Quantitative climate reconstructions based on fossil pollen: novel approaches to calibration, validation, and spatial data analysis

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ACADEMIC DISSERTATION
To be presented, with the permission of the Faculty of Science of the University of Helsinki, for public examination in lecture room D101, Physicum, Kumpula campus, on the 24th of May 2012, at 12 o’clock noon.
Cover photo: from left, a satellite view of northeast Europe in June (data source: NASA, http://visibleearth.nasa.gov), an ice-covered tundra lake in northeast European Russia, a steppe lake in the Central Russian Highland, and an early-Holocene fossil birch pollen grain.

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Abstract

Palaeoclimatic reconstructions from fossil proxies have provided important insights into the natural variability of climate in the late Quaternary. However, major challenges remain in ensuring the robustness of these reconstructions. Multiple factors may introduce variability and biases into the palaeoclimatic estimates. For example, quantitative reconstructions use diverse modern calibration data-sets, and a wide variety of numerical calibration methods. While the choice of calibration data-set and calibration method may significantly influence the reconstructions, the comparison and analysis of these data-sets and methods have received relatively little attention. Further challenges are presented by the validation of the prepared reconstructions and the identification of climatic variables which can be robustly reconstructed from a given proxy.

In this work, summer temperature reconstructions are prepared based on late-Quaternary pollen sequences from northern Finland and northern Russia, covering the Holocene and the early part of the last glacial period (Marine Isotope Stages 5d–c). The major aim of this work is to validate these reconstructions and to identify sources of bias in them. Reconstructions are prepared using a number of different calibration methods and calibration sets, to analyse the between-reconstruction variability introduced by the choice of calibration method and calibration set. In addition, novel regression tree methods are used to test the ecological significance of different climatic factors, with the aim of identifying parameters which could feasibly be reconstructed.

In the results, it is found that the choice of calibration method, calibration data-set, and fossil pollen sequence can all significantly affect the reconstruction. The problems in choosing calibration data are especially acute in pre-Holocene reconstructions, as it is difficult to find representative calibration data for reconstructions from non-analogue palaeoclimates which become increasingly common in the more distant past. First-order trends in the reconstructed palaeoclimates are found to be relatively robust. However, the degree of between-reconstruction variability stresses the importance of independent validation, and suggests that ensemble reconstructions using different methods and proxies should be increasingly relied on.

The analysis of climatic response in northern European modern pollen samples by regression trees suggests secondary climatic determinants such as winter temperature and continentality to have major ecological influence, in addition to summer temperature which has been the most commonly reconstructed variable in palaeoclimatic studies. This suggests the potential to reconstruct the secondary parameters from fossil pollen. However, validating the robustness of secondary-parameter reconstructions remains a major challenge for future studies.
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This thesis is based on the following publications:


The publications are referred to in the text by their roman numerals.
Authors’ contribution to the publications

I  The study was planned by J. S. Salonen, H. Seppä, V. J. Jones, and A. Self. The field work and sampling were conducted by V. J. Jones, A. Self, and H. Seppä. The laboratory work and analyses were performed by J. S. Salonen (pollen analysis and climate reconstructions), A. Self (lithostratigraphy and radiometric dating), M. Väliranta (macrofossil analysis), and H. Yang (radiometric dating). S. Kultti and M. Heikkilä contributed data. J. S. Salonen was responsible for preparing the manuscript, while all authors commented and contributed.

II  The study was planned by J. S. Salonen, L. Ilvonen, H. Seppä, and L. Holmström. The field work and sampling were conducted by J. S. Salonen, H. Seppä, A. Gaidamavicius, M. Stancikaite, and D. Subetto. The laboratory work was performed by J. S. Salonen and A. Gaidamavicius. The analyses were done by J. S. Salonen (pollen analysis and WA/WA-PLS reconstructions), L. Ilvonen (Bayesian reconstructions), R. J. Telford ($\ell$-block cross-validation and significance tests), and A. Gaidamavicius (pollen analysis). J. S. Salonen and L. Ilvonen were responsible for preparing the manuscript, while all authors commented and contributed.

III  The study was planned by all authors. The data were contributed by J. S. Salonen, H. Seppä, A. E. Bjune, and H. J. B. Birks. The analyses were done by J. S. Salonen (data synthesis, GIS analysis, and multivariate regression trees) and M. Luoto (boosted regression trees). J. S. Salonen and M. Luoto were responsible for preparing the manuscript, while all authors commented and contributed.

IV  The study was planned by all authors. All laboratory work and analyses were done by J. S. Salonen. All authors contributed data. J. S. Salonen was responsible for preparing the manuscript, while all authors commented and contributed.
Abbreviations

AMS  accelerator mass spectrometry
BRT  boosted regression tree
cal BP  calibrated radiocarbon years before present
DCA  detrended correspondence analysis
DEM  digital elevation model
GIS  geographic information system
HTM  Holocene thermal maximum
IPCC  Intergovernmental Panel on Climate Change
$K_G$  Gorczynski continentality index
LOESS  locally weighted scatterplot smoothing
MAT  modern-analogue technique
MIS  marine isotope stage
MRT  multivariate regression tree
NECS  North European Calibration Set
$P_{an}$  mean annual precipitation
RMSEP  root-mean-square error of prediction
$T_{an}$  mean annual temperature
$T_{djf}$  December-to-February mean temperature
$T_{mjju}$  May-to-August mean temperature
$T_{jja}$  June-to-August mean temperature
$T_{jul}$  July mean temperature
WA  weighted averaging
WAB  water balance
WA-PLS  weighted averaging-partial least squares

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Fig. 1  Map of fossil and calibration sites
Fig. 2  Holocene climate, treeline and permafrost changes in NE European Russia
1. Introduction

1.1. The need for palaeoclimatic data

Palaeoclimatology is the study of the past variability of Earth’s climate, in time periods of the distant past not covered by instrumental observations. Palaeoclimatic data are derived from a multitude of sources, including ice cores, tree rings, historical records, biological fossils, and various features of geological deposits (e.g., mineralogical or chemical composition). All of these sources can give indirect information (or, proxy data) about past climatic conditions when direct observations are not available.

Palaeoclimatology constitutes one key facet in the study of climate change, not only in terms of describing past variability, but also in assessing the present, and in anticipating future changes. Available instrumental records, which only rarely extend more than 200 years into the past, are insufficient to fully capture the centennial and millennial variability of climate. Consequently, palaeoclimatic data must be relied on to provide the long-term record of natural climatic variability (Bradley, 1999). Thereby palaeoclimatology establishes the baseline against which superimposed anthropogenic effects can be identified (Bradley, 1999; IPCC, 2007a; Kaufman et al., 2009).

Quantitative palaeoclimatic data have been in increasing demand due to their use in validating numerical climate models used to predict future climatic changes (Schmidt, 2010). In addition, the palaeoclimatic record provides an essential body of evidence of the sensitivities, rates of change, and the probability of rapid threshold responses the Earth’s environmental systems can exhibit under different climatic forcings (Alley et al., 2003; Overpeck and Cole, 2006).

1.2. Palaeoclimatic reconstruction from fossil biological proxies – ongoing challenges

Numerical reconstructions from fossil biological proxies are one of the major sources of quantitative palaeoclimatic data. Since the pioneering studies in the mid-19th century, palaeoclimate studies based on fossils preserved in peat and lake sediments have provided major insights into the natural variability of climate, especially during the Holocene and the late-glacial. The past few decades have seen the proliferation of numerical techniques used to infer quantitative palaeoclimate estimates from the variation in fossil assemblages (Birks and Seppä, 2010; Birks et al., 2010).

Despite these achievements, major challenges remain in improving the accuracy and validity of the reconstructions. First, the consistency of the modern calibration sets needs to be improved and tested, including the comparison of the available modern climate data-sets (Daly, 2006; Peterson and Nakazawa, 2008; Kriticos and Leriche, 2010), and exploring the principles of site selection for calibration sets and the effects of site selection on the reconstructions (Bjune et al., 2010; Velle et al., 2011).

Second, different reconstruction methods need to be further analysed to identify their strengths and weaknesses in different situations, such as specific spatial or temporal scales (e.g., Köster et al., 2000; Lotter et al., 2000; Birks, 2003; Guiot et al., 2009; Peyron et al., 2011).

Third, the robustness of reconstructions over longer timescales with climates less analogous with modern ones needs further assessment.
Fourth, multi-proxy studies are increasingly needed to provide data for the validation of reconstructions (Birks and Birks, 2003). Fifth, it has become increasingly clear that more rigorous climatological, biogeographic and ecological consideration needs to be given to which climatic parameters can realistically be reconstructed from each proxy (Birks et al., 2010; Telford and Birks, 2011a).

All of these factors may contribute to the variability seen in palaeoclimatic reconstructions. Critical analysis of these sources of bias and the relative strengths and weaknesses of different methods is thus vital, to establish which features in palaeoclimatic reconstructions are robust, and to ensure the policy-relevancy of palaeoclimate reconstruction studies (see also Telford and Birks, 2011a). Another persistent challenge in palaeoclimatology is the uneven distribution of available reconstructions in both space and time. Pre-Holocene periods and regions outside North America and northern/western Europe remain relatively sparsely sampled (e.g., Bartlein et al., 2011). This is due to, e.g., the lack of suitable depositional environments, erosion of deposits, obstacles to working in remote localities, and the difficulty of transferring established proxy–climate calibrations to environments different from those in which the calibration was originally done.

### 1.3. Aims of this study

In this work, new palaeoclimatic reconstructions are prepared from fossil pollen sequences from northern Finland and the relatively sparsely studied region of northeast European Russia, covering the Holocene (in Finland and Russia) and the early part of the last glaciation (in Finland). The reconstructions are prepared using a new north-European pollen–climate calibration set which is synthesised in this work. All fossil and calibration data-sets are integrated in GIS (geographic information system) with base maps, digital elevation models, and biogeographic and climatological data-sets for mapping, analysis and visualisation of the data.

Apart from preparing the calibration data-set and the reconstructions, a major aim of this study is the validation of palaeoclimatic reconstructions and identification of sources of bias, and testing new methods for these purposes. Several factors which could potentially contribute to reconstruction biases and variability between reconstructions are analysed. First, the effect of the calibration set size on the reconstructions is tested, to examine the largely unexplored problem of optimal spatial dimensions for a calibration set. Second, different calibration methods are tested and compared, to analyse the variability in reconstructions due to calibration model choice. Third, the influence of different climatic factors on pollen assemblage variability is analysed using novel regression tree methods, to assess which climatic features are ecologically significant and could thus potentially be reconstructed. Fourth, the extent to which calibrations based on modern climate and vegetation patterns can be relied on to produce reliable palaeoclimate estimates from the distant past is critically analysed.

By examining these possible sources of bias, the study aims to assess the reliability of palaeoclimatic reconstructions from fossil proxies, and to provide practical suggestions for improving the robustness of future reconstructions.
2. Materials and methods

2.1. Pollen–climate calibration data

In this work, 46 new calibration pollen samples were analysed from European Russia (Fig. 1). In the Russian reconstructions, these samples were combined with previously analysed samples from western Russia, Estonia and Lithuania, to produce northeast European calibration sets extending from the temperate mixed forest to the tundra (I, II). Later, the new samples were synthesised with previously analysed calibration sets from Fennoscandia (Seppä et al., 2004, 2005; Bjune et al., 2010) to produce a cohesive, 583-sample North European Calibration Set (NECS; III), spanning from the Atlantic coast of Norway to the Urals (Fig. 1).

The climate data for transfer function calibration are based on the WorldClim climate grids (Hijmans et al., 2005), interpolated at 30-arc-second resolution, and available for the monthly temperature and precipitation means. Based on the WorldClim monthly grids, grids for further parameters were calculated using ArcGIS Spatial Analyst, including temperature means for June-to-August \((T_{jja})\), May-to-August \((T_{mjja})\), December-to-February \((T_{djf})\), and annual \((T_{ann})\) periods, as well as mean annual precipitation \((P_{ann})\), water balance \((WAB;\) calculated as in Skov and Svenning, 2004), and continentality index \((K_G;\) Gorczynski, 1920, 1922). To correct possible errors due to insufficient spatial resolution in the climate grids, the temperature values for calibration sites were lapse-rate corrected based on the difference between the mapped elevation of the calibration site and the value of the DEM.
underlying the WorldClim interpolation.

To analyse the spatial patterns of the calibration data in relation to topographic, biogeographic, and climatic features of northern Europe, the calibration data set was imported into ArcInfo GIS software and overlain with a vector base map (imported from Generic Mapping Tools; Wessel and Smith, 1991, 1998), the WorldClim-based gridded climate datasets, a DEM (ETOPO1; Amante and Eakins, 2009), vegetation data (Olson et al., 2001), and other data layers. All data were transferred into a map projection with acceptable distortions in both area and shape over northern Europe (Lambert conformal conic projection, standard parallels 40°N and 70°N).

2.2. Analysis of the climate signal in modern pollen assemblages

GIS tools and regression trees (De’ath and Fabricius, 2000) were used to analyse the climatic response of taxa to different climatic parameters (III). Gridded pollen maps were interpolated for the most common pollen and spore taxa to visualise spatial patterns. Two varieties of regression trees were used to model the climatic signal in modern pollen assemblages.

Boosted regression trees (BRTs; Elith et al., 2008) were used to model the response of each taxon to $T_{\text{jas}}, T_{\text{djf}}, WAB$, and $K_G$. BRTs are a relatively recent statistical modelling tool which combines two algorithms: regression trees and boosting, a machine-learning method in which many simple models are combined to improve predictive accuracy. In BRTs boosting is used to produce a combined model from many simple regression trees models (Elith et al., 2008). BRTs were used to model the shape of response of each taxon to $T_{\text{jas}}, T_{\text{djf}}, WAB$, and $K_G$, as well as to estimate the relative influence of each of the four parameters on each taxon.

The climatic response of the modern pollen samples was also studied at assemblage level using multivariate regression trees (MRTs; De’ath, 2002). In this method, $T_{\text{jas}}, T_{\text{djf}}, WAB$, and $K_G$ were used as explanatory variables and all pollen types as response variables. MRTs were thus used as a clustering tool for the pollen samples in the modern climate space, with the clustering based on hierarchical binary splits. To analyse the spatial structure in the resultant MRT, the modern pollen samples were finally mapped in GIS according to their MRT terminal node membership.

2.3. Fossil pollen data

Reconstructions were prepared from five fossil pollen sequences (Fig. 1). Two of the sequences were first analysed in this work: Holocene sequences from Lake Kharinei (I), in northeast European Russia near the Arctic Urals, and from Lake Loitsana, Sokli, northern Finland (IV). Three previously analysed fossil pollen sequences were also used: Holocene sequences from Lake Tumbulovaty (Kultti et al., 2004) and Lake Llet-Ti (unpublished data, A. Klimaschewski) in northeast European Russia, and an early-Weichselian (Marine Isotope Stage (MIS) 5d–c) sequence from Sokli, northern Finland (Helmens et al., submitted).

The new Lake Kharinei and the Sokli Holocene core sequences were dated with AMS radiocarbon ($^{14}$C) dates from terrestrial plant macrofossils. The top of the Lake Kharinei sequence was additionally dated with lead ($^{210}$Pb). The $^{14}$C dates were calibrated using the IntCal09 calibration
curve (Reimer et al., 2009) in OxCal 4.1 software (Bronk Ramsey, 1995, 2009). Cubic-smooth-spline age-depth models were fitted to the calibrated dates using the method of Heegaard et al. (2005) in the R statistical software (R Development Core Team, 2009).

2.4. Palaeoclimatic reconstructions

Pollen-based summer temperature reconstructions (I, II, IV) were prepared using weighted averaging-partial least squares regression (WA-PLS; ter Braak and Juggins, 1993) transfer functions, calculated in the C2 software (Juggins, 2007). Calibration data-sets for transfer functions were selected from the calibration data presented in Fig. 1. Generally, subsets of 58–218 samples were selected, located around the fossil site, to represent the climate–vegetation relationships in the region surrounding the fossil site. In II and IV, two calibration sets were used in the reconstruction, to explore the effects of calibration set selection on reconstructions. In II, the second calibration set was a spatially restricted version of the base set, to study the effect of the gradient length represented in the calibration data. In IV, the base set surrounded the fossil site, while the second set was selected from a more continental climatic regime, in an attempt to improve the robustness of reconstructions from highly continental palaeoclimates.

In II, WA-PLS-based reconstructions were also compared with reconstructions based on simple weighted averaging regression (WA) and a Bayesian reconstruction method, to study the effect of calibration-model choice on the reconstructions. The Bayesian algorithm used here is Bummer, originally described by Vasko et al. (2000) and previously applied by Korhola et al. (2002).

2.5. Validation of palaeoclimatic reconstructions

Several methods were used to assess the robustness of the prepared reconstructions. First, the statistical performance of the used calibration model was evaluated by traditional leave-one-out cross-validation methods (I, II, IV). When diagnosing the differences found in reconstructions from different calibration methods (II), special attention was paid to biases shown by different methods in specific environmental types (see also Telford and Birks, 2011b). Second, to evaluate the role of spatial autocorrelation in inflating leave-one-out cross-validation performance, h-block cross-validation (Telford and Birks, 2009) was also performed (II). In this approach, nearby sites are left out in cross-validation to prevent predictions based on nearby sites which may have similar species assemblages for non-climatic reasons. Third, for independent validation of reconstructions, the pollen-based reconstructed palaeoclimates were compared with macrofossil-based minimum temperature estimates from the same core (I, II, IV; cf. Birks and Birks, 2003), as well as other published reconstructions from the same region (I, II). Fourth, the statistical significance of the reconstructions was tested (II, IV) using the method of Telford and Birks (2011a). In this method, redundancy analysis is used to test if the reconstruction of the chosen climatic variable explains more of the variance in the fossil data compared with reconstructions using random climate data (white noise). The reasoning is that if reconstruction of the chosen variable is ecologically feasible, the reconstruction should explain more of the fossil variance than reconstructions using random climate data. Fifth, the fit between the fossil data
and different calibration data-sets was tested using detrended correspondence analysis (DCA) and the squared-chord distance (Overpeck et al., 1985) between the fossil and calibration samples (IV). The assumption is that reconstructions are more likely to be robust if the calibration set includes samples with similar assemblages compared to the fossil samples.

3. Summary of original publications

3.1. Paper I

In I, WA-PLS-based summer temperature ($T_{mjja}$) reconstructions were prepared based on fossil pollen sequences from Lake Kharinei and Lake Tumbulovaty, located in the tundra of NE European Russia. The calibration set used in I included 58 samples from northern Russia. In addition, treeline dynamics in the region were analysed based on a plant macrofossil and stomata record from Lake Kharinei. The macrofossil record was additionally used to validate the pollen-based reconstructions.

The results suggest that the early-Holocene summer temperatures from 11,500 cal BP onwards were already slightly higher than at present, followed by a stable Holocene thermal maximum (HTM) at 8000–3500 cal BP when summer temperatures in the tundra were ca. 3°C above present-day values. A Picea forest surrounded Lake Kharinei during the HTM, reaching 150 km north of the present taiga limit. The HTM ended with a temperature drop at 3500–2500 cal BP associated with permafrost initiation in the region. Mixed spruce forest began to disappear around Lake Kharinei at ca. 3500 cal BP, with the last tree macrofossils recorded at ca. 2500 cal BP, suggesting that the present wide tundra zone in the NE European Russia formed during the last ca. 3500 years.

3.2. Paper II

In II, the focus was on comparing different calibration methods and different-sized calibration data-sets. To this end, summer temperature ($T_{mjja}$) reconstructions were prepared based on the Lake Kharinei pollen sequence using three different calibration methods: WA-PLS, WA, and the Bayesian method. In addition, to test the effect of calibration set size, all three calibration methods were run with two different calibration sets. The first set included 113 samples, consisting of all Russian, Estonian, and Lithuanian samples of NECS. The second set was a spatially restricted subset of the first set, including 58 samples (same as in I).

WA-PLS was found to outperform WA in leave-one-out cross-validation, probably because of smaller edge-effect biases at the ends of the calibration set gradient. The Bayesian-based calibration models showed further improved performance compared with WA-PLS. Additional $h$-block cross-validation showed spatial autocorrelation to have a relatively small effect on calibration model performance with all three methods. Comparison with independent climate proxies revealed, however, some clear biases in the Bayesian palaeotemperature reconstructions. The reasons for the biases in the Bayesian reconstructions remain uncertain. It is possible that the Bayesian method proved sensitive to spatial gaps in the calibration data-sets, causing biases in reconstructions from environments which
are poorly sampled in the calibration data. Thus the reconstruction biases would reflect limitations of the available calibration data. Alternatively, it is possible that the used prior parameters in the Bayesian algorithm may need to be revisited. As the selected prior parameters can significantly affect both Bayesian cross-validation performance and reconstructions, there is a clear need to further test Bayesian reconstructions in different geographic contexts and over different timescales, with special attention given to the selection of the most realistic priors in each reconstruction scenario.

Some smaller cross-validation biases were found with the smaller calibration data-set. This is likely because of complex, partially bimodal responses of several taxa along the longer temperature gradient. Such complex responses are ill-suited for calibration methods assuming unimodal responses to climate. This demonstrates the importance of analysis of taxon responses over different spatial scales when selecting calibration data-sets for reconstruction methods. In general, it is seen in II that statistically well-performing calibration methods may produce clearly differing palaeotemperature reconstructions, urging caution in the interpretation of reconstructions.

### 3.3. Paper III

In III, all the modern calibration samples used in this study (Fig. 1) were synthesised into a cohesive North European Calibration Set (NECS). As a pollen–climate calibration set, NECS is characterised by high taxonomic resolution (167 taxa) and homogenous taphonomy, as all pollen samples are from small-to-medium-sized lakes. Modern temperature values for the samples were derived from the WorldClim climate grids for numerous climatic parameters (see 2.1.).

Gridden pollen maps were interpolated for 15 common taxa. In addition, to assess the potential of NECS for the reconstruction of different climatic parameters, regression tree methods were used to analyse the effect on pollen composition and variability of four parameters: summer temperature ($T_{jja}$), winter temperature ($T_{djf}$), water balance ($WAB$), and continentality index ($K_G$). MRTs were used to analyse the variation in pollen assemblages in modern climate space. BRTs were used to analyse the relative influence of different climatic parameters on each taxon.

In BRT analysis, taxon responses to the four climatic parameters were found to be highly individualistic. While most taxa (65%) were most responsive to $T_{jja}$, other parameters were found to be either primary determinants or significant secondary determinants for many taxa. In analysis at the assemblage level using MRTs, significant variation was found in assemblages from similar $T_{jja}$ regimes, with distinct clusters of assemblages also identified along the $K_G$ gradient. Thus the results from BRTs and MRTs suggest that secondary climatic determinants like continentality and winter temperature may have major ecological influence on the vegetation and pollen assemblages in northern Europe. This further suggests the potential to reconstruct these secondary parameters from fossil pollen sequences. However, it is cautioned in III that confounding factors may make the validation of secondary-parameter reconstructions challenging. BRTs were found to be a highly effective multivariate method in describing and modelling modern climate–taxon relationships.
3.4. Paper IV

In IV, WA-PLS-based summer temperature ($T_{jul}$) reconstructions were prepared based on the Sokli sequence which extends from the Holocene into the early Weichselian glaciation (MIS 5d–c). The main focus was on examining the robustness of reconstructions over long, glacial–interglacial timescales. A key problem over long timescales is to find calibration data applicable to increasingly non-analogue climates of the past. To improve the robustness in highly continental palaeoclimates, $T_{jul}$ reconstructions were prepared using two calibration sets. The first calibration set was selected from eastern Fennoscandia, representing the modern-day continentality regime of Sokli, and the second from Russia, representing a higher-continentality regime. The robustness of the two reconstructions based on different calibration sets was assessed by estimating the compositional fit (using DCA and squared-chord distance) between the fossil samples and each of the two calibration data-sets. In addition, the two reconstructions were assessed by comparing them with independent, macrofossil-based reconstructions, and by performing the Telford and Birks (2011a) significance test.

In the results, it was found that the fossil samples fit the extra-regional, high-continentality calibration set better during the early Holocene and MIS 5d–c. Thus the approach of increasing the robustness of reconstruction with a second calibration set seems generally valid. However, especially in MIS 5d–c even the high-continentality calibration set fits the fossil samples poorly compared to the fit achieved in the mid and late Holocene. Also, during MIS 5d–c the reconstructions fail the Telford and Birks (2011a) significance test, while the Holocene reconstructions test as significant. These results highlight the problem of finding applicable calibration data for reconstructions of glacial palaeoclimates. However, some general features of the reconstructions were found relatively robust to the choice of calibration set. These robust features also showed significant fit with the independent, macrofossil-based reconstructions, suggesting that the choice of calibration data may not be critical for reconstruction of some general palaeoclimatic trends. It is further suggested in IV that this robustness over long timescales may be a general feature of methods based on estimating taxon-specific climate response models (e.g., WA/WA-PLS transfer functions, indicator species methods). However, in reconstruction from non-analogue palaeoclimates, the new methods based on inverting vegetation models may have considerable advantages over all traditional reconstruction methods.

4. Discussion

4.1. Holocene climate changes and environmental sensitivity in the treeline zone of NE European Russia

The arctic and subarctic region have become under increasing scrutiny in the assessment of modern climate change for two reasons (MacDonald, 2010). First, anthropogenic warming is expected to be especially strongly expressed in the northern regions. The arctic and subarctic regions have thus been considered “a canary in the coal mine” in the assessment of modern climate change (MacDonald, 2010). Second, possible
Figure 2. Holocene shifts in temperature, treeline and permafrost in NE European Russia. A) Reconstructed Mayto-August mean temperature ($T_{maj}$) based on pollen sequences from Lake Kharinei (I), Lake Tumbulovaty (Kultti et al., 2004), and Lake Llet-Ti (unpublished data, A. Klimaschewski), using a WA-PLS calibration model (I). Error bars show bootstrap-estimated standard errors. All reconstructions are expressed as deviations from the reconstruction-specific mean. A LOESS smoother (span 0.25, one robustifying iteration) is fitted to all points. B) Change in treeline and permafrost in 5000 cal BP compared to present. Green lines show the present-day northern limits of taiga (solid line) and forest tundra (dashed line) based on Rekacewicz (1998). Red lines show the estimated northern limits for 5000 cal BP based on vegetation reconstructions for 5000 cal BP from $^{14}$C-dated stratigraphic sequences (red symbols) and localities with tree megafossils dating to 6000–4000 cal BP (plus signs; Kremenetski et al., 1998; MacDonald et al., 2000). Presence of taiga is reconstructed at Lake Kharinei (site 7) based on abundant Picea stomata and macrofossils and high Picea pollen accumulation rates, while for the other sites the reconstructions are cited from literature. Current extent of permafrost (dashed blue lines; generalized from Mazhitova and Oberman, 2003) in the Usa river basin (highlighted) and a fossil site suggested as permafrost free at 5000 cal BP (blue triangle; Oksanen et al., 2001) are also shown. Names and references for the numbered sites: 1. Timan Ridge: Paus et al., 2003; 2. Ortino: Väliranta et al., 2003; 3. Llet-Ti: Väliranta et al., 2006; 4. Tumbulovaty: Kultti et al., 2004; 5. Khaipudurskaya Guba: Andreev and Klimanov, 2000; 6. Rogovaya: Oksanen et al., 2001; 7. Lake Kharinei: Paper I; 8. Cape Shpindler: Andreev et al., 2001; 9. Lyadhej-To: Andreev et al., 2005; 10. Baidaratskaya Guba: Andreev and Klimanov, 2000. Any uncalibrated $^{14}$C dates in the cited sources were calibrated using the IntCal09 calibration curve (Reimer et al., 2009) in OxCal 4.1 software (Bronk Ramsey, 1995, 2009).
positive net feedback due to northward treeline shift and associated changes in surface albedo may cause further regional and global warming (Foley et al., 1994, 2003; Betts, 2000; Chapin et al., 2005; Swann et al., 2010). A major geographic shift of the Eurasian arctic treeline is expected to occur due to anthropogenic warming, with the treeline projected to reach the Arctic Ocean coast over much of the region (ACIA, 2004; IPCC, 2007b).

To provide a palaeoclimatic viewpoint on the future projections, Holocene changes in temperature, vegetation and permafrost in NE European Russia are summarised in Fig. 2. In Fig. 2A an ensemble $T_{mjia}$ reconstruction is shown based on the fossil sequences on Lake Kharinei and Lake Tumbulovaty, as well as unpublished pollen data (A. Klimaschewski) from Lake Llet-Ti. Based on the reconstructions, the NE European tundra zone has seen a summer temperature fall of ca. 2.5°C since the HTM at ca. 8000–3500 cal BP (Fig. 2A). This estimate for the cooling since the HTM is likely to be relatively robust, as it agrees with results from several other studies in NE European Russia, using different climate proxies and calibration methods. A cooling of ca. 2–3°C has been suggested based on the geographical shift of vegetation and permafrost zones (Kremenetski et al., 2000; MacDonald et al., 2000; Oksanen et al., 2001; Kultti et al., 2003, 2004; Väliiranta et al., 2003), indicator species macrofossils (Kultti et al., 2004), and quantitative reconstructions based on pollen (Andreev and Klimanov, 2000; Andreev et al., 2005) and chironomids (Andreev et al., 2005). Fig. 2B summarises available fossil data on the mid-Holocene (5000 cal BP) treeline in the region, assembled from this work and from literature. The data points suggest a major southward displacement of the treeline zone by ca. 150 km during the late-Holocene cooling. The shift in treeline during the late Holocene was associated with a major southward expansion of the permafrost zone in northern Russia, measuring in hundreds of km while being widely variable between different regions (Kondratjeva et al., 1993). At a fossil site just south of the northern taiga limit at 5000 cal BP, no presence of permafrost is suggested at that time, while currently permafrost is widespread around the site (Fig. 2B; Oksanen et al., 2001).

Considering the magnitude of the treeline and permafrost shifts associated with the reconstructed temperature fall of 2.5°C, the weight of the fossil evidence suggests an alarming sensitivity of the Russian arctic treeline region environment under climatic warming. According to an IPCC multi-model ensemble projection (A1B emission scenario), European Russia around the Arctic circle is expected to see a summer surface air temperature ($T_{jja}$) rise of ca. 2.5–3°C by 2080–2099 AD (IPCC, 2007c), thus returning summer temperatures to the estimated HTM level. The projected rise in winter temperature ($T_{djf}$) is projected to be significantly larger, exceeding 7.5°C by 2080–2099 AD (IPCC, 2007c).

While the large treeline and permafrost shifts of the Holocene serve as a cautionary tale, there are numerous uncertainties in employing the HTM as an analogue for the future. First, the rates of treeline advance to be expected under climatic warming remain highly uncertain (Rupp et al., 2001; Chapin et al., 2005; Harsch et al., 2009; MacDonald, 2010). Also, precise quantification of past treeline and permafrost changes in climatologically
significant terms like permafrost volume, biomass, or canopy cover is unlikely to be achieved from fossil observations which are available from a limited number of sites. The sensitivity of the arctic treeline zone may be best explored with methods in which the fossil data are paired with modelling (cf. Anderson et al., 2006; Miller et al., 2008). In this approach, the magnitudes and rates of environmental change and the significance of different feedbacks under different climatic scenarios can be studied with coupled climate–vegetation models, while model–data comparisons for periods such as the HTM are used to tune the sensitivity and parametrization of the models.

Finally, while the projected late-21st century summer temperatures are similar with reconstructed HTM temperatures, the HTM may not be a close analogue for the future in terms of other seasons. While numerous fossil proxies document the past summer temperature changes in NE European Russia, as summarised above, only sparse data is available on palaeoclimatic variability in other seasons. While summer temperature is a major control on both permafrost active-layer depth and the Eurasian arctic treeline vegetation, the variation in both permafrost and treeline is likely partially determined by the full, year-around distributions of temperature and precipitation (MacDonald et al., 2008; Schuur et al., 2008). In terms of this full spectrum of seasonal climates, the possible anthropogenically warmed future in the northern Eurasian treeline zone is unlikely to be a close analogue of the HTM (MacDonald et al., 2008; MacDonald, 2010). Rather, the projected greater rise in winter temperature compared with summer temperature in the 21st century may continue and speed up the Holocene trend towards lower seasonality. This could take northern Eurasia towards a novel, low-seasonality climatic regime without a close analogue during the late Quaternary, causing unpredictable trajectories in the environmental conditions of the arctic treeline zone.

### 4.2. Robust and non-robust features – how reliable are the reconstructions?

In this work, many reconstructions of summer temperature have been prepared from the late-Quaternary pollen assemblages of northern Europe, including several different reconstructions from same lakes. In these reconstructions, the effects of many different methodological decisions on the inferred temperature curve have been tested, including the choice of calibration method (II), the choice of calibration data-set (II, IV), the effect of reconstructing from a different fossil series from the same region (Fig. 2; I). To summarise these reconstructions, relatively large between-reconstruction variability is seen. For example, a major feature of interest in the northern Russian reconstructions – the magnitude of late-Holocene cooling (see 4.1., above) – is not a robust feature in the reconstructions, but is affected significantly by the choice of calibration method (variation of 2°C in the magnitude of cooling; II) and the choice of lake in the same region (variation of 1.5°C; see individual reconstructions in Fig. 2) and to a lesser degree by the spatial extent of the calibration set (variation of 0.5°C; II).

The above discrepancies are noteworthy, as these reconstructions likely represent a relatively “easy” reconstruction scenario. For example, the reconstructions have a sound
ecological basis as the impact of growing season temperature on the northern Eurasian treeline vegetation is well established, the pollen samples have highly consistent taphonomy and limited anthropogenic effects, and the used calibration models have good predictive performance in cross-validation.

Some differences in the reconstructions are inevitable. In calibration models for fossil biological proxies, biases always remain in cross-validation, due to influence of other factors apart from the climatic variable being reconstructed. In Holocene reconstructions, even with the best-performing calibration models the root-mean-square of the cross-validation residuals invariably covers a significant part of the expected range of climatic variability. Typically, distinct patterns can be observed in the residuals, with the sign and magnitude of bias varying between different segments of the gradient. Furthermore, it is found that well-performing calibration models may have surprisingly large biases in specific environmental types, possibly significantly larger than the RMSEP (\( II \); see also Telford and Birks, 2011b).

As these residual patterns vary between methods, one method may produce systematically different temperatures from a specific vegetation type compared to another method, contributing to the differences seen in the reconstructions. For example, a method with a negative bias in the taiga and/or a positive bias in the tundra would reconstruct a significantly smaller temperature drop during the late-Holocene taiga–tundra transition (e.g., the WA model in \( II \)). When reconstructing from multiple sites in the same region, differences are typically seen the fossil pollen sequences due to, e.g., varying positions of the fossil sites along the vegetation zones, non-climatic variation in the regional vegetation, or local effects. The variable biases of the calibration methods in different environmental types and with different pollen assemblages then guarantee that the palaeoclimate curves will have different shapes between fossil sites.

Despite the major variability seen between reconstructions in this study, certain key features are found to be highly robust. Especially, all the northern Russian reconstructions show very similar HTM timing. In other studies synthesising pollen-based reconstructions, the first-order trends in reconstructed palaeoclimates have also proved highly robust to the choice of calibration method (e.g., Lotter et al., 2000; Klotz et al., 2003; Peyron et al., 2005, 2011; Brewer et al., 2008; Bartlein et al., 2011) and the choice of fossil sequence when using the same calibration method with multiple sites (e.g., Klotz et al., 2003; Seppä et al., 2009; Peyron et al., 2011). But considering the magnitude of between-reconstruction variability, it seems that any single reconstruction should not be interpreted in more than broad, qualitative terms (e.g., warmer vs. colder periods, periods of rapid vs. gradual change). For robust quantitative estimates of absolute temperature shifts, ensembles of reconstructions (Fig. 2; see also Davis et al., 2003; Brewer et al., 2008; Kaufman et al., 2009; Seppä et al., 2009; Bartlein et al., 2011) and coinciding lines of evidence from different proxies and calibration methods should be relied on (see 4.1., above).

While biases are inevitable in any reconstruction, there are also fundamental differences in the quantitative basis of different calibration methods (cf. Birks et al., 2010). For example, multivariate transfer
functions and indicator species methods employ taxon response models while MAT is based on analogue-matching of assemblages. Among methods based on taxon response models the assumed shape of response varies. Some methods consider taxon abundances while others only consider presence or absence of taxa. Different methods may exhibit varying sensitivity to taxa occurring at large vs. small abundances. Some methods may be more susceptible to calibration model over-fitting than others. New methods based on inverting vegetation models differ fundamentally from all traditional calibration methods, as model-inversion reconstructions are not based on observing modern climate and vegetation patterns.

Different methods are thus likely to be more robust in specific reconstructions scenarios, considering, e.g., the timescale and the likelihood of non-analogue assemblages (IV), considering the relative ecological influence of the reconstructed climatic parameter and the sensitivity thus required, and considering the characteristics of the available calibration data. Consequently, the analysis and comparison of different calibration methods remains a critical area of research.

4.3. Reconstructing seasonal changes for a dynamic view of late-Quaternary climates

In palaeoclimatic reconstructions from fossil proxies in the northern latitudes, the main focus has traditionally been on reconstructing changes in summer temperature, a likely major determinant of ecological variability in the region. Especially in pollen-based reconstructions using the modern-analogue technique (MAT), other variables like winter temperature or mean annual precipitation are also often reported, as any number of climatic parameters can be relatively easily attached to modern pollen samples for MAT-based inference of past values. The continuing, widespread limitation of reconstructions to summer temperature is unsatisfactory, as climatic variability in the northern hemisphere involves widespread changes in the full seasonal distributions of temperature and precipitation. The changes in the seasonal parameters do not necessarily correlate, as they are partially under independent forcings (seasonal insolation: Berger and Loutre, 1991; see also Jackson and Overpeck, 2000; Davis et al., 2003). Shifts in gradients other than summer temperature have been identified as major components in past climatic variability over Milankovitch timescales (e.g., Davis et al., 2003). Robust reconstructions of the seasonal distributions of temperature and precipitation would facilitate the analysis of the mechanisms of past climate change and the relative significance of different forcing factors. Reconstructions of seasonal differences would also shed light on the involved changes in atmospheric and oceanic circulation, providing a more dynamic view of palaeoclimatic variability. By extension, the reconstruction of atmospheric and oceanic dynamics under late-Quaternary climatic forcings might help elucidate the sensitivities involved.

The analysis of climatic response by regression trees (III) suggests that there is major variability in northern European pollen assemblages related to variables other than summer temperature. Substantial signal of secondary climatic factors is thus suggested. However, careful consideration must be given to possible confounding variables such as intercorrelated, non-climatic factors.
with possible ecological influence (Birks et al., 2010). Due to the likely presence of confounding variables, traditional cross-validation with modern samples cannot be relied on to identify parameters which can be reconstructed from a given proxy (see also Telford and Birks, 2005, 2009). Validating reconstructions of secondary parameters by other means such as statistical testing (Telford and Birks, 2011a), comparison to independent proxies, or, when possible, against instrumental data (Self et al., 2011) is thus vital. As discussed above, reconstructions of primary gradients have proven relatively robust to calibration model selection in terms of first-order palaeoclimatic trends, increasing the confidence in these reconstructions (cf. Birks et al., 2010). Whether such robustness can be achieved with secondary climatic determinants remains largely untested. The identification of ecologically significant secondary climatic parameters, assessing the suitability and sensitivity of different methods for reconstructing these parameters, and testing the robustness of the reconstructions are key challenges in future palaeoclimatic reconstructions.

5. Conclusions

- Pollen-based summer temperature reconstructions are found to show significant between-reconstruction variability with different calibration methods, different calibration sets, and different fossil sites. Contributing to these differences are factors such as the variable biases in different calibration methods, the inherent noisiness of fossil data-sets, and the inevitable non-climatic local and regional effects in fossil assemblages. These results emphasise the value of multi-proxy studies and ensemble reconstructions combining different calibration methods and fossil sites, to identify robust palaeoclimatic features.

- As the choice of calibration data is found to significantly affect the reconstructions, principles of calibration set selection require further analysis. The effects of the selection of modern climate data, calibration set sample size, spatial orientation, and spatial extent, and the applicability of modern calibration sets over long timescales have received relatively little attention in past studies. Assessment of these factors and their effects on reconstructions is vital to increase objectivity in calibration set selection.

- Over long glacial–interglacial timescales, the fossil samples and the modern calibration samples are found to become increasingly dissimilar through time, with especially poor fit during glacial times. This suggests an increasing likelihood of palaeoclimates without modern analogues. This presents major challenges to traditional calibration methods, as calibration sets may produce significantly biased reconstructions from palaeoclimatic regimes different from the climatic regime of the calibration data.

- Pollen-based summer temperature reconstructions of summer temperature in northeast European Russia show a long, steady HTM at around 8000–3500 cal BP, followed by a temperature fall of ca. 2.5°C to the present day. The cooling since the HTM was associated with significant environmental shifts, including treeline withdrawal of ca. 150 km and major permafrost aggradation, suggesting great sensitivity of the Eurasian arctic treeline zone under climatic warming.
Analysis of climate response in northern European modern pollen samples by regression trees suggests secondary climatic determinants such as winter temperature and continentality, in addition to summer temperature, to have major ecological influence. This suggests the potential to reconstruct these parameters from fossil pollen, but validating the robustness of secondary-parameter reconstructions remains a major challenge for future studies.

References


