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Calculating uncertainties on predictions of palaeoprecipitation from the magnetic properties of soils

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ABSTRACT

Quantitative predictions of past climate states based on calibrated proxy data are key to the reconstruction of palaeoenvironments and are essential for climate model validation. Magnetic climofunctions have been used to make predictions concerning past climates based on soil magnetic mineral assemblages. For example, detailed time series of Quaternary mean annual precipitation and palaeoprecipitation gradients across wide geographic regions have been predicted from the rock magnetic properties of Chinese loess and palaeosol units. Quantitative prediction requires full assessment of the uncertainties associated with predictions. However, little attention has been given to this important aspect of climofunction prediction. We present an analysis of an ensemble of published rock magnetic climofunctions and estimate the uncertainty of the associated predictions. We find that existing climofunctions have associated uncertainties that are so large that their subsequent predictions are effectively invalid. Thus, palaeoprecipitation reconstructions must be treated with extreme caution. In the future climofunctions that are constrained geologically through the inclusion of theoretical models of soil development may provide predictions with lower uncertainties.

1. Introduction

Numerous studies have demonstrated a relationship between climate and the magnetic properties of soils (see Orgeira et al. (2011) and Liu et al. (2012) for recent reviews). Different mechanisms, such as magnetic mineral formation during natural fires (Le Borgne, 1960; Kletetschka and Banerjee, 1995) and mixing of magnetic and non-magnetic sediments (Kukla et al., 1988; Porter et al., 2001), have been proposed to explain this relationship. It is now widely agreed, however, that the inorganic formation of secondary ferrimagnetic minerals during pedogenesis is responsible for the magnetic enhancement of soils (Maher and Taylor, 1988; Zhou et al., 1990; Maher and Thompson, 1991; Zheng et al., 1991). A link therefore exists between the climate parameters (e.g., precipitation, evaporation and ambient temperature variations) that influence soil formation and the properties of pedogenically enhanced magnetic mineral assemblages. Soil formation is, however, a complex process and the mechanisms that control the formation and destruction of magnetic minerals during pedogenesis remain a matter of debate (Orgeira et al., 2011; Liu et al., 2012).

Studies of links between magnetic properties and soil formation go beyond solely attempting to understand pedogenic processes. By quantifying the relationship between modern climate parameters and carefully selected magnetic properties of recent soils, it may be possible to develop a calibrated transfer function with which to make quantitative palaeoclimate predictions. Such magnetic "climofunctions" were pioneered by Maher et al. (1994), who considered the relationship between magnetic susceptibility and rainfall for loess–palaeosol sequences of northwest China. To isolate the portion of the magnetic mineral assemblage attributable to soil formation, Maher et al. (1994) used the pedogenic magnetic susceptibility (χ_{ped}), which is simply the difference between the magnetic susceptibility (χ) of pristine parent material (loess) and pedogenically enhanced subsoil. By comparing χ_{ped} of 9 modern soils from the Chinese Loess Plateau with meteorological data, Maher et al. (1994) showed that the logarithm of χ_{ped} correlates strongly with mean annual precipitation (MAP), whilst other factors, such as temperature and the time required for soil development, are of secondary importance. By assuming that this relationship does not vary with time, the derived climofunction was applied to ancient soils to make quantitative predictions of past rainfall levels and precipitation gradients across the Chinese Loess Plateau (Maher et al., 1994; Maher and Thompson, 1995; Maher and Hu, 2006).

Subsequent studies have adopted the magnetic climofunction concept of Maher et al. (1994) and have investigated the relationship between the magnetic properties of modern soils and the rainfall/temperature regime in which they developed. Some studies have used less discriminative magnetic properties, such as bulk magnetic susceptibility (Balsam et al., 2011), whilst others have developed specific parameters to quantify the abundance of fine-grained ferrimagnetic minerals that are characteristic of pedogenesis (Geiss and Zanner, 2006; Geiss et al., 2008). Irrespective of their differences in approach, the motivation behind these studies is to make quantitative predictions of past climate states based on climofunctions derived

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from the magnetic properties of modern soils. Limited geological consideration has been given to the form of the climofunctions. Instead, empirical model selection has been adopted by identifying magnetic parameters that exhibit a strong correlation with rainfall and temperature values.

Quantitative prediction of past climate states has involved determination of a regression-based calibration that links magnetic properties of modern soils to MAP or mean annual temperature (MAT) (Maher et al., 1994, 2002; Han et al., 1996; Geiss et al., 2008; Balsam et al., 2011). The calibration can then be inverted to determine a climofunction with which the magnetic properties of ancient soils provide a basis to make predictions of the environmental conditions under which a soil formed. The quality of empirical climofunctions is most often assessed using the coefficient of determination (r^2) between a given magnetic parameter and MAP or MAT. Given that the aim of climofunction development is to produce quantitative predictions, the r^2 statistic is difficult to interpret. For example, if a study quotes a predicted MAP of 600 mm/yr obtained from a climofunction with $r^2 = 0.7$, the uncertainty on the predicted MAP is not apparent in mm/yr. Some studies have attempted to quantify uncertainties associated with predictions made from empirical climofunctions. Maher and Hu (2006) and Balsam et al. (2011) presented errors in mm/yr calculated from the estimated quality of the regression-based calibration. These authors did not, however, consider additional uncertainties that arise when making predictions for samples that were not included in the original calibration data set.

The aim of this study is to demonstrate an approach with which the uncertainty associated with climofunction predictions can be quantified. Through the use of so-called discrimination intervals (Lieberman et al., 1967), the predictive power of a given climofunction can be judged. As was the case in the original cited studies, we focus on a statistical analysis that does not take into account geological constraints. The key issue is that quantification of uncertainties associated with climofunctions is essential if meaningful comparisons between predicted climate states are to be made.

2. Materials and methods

We analyse here a number of published climofunctions. These climofunctions all aim to predict MAP and are considered in sequence according to the complexity of the magnetic parameter used. As mentioned above, we do not consider the appropriateness of a given magnetic parameter to predict past rainfall levels. We focus instead on the empirical predictive power that is claimed to be associated with each climofunction in the respective cited studies.

Two data sets are taken from Balsam et al. (2011), who considered the relationship between the logarithm of χ in modern soils and MAP. The first data set is composed of data from Mali ($n = 38$), whilst the second data set comprises the western subtransect ($n = 19$) subset of the Mali data.

Maher et al. 1(994) developed a climofunction for the Chinese Loess Plateau ($n = 9$) to predict MAP from the logarithm of χ_{ped}. This work was later extended by Maher et al. (2002) to include additional soils from the Chinese Loess Plateau ($n = 31$, Porter et al. (2001)) and the Russian steppe ($n = 22$). From a statistical analysis, Maher et al. (2002) demonstrated that their models that relate MAP and χ_{ped} in Chinese and Russian soils match closely.

A study of modern loessic soils ($n = 76$) from the midwestern United States by Geiss et al. (2008) related linearly the magnetic enhancement of soil horizons (quantified by the ratio of susceptibility of anhysteretic remanent magnetisation to isothermal remanent magnetisation, χ_{ARM}/IRM) to MAP. A statistical analysis of χ_{ARM}/IRM revealed that it was a better predictor of regional MAP than any other previously studied magnetic parameter (Geiss et al., 2008).

Proxy calibration is assessed here for all of the selected data sets using the same form of climofunction used by the authors of the original studies (e.g., linear, log-linear). On the basis of these calibration models the power of a given magnetic parameter to predict MAP is then assessed using discrimination intervals (Lieberman et al., 1967).

2.1. Proxy calibration

Climofunction estimation is based on a process of inverse calibration, which allows predictions of an independent variable on the basis of a dependent variable (Osborne, 1991). In such calibration problems it is essential to consider if the derived climofunction will be used only once (i.e., to predict palaeoprecipitation from a single sample) or repeatedly (i.e., multiple palaeoprecipitation predictions from a collection of samples). It is reasonable to assume that after a climofunction is developed it will be used repeatedly to make numerous predictions of palaeoprecipitation at single or multiple locations as a function of time (Maher and Thompson, 1995). We therefore employ the approach of Lieberman et al. (1967) where the number of predictions to be made on the basis of an inverse calibration is considered to be arbitrarily large.

For n calibration data points included in the development of a climofunction, it is assumed that the dependent parameter, y, can be related to the independent parameter, x, by the linear regression model:

$$y = a + bx + \epsilon, \tag{1}$$

where ϵ represents a collection of error terms. The ordinary least-squares estimator of the regression coefficients is given by:

$$b = \frac{\sum(x-\bar{x})(y-\bar{y})}{\sum(x-\bar{x})^2} \quad \text{and} \quad a = \bar{y} - b\bar{x}. \tag{2}$$

Predictions of y for the independent parameter values in x are then given by:

$$\hat{y} = a + bx. \tag{3}$$

The misfit between the data (y) and the regression predictions ($\hat{y}$) can be quantified by the *estimated residual variance*:

$$s^2 = \frac{\sum(y-\hat{y})^2}{n-2}. \tag{4}$$

The relationship between x and y obtained from the n calibration data points forms a climofunction from which numerous predictions of x will be made on the basis of y. This relationship is, however, only an estimate of the true relationship because it is based on a statistical sample of n points rather than the entire population. Given this limitation, it is essential to assess the uncertainty associated with the estimated regression line. Working and Hotelling (1929) showed how a confidence band for the location of the true regression line (i.e., that of the entire population) can be determined across the range of the data. This band is based on the estimated regression line and is constructed in a point-wise manner. For example, at the point x_a the confidence band is:

$$\hat{y}_a \pm \left\{2F_{(1-\alpha;2,n-2)}\right\}^{\frac{1}{2}} s\left(\frac{1}{n} + \frac{(x_a-\bar{x})^2}{\sum(x-\bar{x})^2}\right)^{\frac{1}{2}}, \tag{5}$$

where $F_{(1-\alpha;2,n-2)}$ is the value of a F distribution with $(2, n-2)$ degrees of freedom at the $1-\alpha$ level. For a given value of α there is a $1-\alpha$ probability that the confidence band contains the true regression line for the population.

A second source of uncertainty originates from the ability of the parameter y to make predictions of x. A non-zero value of s^2