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Near-infrared spectrometry (NIRS): a new tool for inferring past climatic changes from lake sediments

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Abstract: This study tests the hypothesis that lake sediments contain climate-related information that can be detected by near-infrared spectrometry (NIRS), and that NIRS can be used to infer past climatic changes from analysis of sediment cores. NIRS is a rapid and non-destructive technique that measures attributes of the chemical composition of organic materials. A training set of 76 lakes from northern Sweden, spanning a broad altitudinal gradient, was used to assess whether lake altitude and vegetation zones can be modelled from NIR spectra of surface sediments (0–1 cm) using partial least squares (PLS) regression and soft independent modelling of class analogies (SIMCA) classification. Lake altitude served as a surrogate variable reflecting differences in climatic conditions among sites. After spectral filtering using orthogonal signal correction (OSC), cross-validated predictions explained 86% of the variance in altitude and the prediction error (root mean square error) was 78 m, corresponding to 8.3% of the gradient (390–1250 m above sea level). To evaluate the significance of NIR spectral differences between surface sediments of lakes in different vegetation zones (mountain-birch forest, dwarf shrub and alpine heath), principal component analysis (PCA) models were developed separately for lakes in each vegetation zone. Multivariate classification analysis demonstrated that NIR spectra of surficial sediments differed between lakes located in different vegetation zones. A separate sediment data set from 56 lakes was used to assess sediment ageing effects on NIR signals. Marked similarities between NIR spectra in surface sediments (0–1 cm) and sediments from 1–2 cm depth indicated that degradation of organic material following sediment consolidation resulted in little loss or change of climate-related information. Finally, to assess the ability of NIRS methods to reconstruct past climatic changes over Holocene timescales, we applied the NIRS-altitude model to sediments in a core from a small mountain lake. Estimates of mean July air temperature based on the NIRS-altitude transfer function showed similar trends compared with inferences from chironomids, diatoms and pollen from the same core. Overall, the results indicate that changes in NIR spectra from lake sediments reflect differences in climate, and that NIRS models based on surface-sediment samples can be applied to sediment cores for retrospective analysis.

Key words: Near-infrared spectrometry, NIRS, climatic change, lake sediments, July temperature, northern Sweden, transfer function, Holocene.

Introduction

Concerns about global warming have focused increasing scientific attention on sedimentary records, and particularly on the opportunities they provide for quantifying past climates and climate variability. Lakes situated at ecotonal boundaries, such as the alpine tree-line, are of particular interest for climate reconstructions because small changes in climate can result in large changes

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in environmental conditions and biological communities (MacDonald *et al.*, 1993; Körner, 1998). Several techniques are available for inferring past climatic conditions from biological remains in sediments; for example, chironomids (Walker *et al.*, 1991), diatoms (Pienitz *et al.*, 1995; Lotter *et al.*, 1997), and pollen (Bartlein and Webb, 1985; Bartlein and Whitlock, 1993). Each of these techniques has their own advantages and limitations. As a consequence, there is a need for new, independent methods and multiproxy approaches to facilitate interpretation of palaeorecords and to improve our understanding of the dynamics of climatic change.

Near-infrared spectrometry (NIRS) is a rapid and non-destructive technique that measures attributes of the chemical composition of organic materials (Norris *et al.*, 1976; Osborne and Fearn, 1988; McClure, 1994; Bokobza, 1998). NIR is widely used in industry for process monitoring and quality control (Davis and Williams, 1997) and has found some ecological applications (Nilsson *et al.*, 1992; Foley *et al.*, 1998; McTiernan *et al.*, 1998). Previous applications of NIRS to lake sediments include: quantitative inferences of lake-water pH, total phosphorus concentration and total organic carbon concentration (Korsman *et al.*, 1992; Nilsson *et al.*, 1996); inferences of C, N, P and diatoms in lake sediments (Malley *et al.*, 1996; 1999); assessment of the origin and spatial variability of sediments (Korsman *et al.*, 1999); and assessment of sampling reproducibility and error estimation in NIRS calibration of lake sediments (Dåbakk *et al.*, 1999).

We hypothesize that lake sediments also contain climate-related information that can be detected using NIR spectrometry. This seems likely, since the composition of the sediments is determined by a variety of catchment and lake processes, of which many are directly or indirectly influenced by climate. In this first attempt to assess whether NIR spectrometry of lacustrine sediments has the potential to become a method for inferring past climatic conditions, we address the following three questions.

(1) Can relationships be established between NIR spectra of surface sediments (0–1 cm) and contemporary climate-related variables using partial least squares (PLS) modelling? A training set comprising 76 lakes was collected from the Swedish mountains, and two approaches were used to answer this question: (a) statistical modelling of lake altitude from NIR spectra; and (b) statistical modelling of catchment vegetation from NIR spectra. Lake altitude is used as a surrogate for climate data in this first test. For example, altitude and summer temperature are closely linked (Laaksonen, 1976), and summer temperature is very important for both limnic and terrestrial ecosystems and thus for the properties of the sediment. However, other factors that may affect temperature conditions at the lakes are exposure and geomorphological conditions. Further work should develop more reliable climate data. The training set spanned lakes from the mountain-birch forest (*Betula pubescens* ssp. *tortuosa* Led.), through the dwarf-shrub zone, and up into the alpine-heath zone. This zonation is well known to be driven by climate (Körner, 1998). It is likely that direct influx of organic matter from the terrestrial ecosystems to the sediment, or influences on the lake ecosystem from catchment vegetation and soils, may affect the sediment properties.

(2) If models between NIR spectra of surface sediments and contemporary climate data, or climate-related variables, can be established, are these models useful for retrospective analysis of climate using NIRS analysis of sediment cores? A potential problem is degradation of organic material at the sediment-water interface, and loss or change of climate signals during processes of diagenesis and consolidation of the sediment. We address this potential ageing-effect problem by comparing NIR spectra from the surface sediments (0–1 cm) with spectra from a lower horizon (1–2 cm) from 56 lakes. These two topmost centimetres typically represent approximately 10 and 20–30 years, respectively. It is assumed that differences in NIR spectra between these two levels mainly derive from changes in the chemical composition of the sediment due to microbial degradation and not from climate or vegetation change, since climate and vegetation have not changed significantly during the last few decades in the region (Holmgren and Tjus, 1996). Microbial degradation of complex organic material normally occurs according to a negative exponential function, i.e., most rapidly during the first months or years (see, for example, Ågren and Bosatta, 1996). If the degradation occurs over a period of years this would be reflected by differences in the NIR spectra between the 0–1 cm and 1–2 cm intervals. To the contrary, very similar NIR spectra from 0–1 and 1–2 cm respectively indicate that nearly all changes in the sediment composition, due to degradation, occur during the first months or years after deposition, i.e., most of the sediment from 0–1 cm is already chemically altered and therefore similar to the sediment from 1–2 cm.

(3) Finally, to test the predictive ability of the NIRS-altitude (temperature) model, we apply the NIRS-altitude model from the training data set to a sediment core from Lake Sjuodjijaure, and compare the results with past climate inferences obtained using chironomids, diatoms and pollen.

Study area

The training set (76 lakes) used to assess relationships between NIR spectra of surface sediments and lake-altitude and catchment vegetation, and a separate data set (56 lakes) used to investigate the potential ageing effect on NIR spectra, are from northern Sweden 64°00′–68°30′N. The lakes span a climatic gradient from 7°C to 12°C in mean July air temperature, and altitude from 390 to 1250 m above sea level. Precipitation ranges from 500 to 1900 mm per year with the highest precipitation at high-elevation sites (Alexandersson *et al.*, 1991). The lakes are mainly small (typically ~5 ha; range 0.5–130 ha), headwater lakes situated on similar bedrock (mainly granite and gneiss), and with maximum depth 2–30 m. There is a good correlation ($r = 0.94$) between mean July air temperature and altitude in Fennoscandia ($n = 612$ climate stations), with decreasing temperature with increasing altitude (Laaksonen, 1976).

Lake Sjuodjijaure (unofficial name, 67°22′N, 18°04′E), in which down-core reconstructions were applied, is a small (6 ha) headwater lake situated at 826 m a.s.l. and ~100 m above present tree-line in Sarek National Park. The lake is situated on granite and syenite rock and is an oligotrophic, slightly acidic (pH 6.3), clear-water lake.

Methods

Field and laboratory methods

Surface sediment samples (0–1 cm) for the 76-lake NIRS-altitude training set were collected during 1989–90 and 1996–97, whereas sediment samples for the assessment of diagenetic processes (0–1 cm and 1–2 cm) were collected from an additional 56 lakes during 1998. Sediment samples were collected from the deepest part of each lake using a gravity corer (HTH-Teknik, Vårvägen 37, SE-951 49 Luleå). The cores were extruded in the field and stored in the dark until placed in a freezer (–18°C) within a few days. Each lake was classified as located within one of three vegetation zones (mountain-birch forest, dwarf-shrub zone or alpine-heath zone) during field reconnaissance, based on the dominant vegetation in the catchment.

About 2 cm^3 of wet sediment was used for NIRS analysis. Samples were freeze-dried, ground in a mortar and stored at +4°C in a dessicator before analysing with a NIRS instrument. From

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Lake Sjuodjijaure, samples were taken at 5 cm intervals from the 255 cm long Holocene sequence. The samples were treated in the same way as samples in the training set. NIR spectra were recorded using a NIRSystems 6500 instrument (FOSS NIRSystems Inc., Silver Spring, MD, USA). The instrument measured diffuse reflectance (R) which was transformed to apparent absorbance values (A) according to A = log(1/R). Data were collected at 4 nm intervals between 400 and 2500 nm yielding 525 data points per sample.

Numerical analyses

Principal component analysis (PCA) (cf. Jackson, 1991) was used to get an overview of the spectral variability of the lakes and as a basis for outlier detection. Prior to PCA, spectral variation arising from varying effective pathlengths and particle size was removed using multiplicative signal correction (MSC) (Geladi *et al.*, 1985; Martens and Næs, 1989). Partial least square regression (PLS) (e.g., Martens and Næs, 1989) was used to develop a transfer function between NIR spectra of surface sediment (0–1 cm) and lake altitude. PLS is a multivariate regression method capable of handling the numerous correlated variables (absorbance values in the NIR spectra) by summarizing them into a few components that maximize covariance with the dependent variable. Prior to the PLS regression, we used orthogonal signal correction (OSC) (Wold *et al.*, 1998) as a spectral pretreatment to remove signals in the NIR spectra which were not related to lake altitude.

Classification of the lakes into vegetation zones, based on the information in the NIR spectra, was performed using a supervised multivariate classification technique (SIMCA) (Wold *et al.*, 1983). The class 'mountain birch' here refers to lakes with mountain birch in the drainage area; the class 'dwarf shrubs' refers to lakes where the main part of the drainage area is covered by dwarf birch (*Betula nana*), willows (*Salix* spp.) and heather vegetation (Ericaceae); and the class 'alpine heath' refers to lakes with sparse catchment vegetation (mainly lichens and mosses) and little or no soil. In this analysis, each class (i.e., lakes from the same vegetation zone) was modelled by a separate PCA. Lakes were then projected onto these PCA models and classified as belonging to one class, to no class or to more than one class. Finally, comparisons between classifications based on NIRS and classifications determined during field reconnaissance were visualized using Cooman plots (Wold *et al.*, 1983).

The number of significant components in PCA and PLS was assessed by cross-validation with ten groups. Root mean squared error of calibration (RMSEC) was used as an estimate of model error and root mean squared error of cross-validation (RMSECV) was used as an estimate of prediction error. RMSECV was calculated according to:

$$RMSECV = \sqrt{\frac{\sum_{i=1}^{I}(y_i - \hat{y}_i)^2}{I-1}}$$

where I is the number of lakes, y_i is the measured altitude for lake i, and $\hat{y}_i$ is the mean altitude for all lakes and $\hat{y}_i$ is the predicted altitude. RMSEC was calculated similarly, except that y is the best estimate and not the value predicted by the cross-validation procedure. The Unscrambler 6.11 software (CAMO ASA, Trondheim, Norway) was used for all multivariate data analysis, except OSC, which was performed using SIMCA-P 7.01 (Umetrics AB, SE-907 19 Umeå, Sweden).

In an attempt to assess differences between NIR spectra of sediments from depths of 0–1 cm and 1–2 cm, spectra were pretreated with OSC to remove information not related to sediment depth. In this analysis, partial least squares discriminant classification (PLS-DA: Wold *et al.*, 1983; Sjöström *et al.*, 1986) was applied to NIR spectra of the two sediment depths, using depth levels as discrete class indicators (specifically, the 0–1 cm samples were assigned a value of 0, whereas 1–2 cm samples were assigned a value of 1).

In order to compare the NIRS-inferred altitude in the down-core reconstruction from Lake Sjuodjijaure with mean July air temperatures inferred from available chironomid, diatom and pollen data, we converted NIRS-inferred altitude to NIRS-inferred mean July air temperature using the equation:

$$\textit{July temperature} = 9.8 - 0.0057(\textit{altitude} - 826)$$

where *9.8* is the present-day mean July air temperature for Lake Sjuodjijaure. This value was extrapolated and corrected for altitude from a nearby climate station. The value *0.0057* represents the altitudinal change in temperature per metre rise in elevation (Laaksonen, 1976). The term *altitude* is the inferred altitude from NIRS, whereas the term *826* is the altitude for Lake Sjuodjijaure according to a topographic map. The mean July air temperatures were inferred from: (a) chironomids using a weighted average (WA) model and inverse deshrinking on a 40-lake training set ($R^2_{\text{jack (=leave-one-out jack-knifing)}} = 0.44$, root mean square error of prediction (RMSEP) = 1.02°C (18.9% of gradient)); (b) diatoms using a weighted average partial least square (WA-PLS) model with three components on a 52-lake training set ($R^2_{\text{jack}} = 0.62$, RMSEP = 0.86°C (12.6% of gradient), Rosén *et al.*, 2000); (c) pollen using a WA model and inverse deshrinking on a 55-lake training set ($R^2_{\text{jack}} = 0.33$, RMSEP = 1.20°C (16.0% of gradient)). The climatic assessment of all results will be presented in a separate paper.

Results and discussion

A statistically significant relationship was observed between measured altitude and altitude inferred from NIR spectra of surface sediments (0–1 cm) in our 76-lake training set (Figure 1), with $R^2 = 0.88$, R^2_{cv}(cross-validated) = 0.86, RMSEC = 75 m (7.9% of gradient) and RMSECV = 78 m (8.3% of gradient).

Based on the SIMCA classification, NIR spectra of surficial sediments from most lakes situated within the alpine-heath vegetation zone could be distinguished from lakes within both the mountain-birch forest and the dwarf-shrub zone (Figure 2). Although the Cooman plot shows a separation of sites between mountain-birch forests and dwarf-shrub zones, statistical classi-

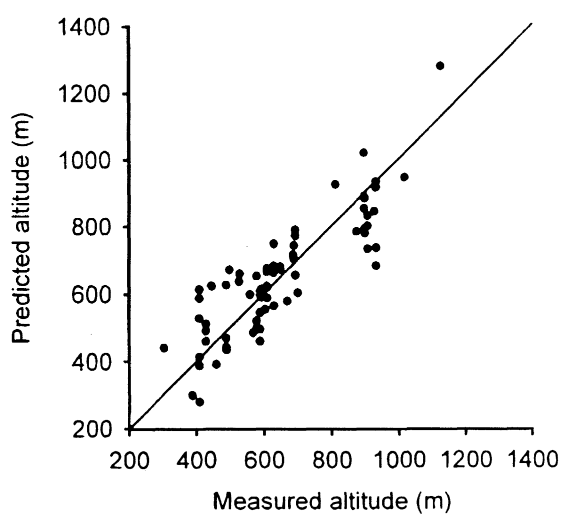

Figure 1 Altitude inferred from near-infrared (NIR) spectra from surface sediments (0–1 cm) of 76 lakes in northern Sweden versus measured altitude. Predictions are based on leave-one-tenth-out cross-validation.

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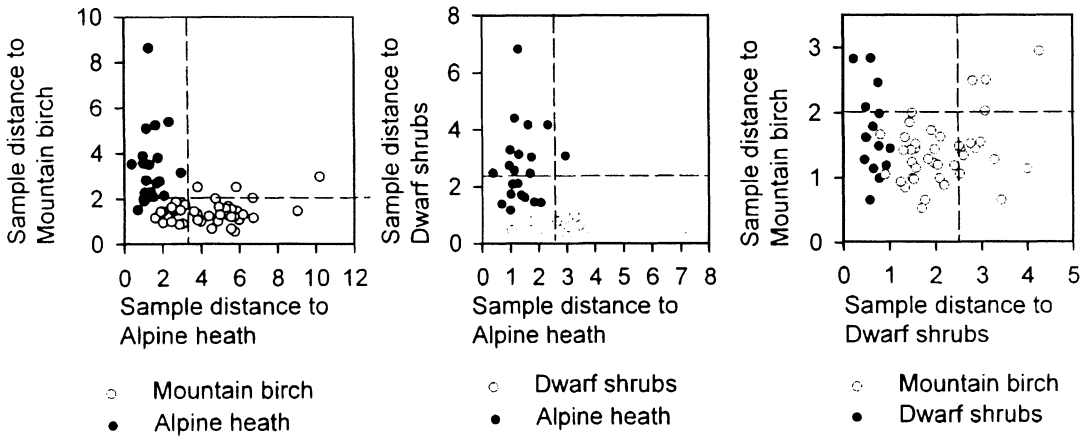

Figure 2 Cooman plots showing results of classification of the lakes according to the three vegetation zones based on analysis of near-infrared (NIR) spectra in surficial sediments (0–1 cm) from 76 lakes in northern Sweden. Sample distances of individual lakes are plotted pairwise against their own principal component (PC) class model and the PC model for the other class. Dashed lines indicate 95% confidence intervals. Samples having values within the 95% confidence interval of their own class were statistically distinguished as belonging to that lake classification. For example, in the left-hand panel alpine-heath lakes with values less than the 95% confidence limit on the x-axis (vertical dashed line) were correctly classified as belonging to the alpine-heath class. Similarly, mountain-birch lakes with values less than the 95% confidence limit on the y-axis (horizontal dashed line) were correctly classified as belonging to the mountain-birch class. Lakes located within both 95% confidence limits (lakes in the bottom left quadrant) were correctly classified according to both vegetation classes and could not be statistically separated. Lakes positioned outside the 95% confidence limits could not be classified to either of the vegetation zones.

fication was poor (Figure 2, right-hand panel). Many lakes were classified as belonging to two classes, but this is hardly surprising when considering that the *a priori* classification relies on field reconnaissance of vegetation zones that change gradually from one zone into the other.

Overall, results from the NIRS-altitude model, as well as the NIRS classification of vegetation type, clearly indicate that NIR spectra of surficial sediments of lakes contain climate-related information, which can be described by statistical models.

The comparison of NIR spectra in surface sediments (0–1 cm) with spectra from a lower depth interval (1–2 cm) indicated no significant effect of sediment ageing (microbial degradation, compaction, etc.) on NIR properties of the sediments (Figure 3). Modelled values for both sediment depths vary between the two discrete levels 0 (0–1 cm) and 1 (1–2 cm), with a rather similar distribution and a mean of 0.5. This result indicates that sediment depth cannot be modelled, and that the differences between NIR spectra from sediment taken from 0–1 cm and from 1–2 cm were small compared to the differences in NIR spectra between lakes. Overall, these results indicate that important degradation processes, or ageing effects, that may influence NIR spectra in these sediments are completed within the uppermost part of the top centimetre of sediment and do not significantly affect NIR spectra in deeper layers. We conclude, therefore, that the model between NIR spectra of surface-sediment samples (0–1 cm) and lake altitude can be used for retrospective analysis of altitude and by extension temperature using sediment cores.

Mean July air temperatures, obtained when applying the present NIRS-altitude model to the sediment core from Lake Sjuodjijaure, show similar trends to preliminary values inferred from transfer functions based on chironomids, diatoms and pollen (Figure 4). Also, the NIRS-inferred altitude (839 m) from the surface-sediment sample of Lake Sjuodjijaure, which was not included in the training set, corresponds well with the real altitude (826 m) for Lake Sjuodjijaure. These results indicate that NIR spectra of sediment cores contain information about past climate-related variables. However, the NIRS-inferred temperature curve also shows a coarse similarity with the loss-on-ignition (LOI) curve (Figure 4). Based on this coarse similarity, it could be argued that the NIRS modelling reflects largely the LOI of the sediment, because NIRS may be sensitive both to the concentration of organic material and the composition of this material. This must be studied further, for example, by analyses of the organic material of the samples of the calibration data set (e.g., C and N analyses, since remaining samples are too small and valuable to

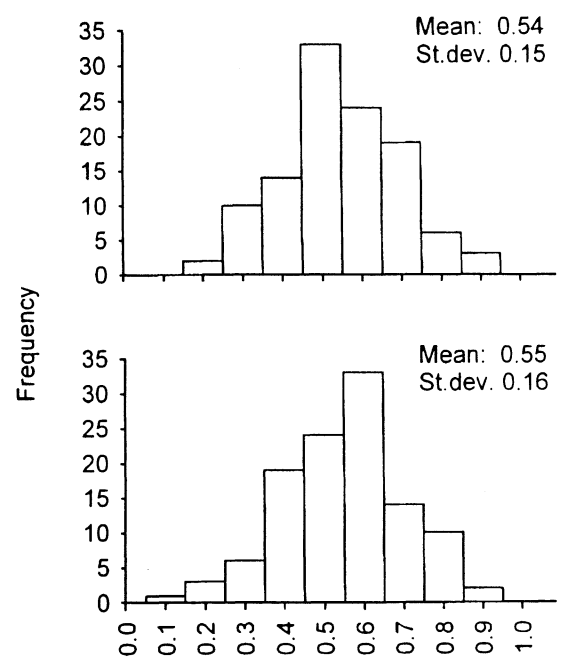

Figure 3 Distributions of modelled class membership for sediment samples from 0–1 cm depth (class 0, lower panel) and 1–2 cm depth (class 1, upper panel) using partial least squares discriminant (PLS-DA) classification on orthogonal signal correction (OSC) filtered spectra. Modelled values for both sediment depths vary between the two discrete levels 0 and 1, and demonstrate rather similar histograms with means of 0.54 and 0.55 and standard deviation of 0.15 and 0.16. The similarity of the histograms indicates that the difference in NIR spectra from sediment taken from 0–1 cm and 1–2 cm was small compared to the difference in NIR spectra between lakes.

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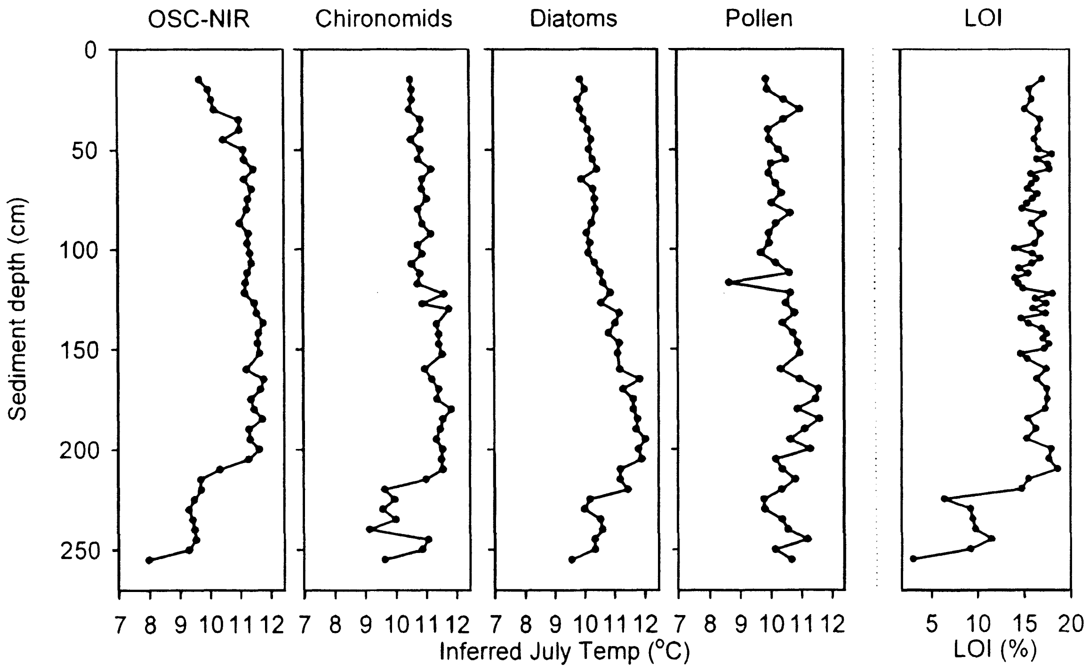

Figure 4 Mean July air temperatures as inferred from NIR spectrometry, chironomids, diatoms and pollen and to the right loss-on-ignition (LOI) in a sediment core from Lake Sjuodjijaure (826 m a.s.l.) in Sarek National Park. The 2.55 m long sediment core covers, according to calibrated radiocarbon dates, approximately 9500 years. Notice that the top 15 cm were not analysed due to shortage of sediment.

use for LOI measurements). Besides the well-established fact that attributes of organic material are important for NIR signals, there are two arguments pointing to the importance of the organic material composition. One argument is the poor correlation between LOI and NIRS-inferred temperature for the sediment down to 210 cm depth ($R^2 = 0.1$); if all sediment samples (down to 255 cm) are included in the analysis the correlation increases ($R^2 = 0.49$), but then the low LOI values at the bottom of the core have a strong leverage effect on the regression. The other argument is that Korsman *et al.* (1999), in a whole-basin study including many surface-sediment samples with highly variable LOI values, demonstrated that NIR spectra reflected properties that could not be accounted for by LOI.

Conclusions

The relationships between NIR spectra of surface sediments of lakes and lake-altitude and catchment vegetation clearly indicate that lacustrine sediments contain climate-related information in the organic material that can be detected using NIRS. It is also demonstrated that decomposition processes within surface sediments do not destroy these climate-related signals, which can be seen from the PLS-DA analysis of 0–1 cm versus 1–2 cm sediment samples. The results demonstrate that predictive transfer functions can be established between NIR spectra of surface sediments and climate variables, and that they may provide useful quantitative inferences of past climatic conditions from analyses of sediment cores. Preliminary inferences of mean July air temperature at Lake Sjuodjijaure during the past 9500 years show some similarity with quantitative inferences based on other climate proxies and encourage further work towards developing NIR spectrometry of lake sediments as a tool for studies of past climate.

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