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A theory of palaeoclimate reconstruction

Mengmeng Liu[1], Iain Colin Prentice[1], Cajo ter Braak[2], and Sandy Harrison[3]
[1]Imperial College London, Ascot, Berkshire, United Kingdom of Great Britain and Northern Ireland
[2]Wageningen University & Research, Wageningen, Netherlands
[3]University of Reading, Reading, United Kingdom of Great Britain and Northern Ireland

Past climate states can be used to test climate models for present-day changes and future responses. Past states can be reconstructed from fossil assemblages, and WA-PLS (weighted averaging–partial least squares) is one of the most widely used statistical methods to do this. However, WA-PLS has a marked bias. Whatever biotic indicator is being used, reconstructed climate values are artificially compressed and biased towards the centre of the range used for calibration.

Here we developed an improvement of the method, derived rigorously from theory. It makes three assumptions:

a) the theoretical abundance of each taxon follows a Gaussian (unimodal) curve with respect to each climate variable considered;

b) the abundances of taxa are compositional data, so they sum to unity and follow a multinomial distribution;

c) the best estimate of the climate value at the site to be reconstructed maximizes the log-likelihood function – in other words, it minimizes the difference between theoretical and actual abundances as assessed by the likelihood criterion.

The best estimate of the climate value is approximated by a tolerance-weighted version of the weighted average in which the abundances of taxa are weighted by the inverse square of their tolerances (a measure of the range of environments in which a taxon is found). WA-PLS thus corresponds to the special case when all taxon tolerances are equal. The fact that this special case is far from reality generally is part of the the cause of the “compression and bias”. The new method can be applied using the existing functions for WA-PLS in the R package rioja. We show that it greatly reduces the compression bias in reconstructions based on a large modern pollen data set from Europe, northern Eurasia and the Middle East.