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A robust least-squares Gondwanan apparent polar wander path and the question of palaeomagnetic assessment of Gondwanan reconstructions

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Two hundred and nineteen palaeomagnetic results are combined in calculating Gondwanan apparent polar wander paths, their confidence intervals, and the residual mean square errors about the paths, for six reconstructions.

A quantitative assessment of the six reconstructions of Gondwanaland is made on the basis of the consistency of palaeomagnetic pole positions using a new statistical technique. Smith and Hallam's [1] Gondwanan reconstruction is the most effective in accounting for the distribution of the palaeomagnetic data and is used in calculating our preferred apparent polar wander path.

1. Introduction

Several reconstructions of Gondwanaland have been proposed. The first reconstructions (e.g. [1,2]) were based on the shape of the continental margins and the continuity of geological features. Later workers have been able to use information from the magnetic anomalies produced by sea-floor spreading in the southern oceans (e.g. [3,4]) and from palaeomagnetic data (e.g. [5,6]) to help constrain their reconstructions. Despite advances in the quality and quantity of data on which to base reconstructions, debate continues as to which reconstruction is the most likely [7,8]. In particular the relationship between West Gondwanaland (South America and Africa) and East Gondwanaland (Antarctica, Australia and India) remains unresolved.

Previous investigations of Gondwanan palaeomagnetic data (e.g. [8,9]) have tended to be qualitative or semi-quantitative. Sufficient palaeomagnetic data are now available for a Gondwanan apparent polar wander (APW) path to be constructed by reproducible mathematical methods. Our mathematical approach permits statistical analysis of the APW path and a simple quantitative palaeomagnetic assessment of Gondwanan reconstructions.

2. Construction of apparent polar wander paths

Gondwanan palaeomagnetic data published prior to 1979 were obtained from the following GJRAS lists: summary in McElhinny [10,11], McElhinny and Cowley [12–14]. Additional data were added from lists for Africa in McWilliams [15] and Brock [16]; for India in Athavale et al. [17]; and for Australia in Goleby [18] and Embleton [19]. The data are in the form of palaeomagnetic pole positions, computed under the usual assumption that the geomagnetic field has been, on the time average, geocentric, axial and dipolar. Ages were assigned to all the palaeomagnetic pole positions using the time scale of the Geological Society of London [20]. The minimum criteria of McElhinny [10] were used as a first stage filter in order to separate unreliable results from the main body of the data. The additional second minimum criterion of Irving et al. [21] for their A category data was also applied for this purpose. After application of these minimum criteria 219 palaeomagnetic pole positions spanning the period from 550 to 150 Ma ago remained for analysis.

The approach generally followed by others at this point, in the analysis of palaeomagnetic data, has been to carry out further data selection using additional information such as the behaviour of natural remanent magnetization during detailed partial demagnetization analyses, or from judgement of the possibility of geological biasing (e.g. by local rotations or remagnetization). Then an APW path has either been produced by free-hand drawing or else been defined by a series of disjoint points [22–24].

In contrast, our method automatically allows for the presence of local aberrant or outlying observations by employing the technique of bi-square weighting [25]. This technique is a robust reproducible method of assigning weights to each observation in such a way that any outlying observation is given a low weight defined in terms of its deviation from the main body of the data. Our APW path is fitted by a statistical method based on weighted least-squares regression using the iteratively-computed bi-square weights [26].

The main assumptions in our APW path construction are as follows:

(1) The palaeomagnetic pole positions have a Fisherian [27] distribution about the true APW path.

(2) The APW path is mathematically smooth in that its first and second derivatives are continuous. (However, since we do not impose bounds on these derivatives, the fitted APW path can still contain relatively sharp kinks, e.g. at 190 Ma, Fig. 1.)

(3) The age of magnetization is known within 10 Ma for each palaeomagnetic pole position. (Numerical experiments indicate that errors in age of up to 15% have little effect on the mathematical stability of our curve fitting procedure.)

Our APW path is calculated in terms of cubic splines [28]. (Cubic spline functions are defined as piece-wise cubic polynomial functions subject to continuity conditions on the function and its first two derivatives at the knots (points where the polynomials join each other).) Our procedure in constructing APW paths for different Gondwanan reconstructions is as follows:

(1) The palaeomagnetic pole positions for each Gondwanan continent are rotated back to their proposed Gondwanaland locations.

(2) Cubic splines are fitted by weighted least-squares to the latitudinal and longitudinal data separately, using the method of Thompson and Clark [26] based upon a normal approximation [29] to the Fisher distribution.

(3) The knot spacing for the splines is determined by cross validation (e.g. [30,31]). For the Gondwanaland data, cross validation consistently indicates that five equally-spaced knots are adequate for both longitude and latitude.

(4) Iterative bi-square weighting [25], based on the residuals to the spline functions, is applied until the solution stabilizes (Fig. 1).

(5) Confidence bands are calculated for the APW paths based on the fitted spline functions using the method of Clark and Thompson [31] and the normal approximation to the Fisher distribution [29].

An additional temporary transformation of the directional data is applied after step 1. In order to improve the accuracy of the normal approximation on which the curve fitting and confidence bands are based, the data set is rotated so that the bulk of the data lie along the equator. After fitting is completed, the data, fitted path and confidence bands are rotated back to the original co-ordinate system.

Our final Gondwanan APW path from 550 to 150 Ma is shown in Fig. 1 for the Smith and

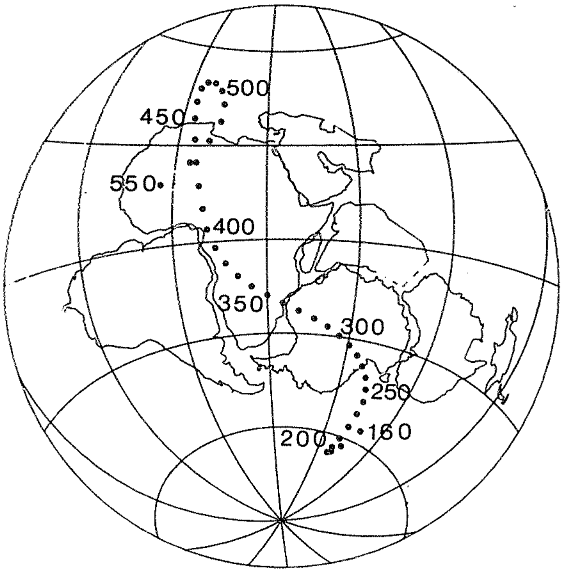

Fig. 1. Gondwanaland apparent polar wander path 550–160 Ma for Smith and Hallam's [1] reconstruction with Africa held stationary. The path is defined continuously but is only plotted at 10-Ma intervals.

Hallam [1] reconstruction with Africa held stationary. The pole positions of this path are listed every 10 Ma in Table 1. 95% confidence limits for the APW path are plotted as circles at 10-Ma intervals in Fig. 2 and listed in Table 1. Because of the poor quality of some of our data, these 95% confidence bands should be treated as a practical guide to the reliability of the fitted APW path rather than as strict limits.

Our final path is broadly similar to previously published paths. It exhibits a particularly sharp "hairpin bend" at 190 Ma. However, it contains less high-frequency variation than paths based on disjoint Fisherian means or key poles. The overlap of our confidence limits between 410 and 550 Ma indicates that with the presently available Gondwanan palaeomagnetic data it is not possible to distinguish between an open loop and a sharp bend in the Lower Palaeozoic section of the APW path. The relatively large confidence limits around 400 and 450 Ma reflect the sparsity of well-grouped palaeomagnetic results from these periods. Further palaeomagnetic studies are needed to constrain the Gondwanan APW path at these times.

TABLE 1

Robust least-squares Gondwanan APW path

Age (Ma)	Latitude (°N)	Longitude (°E)	Confidence interval (°)
160	−56.2	78.8	8.0
170	−62.4	72.8	4.2
180	−65.2	68.8	3.9
190	−65.4	67.5	4.1
200	−63.6	68.4	3.9
210	−60.4	70.2	3.4
220	−56.3	72.0	3.4
230	−51.9	73.0	3.9
240	−47.7	73.0	4.4
250	−43.9	72.0	4.4
260	−40.6	70.1	4.2
270	−37.6	67.5	4.1
280	−34.8	64.3	4.3
290	−32.1	60.5	4.9
300	−29.7	56.2	5.5
310	−27.3	51.4	6.0
320	−25.1	46.3	6.2
330	−22.9	40.8	6.1
340	−20.5	35.2	6.1
350	−17.9	29.8	6.3
360	−14.7	24.8	6.8
370	−11.0	20.3	7.5
380	−6.8	16.5	8.1
390	−1.8	13.4	8.3
400	4.0	11.1	8.1
410	10.6	9.5	7.5
420	17.7	8.1	7.0
430	24.9	6.7	6.9
440	31.9	5.4	7.3
450	38.3	4.1	8.0
460	43.6	3.3	8.5
470	47.6	3.5	8.4
480	49.6	5.3	7.6
490	49.4	8.5	6.3
500	47.1	11.7	5.6
510	43.1	13.6	5.7
520	37.7	13.3	6.1
530	31.5	10.5	6.2
540	24.9	4.8	6.8
550	18.4	355.8	10.3

The latitude and longitude of the Gondwanan south pole positions are listed for Africa in its present geographic position. The confidence intervals tabulated are the radius for each confidence circle in degrees.

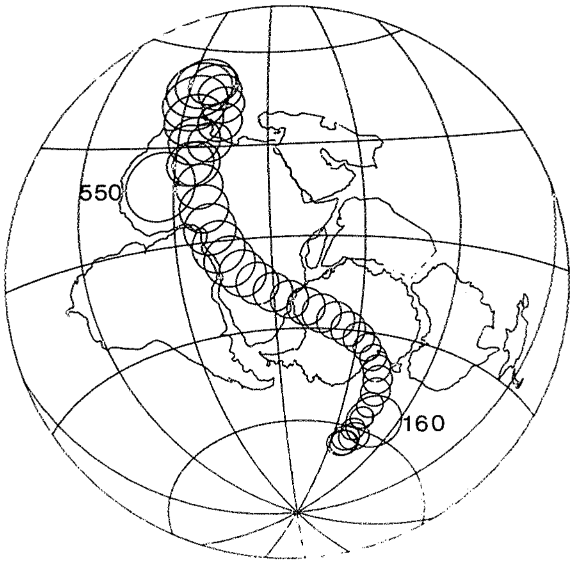

Fig. 2. 95% confidence limits for the APW path of Fig. 1 drawn at 10-Ma intervals.

3. Palaeomagnetic assessment of Gondwanan reconstructions

The distribution of palaeomagnetic pole positions about our APW paths can be used to assess the different reconstructions on which the paths are based. The goodness of fit of the reconstructions is judged by a single number, namely the residual mean square error (RMSE) of the palaeomagnetic pole positions about the APW paths. A low RMSE is taken to indicate a good reconstruction. Table 2 summarizes our results for six different reconstructions and shows that Smith and Hallam's 1970 [1] reconstruction gives the best fit to the palaeomagnetic data, as judged by our RMSE criterion.

TABLE 2

Residual palaeomagnetic mean square error about the APW paths calculated for six possible Gondwanan reconstructions

Reconstruction	RMSE	DF
	$\sum_{i=1}^{219} \frac{(\psi_i)^2}{W_i}/\text{DF}$	
Smith and Hallam [1]	394	184
Norton and Sclater [4]	441	183
Tarling [5]	465	184
Barron et al. [3]	475	183
Rickard and Belbin [7]	481	182
Powell et al. [8]	486	182

RMSE = residual mean square error (measured in degrees squared); ψ_i = solid angle in degrees of ith actual pole position from its predicted position on fitted APW path corresponding to given reconstruction; DF = degrees of freedom (this varies between reconstructions due to the bi-square weighting method and is given by the total weight [25] minus the order of the spline minus the number of internal knots); W_i = bi-square weight of Mosteller and Tukey [25].

4. Comparison of the residual mean square errors

We now examine the question: do the differences in the RMSEs in Table 2 correspond to real differences in the compatibility of the data with the six reconstructions, or are these differences simply due to an inherent random component in the RMSEs? Unfortunately, for reasons given below, we cannot give an unequivocal answer to this question. But the indications are that the differences in the 6 RMSEs are due primarily to their inherent random variability.

Table 2 shows that Smith and Hallam's [1] reconstruction gives the best fit to our data. However, it must be remembered that each of the six fitted curves and six corresponding RMSEs are derived from the 219 measured apparent pole positions, each of which is subject to "random noise" or random variability to a greater or lesser extent. This "random noise" in the data is due partly to inherent variability in the process of measuring a remanence and in orientating samples and partly due to the intrinsic variability in remanent magnetization due to such factors as partial remagnetization and inhomogeneity and anisotropy of the rock samples. Hence each of the 6 RMSEs in Table 2 is subject to random variability to some extent.

Our statistical examination of the differences in the RMSEs is based on the following extension of an approximation given in various forms by Watson [32], Gould [33], Stephens [34] and Mardia [35, sections 8.5.4(c), 8.7.2(b)]. Suppose, as we have done in fitting our smooth curves, that we have N independent observations (θ_i, ϕ_i) denoting the polar co-ordinates of the ith pole position with corresponding age t_i. Also assume that (θ_i, ϕ_i) has the Fisher distribution with concentration parameter κ and mean direction specified by polar co-ordinates $(\theta_0(t_i), \phi_o(t_i))$. Then if each of the functions $\theta_0(t)$ and $\phi_0(t)$, which specify the "true" mean direction t years ago, and involve k unknown parameters, are subsequently estimated by the method of ordinary unweighted least squares, it follows that if κ is fairly large, say 10 or greater, that the statistic:

$$Q = \kappa \sum_{i=1}^{N} (\psi_i)^2$$

is approximately distributed as χ^2 on $2N - 2k$ degrees of freedom (DF), with the solid angles (ψ_i) expressed in radians. An implicit assumption here is that the fitted functions $\theta_0(\cdot)$ and $\phi_0(\cdot)$ are of the correct form, i.e., there is no systematic component in the residuals, or equivalently, the major component of Q is due to inherent variability of the data, not a poor reconstruction. The $2N$ term in the DF arises because there are essentially two independent measurements (θ and ϕ) at each of the N data points. For our data, $N = 219$ and $k = 9$, so that $2N - 2k = 420$.

To estimate κ, we equate the average RMSE from Table 1 to the theoretical average value of χ^2 on 420 DF, adjusting for the RMSEs being computed in terms of the bi-square weights and with the solid angles expressed in degrees. This gives $\hat{\kappa} = 16.5$. With this estimate of κ and using the formula by Fisher [36] for the percentiles of the χ^2 distribution, the corresponding 95% probability limits for the RMSE (as defined in Table 2) are 397 to 521. In other words, the RMSE could range from 397 and 521 with 95% probability, due solely to random noise in the original observations $\{(\theta_i, \phi_i)\}$.

An implicit assumption in the preceding theory and above calculation is that the functions θ_0 and ϕ_0 are fitted by ordinary unweighted least squares. To adjust for our use of weighted least squares, we follow the recommendation of Mosteller and Tukey [25, section 14F] and repeat the previous calculation but with the DF set equal to the sum of the bisquare weights. This gives $\hat{\kappa} = 14.4$, and 95% probability limits for the RMSE of 393 to 525.

In both cases, the last 5 RMSEs in Table 2 lie well within these 95% prediction limits, while the RMSE for the Smith and Hallam reconstruction is extremely close to the lower limit. This suggests that there is no statistically significant difference between these six alternative Gondwanaland reconstructions in their ability to explain the distribution of the palaeomagnetic data.

However, our calculations should be treated with some caution. First, the same set of 6 RMSEs is used both to estimate the likely range of the RMSE and then to compare the actual range with this predicted range. This "double-use" of the data is not necessarily wrong in itself; when assessing the goodness-of-fit of data to a model, it is clearly sensible to estimate any necessary parameters from the data, and then compare the actual data with the predictions of the model using the estimated parameter. This approach is valid statistically, provided one allows (usually by adjusting the DF) for this estimation of the parameters. We have not made such an allowance, and it does not seem possible to do so. This is because the 6 RMSEs in Table 2 are not statistically independent, since they are all derived from essentially the same data on the same 219 apparent pole positions. The usual methods for adjusting statistical analyses for the estimation of parameters rely heavily on the presumption that the observations on which the estimation is based are statistically independent.

Secondly, our estimation of κ involves an implicit assumption that the major component in the RMSEs is random variability, and not possible systematic differences between the subgroups of the data corresponding to continental blocks, or between different reconstructions.

In addition, the theory underlying our calculations assumes that observations (θ_i, ϕ_i) follow the Fisher distribution with the same concentration parameter throughout, and that the ages assigned to the pole positions are correct and exact. Although the observations do not have equal variability (those older than 450 Ma being considerably more variable than the rest), the use of Mosteller and Tukey's bi-square weights compensates automatically for this. Since the probability distribution of the observations $\{(\theta_i, \phi_i)\}$ may be expected, from both theoretical and practical grounds, to be close to the Fisher distribution, the main factor affecting the validity of our calculations is that the ages t_i are of course known only approximately. Experiments with similar data [26] indicate that both the fitted curve and the corresponding RMSE are subject to only negligible error if the t_i's are in error by at most 15%.

Because of the above difficulties, any calculations in assessing the RMSEs must remain to some extent approximate. Nevertheless, it seems clear that there is no significant difference in the goodness-of-fit to the palaeomagnetic data of the last five reconstructions in Table 2 as their RMSEs lie within our 95% probability limits. This means that the differences between the RMSEs of these five reconstructions can be accounted for quite satisfactorily by random errors in the palaeomagnetic data rather than by any significant differences in the ability of the various reconstructions to explain the distribution of palaeomagnetic pole positions. It is possible that Smith and Hallam's [1] reconstruction is significantly better than the other five in its explanation of the data. But the situation is not entirely clear as Smith and Hallam's [1] reconstruction has a RMSE lying very close to our lower 95% probability limit. So the present palaeomagnetic data do not appear to be quite of sufficient quality to demonstrate unequivocally any significant superiority.

5. Summary

Our mathematical approach to constructing apparent polar wander paths allows continental reconstructions to be ranked according to their ability to explain the distribution of palaeomagnetic data. The residual mean square error (RMSE) of the palaeomagnetic pole positions about our paths provides a simple quantitative measure of the goodness of fit of different Gondwanan reconstructions. Of six reconstructions examined Smith and Hallam's [1] explains the distribution of palaeomagnetic data most effectively. Smith and Hallam's [1] reconstruction is therefore used in our construction of a Gondwanan APW path. Our robust, weighted least-squares spline fitting method produces an APW path, rate of apparent polar movement, and apparent polar acceleration which are all defined continuously for the whole length of the path. The resulting Gondwanan APW path is not as well defined as the European or North American paths calculated using the same approach [26], although similar amounts of data are available for constructing all three paths. The Gondwanan path is particularly poorly defined around 450 and 400 Ma ago mainly due to the sparcity of data of these ages. Our Gondwanan APW path exhibits a sharp turn at 190 Ma but otherwise is very smooth. The fastest rate of Gondwanan apparent polar movement occurred in the Cambrian.

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