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Invited review

Quantitative reconstructions in palaeolimnology: new paradigm or sick science?

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ABSTRACT

Quantitative reconstructions from biological proxies have revolutionised palaeolimnology but the methodology is not without problems. The most important of these result from attempts to reconstruct non-causal environmental variables and from the effects of secondary variables. Non-causal variables act as surrogates for often unknown or unquantified ecological factors and the method assumes that these relationships are invariant in space and time. This assumption is almost never met and examples of diatom models for water depth and summer temperature demonstrate how violation leads to spurious and misleading reconstructions. In addition, comparison of published species optima indicate that a number of models have little or no predictive power outside their current spatial setting. Finally, experiments using simulated training sets of known properties demonstrate how changes in secondary "nuisance" variables can lead to large, consistent, and interpretable trends in a reconstruction that are completely spurious and independent of any real change in the reconstructed variable. These problems pervade many quantitative reconstructions in palaeolimnology and other disciplines. Palaeoecologists must give greater attention to what can and cannot be reconstructed and explicitly address the dangers of reconstructing surrogate and confounded variables if our reconstructions are to remain credible.

1. Introduction

It is not an overstatement to say that quantitative reconstructions from biological proxies using so-called "transfer functions" have revolutionised palaeolimnology. The methodology was originally used to quantify the impact of recent acidification and eutrophication on lakes using diatoms (e.g. Renberg and Hellberg, 1982; Charles and Smol, 1988; Birks et al., 1990a; Bennion et al., 1996) but has since been used to reconstruct a wide range of variables using a number of different proxies, and plays an increasingly important role in palaeolimnology, especially in studies of past climate change (e.g. Samartin et al., 2012) and in the identification of reference conditions for lake management (e.g. Bennion et al., 2004). There are a number of reviews that describe the rationale, numerical techniques, and assumptions of the approach (Birks, 1995; Ter Braak, 1995; Birks et al., 2010; Juggins and Birks, 2012). These and other recent papers have also identified serious problems and limitations, either in reconstructing particular variables (e.g. temperature: Anderson, 2000; Battarbee et al., 2002; Brodersen and Anderson, 2002; Velle et al., 2010, or nutrients: Fritz et al., 1993; Arnett et al., 2012), in applications to particular systems (e.g. shallow lakes: Sayer, 2001), or with particular training-set designs, such as within-lake (e.g. Cwynar et al., 2012) or other spatially dependent calibrations (Telford and Birks, 2005, 2009; Belyea, 2007; Velle et al., 2012). It is not my intention here to review the pros and cons of individual numerical methods, proxies or environmental variables. Instead, I use a small number of examples of real and simulated data to demonstrate that these problems are more widespread and the result of violating two of the basic assumptions of the approach.

These assumptions were first elaborated by Imbrie and Kipp (1971) and Imbrie and Webb (1981) and refined by Birks et al. (1990a, 2010) and Birks (1995). They are:

1. The taxa in the modern training-set are systematically related to the environment in which they live.
2. The environmental variable(s) to be reconstructed is, or is linearly related to, an ecologically important determinant in the system of interest.
3. The taxa in the training-set are the same biological entities as in the fossil data and their ecological responses to the environmental variable(s) of interest have not changed over the time represented by the fossil assemblage.
4. The mathematical methods adequately model the biological responses to the environmental variable(s) of interest and

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yield numerical models that allow accurate and unbiased reconstructions.

5. Environmental variables other than the one of interest have negligible influence, or their joint distribution with the environmental variable does not change with time.

Assumption 1 essentially follows from assumption 2. Assumption 3 invokes the principles of uniformitarianism and space-for-time substitution. Birks (1995) and Juggins and Birks (2012) discuss criteria for assessing assumption 4. Assumptions 2 and 5 are critical but rarely challenged. I will show that by ignoring these assumptions palaeolimnologists have developed predictive models with little predictive power that lead to misleading reconstructions. The title of this paper was prompted by an article by the ecologist Daniel Simberloff in which he bemoaned the state of ecology for, in part, a reliance on untested models "… as remote from biological reality as are faith-healers" (Simberloff, 1980). I will show that a number of quantitative reconstructions in palaeolimnology are open to the same criticism and argue that palaeolimnologists must pay far more attention the consequences of violating assumptions 2 and 5 if our reconstructions are to remain credible.

2. Are we reconstructing ecologically important variables?

In palaeolimnology, quantitative reconstructions using diatoms and chironomids have been developed for a wide range of environmental variables. Early models attempted to quantify long-observed relationships between organisms and pH and salinity (e.g. Battarbee, 1984; Fritz et al., 1991) but since then the range of reconstructed variables has been greatly expanded to include nutrients, dissolved organic carbon, various heavy metals, water depth and various climatic and hydrological variables including summer temperature, ice and snow cover, wind activity, stream flow and hydroperiod (see Appendix A for list and references). These variables are chosen either *a priori* and the training set designed to capture variation along the variable of interest, or *post hoc*, after a variable is found to be statistically correlated to taxon distribution in subsequent analyses. For some variables there may be some experimental or other data demonstrating a physiological response (e.g. diatoms and nutrients: Kilham et al., 1986) or a long history of observational data that suggests a direct ecological effect (e.g. diatoms and pH: Hustedt, 1937–1939). In many cases the ecological basis for the reconstruction is poorly understood and is seldom explicitly addressed. Indeed, assumption 2 only actually requires a correlation, not a causal effect. Consequently, most quantitative reconstructions are justified by demonstrating a significant statistical relationship rather than a direct ecological effect, and by using some form of internal cross-validation to demonstrate the (hopefully high) predictive power of the model (Juggins and Birks, 2012).

2.1. Diatoms and water depth

Fig. 1 illustrates the above procedure and its limitations using an example of diatoms and water depth from Denmark. The training set consists of 67 surface-sediment samples and associated water chemistry and other environmental data sampled from a range of

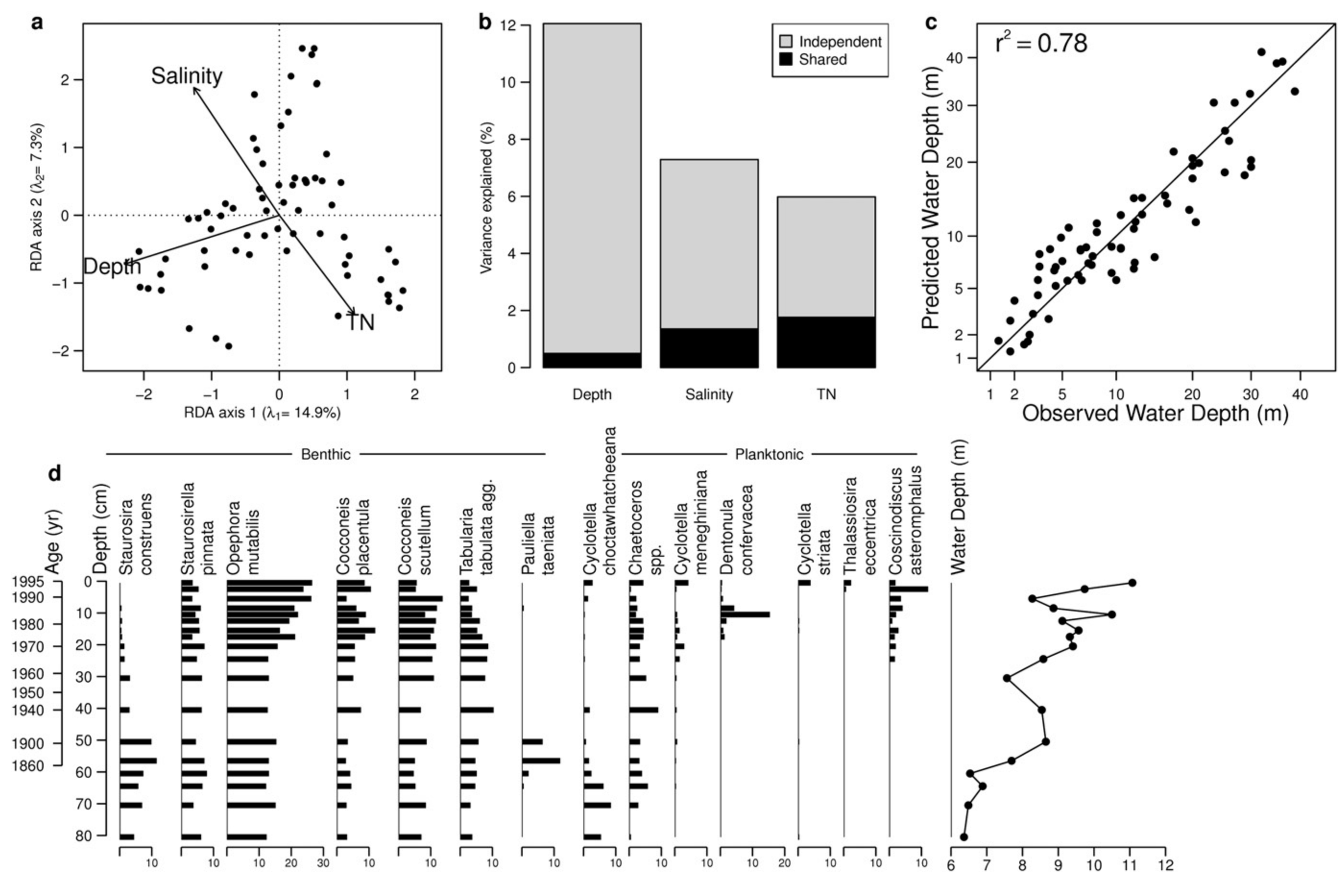

Fig. 1. Analysis of the Danish coastal dataset showing (a) RDA ordination biplot with sites and selected environmental variables for the training set, (b) variance partitioning of the training-set diatom data showing the independent and shared components of variance explained by selected environmental variables, (c) relationship between observed and predicted water depth under leave-one-out cross validation, and (d) diatom stratigraphy and water depth reconstruction for Roskilde Fjord. Fractions of variance in (b) are adjusted for the number of explanatory variables using the method described in Peres-Neto et al. (2006).