in paleomagnetism concerns the analysis of samples carrying a large proportion of low coercivity or low unblocking temperature grains. Often the remanence residing in these grains is of a secondary nature and has an intensity such that it completely dominates the paleomagnetic signature of the sample. Remanence components of interest, carried by higher coercivity or higher unblocking temperature grains may be initially masked by such large components and are only revealed as progressively more remanence is removed by alternating field or thermal demagnetization. For example, diabase dyke samples distant from chilled margins often display this behaviour, due to increasing size of titanomagnetite grains towards the intrusion centre. Likewise, partial oxidation of magnetite may create a secondary CRM in a sample where the bulk of the primary remanence resides in original magnetite.

If in either example the smaller component is sought, it may be impossible to isolate it either because of spectral overlap between the two components or because large demagnetized grains contribute sufficient magnetic noise to prevent attainment of an acceptable stable end-point.

Therefore, within a suite of samples collected from a site we may expect that only a fraction will yield stable end points. Assuming a two-component system, the remaining samples will exhibit remagnetization circles along which the resultant remanence vector continues to move until the background or intrinsic noise level of the samples becomes comparable to the remaining remanence signal. At this stage the resultant remanence behaves erratically in direction and intensity, and a coherent demagnetization path is lost. However, prior to the onset of such disturbance, the remagnetization circle is clear and defines a trajectory along which the component of interest would lie in the absence of measurement errors.

While such samples thus do not yield stable endpoints, they are obviously providing a measure of constraint on the direction of the desired component. Until now such samples have been discarded when in fact they are providing valid additional information.

The common practice in paleomagnetism is to collect at least five independently oriented samples per site. In many instances, particularly for rocks having low median destructive fields or unblocking temperatures, a significant proportion of the collection may be severely contaminated by large, viscous or temporary components, lightning strikes or by large secondary overprints of chemical or thermal origin. In conventional paleomagnetic analysis relying on stable end points, the number of usable samples per site may be reduced sufficiently such that the site must either be discarded or recollected. By increasing the amount of usable data, the analysis presented in this paper will not only lead to paleomagnetic site data of improved quality but may allow retrieval of site information that would otherwise have been omitted in the final site mean estimate.

Appendix

We want the probability distribution of the remagnetization circle pole **p**, given the direction of the undispersed or "true" component **t**. The dispersed version of **t** will be called **e**. It is actually easier to compute the

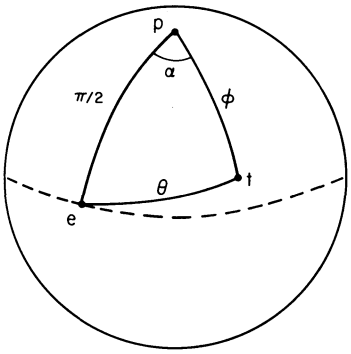

Fig. 4. Spherical triangle on unit sphere defining angular relations between a pole to measured remagnetization circle p, the true mean component direction t, and the measured dispersed version, e of t

distribution of **t**, given **p**. The distribution of **p** conditional on **t** is the same as the distribution of **t** conditional on **p** if the marginal distributions of **t** and **p** on the sphere are constant. As we place no a priori restrictions on where poles or components might lie, these marginal distributions are in fact constant and both equal to $1/(4\pi)$ per unit solid angle.

For convenience, let **p** lie at the North pole of the unit sphere as shown in Fig. 4. This leads to no loss of generality. The corresponding component direction **e** for the specimen must lie on the equator. The specimen component **e** and the "true" or undispersed component direction **t** are separated by an angle θ as shown, where θ is governed by the Fisher distribution. That is, the probability that **e** lies in solid angle dA at angle θ from **t** is given by

$$dP=\frac{k}{4\pi \sinh k}\exp[k\cos\theta]\,dA. \tag{A.1}$$

Referring to Fig. 4, we can replace $\cos\theta$ by $(\sin\phi\cos\alpha)$, where ϕ and α are respectively the colatitude of **t** and the longitude of **e**, assuming without loss of generality that **t** has zero longitude. Then

$$dP=\frac{k}{4\pi \sinh k}\exp[k\sin\phi\cos\alpha]\,dA. \tag{A.2}$$

Now **p** is an experimentally determined direction. We know that the specimen component **e** lies on the equator of **p**, but do not know its longitude with respect to **t**. Thus the distribution of the angle between **p** and **t** is given by averaging the above probability over all longitudes α.

It might be argued that not all values of α are equally likely. Some values may be excluded by the original data. For large k, however, as will often be the case, most of the integral is contributed when α is small. The integration gives

$$dP=\frac{1}{2\pi}\int_0^{2\pi}\frac{k}{4\pi \sinh k}\exp(k\sin\phi\cos\alpha)\,d\alpha\,dA \tag{A.3}$$

or

$$dP=\frac{k}{4\pi \sinh k}I_0(k\sin\phi)\,dA \tag{A.4}$$

where I_0 is the modified Bessel function of the first kind of order zero. This is a girdle distribution with **p** as the pole. It is a special case of the small circle distribution derived as Eq. (4.4) in Mardia and Edwards (1982) in a different physical context. It can be expressed in terms of the unit vectors **p** and **t** as

$$dP=\frac{k}{4\pi \sinh k}I_0(k(1-(\mathbf{p}\cdot\mathbf{t})^2)^{\frac{1}{2}})\,dA. \tag{A.5}$$

This expression is rather intractable as it stands. If one considers good data where k is large and as a consequence **p** and **t** are nearly at right angles, a much simpler expression results. Using the approximations

$$\sin\phi=(1-(\mathbf{p}\cdot\mathbf{t})^2)^{\frac{1}{2}}\simeq 1-\tfrac{1}{2}(\mathbf{p}\cdot\mathbf{t})^2 \tag{A.6}$$

since $\mathbf{p}\cdot\mathbf{t}$ is small and

$$I_0(x)=\frac{1}{(2\pi x)^{\frac{1}{2}}}\exp(x)+O\left(\frac{e^2}{x}\right) \tag{A.7}$$

since $x\simeq k$ and k is large, we obtain

$$\frac{dP}{dA}=\frac{k^{\frac{1}{2}}\exp(k)}{4\pi \sinh k}\,\frac{\exp(-\frac{1}{2}k(\mathbf{p}\cdot\mathbf{t})^2)}{(2\pi)^{\frac{1}{2}}}+\varepsilon. \tag{A.8}$$

If k is large, the error term ε is small, typically a factor k smaller than the term it accompanies and may be neglected.

References

Bailey, M.E., Hale, C.J.: Anomalous magnetic directions recorded by laboratory induced chemical remanent magnetisation. Nature **294**, 739–741, 1981

Creer, K.M.: A statistical enquiry into the partial remagnetization of folded Old Red sandstone rocks. J. Geophys. Res. **67**, 1899–1906, 1962

Halls, H.C.: A least-squares method to find a remanence direction from converging remagnetization circles. Geophys. J.R. Astron. Soc. **45**, 297–304, 1976

Halls, H.C.: The use of converging remagnetization circles in paleomagnetism. Phys. Earth Planet. Inter. **16**, 1–11, 1978

Halls, H.C.: Separation of multicomponent NRM: combined use of difference and resultant magnetization vectors. Earth Planet. Sci. Lett. **43**, 303–308, 1979

Hoffman, K.A., Day, R.: Separation of multicomponent NRM: a general method. Earth Planet. Sci. Lett. **40**, 433–438, 1978

Jones, D.L., Robertson, I.D.M., McFadden, P.L.: A paleomagnetic study of Precambrian dyke swarms associated with the Great Dyke of Rhodesia. Geol. Soc. S. Afr. **78**, 57–65, 1975

Khramov, A.N.: Paleomagnetism and stratigraphic correlation, Gastoptechizdat (Leningrad, 218 p., transl. Lojkine, A.J.). Geophysics Department, Australian National University, 1960, 1958

Khramov, A.N.: Paleomagnetic directions and paleomagnetic poles. McElhinny, M.W. (Ed.) and Brown, D.A. (Transl.). Australian National University, RSES Publ. No. 990, 1973, 1971

Kirschvink, J.L.: The least squares line and plane and the analysis of paleomagnetic data. Geophys. J.R. Astron. Soc. **62**, 699–718, 1980

Mardia, K.V., Edwards, R.: Weighted distributions and rotating caps. Biometrika **69**, 323–330, 1982

McFadden, P.L.: Comments on "a least-squares method to find a remmanence direction from converging remagnetization circles" by H.C. Halls. Geophys. J.R. Astron. Soc. **48**, 549–550, 1977

Onstott, T.C.: Application of the Bingham distribution function in paleomagnetic studies. J. Geophys. Res. **85**, 1500–1510, 1980

Palmer, H.C., Halls, H.C., Pesonen, L.J.: Remagnetization in Keweenawan rocks. Part I: Conglomerates. Can. J. Earth Sci. **18**, 599–618, 1981

Ramsay, J.G.: Folding and fracturing in rocks. New York: McGraw-Hill, 1967

Watson, G.S.: More significant tests on a sphere. Biometrika **47**, 87–91, 1960

Watson, G.S.: Equatorial distributions on a sphere. Biometrika **52**, 193–201, 1965

Zijderveld, J.D.A.: A.C. demagnetization in rocks: analysis of results. In: Methods in paleomagnetism, D.W. Collinson, K.M. Creer, S.K. Runcorn, eds. New York, Elsevier, 254–286, 1967

Received April 19, 1983; Revised version February 17, 1984
Accepted February 17, 1984