Key Points:

- The similarity between paleomagnetic poles is quantified with information-theoretic metrics
- A Bayes error is derived to measure pole similarity in a probabilistic framework
- This approach enables quantitative comparison of new and published paleomagnetic poles

Correspondence to:

D. Heslop,
david.heslop@anu.edu.au

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Quantifying the Similarity of Paleomagnetic Poles

D. Heslop¹ and A. P. Roberts¹

¹Research School of Earth Sciences, The Australian National University, Canberra, Australia.

Abstract An ability to compare paleomagnetic poles quantitatively is fundamental to paleogeographic reconstruction. The Fisher distribution provides a statistical framework for both constructing and relating paleomagnetic poles to enable comparison of estimated pole positions in paleomagnetic reconstructions. However, Fisher distribution-based confidence regions for paleomagnetic poles are often compared using empirical rules of thumb rather than by quantitative analysis of their full structure. Here we demonstrate potential shortcomings of such comparisons and propose continuous metrics for quantitative comparison of paleomagnetic poles. These metrics are simple to apply for Fisher distributions and can be modified readily for a broad range of alternative distributions that may be more appropriate for representing some paleomagnetic data sets. We demonstrate how our proposed metrics provide both quantitative and probabilistic approaches to common tasks in paleomagnetic reconstruction, such as comparing estimated mean pole positions with apparent polar wander paths.

1. Introduction

In many paleomagnetic reconstructions, individual specimen directions are combined to provide site mean directions, which in turn are combined to yield mean directions for geological units or formations to provide paleomagnetic poles (McElhinny & McFadden, 2000). Thus, it is essential to have an appropriate statistical framework to compare paleomagnetic poles in a quantitative manner that takes into consideration their associated uncertainties. For example, an ability to make such a comparison quantitatively is crucial when comparing estimated poles with apparent polar wander paths (APWPs). As a case in point, van der Voo (1990) developed a set of seven reliability criteria to classify paleomagnetic poles, including the criterion “No resemblance to paleopoles of younger age”, which is designed to protect against unidentified remagnetization. However, how can “resemblance” between paleopoles be judged without a framework to measure similarity quantitatively?

Fundamental to any comparison of paleomagnetic directions is a model that enables inferences to be drawn concerning a population (i.e., the magnetization direction of a geological formation or unit) based on the information obtained from a statistical sample (i.e., remanence directions from a collection of paleomagnetic specimens). The Fisher (1953) distribution forms the foundation of paleomagnetic statistics and is the focus of this study. The probability density function (pdf) of the Fisher (1953) distribution is given by

$$f_F(\omega|\mu, \kappa) = \begin{cases} \frac{1}{4\pi} & \text{for } \kappa = 0, \\ \frac{\kappa}{4\pi \sinh \kappa} \exp(\kappa \mu^T \omega) & \text{for } \kappa > 0, \end{cases} \quad (1)$$

where ω is a unit vector, κ is the concentration parameter, and μ is a unit vector corresponding to the mean direction of the distribution. Employing a Cartesian (x , y , and z) coordinate system, the resultant length, R , of N unit vectors representing a collection of paleomagnetic directions is given by

$$R = \sqrt{\left(\sum_{i=1}^N x_i\right)^2 + \left(\sum_{i=1}^N y_i\right)^2 + \left(\sum_{i=1}^N z_i\right)^2}. \quad (2)$$

Fisher (1953) demonstrated that the maximum likelihood estimate of the true mean direction is simply the direction of the unit resultant vector given by

$$\bar{x} = \frac{1}{R} \sum_{i=1}^N x_i, \quad \bar{y} = \frac{1}{R} \sum_{i=1}^N y_i, \quad \text{and} \quad \bar{z} = \frac{1}{R} \sum_{i=1}^N z_i \quad (3)$$

and provided an approximation of the concentration parameter (when $\kappa > 3$):

$$\kappa \approx \frac{N-1}{N-R}. \quad (4)$$

Additionally, Fisher (1953) demonstrated that the mean direction is distributed according to equation (1) with concentration κR and defined the semiangle of a circular cone centered on the estimated mean direction that contains the true population mean direction with 95% probability:

$$\alpha_{95} = \arccos \left(1 - \frac{N-R}{R} \left[20^{\frac{1}{N-1}} - 1 \right] \right). \quad (5)$$

A common approach to averaging paleomagnetic directions is to first transform them into virtual geomagnetic poles (VGPs). The use of VGPs has a number of advantages, including the ability to compare poles from geographically disparate sites and the suggestion that VGPs may conform more closely to a Fisher (1953) distribution than paleomagnetic directions (Deenen et al., 2011). The mean of VGP positions and uncertainties can be estimated using the same approach as outlined above, with upper case symbols indicating the use of VGPs (i.e., κ and α_{95} become K and A_{95} , respectively).

Assuming that paleomagnetic directions or VGPs are Fisher (1953) distributed, paleomagnetists adopt the framework above to estimate pole positions and their associated uncertainties. As such, a paleomagnetic pole is not a single point, but rather a Fisher (1953) distribution with a concentration of κR . Therefore, in a statistical setting, it is appropriate to consider paleomagnetic poles as pdfs.

A common task in paleomagnetic reconstructions is to consider the similarity of poles, such as when comparing an estimated pole position to poles in an APWP. A range of hypothesis tests are available to compare the means of two sets of directions (Heslop & Roberts, 2018; McFadden & Lowes, 1981; McFadden & McElhinny, 1990; Tauxe, 1998; Watson, 1956, 1983, 1984). While the common mean test is appropriate for comparing directions in certain settings, for example, polarity zones within a sediment core (e.g., Hong et al., 2013) or a succession of geological units (e.g., Strik et al., 2003; Swanson-Hysell et al., 2014), such a hypothesis test may be too stringent when comparing estimated pole positions for sites separated by large distances. Furthermore, the common mean test requires comparison of ensembles of directions and cannot be applied readily to estimated poles. If appropriate ensembles of directions are available, then performing a common mean test may be desirable. More commonly, however, derived poles are compared directly.

Gordon and Cox (1980) developed a null-hypothesis significance test to compare paleomagnetic poles, where two observed poles and their uncertainties are used to estimate a best fit (in a maximum likelihood sense) hypothetical mutual pole. A χ^2 statistic is then used to test if the observed poles are inconsistent with the hypothetical mutual pole at a given significance level. If there is insufficient disagreement between the observed and hypothetical poles, then the null hypothesis of common directions cannot be rejected. Acton and Kettles (1996) outlined a rule-of-thumb approach to the Gordon and Cox (1980) test based on interpreting the similarity of mean directions via their α_{95} (or equivalent A_{95}) angles. These rules are summarized in Figure 1. In the first case, if one α_{95} contains the mean of the other set of observations, their means are deemed to be indistinguishable (Figure 1a). Alternatively, if the α_{95} for each set of observations do not overlap, it is concluded that their mean directions are discernibly different (Figure 1b). McElhinny and McFadden (2000) commented that although this criterion is correct, it is conservative because it is possible for sets of observations with overlapping α_{95} circles to have different means. This highlights a third possibility, where there is α_{95} overlap but the distribution means are not included in the overlap (Figure 1c). Tauxe (1998) defines this as a “gray zone” where it cannot be inferred if the mean directions are indistinguishable in the absence of a statistical test.

Such empirical rules appear to make sense intuitively and can be applied readily. It is possible, however, to envisage cases where these rules result in inappropriate conclusions. Such a scenario is demonstrated in Figure 1d, where the α_{95} of one set of observations contains the mean of the second set of observations, and, thus, it would be concluded that the mean directions are indistinguishable. In this case, however, most of the larger (black) α_{95} does not overlap with the smaller α_{95} (blue), which suggests that agreement between the mean directions may be low. Furthermore, preferred methods for representing α_{95} visually (e.g., stereoplots) give the impression that the pole pdf is flat. Given that the estimated mean direction of a Fisher (1953) distribution is also Fisher (1953) distributed with a concentration of κR , this is not the case (except in the extreme of $\kappa R = 0$). Rather, regions close to the center of the α_{95} circle have higher probability densities.

Figure 1. Examples of the empirical approach that is typically employed to compare two paleomagnetic poles. In this illustration, Fisher (1953) distributions are represented by mean directions (square symbols) and their corresponding α_{95} circles (lines). (a) The mean direction of the blue distribution resides inside the α_{95} circle of the black distribution; therefore, the two directions are deemed to be indistinguishable. (b) The α_{95} circles do not overlap; therefore, the directions are considered to be distinguishable. (c) Overlapping α_{95} circles that do not include the mean direction of the other distribution are considered as a “gray zone” where it cannot be inferred whether the mean directions are indistinguishable. (d) The mean direction of the blue Fisher (1953) distribution resides within the α_{95} circle of the black distribution. Such an overlap would typically be taken as an empirical indication that the blue and black directions are indistinguishable. (e) When plotted as a function of inclination (at a constant declination of 270°), it is apparent that the probability density functions in (d) do not overlap strongly. (f) The approach of Gordon and Cox (1980) would posit the existence of two separate common mean poles between the blue-black and red-black pairs of distributions. This results in a paradox, whereby the black pole is deemed to be indistinguishable from both the blue and red poles, while the blue and red poles are clearly distinguishable. (g) The scenario illustrated in (f) is demonstrated further when the pole pdfs are plotted as a function of inclination (at a constant declination of 270°). The blue and red poles share an equal level of overlap with the black pole; however, it is apparent that in both cases the overlap is not strong. Additionally, lack of overlap between the blue and red distributions means that it is infeasible for the black pole to be deemed indistinguishable with both.

This point is illustrated by comparing cross sections through the Fisher (1953) distributions that represent the mean directions (Figure 1e). Two issues are highlighted by this example. First, pole comparisons should not focus solely on overlap (i.e., agreement) but also on the extent to which the α_{95} s do not overlap (i.e., disagreement). Second, paleomagnetic poles are best considered as pdfs and comparisons can exploit this property.

The approach of Gordon and Cox (1980) may also result in contradictions when making multiple comparisons to a reference pole or APWP. The test of Gordon and Cox (1980) is based on estimating the position of a hypothetical true pole that may or may not be consistent with the two empirical poles under consideration. This appears reasonable until one considers the scenario of multiple studies making comparison to the same reference pole. This scenario is illustrated in Figure 1f, where the black distribution represents a reference pole with its associated α_{95} . A given study may produce the blue pole, which according to the framework of Gordon and Cox (1980) would be deemed indistinguishable from the reference pole, with a hypothetical true pole located between the centers of the black and blue distributions. A second study may then use the same black reference pole in comparison to the red pole. In this case, the Gordon and Cox (1980) framework would deem the black and red poles to also be indistinguishable on the basis of a hypothetical true pole positioned between their centers. When these two independent comparisons are considered in combination, it can be seen that each study produced a hypothetical true pole that was inconsistent with the alternative study and two clearly separated poles have been ruled to be indistinguishable from the reference, while they are distinguishable from each other. Thus, a statistical framework that results in a binary decision that rules paleomagnetic poles to be either indistinguishable or distinguishable may produce contradictions when multiple comparisons are made.

The challenge of quantitative comparison of paleomagnetic poles based on Fisher (1953) distributions was considered by Bazhenov et al. (2016), who showed how comparisons based on α_{95} -derived statistics can yield conflicting results. To address this problem, Bazhenov et al. (2016) recommended the use of “alarm-bands” that envelope APWPs. Poles that fall within the alarm-band would be deemed not to be different from the APWP, which provides an indication of potential remagnetization consistent with the reliability criterion of van der Voo (1990). While such an alarm-band can indicate similarity to a reference APWP, it does not take into consideration the uncertainty associated with the pole that is being evaluated. For example, should the entire α_{95} of the estimated pole reside within the alarm-band, or is it sufficient for the center or only a small segment of the α_{95} to overlap the alarm-band?

In this paper, we demonstrate how the level of similarity between Fisher (1953) distributions and thus paleomagnetic poles can be quantified using readily calculated information-theoretic metrics. These metrics provide continuous measures that can be placed into a probabilistic context. We argue that such a quantitative approach provides a more informative framework for comparing paleomagnetic poles, which avoids the contradictions arising from hypothesis tests that are interpreted as providing binary “yes” or “no” outcomes.

2. Quantifying the Similarity of Fisher (1953) Distributions

It is intuitive to measure the similarity of paleomagnetic poles based on the extent of their overlap. In paleomagnetism, overlap has traditionally been assessed by α_{95} comparison; however, as discussed above, this can result in inconsistencies because the probability density within an α_{95} circle is not expected to be constant. A more informative way to consider the similarity between mean directions is in terms of their Fisher (1953) pdfs. We now present three related information-theoretic measures of similarity for Fisher (1953) distributions.

2.1. Bhattacharyya Coefficient

Bhattacharyya (1943) developed a generalized approach to measure the similarity of any two pdfs. The Bhattacharyya (1943) coefficient, B , between continuous pdfs p and q is given by

$$B(p : q) = \int \sqrt{p(x)q(x)} dx. \quad (6)$$

In equation (6), B has a maximum of 1 for identical pdfs (by definition, p and q have integrals of 1; therefore, if $p(x) = q(x)$ at all values of x , the integral in equation (6) will also be 1). In turn, B has a minimum value of 0 for completely dissimilar distributions (i.e., $p(x) = 0$ at any x value where $q(x) \geq 0$ and *vice versa*). Therefore, the

Bhattacharyya (1943) coefficient provides an intuitive metric, which lies between 0 (completely dissimilar) and 1 (identical), for comparing two pdfs.

Given the mean directions, μ_p and μ_q (in Cartesian coordinates), and concentrations, κ_p and κ_q , of two Fisher (1953) distributions, the Bhattacharyya (1943) coefficient is given by (derivation in Appendix A):

$$B(p : q) = \frac{\sinh(\kappa_{pq})}{\kappa_{pq}} \sqrt{\frac{\kappa_p \kappa_q}{\sinh(\kappa_p) \sinh(\kappa_q)}}, \quad (7)$$

where

$$\kappa_{pq} = \left\| \frac{\mu_p \kappa_p}{2} + \frac{\mu_q \kappa_q}{2} \right\|, \quad (8)$$

with $\|\cdot\|$ indicating the vector length. As discussed above, when paleomagnetic directions are averaged assuming that they are Fisher (1953) distributed, the resulting mean direction is also Fisher (1953) distributed with concentration κR . Thus, equation 7 can be extended to measure the similarity between two paleomagnetic poles. Assuming that the poles are based on combining VGPs, which yield mean directions of M_p and M_q , concentrations of K_p and K_q , and resultant vector lengths of R_p and R_q , equation (7) becomes

$$B(p : q) = \frac{\sinh(K_{pq} R_{pq})}{K_{pq} R_{pq}} \sqrt{\frac{K_p R_p K_q R_q}{\sinh(K_p R_p) \sinh(K_q R_q)}}, \quad (9)$$

where

$$K_{pq} R_{pq} = \left\| \frac{M_p K_p R_p}{2} + \frac{M_q K_q R_q}{2} \right\|. \quad (10)$$

2.2. Bayes Error

The Bhattacharyya (1943) coefficient provides a measure of the similarity between two Fisher (1953) distributions, but it lacks a clear probabilistic interpretation. To overcome this, we adopt a Bayesian framework (Bayes, 1763) focused on the classification problem of assigning a random observation, x , to either p or q (Cover & Thomas, 2006). Within a Bayesian framework the upper bound on the probability that x is misclassified (i.e., incorrectly attributed to either p or q), which is referred to as the Bayes error (Nielsen, 2014), is given by (derivation provided in Appendix B):

$$E^* \leq \frac{C_\alpha^*(p : q)}{2}, \quad (11)$$

where α lies in the interval (0, 1), and minimizes

$$C_\alpha(p : q) = \left[\frac{\sinh(\kappa_p)}{\kappa_p} \right]^{-\alpha} \left[\frac{\sinh(\kappa_q)}{\kappa_q} \right]^{\alpha-1} \left[\frac{\sinh(\kappa_{pq})}{\kappa_{pq}} \right], \quad (12)$$

with

$$\kappa_{pq} = \|\alpha \mu_p \kappa_p + (1 - \alpha) \mu_q \kappa_q\|. \quad (13)$$

The Bayes error can range between 0.5 (the distributions are identical; therefore, the probability of misclassifying a random observation is 50%) and 0 (the distributions are completely dissimilar; therefore, the probability of misclassifying a random observation is 0%). As is the case for the Bhattacharyya (1943) coefficient, equation (12) can be adapted to consider paleomagnetic poles:

$$C_\alpha(p : q) = \left[\frac{\sinh(K_p R_p)}{K_p R_p} \right]^{-\alpha} \left[\frac{\sinh(K_q R_q)}{K_q R_q} \right]^{\alpha-1} \left[\frac{\sinh(K_{pq} R_{pq})}{K_{pq} R_{pq}} \right], \quad (14)$$

with

$$K_{pq} R_{pq} = \|\alpha M_p K_p R_p + (1 - \alpha) M_q K_q R_q\|. \quad (15)$$

Figure 2. Example of two Fisher (1953) distributions that share a common mean but have substantially different precisions. (a) The entire α_{95} circle of the blue distribution resides within the α_{95} circle for the black distribution; however, (b) plotting the pdfs as a function of inclination (at a constant declination of 270°) reveals the disagreement between the two pdfs.

2.3. Kullback-Leibler Divergence

The Kullback and Leibler (1951) divergence provides a measure of the similarity of a given pdf, q , to a reference pdf, p . This enables quantitative comparison of an estimated pole to a reference pole. For example, the Kullback-Leibler divergence can be used to compare a pole of unknown age to reference poles in an APWP. The Kullback and Leibler (1951) divergence, $D_{KL}(p, q)$, is given by

$$D_{KL}(p, q) = \int p(x) \log \left(\frac{p(x)}{q(x)} \right) dx. \quad (16)$$

For the specific case of Fisher (1953) distributions, $D_{KL}(p, q)$ is given by (Ćesić et al., 2016):

$$D_{KL}(p, q) = \log \left[\frac{\kappa_p \sinh(\kappa_q)}{\kappa_q \sinh(\kappa_p)} \right] - \left(\frac{1}{\tanh(\kappa_p)} - \frac{1}{\kappa_p} \right) \mu_p^T (\kappa_q \mu_q - \kappa_p \mu_p) \quad (17)$$

and can be applied to paleomagnetic poles in the form (derivation provided in Appendix C):

$$D_{KL}(p, q) = \log \left[\frac{K_p R_p \sinh(K_q R_q)}{K_q R_q \sinh(K_p R_p)} \right] - \left(\frac{1}{\tanh(K_p R_p)} - \frac{1}{K_p R_p} \right) \mu_p^T (K_q R_q \mu_q - K_p R_p \mu_p). \quad (18)$$

As indicated by its name, $D_{KL}(p, q)$ quantifies the divergence (i.e., dissimilarity) between two probability distributions. Thus, if two paleomagnetic poles are identical, that is, $p(x) = q(x)$ at all values of x , then $D_{KL}(p, q) = 0$. Correspondingly, D_{KL} increases with growing dissimilarity between the poles.

2.4. Advantages of Similarity Metrics

As discussed, paleomagnetic poles are best considered as pdfs, and it is necessary to compare them in terms of both their similarities and dissimilarities. This is demonstrated in equations (9), (14), and (18), where the Bhattacharyya (1943) coefficient, Bayes error, and Kullback and Leibler (1951) divergence consider both mean directions and precisions. Thus, it is feasible to have two pdfs with the same mean direction, but their similarity is lowered by their different precisions (Figure 2). This may appear to be a potential drawback when comparing poles, but as discussed above, poles are best considered as Fisher (1953) distributions. Specifically, the pole pdf provides us with a probabilistic representation (constructed from the observed paleomagnetic directions) for the true pole position. Thus, differences in precision must be considered.

Our approach also resolves the contradiction illustrated in Figure 1f, where two clearly different poles are both inferred to be indistinguishable from a third pole. This issue can be resolved by use of continuous, rather than binary, similarity metrics that consider the probabilistic nature of paleomagnetic poles. We return to Figures 1f and 1g to illustrate this point. Comparison of the blue and black poles yields $B = 0.42$ and $E^* = 0.19$. Where use of existing binary classification schemes would conclude that the poles are indistinguishable, the Bayes error indicates only a 19% probability of misclassification. Similarly, the red and black poles yield

Table 1*Collection of Northwest Africa Paleomagnetic Poles Collated by Palencia-Ortas et al. (2011) for the Age Interval 190 to 210 Ma*

Pole code	Plat. [°]	Plon. [°]	<i>R</i>	<i>K</i>	Study
IG ⁽¹⁾	78.4	238.2	10.79	47.4	Palencia-Ortas et al. (2011)
FZ ⁽¹⁾	67.9	247.9	11.91	124.8	Palencia-Ortas et al. (2011)
IG+FZ ⁽¹⁾	73.0	244.7	22.60	55.5	Palencia-Ortas et al. (2011)
S2006 ⁽¹⁾	67.8	250.3	5.99	780.4	Silva et al. (2006)
HM1971 ⁽¹⁾	58.0	259.0	4.99	366.9	Hailwood and Mitchell (1971)
T2008 ⁽²⁾	69.9	236.9	34.42	58.4	Torsvik et al. (2008)
BC2002 ⁽²⁾	63.4	250.1	18.71	61.9	Besse and Courtillot (2002)
H1999 ⁽³⁾	82.9	212.7	12.78	55.8	Hargraves et al. (1999)
B1973 ⁽¹⁾	71.0	216.0	25.45	16.7	Bardon et al. (1973)
K2004 ⁽¹⁾	77.2	240.9	61.78	15.4	Knight et al. (2004)
M1978 ⁽⁴⁾	50.6	251.4	19.26	7.7	Martin et al. (1978)
K1995 ⁽⁵⁾	70.9	235.1	7.99	581.0	Kies et al. (1995)

Note. Plat. and Plon. correspond to pole latitude and longitude, respectively. Definitions of *R* and *K* are provided in the main text. Superscript indices denote the origin of the paleomagnetic pole, corresponding to (1) Central Atlantic Magmatic Province; (2) northwest Africa apparent polar wander path running mean; (3) Freetown Layered Igneous Complex, Sierra Leona; (4) Moroccan red beds; and (5) Zarzaitine Formation, Algeria.

$B = 0.42$ and $E^* = 0.19$ and would again be ruled indistinguishable with existing binary schemes. Adoption of continuous metrics means that the relationship between poles can be judged purely on their quantified similarity. Thus, contradictions are avoided because it is not necessary to reduce quantitative evidence down to a hard designation of directions being simply different or indistinguishable.

While the Fisher (1953) distribution currently underpins paleomagnetic analysis, various alternative probability distributions have been proposed for paleomagnetic directional analysis (Bingham, 1974; Kent, 1982; Wood, 1982). The complicated form of some of these distributions means that they may not lend themselves to derivation of closed-form representations of the presented information-theoretic metrics. Instead, these metrics can be estimated readily via numerical integration across the surface of a unit sphere using schemes such as Lebedev and Laikov (1999) quadrature. Regardless, our proposed approach for quantifying paleomagnetic pole similarity is not restricted to Fisher (1953) distributions and can be adapted readily to other probability distribution types.

3. Case Studies

To demonstrate our proposed metrics, we provide two case studies that are underpinned by a comparison of Fisher (1953) distributions that represent paleomagnetic poles. We show how our approach can place such comparisons into a quantitative framework. These examples are used solely for illustrative purposes and are not presented as critiques of the studies in which they were published. The case studies involve comparison of poles and APWPs. It should be noted that APWPs are typically constructed by estimating a running mean through a collection of poles with different ages. The ensemble of poles in a given time interval, however, may not be Fisher (1953) distributed because of plate motion, and so forth. This is an important consideration; however, the current approach for reporting APWPs assumes that points along the running mean can be represented with Fisher (1953) distributions. We, therefore, follow this approach and employ published APWPs based on an assumption of Fisher (1953) distributions.

Paleomagnetic poles are commonly published in terms of their direction, α_{95} , and N . R and κ (or equivalently K) are required for equations (9), (14), and (18). Rearranging equation (5) enables determination of R as follows:

$$R = \frac{\left[20^{\frac{1}{N-1}} - 1\right] N}{20^{\frac{1}{N-1}} - \cos(\alpha_{95})}, \quad (19)$$

and κ (or K) can be determined using equation (4).

Table 2

Common Mean Test Results From Palencia-Ortas et al. (2011) and Pole Comparison From This Study

Pole code	IG	FZ	IG+FZ	S2006	HM1971	T2008	BC2002	H1999	B1973	K2004	M1978	K1995
IG	–	0.03/0.01	0.38/0.18	0.01/0.00	0.00/0.00	0.09/0.03	0.00/0.00	0.43/0.22	0.22/0.11	0.91/0.46	0.00/0.00	0.08/0.02
FZ	N	–	0.24/0.12	0.80/0.39	0.00/0.00	0.28/0.14	0.35/0.17	0.00/0.00	0.03/0.01	0.02/0.01	0.03/0.01	0.07/0.03
IG+FZ	B	B	–	0.08/0.03	0.00/0.00	0.39/0.19	0.01/0.01	0.01/0.00	0.12/0.05	0.48/0.23	0.00/0.00	0.30/0.14
S2006	N	A	N	–	0.00/0.00	0.005/0.02	0.20/0.09	0.00/0.00	0.01/0.00	0.00/0.00	0.01/0.00	0.00/0.00
HM1971	N	N	N	N	–	0.00/0.00	0.07/0.04	0.00/0.00	0.00/0.00	0.00/0.00	0.24/0.09	0.00/0.00
T2008	N	B	B	N	N	–	0.02/0.01	0.00/0.00	0.20/0.08	0.06/0.03	0.01/0.00	0.79/0.39
BC2002	N	B	N	B	N	N	–	0.00/0.00	0.00/0.00	0.00/0.00	0.12/0.04	0.00/0.00
H1999	B	N	N	N	N	N	N	–	0.05/0.03	0.19/0.09	0.00/0.00	0.00/0.00
B1973	C	N	N	N	N	B	N	N	–	0.15/0.07	0.00/0.00	0.18/0.06
K2004	B	N	B	N	N	N	N	N	N	–	0.00/0.00	0.06/0.02
M1978	N	N	N	N	C	N	C	N	N	N	–	0.00/0.00
K1995	N	N	B	N	N	A	N	N	B	N	N	–

Note. Results of the common mean tests performed by Palencia-Ortas et al. (2011) are provided in the lower triangle of the table. Test results are classified according to the scheme of McFadden and McElhinny (1990) and are taken directly from Table 4 of Palencia-Ortas et al. (2011). The upper triangle of the table contains B/E^* results for each pole-pole comparison.

3.1. A 200 Ma Paleomagnetic Pole for Africa

Motivated by a disagreement between different APWPs for the 200 Ma configuration of Pangaea, Palencia-Ortas et al. (2011) estimated paleomagnetic poles from the Ighrem and Fom Zguid dykes in Morocco. Their final analysis included 188 samples from 23 sites across the Ighrem and Fom Zguid dykes, which are part of the Central Atlantic Magmatic Province. Palencia-Ortas et al. (2011) assessed the fidelity of measured paleomagnetic directions based on demagnetization behavior and standard field tests. Paleomagnetic directions were transformed into VGPs, which were concluded to be Fisher (1953) distributed based on quantile-quantile plots (Fisher et al., 1987) and averaged to provide individual poles for the Ighrem (IG) and Fom Zguid (FZ) dykes and a combined pole (IG+FZ). Palencia-Ortas et al. (2011) then utilized a series of common mean tests to compare a collection of paleomagnetic poles and African APWPs (Table 1). Results of the common mean tests are represented using the quality classification scheme of McFadden and McElhinny (1990), where positive tests (interpreted as indistinguishable mean directions) are graded

“A,” “B,” “C,” or “Indeterminate,” which represents a sequence of decreasing reliability. Cases of failed tests (interpreted as different mean directions) are given a “Negative” classification (Table 2).

Calculation of Bhattacharyya (1943) coefficients and Bayes errors for the pole comparisons of Palencia-Ortas et al. (2011) demonstrates broad consistency with the common mean test classifications (Figure 3; Table 2). Higher-quality test results typically have higher B and E^* values, which demonstrates greater pole similarity. Similarly, lower quality tests and negative results are associated with reduced B and E^* values. This is to be expected, but it is important to stress that cutoff values of B and E^* corresponding to different common mean test classifications do not exist. The null hypothesis testing paradigm of the common mean test and the information-theoretic measures presented here are fundamentally different and attempting to unify these approaches is inappropriate (Burnham & Anderson, 2002). We do not provide an ad hoc classification scheme to categorize different values of B and E^* . Rather, we view the metrics as providing quantitative continuously varying evidence that may be interpreted according to the question being asked.

Figure 3. Values of B and E^* for the pole-pole comparisons performed by Palencia-Ortas et al. (2011). Points are coded according to their McFadden and McElhinny (1990) common mean test classification as given by Palencia-Ortas et al. (2011). Detailed results of this comparison are given in Table 2.

Figure 4. (a) Comparison of poles FZ (red) and S2006 (blue), represented by their mean directions (square symbols) and their corresponding α_{95} circles (lines). The black line plotted through the pole mean directions corresponds to a great circle along which the pdf profiles in (b) are plotted (centered on the mean of FZ). (c) Comparison of poles IG+FZ (red) and K1995 (blue), including pdf profiles (d) plotted along a great circle centered on the mean of IG+FZ. (e) Comparison of poles HM1971 (red) and M1978 (blue) including pdf profiles (f) plotted along a great circle centered on the mean of HM1971. Details of the poles used in this figure are provided in Tables 1.

We have selected specific pole comparison examples from Palencia-Ortas et al. (2011) to demonstrate the performance of B and E^* . The first example compares the FZ pole of Palencia-Ortas et al. (2011) with the S2006 pole from the Fom Zguid dyke (Silva et al., 2006). A common mean test applied to these poles results in an “A” classification; visual inspection of the poles (Figures 4a and 4b) demonstrates their high level of overlap. The similarity of the poles is quantified as $B = 0.80$ and $E^* = 0.39$. The second example compares the combined IG+FZ pole of Palencia-Ortas et al. (2011) with the K1995 pole from the Zarzaitine Formation in Algeria reported by Kies et al. (1995). The center of the K1995 pole resides within the A_{95} of the IG+FZ pole and the corresponding common mean test result received a “B” classification. Visual inspection (Figures 4c and 4d) suggests that overlap of the pole distributions is limited and is quantified as $B = 0.30$ and $E^* = 0.14$.

Figure 5. (a) The Irish Midlands paleomagnetic pole of Wilkinson et al. (2017); triangular symbol and white A_{95} , compared to the European APWP (square symbols and green A_{95} for each pole) of Torsvik et al. (2012). APWP ages are indicated in Ma. (b) Use of the Kullback and Leibler (1951) divergence to compare the Wilkinson et al. (2017) pole to individual poles in the APWP, where the minimum value occurs at 310 Ma.

The final example (Figures 4e and 4f) compares pole M1978 from the Argana red beds in Morocco (Martin et al., 1978) to pole HM1971 from the Foum Zguid dyke (Hailwood & Mitchell, 1971). M1978 has a large A_{95} , which almost entirely encloses the A_{95} circle of HM1971. Following the interpretational framework of Acton and Kettles (1996), the M1978 and HM1971 poles would be ruled indistinguishable. This conclusion would be supported by a passed common mean test, with “C” classification. As with earlier examples, visual inspection of the poles suggests that although they are similar in some regions, there are larger regions where they appear to be dissimilar. Quantitative comparison of M1978 and HM1971 yields $B = 0.24$ and $E^* = 0.09$, which raises concerns if these poles are ruled as “indistinguishable” using existing approaches. As discussed, we do not attempt to use B and E^* to make a binary decision that directions are “indistinguishable” or “distinguishable.” Reducing quantitative information to a “yes” or “no” outcome is inappropriate in a probabilistic setting. Rather, we encourage the reporting of similarity metrics and the formulation of interpretations based on the quantitative information they provide.

3.2. Dating Irish Regional Remagnetization

In a study of Irish Carboniferous carbonates, Wilkinson et al. (2017) tested the hypothesis that characteristic remanent magnetization (ChRM) directions from sediment-hosted Zn-Pb ores can provide age control for the ore-forming process. Previous paleomagnetic studies had indicated that ores of the Irish Midland Zn-Pb ore field ranged from the early Carboniferous to early Permian (Pannalal et al., 2008a; Pannalal et al., 2008b; Symons et al., 2007). This broad span of paleomagnetic ages, however, contrasts with geological constraints and with results from other dating techniques, which yield ages restricted to the early Carboniferous. Paleomagnetic samples were collected across the Irish Midlands from rocks that are distal to the Zn-Pb mineralization, but of an equivalent age to rocks in the ore host area. ChRM directions from the sampled unmineralized rocks were combined to provide a mean pole position that was found to be consistent with published poles for mineralized and unmineralized zones of the Irish Zn-Pb ore deposits. Wilkinson et al. (2017) state that their mean pole position is “close” to the 310 Ma pole of the European APWP (Torsvik et al., 2012) and hypothesized that the recorded paleomagnetic directions correspond to a remagnetization of older rocks rather than to a mineralization event (Figure 5a; Table 3). This hypothesis is supported by additional independent constraints, and it was concluded that the paleomagnetic dates correspond to a later orogenic overprint.

The Kullback and Leibler (1951) divergence provides a quantitative framework for comparing the mean pole position of Wilkinson et al. (2017) to European APWP reference poles (Torsvik et al., 2012) to assess any ambiguity in their association to the 310 Ma pole (Table 3). Calculation of the Kullback and Leibler (1951) divergence (equation 18) is straightforward (Figure 5b). Our proposed approach provides quantitative confirmation of the comparison made by Wilkinson et al. (2017), where the divergence between the 310 Ma

Table 3
Paleomagnetic poles employed in Fig. 5

Age [Ma]	Plat [°]	Plon [°]	K	R	Study
270	334.8	-51.0	109.9	22.80	Torsvik et al. (2012)
280	342.0	-45.6	78.6	38.52	Torsvik et al. (2012)
290	342.6	-43.1	70.5	59.16	Torsvik et al. (2012)
300	341.2	-42.4	57.8	39.32	Torsvik et al. (2012)
310	336.5	-38.3	39.5	13.67	Torsvik et al. (2012)
320	331.0	-25.6	57.6	5.91	Torsvik et al. (2012)
330	331.1	-17.7	102.2	6.94	Torsvik et al. (2012)
340	336.7	-15.8	255.1	4.98	Torsvik et al. (2012)
NA	332.1	-36.8	62.6	8.81	Wilkinson et al. (2017)

Note. The poles of Torsvik et al. (2012) make up the APWP for Laurussia/Laurasia and include a correction factor for inclination shallowing (see Torsvik et al. (2012) for details). The estimated pole of Wilkinson et al. (2017) does not have an independent age (NA = not available).

pole in the European APWP and their new pole is minimized ($D_{KL}(p, q) = 1.2$). Although this is a simple example, it demonstrates use of the Kullback and Leibler (1951) divergence to compare quantitatively an observed paleomagnetic pole to a reference APWP for dating and for identifying potential remagnetization.

4. Conclusions

An ability to compare poles quantitatively is crucial to paleomagnetism. Existing statistical frameworks for comparing poles are structured to provide binary outcomes where two poles are either deemed indistinguishable or distinguishable. Empirical rules have been developed around these frameworks to compare mean directions based on the overlap of their confidence regions. The information provided by overlapping confidence regions is limited and does not consider fully the nature of paleomagnetic poles, which are best considered as probability distributions. As we have shown, binary decisions based on overlap of α_{95} (or A_{95}) circles can result in inappropriate and contradictory outcomes concerning the relationships between paleomagnetic poles.

We propose three information-theoretic metrics that provide continuous measures of the similarity between paleomagnetic poles while accounting for the uncertainty that is expressed by their probability distributions. Similarity can be measured using the Bhattacharyya (1943) coefficient, which quantifies the overlap of two probability distributions, or in a probabilistic manner using the Bayes error (Cover & Thomas, 2006). The Kullback and Leibler (1951) divergence quantifies the dissimilarity of an observed pole to a reference pole. We have derived simple expressions to calculate the proposed metrics for Fisher (1953) distributions, which can be applied directly to paleomagnetic poles. By design, these measures do not give “yes” or “no” answers but rather provide a quantitative framework for comparing paleomagnetic poles. Two case studies demonstrate how these metrics can be employed in paleomagnetic reconstructions that depend on an ability to compare paleomagnetic poles in a quantitative fashion.

Appendix A: Bhattacharyya (1943) Coefficient for Two Fisher (1953) Distributions

Nielsen (2011) and Nielsen (2013) provided a framework to derive the Bhattacharyya (1943) coefficient for the exponential family of distributions (of which the Fisher (1953) distribution is a member). In the specific case of the Bhattacharyya (1943) coefficient, the Jensen divergence (Rao, 1982) between two exponential distributions, p and q , is given by

$$J_F(p : q) = \frac{F(p)}{2} + \frac{F(q)}{2} - F\left(\frac{p}{2} + \frac{q}{2}\right), \quad (\text{A1})$$

where F is the lognormalizer term of the exponential distribution under consideration. For the Fisher (1953) distribution, the lognormalizer term is given by (Mardia & Jupp, 2000):

$$F = \log \left(\frac{\sinh(\kappa)}{\kappa} \right). \quad (\text{A2})$$

Substitution of equation (A2) into equation A1 for two Fisher (1953) distributions with means of μ_p and μ_q and precisions κ_p and κ_q yields (Česić et al., 2016)

$$J_F(p : q) = \frac{1}{2} \log \left(\frac{\sinh(\kappa_p)}{\kappa_p} \right) + \frac{1}{2} \log \left(\frac{\sinh(\kappa_q)}{\kappa_q} \right) - \log \left(\frac{\sinh(\kappa_{pq})}{\kappa_{pq}} \right), \quad (\text{A3})$$

where

$$\kappa_{pq} = \left\| \frac{\mu_p \kappa_p}{2} + \frac{\mu_q \kappa_q}{2} \right\|. \quad (\text{A4})$$

Based on the form of the Jensen divergence in equation (A1), the Bhattacharyya (1943) coefficient, B , between the two distributions, p and q , is given by (Nielsen, 2011):

$$B(p : q) = \exp(-J_F(p : q)). \quad (\text{A5})$$

Substitution of equation (A3) into equation (A5) provides the final expression of the Bhattacharyya (1943) coefficient for two Fisher (1953) distributions (equation (7) in the main text):

$$B(p : q) = \frac{\sinh(\kappa_{pq})}{\kappa_{pq}} \sqrt{\frac{\kappa_p \kappa_q}{\sinh(\kappa_p) \sinh(\kappa_q)}}. \quad (\text{A6})$$

Appendix B: Bayes Error for Two Fisher (1953) Distributions

Following Nielsen (2011) and Nielsen (2014), a priori probabilities must be defined to represent the probability that x belongs to distribution p or distribution q , before x is observed. These prior probabilities, w , sum to one and are defined as

$$w_p = \Pr(p) > 0, \text{ and} \quad (\text{B1})$$

$$w_q = \Pr(q) = 1 - w_p. \quad (\text{B2})$$

The distribution-specific probabilities of observing a given x conditionally from either p or q are given by

$$p_p(x) = \Pr(x|p), \text{ and} \quad (\text{B3})$$

$$p_q(x) = \Pr(x|q), \quad (\text{B4})$$

which when combined with the a priori probabilities yields the probability of observing x :

$$p(x) = w_p p_p(x) + w_q p_q(x). \quad (\text{B5})$$

The Bayes (1763) rule provides an approach to calculate the probability that a given observation originated from a specific distribution:

$$\Pr(p|x) = \frac{w_p p_p(x)}{p(x)}, \text{ and} \quad (\text{B6})$$

$$\Pr(q|x) = \frac{w_q p_q(x)}{p(x)}, \quad (\text{B7})$$

which defines the Bayesian decision rule where

x is classified as originating from p if $w_p p_p(x) > w_q p_q(x)$, and
 x is classified as originating from q if $w_q p_q(x) > w_p p_p(x)$.

Beyond this probabilistic classification decision, it is possible to consider the probability that a classification error was made. The probability of a classification error, $\Pr(\text{Error})$, for the above decision rule can be obtained by integrating with respect to x :

$$\Pr(\text{Error}) = \int p(x)\Pr(\text{Error}|x) dx, \quad (\text{B8})$$

where $\Pr(\text{Error}|x)$ represents the probabilities of the two possible ways in which misclassification could have occurred. Specifically,

$$\Pr(\text{Error}|x) \begin{cases} \Pr(p|x) & \text{if } x \text{ was incorrectly classified as originating from } q, \\ \Pr(q|x) & \text{if } x \text{ was incorrectly classified as originating from } p. \end{cases} \quad (\text{B9})$$

Referring to equation (B8), the average probability of a misclassification error for the Bayesian decision rule defines the Bayes error, which is given by

$$E^* = \int \min(\Pr(p|x), \Pr(q|x))p(x)dx. \quad (\text{B10})$$

The Bayes error cannot be determined readily, but an upper limit is provided by the Chernoff (1952) bound:

$$E^* \leq w_p^\alpha w_q^{1-\alpha} \int p^\alpha(x)q^{1-\alpha}(x)\delta x. \quad (\text{B11})$$

For ease of notation we adopt the Chernoff (1952) α -coefficient, which is given by

$$C_\alpha(p : q) = \int p^\alpha(x)q^{1-\alpha}(x)\delta x, \quad (\text{B12})$$

where α lies in the interval (0,1).

In Appendix A, the framework of Nielsen (2011) and Nielsen (2013) was used to relate a specific form of the Jensen divergence between two exponential distributions, p and q , to the Bhattacharyya (1943) coefficient. Comparison of equations (6) and (B12) indicates that the Bhattacharyya (1943) coefficient is a specific case of the Chernoff (1952) α -coefficient where $\alpha = 0.5$, that is, $B(p : q) = C_{\frac{1}{2}}(p : q)$. The Jensen divergence can be written in a general form for $0 < \alpha < 1$ as

$$J_F^\alpha(p : q) = \alpha F(p) + (1 - \alpha)F(q) - F(\alpha p + (1 - \alpha)q), \quad (\text{B13})$$

where F is the lognormalizer term in equation (A2). Substitution of equation (A2) into equation (B13) for two Fisher (1953) distributions with means of μ_p and μ_q , and precisions κ_p and κ_q yields

$$J_F^\alpha(p : q) = \alpha \log \left(\frac{\sinh(\kappa_p)}{\kappa_p} \right) + (1 - \alpha) \log \left(\frac{\sinh(\kappa_q)}{\kappa_q} \right) - \log \left(\frac{\sinh(\kappa_{pq})}{\kappa_{pq}} \right), \quad (\text{B14})$$

where

$$\kappa_{pq} = \|\alpha \mu_p \kappa_p + (1 - \alpha) \mu_q \kappa_q\|. \quad (\text{B15})$$

The Chernoff (1952) α -coefficient is obtained from the Jensen divergence as (Nielsen, 2014)

$$C_\alpha(p : q) = \exp(-J_F^\alpha(p : q)), \quad (\text{B16})$$

and substitution of equation (B14) into equation (B16) yields

$$C_\alpha(p : q) = \left[\frac{\sinh(\kappa_p)}{\kappa_p} \right]^{-\alpha} \left[\frac{\sinh(\kappa_q)}{\kappa_q} \right]^{\alpha-1} \left[\frac{\sinh(\kappa_{pq})}{\kappa_{pq}} \right]. \quad (\text{B17})$$

From equation (B11), the lowest value achievable for the upper bound of the Bayes error occurs at the α value that yields the minimum of $C_\alpha(p : q)$. Specifically,

$$C_\alpha^*(p : q) = \min_{\alpha \in (0,1)} \int p^\alpha(x)q^{1-\alpha}(x)\delta x. \quad (\text{B18})$$

Therefore, the best achievable misclassification error, E^* , is given by

$$E^* \leq w_1^\alpha w_2^{(1-\alpha)} C_\alpha^*(p : q). \quad (\text{B19})$$

To provide a probabilistic measure for the similarity of two Fisher (1953) distributions, we set the priors (equations (B1) and (B2)) to be equal, that is, $w_p = w_q = 0.5$; therefore,

$$E^* \leq \frac{C_{\alpha}^*(p : q)}{2}. \quad (\text{B20})$$

Appendix C: Kullback and Leibler (1951) Divergence Between Two Fisher (1953) Distributions

The derivation of the Kullback and Leibler (1951) divergence, $D_{\text{KL}}(p, q)$, for Fisher (1953) distributions is from Česić et al. (2016) and is provided here for completeness with a modified nomenclature and some additional steps to aid exposition. The Kullback and Leibler (1951) divergence is given by

$$D_{\text{KL}}(p, q) = \int p(x) \log \left(\frac{p(x)}{q(x)} \right) dx, \quad (\text{C1})$$

where p is a reference distribution and q is a distribution with which we wish to compare it.

A version of equation (C1) for the specific case of Fisher (1953) distributions can be derived from the relationship between the Kullback and Leibler (1951) and Bregman (1967) divergences, B_F , which is given by

$$B_F(q, p) = D_{\text{KL}}(p, q). \quad (\text{C2})$$

Employing the lognormalizer definition in equation (A2), the Bregman (1967) divergence is

$$B_F(q, p) = F_q - F_p - E[p] \cdot (q - p), \quad (\text{C3})$$

where $E[p]$ indicates the expectation of p . Mardia and Jupp (2000) give the expectation of a Fisher (1953) distribution as

$$\frac{1}{\tanh(\kappa)} - \frac{1}{\kappa}. \quad (\text{C4})$$

Substitution of equations (A2) and (C4) into equation (C3) yields (Česić et al., 2016):

$$D_{\text{KL}}(p, q) = \log \left[\frac{\kappa_p \sinh(\kappa_q)}{\kappa_q \sinh(\kappa_p)} \right] - \left(\frac{1}{\tanh(\kappa_p)} - \frac{1}{\kappa_p} \right) \mu_p^T (\kappa_q \mu_q - \kappa_p \mu_p). \quad (\text{C5})$$

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