Quaternary Science Reviews 88 (2014) 69–81

Contents lists available at ScienceDirect

Quaternary Science Reviews

journal homepage: www.elsevier.com/locate/quascirev

Reconstructing palaeoclimatic variables from fossil pollen using boosted regression trees: comparison and synthesis with other quantitative reconstruction methods

J. Sakari Salonen [a,*], Miska Luoto [a], Teija Alenius [b,c], Maija Heikkilä [d], Heikki Seppä [a], Richard J. Telford [e,f], H. John B. Birks [e,f,g,h]

[a] Department of Geosciences and Geography, PO Box 64, 00014 University of Helsinki, Helsinki, Finland
[b] Department of Philosophy, History, Culture and Art Studies, PO Box 59, 00014 University of Helsinki, Helsinki, Finland
[c] Department of Archaeology, 20014 University of Turku, Turku, Finland
[d] Department of Environmental Sciences, ECRU, 00014 University of Helsinki, Helsinki, Finland
[e] Department of Biology, University of Bergen, PO Box 7083, N-5020 Bergen, Norway
[f] Bjerknes Centre for Climate Research, Allégaten 55, N-5007 Bergen, Norway
[g] Environmental Change Research Centre, University College London, London WC1E 6BT, UK
[h] School of Geography and the Environment, University of Oxford, Oxford OX1 3QY, UK

ARTICLE INFO

Article history:
Received 3 July 2013
Received in revised form
13 January 2014
Accepted 18 January 2014
Available online 11 February 2014

Keywords:
Holocene
Lateglacial
Northern Europe
Weighted averaging
Modern-analogue technique

ABSTRACT

We test and analyse a new calibration method, boosted regression trees (BRTs) in palaeoclimatic reconstructions based on fossil pollen assemblages. We apply BRTs to multiple Holocene and Lateglacial pollen sequences from northern Europe, and compare their performance with two commonly-used calibration methods: weighted averaging regression (WA) and the modern-analogue technique (MAT). Using these calibration methods and fossil pollen data, we present synthetic reconstructions of Holocene summer temperature, winter temperature, and water balance changes in northern Europe. Highly consistent trends are found for summer temperature, with a distinct Holocene thermal maximum at ca 8000–4000 cal. a BP, with a mean T_{jja} anomaly of ca +0.7 °C at 6 ka compared to 0.5 ka. We were unable to reconstruct reliably winter temperature or water balance, due to the confounding effects of summer temperature and the great between-reconstruction variability. We find BRTs to be a promising tool for quantitative reconstructions from palaeoenvironmental proxy data. BRTs show good performance in cross-validations compared with WA and MAT, can model a variety of taxon response types, find relevant predictors and incorporate interactions between predictors, and show some robustness with non-analogue fossil assemblages.

1. Introduction

1.1. Quantitative reconstruction methods: an overview

Quantitative reconstructions based on fossil biological proxies are a major source of information about long-term variability of climate. Since the early 20th century, quantitative palaeoclimatic reconstructions have been based on fossil data using the classical indicator-species method. In recent decades, many new approaches have been developed to derive quantitative reconstructions from Quaternary microfossil assemblages (Birks and Seppä, 2010; Birks et al., 2010; Juggins and Birks, 2012). So-called multivariate calibration functions (or transfer functions), based on regression methods such as weighted averaging regression and calibration (two-way WA; Birks et al., 1990) or weighted averaging-partial least squares regression and calibration (WA-PLS; ter Braak and Juggins, 1993), can be viewed as multivariate extensions of the classical indicator-species approach, adapted to microfossils for which reliable percentage data of taxon abundances are generally available (Birks et al., 2010). In another major approach, the modern-analogue technique (MAT; Overpeck et al., 1985; Simpson, 2012) past climates are reconstructed based on the modern conditions at sites with modern taxon assemblages most similar to the fossil assemblage. Other, less frequently used reconstruction techniques include response surfaces (e.g., Bartlein et al., 1986; Huntley et al., 1993; Gonzales et al., 2009), artificial neural networks (ANNs; e.g., Peyron et al., 1998, 2005; Tarasov et al., 1999a,b), Bayesian approaches (e.g., Vasko et al., 2000; Korhola et al., 2002; Haslett

* Corresponding author.
E-mail address: sakari.salonen@helsinki.fi (J.S. Salonen).

0277-3791/$ – see front matter © 2014 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.quascirev.2014.01.011

et al., 2006; Salonen et al., 2012a), and the so-called model-inversion approach (e.g., Guiot et al., 2000; Garreta et al., 2010). Comparison of these approaches and testing their robustness in different reconstruction scenarios remains a major challenge in modern quantitative palaeoclimatology.

1.2. Boosted regression trees in ecology and palaeoecology

Here we test a new technique, the boosted regression tree (BRT) as a palaeoclimatic calibration and reconstruction tool with fossil pollen assemblage data. The BRT is a state-of-the-art type of regression, representing an ensemble machine-learning method that estimates the relationship between a response variable and its predictors with no *a priori* specification of an underlying response model (De'ath, 2007; Elith et al., 2008). BRTs draw on insights and techniques from both classical statistical and machine-learning traditions. In BRTs, great numbers of simple regression-tree models (De'ath and Fabricius, 2000) are combined to produce a final model optimised for prediction, using cross-validation for model building. The tree models are combined using boosting, a numerical optimisation technique for minimising a loss function (such as deviance) by adding at each step a new model that best reduces the loss function (Ridgeway, 1999; Elith et al., 2008). Boosting methods have been applied, for example, in hydrology (Snelder et al., 2009), soil science (Brown et al., 2006), and ecology (Elith et al., 2006, 2008; le Roux et al., 2013a).

Despite the recent proliferation of BRTs in modern ecology and their success in modelling modern environment–taxon relationships, BRTs are only starting to be used in palaeoecological or palaeoclimatological studies (for a review see Simpson and Birks, 2012). Recent studies have used BRTs to analyse the ecological responses in palaeoecological calibration data-sets, using modern taxon assemblages and contemporary climate or other environmental data (Simpson and Birks, 2012; Zhao et al., 2012; Salonen et al., 2012b). Goring et al. (2010) present pollen–climate calibrations using random forests (Breiman, 2001), a related machine-learning method based on combining multiple tree models. BRTs have several general strengths that encourage their use in palaeoclimatic reconstructions (Simpson and Birks, 2012; Salonen et al., 2012b). *First*, there is increasing empirical evidence that boosting is one of the most useful and robust modelling approaches currently available for complex multivariate data (Elith et al., 2006; Leathwick et al., 2006; Marmion et al., 2009; Heikkinen et al., 2012). *Second*, BRTs automatically include interactions between predictors and are capable of modelling complex non-linear functions. *Third*, variable importance can be estimated, which is an advantage in exploratory analysis and when the variables need to be ranked according to their numerical contributions to the final model (Friedman, 2001; Elith et al., 2008).

1.3. Outline of this study

Here we test BRTs in palaeoclimatic reconstruction, based on northern European Late-Quaternary fossil pollen data. This paper is a follow-up to Salonen et al. (2012b), where we used BRTs to analyse pollen–climatic responses in modern pollen–climate calibration data, and found BRTs highly successful in modelling relationships between different climatic parameters and pollen taxa. Here we "turn around" or invert the BRT method, to reconstruct palaeoclimatic parameter values from fossil pollen assemblages. Three climatic parameters are reconstructed: mean summer temperature (June-to-August mean, T_{jja}), mean winter temperature (December-to-February mean, T_{djf}), and water balance (*WAB*). Reconstructions are presented from six previously published Holocene and Lateglacial fossil pollen sequences, using the North European modern calibration data of Salonen et al. (2012b). The BRT reconstructions are compared with reconstructions prepared with two well-established methods: WA and MAT. We focus on three specific goals:

- We demonstrate and test BRTs as a palaeoenvironmental reconstruction technique based on fossil proxy data, and assess their strengths and weaknesses compared to traditional reconstruction methods based on fitting parametric response models (i.e., WA regression) or based on analogue-matching (i.e., MAT). We hypothesise that given the theoretical strengths and the demonstrated suitability to modelling pollen–climate relationships (Salonen et al., 2012b), BRTs should perform robustly and reliably in reconstruction of climatic parameters from fossil pollen samples, compared with WA and MAT.
- We evaluate the robustness of these reconstructions (Juggins, 2013a) by testing the independent contribution of each climatic parameter in the modern calibration data, by cross-validation tests using the modern calibration data, by testing the statistical significance of the reconstructions (Telford and Birks, 2011), and by analysing the repeatability of the reconstructions as the calibration method or the fossil data-set is changed.
- We present a multi-method and multi-site synthesis of Holocene T_{jja}, T_{djf}, and *WAB* changes in Northern Europe, based on the prepared reconstructions.

2. Materials and methods

2.1. Calibration and fossil data-sets

We use a North European pollen–climate calibration set, described in detail by Salonen et al. (2012b). This calibration data-set consists of 583 modern pollen samples (Fig. 1A) and modern climate data based on the WorldClim 30-arc-second grids (Hijmans et al., 2005). T_{jja} and T_{djf} grids (Fig. 1B) were calculated as the means of the WorldClim monthly grids for the respective three months. A *WAB* grid (Fig. 1B) was calculated by summing the monthly differences between precipitation and potential evapotranspiration (*PET*), following Skov and Svenning (2004), with monthly *PET* calculated as

$$PET = 58.93 \times T_{bio}/12$$

where T_{bio} is the Holdridge biotemperature, defined as the annual mean of monthly temperatures with negative monthly values adjusted to zero (Holdridge, 1967; Lugo et al., 1999). Values for T_{jja}, T_{djf}, and *WAB* were extracted from the WorldClim-based grids for all modern pollen sites, as well as for the fossil sites (see below). The extracted T_{jja} and T_{djf} values and the temperature values used in the *WAB* calculation were lapse-rate corrected, to account for the difference between the real mapped elevation and the value of the WorldClim elevation grid at each pollen site (see Salonen et al., 2012b for details). These modern pollen samples will become available in the upcoming European Modern Pollen Database (EMPD; Davis et al., 2013).

We prepare reconstructions from six previously published fossil pollen sequences, located in northern Europe within the region of our calibration data (see Fig. 1A for locations and Table 1 for other details and references). Five of the sequences have early-Holocene basal ages, while one site that extends into the Lateglacial (Kurjanovas) was selected to test BRTs with fossil assemblages less analogous with modern ones. These sites have been selected as they have comparable pollen deposition environments with our calibration sites (small-to-medium sized lakes), and have high