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THE ESTIMATION OF PALAEOMAGNETIC POLE POSITIONS.(U)

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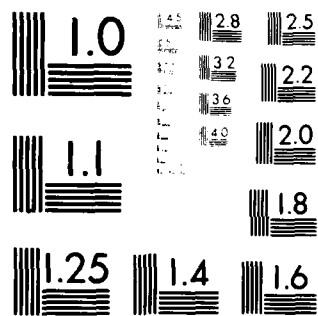
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THE ESTIMATION OF
PALAEOMAGNETIC POLE POSITIONS

by

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ABSTRACT

The use of the Fisher distribution to estimate the mean direction of magnetization of a rock at a sampling site is now standard. Sampling sites are chosen to cover 10^4 to 10^5 years to average out the effect of secular variation. The controversy about how to combine these site means has never been satisfactorily resolved. By using statistical models for secular variation, this paper suggests how methods should be derived. A number of interesting statistical distributions and estimation problems are shown.

Key words: Palaeomagnetism, Fisher distribution, unit vectors, multivariate normal distribution.

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1. INTRODUCTION

When a lava containing iron cools below its Curie point, it becomes magnetized in the direction of the earth's field at that place and time. Sediments containing magnetic particles also acquire (a much weaker) local magnetization as they are formed. The study of palaeomagnetism led to the current revolution in geology - plate tectonics. For assuming that the earth's magnetic field has always been much the same as it is now - except for reversals of polarity - a magnetic measurement gives a good estimate of the latitude of the site when the rock was magnetized. These latitudes make no sense unless one is willing to admit that continental drift has taken place - in fact, they allow continental reconstructions to be made. A full account may be found in the book by McElhinny (1973).

The strength of the magnetization of a specimen may have altered over time and so it is not used in this work - only the direction of natural remanent magnetism, i.e., the original magnetization. Later changes can be "cleaned" out by methods not relevant here. (If the rocks are unstably magnetized, they cannot be used.) If N specimens are taken from one site with directions, the N unit vectors, $r_1, \dots, r_N$, after cleaning, may be assumed to be a sample from Fisher's distribution

$$\frac{\kappa}{4\pi \sinh \kappa} \exp \kappa r' \mu \quad (\kappa \geq 0) \quad (1)$$

where μ is the (unit) mean direction. Fisher (1953) showed that the maximum likelihood estimator of μ is the direction of $R = \sum r_i$, the vector resultant of the sample and, further, that if $|R|$ is the length of R , $\hat{\kappa}$ is the solution of

$$\coth \kappa - (1/\kappa) = |R|/N. \quad (2)$$

An approximation to $\hat{\kappa}$ is κ given by

$$\kappa = \frac{N - 1}{N - |R|} \quad (2)$$

κ measures the precision of the Fisher distribution. Further statistical methods appropriate for palaeomagneticists were given by Watson (1956a, b) and Watson and Irving (1957).

The latter paper gives an approximate within and between sites method of analyzing data from several sites. It is assumed that the within sites distribution is Fisher with $\kappa = \kappa_w$ about the site mean and that the site means are independently Fisher with $\kappa = \kappa_B$ about the true palaeomagnetic direction. Unfortunately, this compound of Fisher distributions is only approximately Fisher. The estimate of κ_B was meant to measure the secular variation since it is supposed that the sites sample the full cycle of secular variations. This is some 10^4 to 10^5 years when the pole moves around its mean position, a short period on continental drift time scales.

In designing this analysis, no real thought was given to modelling secular variation. Furthermore, the immense amount of experimental work done since then has shown that site means often do not vary symmetrically around some mean direction as implied by the Fisher distribution (1), as we supposed.

When the earth's field is averaged over the time period of secular variation, it is found to be approximated, with surprising accuracy, by an earth-centered magnetic dipole currently inclined at about 11 degrees to the rotational axis. From elementary physics, the magnetic force H at a point r from a dipole M (H, M, r are all vectors) is given by

$$H = \left(3 \frac{rr'}{|r|^2} - I \right) \frac{M}{|r|^3} \quad (3)$$

where the prime denotes a transpose, I is the 3×3 identity matrix, and

$|r|$ is the length of r . Of course, the center of the earth is too hot to support a dipole! The field is thought to be due to a self-exciting dynamo made of asymmetric flows of conducting rock (mainly iron and nickel) through stray permanent fields of the rotating earth. Minor changes in the flows and the eastward movement of the crust relative to the interior (core) of the earth cause the secular variation and even the reversals.

Irving and Ward (1964) supposed that the secular variation was due to a smaller geocentric dipole m whose orientation varied uniformly at random over the period but whose magnitude $|m|$ was constant. Then the field at site r at different times in the period is independent and has the representation

$$H = \left(3 \frac{rr'}{|r|^2} - I \right) (M + m) / |r|^3 \quad (4)$$

Here and below we will regard M as fixed and define $\mu = M/|m|$. Creer et al. (1959) assume that the main dipole M has fixed strength $|M|$ but "wobbles" - that the direction of the main dipole is independent from time to time and has a Fisher distribution. Creer et al.'s model says

$$H = \left(3 \frac{rr'}{|r|^2} - I \right) M^* / |r|^3 \quad (5)$$

where $M^* = |M|d$ and d has a Fisher distribution about μ , and some large κ . Cox (1970) supposes that the main dipole oscillates in strength and wobbles in direction and that there is, in addition and independently, a randomly oriented smaller dipole m , as in the Irving and Watson model. In his case

$$H = \left(3 \frac{rr'}{|r|^2} - I \right) (M^+ + m) / |r|^3 \quad (6)$$

where the average value of M^+ is to be M about which M^+ has a rotationally symmetric distribution.

In the last five years some more complex models have been suggested which generate secular variations with dipoles on the surface of the core - see, e.g., Harrison & Watkins (1979). Here we will be content to explore models expressed in (4), (5), and (6), or closely related to them. We will assume that large samples have been taken at each site so that site mean directions are known exactly. Let these directions be $L_1, L_2, \dots, L_N$. The problem is to estimate μ , the direction or mean direction of M, M^*, M^+ .

We will choose, as a unit of length, the earth's radius (assuming it to be a sphere) and set $u = r/|r|$. Then the common factor in (4), (5), and (6) is $3uu' - I$ where u is a fixed but arbitrary unit vector. We will write

$$U = 3uu' - I. \quad (7)$$

Note that $U = U'$, $U^2 = 3uu' + I$ and that

$$U = 2uu' + u_2u_2' + u_3u_3'$$

where u, u_2, u_3 are orthonormal. Hence the eigenvalues and eigenvectors of U are trivially known. Each of the models has the form

$$H = UX$$

where X is a random vector, U is fixed and only the direction of H is observed. In the next section we will explore the distributional and estimation problems this raises. They have some intrinsic statistical interest and may have other applications. In the third section, we return explicitly to our main problem.

2. STATISTICAL PRELIMINARIES

(a) Fisher observed that his distribution may be derived from the Gaussian as follows. If X has a trivariate Gaussian distribution with mean vector μ and covariance matrix $\sigma^2 I$, set $R = |X|$, $L = X/R$,

$\lambda = \mu/|\mu|$. Then the joint density of R and L is

$$\frac{R^2}{(2\pi)^{3/2}\sigma^3} \exp - \frac{1}{2\sigma^2} (R^2 + |\mu|^2) \exp \frac{R|\mu|}{\sigma^2} L \cdot \lambda \quad (8)$$

so that the density of L on the unit sphere, conditional on a fixed R , is proportional to

$$\exp \frac{R|\mu|}{\sigma^2} L \cdot \lambda \quad (9)$$

From (1) we see that L then has a Fisher distribution about the mean direction λ with a κ of $R|\mu|/\sigma^2$. If (9) were appropriate, we know how to estimate λ and $R|\mu|/\sigma^2$ - use Fisher's estimations for (1).

If, however, (8) were appropriate but we were only given the directions $L_1, \dots, L_N$ of $X_1, \dots, X_N$, we would have to use the density f of L ,

$$\int_0^\infty \frac{R^2}{(2\pi)^{3/2}\sigma^3} \exp - \frac{1}{2\sigma^2} (R^2 + |\mu|^2 - 2R|\mu| L \cdot \lambda) dR \quad (10)$$

This is simpler if we set $S = R/\sigma$, $v = |\mu|/\sigma$, since then

$$f(L, \lambda, v) = \int_0^\infty \frac{S^2}{(2\pi)^{3/2}} \exp \left\{ - \frac{1}{2} (S^2 + v^2 - 2SvL \cdot \lambda) \right\} dS \quad (11)$$

with the vector derivative

$$\frac{\partial f}{\partial \lambda} = \int_0^\infty \frac{S^3 v}{(2\pi)^{3/2}} \exp \left\{ - \frac{1}{2} (S^2 + v^2 - 2SvL \cdot \lambda) \right\} L dS, \quad (12)$$

$$= w(L, \lambda, v) L, \text{ say } \quad (12')$$

Since $\lambda \cdot \lambda = 1$, the maximum likelihood (m.l.) estimate of λ requires us to solve

$$\frac{\partial}{\partial \lambda} \left(\sum_{j=1}^N \log f(L_j) + \theta \lambda^{-1} \right) = 0 ,$$

i.e.,

$$\sum_{j=1}^N \frac{J(L_j, \lambda, \nu)}{f(L_j, \lambda, \nu)} L_j + \frac{2\theta \lambda}{\nu} = 0 . \quad (13)$$

If ν is known, (13) may be solved numerically by an iteration. An initial estimate of λ , $\lambda^{(1)}$ would be the direction of $\sum_{j=1}^N L_j$. With computer programs to compute $J(L_j, \lambda^{(1)})$ and $f(L_j, \lambda^{(1)})$, (13) would be used to find $\lambda^{(2)}$, etc. The two integrals have well-behaved integrands so that numerical integration will not be difficult.

To estimate the non-negative parameter ν , we observe that

$$\begin{aligned} \frac{\partial f}{\partial \nu} &= \int_0^\infty \frac{S^2}{(2\pi)^{3/2}} (-\nu + S L^{-1} \lambda) \exp \left\{ -\frac{1}{2}(S^2 + \nu^2 - 2S\nu L^{-1} \lambda) \right\} dS \\ &= -\nu f + L^{-1} \lambda J . \end{aligned} \quad (14)$$

Hence the m.l. equation for $\hat{\nu}$ is

$$\sum_{j=1}^N -\frac{\nu f(L_j, \lambda, \nu) + L_j^{-1} \lambda J(L_j, \lambda, \nu)}{f(L_j, \lambda, \nu)} = 0$$

or

$$\frac{1}{N} \sum_{j=1}^N \frac{L_j^{-1} \lambda J(L_j, \lambda, \nu)}{f(L_j, \lambda, \nu)} = \nu , \quad (15)$$

a form ideal for iteration. It is convenient that no more integrals need be evaluated. To start off the ν iteration we again use the analogy between (8) and (9) and suggest

$$\nu^{(1)} = \frac{N - 1}{N - |\Sigma L_j|} . \quad (16)$$

Thus to solve jointly (13) and (15) for $\hat{\lambda}$ and $\hat{\nu}$, one seesaws between them using the suggested $\lambda^{(1)}$ and $\nu^{(1)}$. Hence given only the directions $L_1, \dots, L_N$ of a sample of N from $G(\mu, \sigma^2 I)$, we may estimate the direction of μ and $\nu = |\mu|/\sigma$. To find the covariance matrix, the second derivatives of the log-likelihood will be evaluated in the usual way. We will leave this calculation for an applied paper to appear elsewhere. This paper will also show the shape of distribution defined by (10) or (11) and compare it with others. This distribution has of course appeared before (see e.g. Kendall (1974) under the names "off-set" or "displaced" normal - I prefer "angular" normal.

(b) If we observed the directions of n copies of $Y = TX$, where X is Gaussian mean μ with known covariance matrix $\sigma^2 I$, and T is a known non-singular 3×3 matrix, we see that we may set $\sigma^2 = 1$ without loss of generality where we wish to estimate the direction of μ . The density of Y is

$$\frac{1}{(2\pi)^{3/2} ||T||} \exp - \frac{1}{2} (Y'(TT')^{-1}Y - 2\mu'T^{-1}Y + \mu'\mu) . \quad (17)$$

Setting $Y = RL$ where $R > 0$ and $|L| = 1$, the joint density of R and L is

$$\frac{R^2}{(2\pi)^{3/2} ||T||} \exp - \frac{1}{2} (R^2 L'(TT')^{-1}L - 2R\mu'T^{-1}L + \mu'\mu) .$$

Thus the density of L is

$$h(L, \mu) = \int_0^\infty \frac{R^2}{(2\pi)^{3/2} ||T||} \exp - \frac{1}{2} (R^2 L'(TT')^{-1}L - 2R\mu'T^{-1}L + \mu'\mu) dR ,$$

so

$$\begin{aligned} \frac{\partial h}{\partial \mu} &= \int_0^\infty \frac{R^2}{(2\pi)^{3/2} ||T||} \exp - \frac{1}{2} (R^2 L'(TT')^{-1}L - 2R\mu'T^{-1}L + \mu'\mu) \\ &\quad \cdot (RT^{-1}L - \mu) dR . \end{aligned}$$

Define

$$\kappa(L, \mu) = \int_0^\infty \frac{R^3}{(2\pi)^{3/2} ||T||} \exp - \frac{1}{2}(R^2 L' (TT')^{-1} L - 2R\mu' T^{-1} L + \mu' \mu) dR .$$

We see that the m.l. equation for μ is

$$\frac{1}{N} \sum_{j=1}^N \frac{\kappa(L_j, \mu)}{h(L_j, \mu)} T^{-1} L = \mu . \quad (18)$$

A natural initial value is $\mu^{(1)} = N^{-1} T^{-1} \sum L_j$ for the iteration to find $\hat{\mu}$.

Then we will take the direction of $\hat{\mu}$. To get the accuracy of $\hat{\mu}$, we may use second derivatives in the usual way.

(c) To go one step further, if $Y = UZ$ where Z is Gaussian with mean vector μ and a known covariance matrix Σ and we wish to estimate the direction of μ given the direction of N Y 's, we may write

$$\begin{aligned} Y &= UZ = U\Sigma^{1/2}\Sigma^{-1/2}Z \\ &= TX \end{aligned}$$

where

$$T = U\Sigma^{1/2}, \quad X = \Sigma^{-1/2}Z$$

and X is Gaussian $(\Sigma^{-1/2}\mu, I)$. Thus we may use the method of subsection (b) to estimate $\Sigma^{-1/2}\mu$. Given an estimate of the latter, we have an estimate of μ , since $\Sigma^{1/2}$ is known, and hence of its direction.

Subsection (c) leads to an algorithm to solve the problem of Section 1 for a model of secular variation where the geocentric dipole has a multivariate Gaussian distribution. This is not a model included in (4) and (5); it is a limiting case in (6).

(d) To deal with model (6) we are led to study the distribution of $Y = X + v$ where X is Gaussian - mean μ , covariance Σ - and v is uniformly distributed over a sphere of radius δ . This leads to a plethora of apparently new multivariate densities.

Because of their intrinsic interest, we consider some *very special cases* not directly relevant to our main problem. In one dimension, the density of y clearly is

$$\begin{aligned} & \frac{1}{\sqrt{2\pi}} \frac{1}{2} (\exp - \frac{1}{2}(y - \mu - \delta)^2 + \exp - \frac{1}{2}(y - \mu + \delta)^2) \\ &= \frac{1}{\sqrt{2\pi}} \exp \left\{ - \frac{1}{2} [(y - \mu)^2 + \delta^2] \right\} \cosh \delta(y - \mu) . \end{aligned}$$

In two dimensions the density of $y = (y_1, y_2)'$ is

$$\begin{aligned} & \frac{1}{(2\pi)^2} \int_0^{2\pi} \exp - \frac{1}{2} (y_1 - \mu_1 - \delta \cos \theta)^2 - \frac{1}{2} (y_2 - \mu_2 - \delta \sin \theta)^2 d\theta \\ &= \frac{1}{2\pi} \exp - \frac{1}{2} \{ (y_1 - \mu_1)^2 + (y_2 - \mu_2)^2 + \delta^2 \} \\ & \quad \cdot \frac{1}{2\pi} \int_0^{2\pi} \exp \{ \delta (y_1 - \mu_1) \cos \theta + \delta (y_2 - \mu_2) \sin \theta \} d\theta \\ &= \frac{1}{2\pi} \exp \left\{ - \frac{1}{2} \{ (y_1 - \mu_1)^2 + (y_2 - \mu_2)^2 + \delta^2 \} \right\} I_0(\delta |y - \mu|) \end{aligned}$$

where $I_0(z)$ is the imaginary Bessel function of zero order.

In three dimensions, a similar averaging of the Gaussian with mean μ and covariance matrix I leads to

$$\frac{1}{(2\pi)^{3/2}} \exp \left\{ -\frac{1}{2}(y - \mu)'(y - \mu) - \frac{1}{2}\delta^2 \right\} \frac{\sinh \delta|y - \mu|}{\delta|y - \mu|}.$$

In each case, as $\delta \rightarrow 0$ the modifying factor tends to unity. The averaging has most effect when $|y - \mu|$ for the basic density is then fallen off very fast. Let us now return to our real problem.

Model (6) requires a general form of the interesting new distributions just given. To put it in neutral notation, let $Y = X + d$ where d is uniformly distributed over a sphere of radius δ , X is Gaussian mean μ and covariance Σ , and the density of Y at y is given by

$$\begin{aligned} \text{Ave}_{|d|=\delta} \frac{1}{(2\pi)^{3/2} |\Sigma|} \exp - \frac{1}{2}(y - d - \mu)' \Sigma^{-1} (y - d - \mu) \\ = \frac{1}{(2\pi)^{3/2}} \frac{1}{|\Sigma|} \exp - \frac{1}{2}(y - \mu)' \Sigma^{-1} (y - \mu) \end{aligned} \quad (19)$$

$$\cdot \text{Ave}_{|d|=\delta} \exp \{ d' \Sigma^{-1} (y - \mu) - \frac{1}{2} d' \Sigma^{-1} d \}.$$

If $\Sigma = H'DH$ where H is orthogonal and D diagonal, $z = \delta D^{-1}H(y - \mu)$, and $E^{-1} = \delta^2 D^{-1}$, the averaging term is

$$\text{Ave}_{|e|=1} \exp \{ e'z - \frac{1}{2} e'E^{-1}e \},$$

which cannot be further evaluated. In fact, with $z = 0$, it is the normalizing constant of the Bingham distribution (see, e.g., the book by Mardia, 1972) and, when $z \neq 0$, of a generalization recently studied by Beran (1979). To get to the working form of the Cox model, we must find the density of the direction of the vector y from (19). Thus the Cox model (6) is hard to deal with mathematically, so estimation schemes based on it do not seem very

practical. However, the Gaussian model without the random smaller dipole seems an adequate approximation since, typically, $|m|/|M|$ is about one-tenth.

(e) The model (4) raises interesting problems. Here M is fixed and m is uniformly distributed over a sphere of radius $|m|$, also fixed. Thus $E m = 0$, $E m m' = |m| I/3$.

First, we consider several related academic problems similar to familiar textbook estimation examples. Suppose that $N \geq 2$ points y are uniformly distributed along a line segment in space, i.e., $y = M + v d$ where v is uniformly distributed on $(0, |m|)$ with M , $|m|$ and d unknown and to be estimated. If, when the points are arranged on the segment, they fall in the order $y_1, y_2, \dots, y_N$, then $\pm d$ is known exactly, and we have $|y_2 - y_1|, |y_3 - y_2|, \dots, |y_N - y_{N-1}|$ as the interior gaps when N points are randomly distributed on $(0, |m|)$. The sufficient statistic is (y_1, y_N) . Simple estimators are (with $m = d|m|$) $y_1 = M$, $y_N = M + m$ or $y_1 = M - m$, $y_N = M$. These will be biased, as are the analogues on the real line. To give another interesting example, suppose we could observe N copies of $y = M + m$ where M and m are as in model (4). For $N \geq 3$, $|m|$ and M can be found *exactly* from the perpendicular bisectors of chords which must intersect at M . As is so often the case, things are simpler on the circle and sphere than on the line.

In practice, we can only observe the directions L of $U(M + m)$. Assuming that $M = |m|\mu/c$, $m = |m|d$, with $c = |m|/|M|$ known and approximately 0.1 and d uniformly distributed over the surface of the unit sphere. It suffices to consider the case of observing L where

$$RL = U(\mu + cd)$$

with known c . M.I. here is very awkward. Since

$$\mu + cd_i = R_i U^{-1} L_i \quad (i = 1, \dots, N),$$

one might use (since $Ed = 0$) the estimator

$$\tilde{\mu} \propto \sum_{i=1}^N U^{-1} L_i. \quad (20)$$

A case of confidence can be obtained from the approximate multivariate distribution of $\sum_{i=1}^N U^{-1} L_i$. To this end we note that

$$R^2 = \mu^2 U^2 + 2c\mu U^2 d + c^2 d^2 U^2 d$$

so

$$ER^2 = 3(\mu^2 U^2) + 1 + 2c^2$$

where $2c^2$ may be ignored. If $\hat{\mu}$ is an approximate pole position, define

$$R^2 = 3(\hat{\mu}^2 U^2) + 1,$$

and write

$$\mu + cd = \bar{R} U^{-1} L.$$

Then

$$\mu \doteq \bar{R} E U^{-1} L$$

$$\bar{R} U^{-1} L - \mu = cd$$

so

$$E(\bar{R} U^{-1} L - \mu)(\bar{R} U^{-1} L - \mu)^T = (c^2/3)I \quad (21)$$

which leads easily to the procedure.

(f) The model (5) of Creer et al. has $M = |M|d$ where $|M|$ is fixed and known, and d has a Fisher distribution about μ with accuracy κ . If the direction of $H = UM$ is known, i.e., the direction L of Ud is known, how to estimate μ ? Since $R_i L_i = U d_i$, $d_i = R_i U^{-1} L_i$, we may compute each $U^{-1} L_i$, reduce to unit length (so not knowing R does not matter) to obtain the d_i . Since these have a Fisher distribution, Fisher's estimator and method of

getting a confidence case for μ may be used. This is, in fact, a standard method of estimating the position of the pole. It is important to observe that the Fisherian method is not applied here to the site means but their transforms. Note that it is related to but different from estimators (20), (18), (15), (13), which are very similar.

3. ESTIMATION OF POLE POSITIONS

We have seen that a rational method of estimating pole positions should follow, by the application of maximum likelihood, from a statistical model for secular variation. In cases where the model makes strict m.l. estimation too difficult, one must try to improve and check the approximations and simplifications made. Since, however, there is unlikely to be any agreement on the model, the chosen method should not be sensitive to model changes within the range of disagreement, i.e., the method should be robust.

The multivariate normal method of Section 2(c) allows a wide variety of models to be tried. These will be tried out in an applied paper to see what model changes are most crucial. The Fisher estimation method has been shown to be robust against deviations from the Fisher distribution but the cone of confidence is not so reliable - Watson (1967).

A counsel of greater perfection is to make a more detailed statistical study of secular variation in the hope of finding a more convincing model. Certainly the newer, more complex models mentioned earlier should be explored. This will be attempted elsewhere. Further, we have here assumed that the site means are known, whereas they will only be estimated, often with different accuracies. This must be taken into account in the final practical method.

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The use of the Fisher distribution to estimate the mean direction of magnetization of a rock at a sampling site is now standard. Sampling sites are chosen to cover 10^4 to 10^5 years to average out the effect of secular variation. The controversy about how to combine these site means has never been satisfactorily resolved. By using statistical models for secular variation, this paper suggests how methods should be derived. A number of interesting statistical distributions and estimation problems are shown.		

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