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A diatom-inference model for nutrients screened to reduce the influence of background variables: Application to varved sediments of Greifensee and evaluation with measured data

S. Hausmann [a,*], F. Kienast [b]

[a] *Institute of Plant Sciences, University of Bern, Altenbergrain 21, CH-3013 Bern, Switzerland*
[b] *Swiss Federal Institute WSL, Zürcherstrasse, CH-8903 Birmensdorf, Switzerland*

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Abstract

Palaeoenvironmental reconstructions of lake sediment records have been greatly facilitated by statistical comparisons with microfossil assemblages from the surface sediments of modern lakes. These modern sub-fossil assemblages from different lakes, which are often referred to as "training-sets", attempt to incorporate gradients of environmental parameters, such as e.g., temperature and phosphorus, are of interest for paleoenvironmental reconstruction. One major assumption of quantitative palaeoenvironmental reconstructions requires that the environmental variable to be reconstructed is, or is linearly related to, an ecologically important determinant in the ecological system of interest, and that the joint distribution with other variables in the fossil set is the same as in the training-set. The motivation for this paper is that present-day diatom species abundances in surface-sediment samples are often influenced by several environmental gradients. Partial least squares (PLS) or weighted-averaging partial least squares (WA-PLS) regression methods can be used to adjust species optima, if the additional PLS components, which are orthogonal to previous PLS components, are included.

This paper tests a reproducible approach for reducing the influence of background variables within a diatom training-set to produce a "screened" training-set, which focuses on the variable of interest. In our example total phosphorus (TP) is the variable of interest. The initial training-set consists of modern Swiss lakes along an elevation gradient spanning 2005 m (334 to 2339 m a.s.l.), which follows a TP gradient from 522 to 3 $\mu g\ L^{-1}$. However, high-elevation lakes are not distributed equally along the TP gradient. They are meso-oligotrophic because high-elevation eutrophic lakes are rare in Switzerland. This leads to a potential confounding effect between the elevation and the nutrient gradients. These higher elevation lakes were selectively excluded, using Monte Carlo permutation tests, until the conditional effect with respect of covariables of elevation was no longer significantly related to the relative abundance of diatoms. The initial and screened inference models for log TP were applied to fossil assemblages from varved sediments at Greifensee (Switzerland), which cover the past century. The evaluation of the reconstructions with measured TP (1954–1994) demonstrates that the smaller (screened) subset performs better than the larger, more heterogeneous, initial data-set when the same number of components are included. The slope of the relation between measured and inferred log TP changed significantly for the reconstructions using partial least squares, with one and two components, and for reconstruction using weighted averaging partial least squares with two components. According to our interpretation, the accuracy of the reconstructions improved because modern diatom abundances of the

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* Corresponding author. Present address: Laboratoire de paléolimnologie et paléoécologie, Centre d'études nordiques, Université Laval Québec (Québec), Canada G1K 7P4. Tel.: +1 418 6562131x8298; fax: +1 418 6562978.
E-mail address: Sonja.Hausmann@cen.ulaval.ca (S. Hausmann).

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smaller subset are controlled mainly by log TP and lakes are more equally distributed along the log TP gradient. This approach of reducing the influence of background variables is applicable to other heterogeneous training-sets, such as merged training-sets, in order to homogenise the background variables and to maintain the gradient of interest.

Keywords: Diatoms; Training-set; Secondary gradients; Total phosphorus; Evaluation

1. Introduction

Quantitative reconstruction techniques of past environments, such as transfer functions, based on known, present-day controlling factors of species distributions and relative abundances have revolutionized palaeoecology (Imbrie and Kipp, 1971; Birks, 1998). If we wish to understand the controls differentiating two or more systems, in our case diatom assemblages, and we keep all other features constant, then the difference may then be attributed to the only factor which we have allowed to vary (*Ceteris paribus* "all other things being equal": This primary strategy of the experimental method in science has been known since Roman times). However, in real life several environmental variables may be important for controlling the distribution of the organisms under investigation. Secondary gradients thus are a common issue in creating transfer functions. In reducing the variation in the background variables, we are not concerned about the ecologically meaningful correlation of variables within a given lake, which is assumed to be the same today as it was in the past; rather, we are interested in the influence of potential confounding variables within the training-set lakes, such as nutrients and lake altitude which largely represents climate (Fig. 1). One major assumption of quantitative paleoenvironmental reconstructions is that the joint distribution with the environmental variable in the fossil set is the same as in the training-set (Birks, 1995). For example, in Switzerland eutrophication throughout the 20th century is independent of climate warming at lower elevations (Gächter and Furrer, 1972) and therefore we would not necessarily expect to find the same relationship in a fossil record. Often, diatom-inference models for several parameters have been established from the same set of lakes (Philibert and Prairie, 2002), because more than one parameter may be statistically important for the distribution and abundance of diatoms (pH, CO_2, TP, TN and DOC). Rosén et al. (2000) published from the same set of lakes diatom-inference models for temperature, pH and total organic carbon (TOC). Within these lakes TOC might be collinear to temperature, since lakes at lower altitude often have high TOC content. Weckström et al. (1997) created diatom-inference models for pH and temperature, which are possibly not independent, because their training-set lakes with temperature above 13.5 °C have on average 0.66 units lower pH than the mean. Lotter et al. (1997b, 1998a) used almost the same data-set to create a diatom-inference model for air temperature and total phosphorus, because both elevation and nutrients were important statistically in explaining the distribution of diatoms. However, using simulated biological species abundance data, Le and Shackleton (1994) demonstrated that taxa that are subject to several kinds of different environmental variables reduce the accuracy of transfer functions.

This paper is concerned with the diatom-inference model for nutrients developed by Lotter et al. (1998), which was applied to diatoms of varved sediments of Baldeggersee (Lotter, 1998) and compared with measured data. By selecting lakes only in calcareous bedrock regions, they tried to minimize the effect of low pH, which might override nutrient effect; however, pH still explained a significant amount of variation in the diatom assemblages (Lotter et al., 1997b, 1998). In addition, many lake surface-sediments came from high-elevation lakes (Fig. 1). Consequently, in a statistical sense, climate also played an important role in explaining patterns of diatom composition and abundance (Lotter et al., 1997b, 1998). It is important to note that lakes having TP concentrations below 50 μg L^{-1}, elevation, total nitrogen, forest cover and impact of glaciers had a higher variance than lake with TP concentrations above 50 μg L^{-1} (Fig. 1).

In order to make background variables, such as elevation more comparable, one possibility would have been to increase the number of eutrophic high-altitude lakes. However, nutrient-rich lakes are rare at higher elevations in Switzerland, because industry and agriculture are concentrated in the lowlands (Ammann et al., 1996). Therefore, we reduced variation in background variables by excluding high-elevation lakes.

In practice, it is difficult to avoid the inclusion of additional environmental gradients in a training-set a priori, because often only limited information about the sampling sites is available before sampling. However, if additional environmental gradients, determined or not,

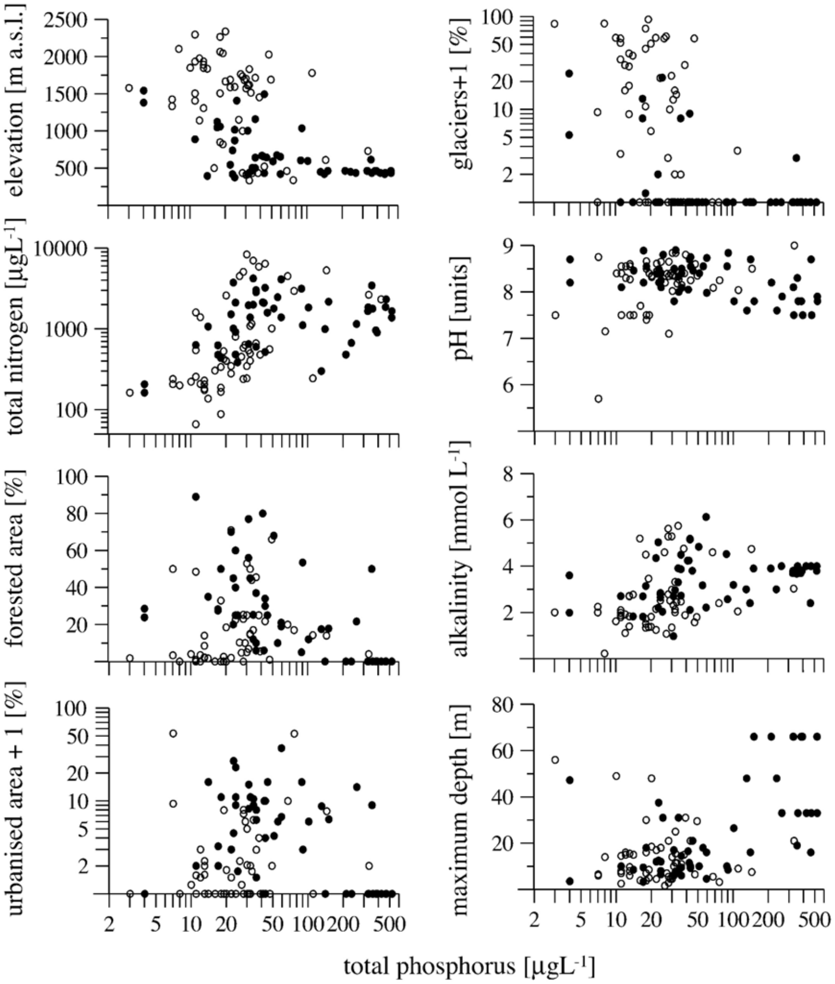

Fig. 1. Relationships between the environmental variables for the modern training-set. Samples with hollow circles were excluded when the influence of background variables was reduced.

are orthogonal to earlier components, they can be used to update species optima, by including additional components in partial least squares and weighted averaging partial least squares (ter Braak et al., 1993). A list of basic requirements for quantitative palaeoenvironmental reconstructions, such as consistent taxonomy and robust statistical tools is provided by Birks (1995).

The objective of this paper is to determine which model performs better: the initial full diatom-inference model, where several environmental variables significantly explain the diatom distribution, versus a smaller subset of lakes, where only the conditional effect with respect to covariables of the variable of interest, and ecologically meaningful correlated variables, are significantly related to the diatom abundance in a partial CCA. In our case TP is the variable of interest and an importance of e.g., chlorophyll *a* would be reasonable too. However enhanced total nitrogen concentrations do not necessarily have to be related to higher TP concentrations. As, Catalan et al. (2002) described high nitrate levels as a typical feature of mountain lakes as sparsely developed soils and vegetation in the catchment cannot take up atmospheric nitrogen, which leads to nitrogen accumulation in lakes. The understanding of modern processes of the ecological system of interest is essential for the approach outlined in this paper. We hypothesize that background variables can strongly alter the estimated species responses to the variable of interest. As in our case all lakes above the tree line had relatively low TP concentrations (Fig. 1). A dominance of one species in a lake above tree line can be driven by low TP concentrations and/or by an ability to cope with harsher climate. In order to address this hypothesis, we reduced the range of other important variables by eliminating lakes. The initial and the screened diatom-inference models for nutrients were applied to diatom assemblages from varved sediments of Greifensee and the resulting reconstructions were evaluated with measured data (1954–1994; EAWAG, unpublished data). In the 1970s Greifensee was reputed to be one of the most polluted lakes in Europe. Since then several efforts have been made to reduce the nutrient load to background conditions. Paleolimnological techniques are beneficial to define former conditions, which are a useful goal for lake management. In order to interpret fossil diatom assemblages modern data-sets of high quality are needed.

2. Methods

2.1. Modern data

A training-set of 77 samples from Switzerland (Lotter et al., 1998) was extended by 7 samples from well-dated varve sequences in monitored lakes with high TP concentrations, which were included to cover the expected past TP range. In addition, 21 surface sediments mainly from lakes around 1400 m a.s.l. (Fig. 1) were added, since surface-sediment samples from this altitude were underrepresented in the initial training-set. The TP of the extended training-set ranges from 3 to 522 $\mu g\ L^{-1}$ and elevation from 2339 to 334 m a.s.l.

Before each surface sample was collected, temperature and conductivity profiles were taken to estimate the depth to the thermocline, since spring overturn concentrations of TP, total nitrogen and alkalinity were estimated as depth-weighted averages of four water samples. Water samples were taken at the surface, one metre above and below the thermocline, and one metre above the bottom of the lake. This approach to estimate spring overturn TP values was evaluated for five years (59 months) at Greifensee using the monthly measured TP records (EAWAG, unpublished data). From this data-set, the thermocline depth was assessed for this study. Four water samples were selected, as in the lake sampling protocol for the training-set, and the monthly depth-weighted averages were compared by linear regression with the measured TP during spring overturn. The depth-weighted averages of the Greifensee data-set closely estimated the spring overturn TP (slope = 0.62; $r^2 = 0.86$). Therefore, depth-weighted averages were calculated for TP, alkalinity and total nitrogen to estimate spring overturn concentrations. Lake pH was measured in the field. See Müller et al. (1998) for methodological details of the water analyses.

Weighted averaging is known to be sensitive to the distribution of the environmental variable in the training-set (ter Braak and Looman, 1986). Total phosphorus (TP), total nitrogen (TN) and the percentage of catchments which were covered with glaciers or subject to urban land-use were $\log_{10}(x+1)$ transformed, because they met the following criteria for log transformation (Jongman et al., 1987), as the standard deviation exceeded the mean and the maximum value of a variable is 20 times greater than the smallest value (Table 1). However, canonical correspondence analysis (CCA) does not require a normal distribution of environmental variables.

The surface sediments were sampled using a gravity corer (Renberg, 1991). The top first centimetres were extruded in the field and were prepared for diatom analysis with 10% HCl and 30% H_2O_2. A minimum of 500 diatom valves per sample was identified to the species. Diatom nomenclature was adapted to the nomenclature of the 77 samples of the previously published training-set (Lotter et al., 1997b, 1998), which mainly followed Krammer and Lange-Bertalot (1986, 1988, 1991a,b), although a variety of other sources was consulted.

2.2. Screening of training-set samples by reduction of the influence of background variables

The aim of reducing the influence of background variables is to obtain a training-set with a long gradient

Table 1
Statistics of the modern samples of the initial (105 samples) and the screened training-set (50 samples)

		Min	Max	Mean	Median	SD
Elevation [m a.s.l.]	Initial	334	2339	1057	887	602
	Screened	374	1543	655	502	304
TP [$\mu g\ L^{-1}$]	Initial	3	522	83	31	126
	Screened	4	522	128	44	160
TN [$\mu g\ L^{-1}$]	Initial	0	8353	1464	801	1641
	Screened	0	4221	1581	1451	1058
Max depth [m]	Initial	1.6	66.0	19.0	12.5	17.3
	Screened	3.3	66.0	24.5	16.0	20.5
pH [units]	Initial	5.7	9.0	8.3	8.4	0.5
	Screened	7.6	8.9	8.3	8.4	0.3
Glaciers [%]	Initial	0	92	12	0	22
	Screened	0	23	1	0	4
Alkalinity [mmol L^{-1}]	Initial	0.2	6.1	3.0	2.7	1.3
	Screened	1.0	6.1	3.4	3.6	1.0
Forested [%]	Initial	0	89	20	14	22
	Screened	0	89	26	21	25
Urban [%]	Initial	0	52	5	1	9
	Screened	0	36	6	3	8

Variables are ranked following their importance in explaining diatom data, as assessed by CCA.

for the environmental variable of interest, but a small gradient of background variables. Background variables are variables which are not functionally related to the variable of interest. The variation of background variables should be equally distributed along the gradient of interest in order to avoid creating confounding variables. This goal was approached by excluding lakes with highest and lowest values of background variables at the ends of the gradients.

The influence of background variables was reduced using following steps:

Step 0 The variables used for this elimination of lakes were selected, from a set of 43 environmental variables, by forward selection with significance levels adjusted by a Bonferroni-adjustment, using canonical correspondence analysis (CCA). Variance Inflation Factors (VIFs) were below 5, indicating a low correlation of variables. Functionally related variables to log TP should be highly correlated. CCA is a direct ordination method to explore the relation between species and environmental variables. Elevation was used as a surrogate for climate, as it was highly inversely correlated with degree-days ($r = -0.96$) and July air temperature ($r = -0.97$). Percentages were square-root transformed and rare taxa were down-weighted, as implemented in the program CANOCO for Windows (version 4.0; ter Braak and Šmilauer, 1998).

Step 1 The most important secondary gradient, which explained second to the variable of interest (in our study log TP) most of the biological variance, was identified according to the eigenvalues of the CCA axis one. In our case it was mainly elevation (Fig. 2).

Step 2 A scatter plot of the variable of interest and the second important environmental variable was explored in order to identify which lake represented the most extreme value of the second important environmental variable, compared to the other lakes of the log TP gradient (Fig. 2). This lake was excluded.

Step 3 The significance of the conditional effect with respect to covariables of each environmental variable was assessed using an unrestricted Monte Carlo permutation test (999 permutations) in separate partial CCAs where all environmental variables initially selected by forward selection other than the one to be tested were used as covariables. Square-root transformed rare taxa were down weighted. If the same initial seed generators for the random number generator are used in CANOCO it is a reproducible method.

Steps 1 to 3 were repeated until a subset of lakes was identified in which only the conditional effect with respect to covariables of the variable of interest, and functionally related variables, remained significantly related to the distribution and abundances of diatoms (Fig. 3).

2.3. Diatom-inference models for log TP

Non-linear diatom-inference models are recommended by ter Braak (1995) if the length of the floristic gradient exceeds 2 standard deviation (SD)-units of a

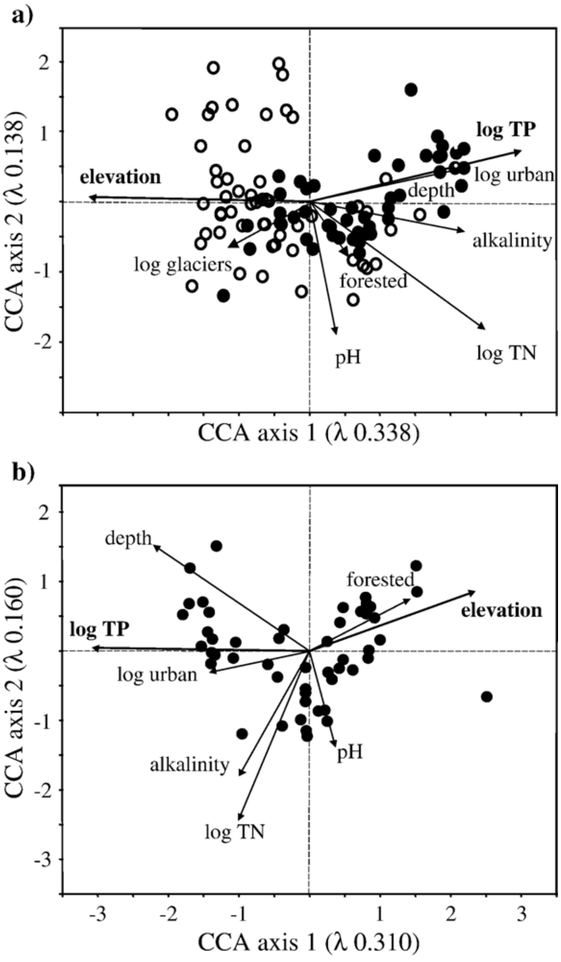

Fig. 2. Biplot of a canonical correspondence analysis (CCA) showing environmental variables (arrows) and modern diatom surface samples (circles). (a) CCA of the initial training-set. Excluded samples are indicated by hollow circles. (b) CCA of the screened training-set.

detrended correspondence analysis (in our case it was 3.3 SD-units for the initial and 3.4 SD-units for the screened training-set). In order to consider non-linear species responses we used weighted averaging partial least squares (WA-PLS), with one and two components, weighted averaging with down-weighting by tolerances and inverse deshrinking (Birks et al., 1990). Reconstructions using WA-PLS models using two components were not made because the inclusion of a second component did not improve the jackknifed error statistics (Table 3). WAtol was considered, because the tolerance of taxa is an important characteristic of the usefulness of a taxon as a bio-indicator for the variable of interest.

In addition, the significance of the individual diatom taxon response models to log TP was tested by means of a hierarchical series of response models (skewed unimodal, symmetric unimodal, monotonic sigmoidal and flat null model) fitted by generalized linear modelling (Huisman et al., 1993) using the program HOF (version 2.3, Oksanen and Minchin, 2002). The HOF models were based on square-root transformed relative abundances of taxa and we assumed a Poisson error structure. Significant responses were assessed for all taxa which occurred at occurred at least 5 times. In the initial training-set, 30% of the taxa showed unimodal responses to log TP and 29% showed monotonic sigmoidal responses to log TP. In the screened training-set, 29% of the taxa showed unimodal responses and 28% showed monotonic sigmoidal responses to log TP (Table 2). We wanted to consider the linear and non-linear response of the diatoms towards log TP. Therefore we used also partial least squares (PLS), which assumes linear species responses. All models were established using the program CALIBRATE (version 0.82; Juggins and ter Braak, unpublished program). In order to better understand the impact of reducing the influence of background variables on the reconstructions samples with high residuals or high leverage were not removed from the diatom-inference models.

Table 2
Species responses towards total phosphorus according to HOF using taxa occurring in the initial training-set, only in the eliminated lakes and the screened training-set

	Initial (%)	Eliminated (%)	Screened (%)
Null model	34	35	37
Monotonic	29	32	28
Symmetric	30	25	29
Skewed	7	7	7

2.4. Sediment core analysis

A freeze-core (Lotter et al., 1997a) was taken from the deepest part of Greifensee in 1995. Greifensee is located 10 km east of Zurich at an elevation of 435 m a.s.l. It has a maximum depth of 33 m, a catchment area of 147.8 km^2, and a water renewal time of 1.1 years. In 1916, continuous varve formation started due to anoxic conditions. Until 1911, Greifensee had a natural abundance of whitefish (*Coregonus lavaretus*; Züllig, 1982). Whitefish is a bio-indicator of lake trophic status, because its eggs need a dissolved oxygen concentrations at the sediment-water interface. The yearly layers in the sediment core could be distinguished by their colours (spring grey, autumn black), thus permitting visual varve couplet counting of the core (Stoll et al., 1997).

Varves were individually sub-sampled at −15 °C to prevent the freeze core from melting. Microspheres were added to a known volume of sediment to estimate diatom accumulation rates (Batterbee and Kneen, 1982). The diatom–microsphere suspension was treated like that of the modern sample using the same taxonomy and nomenclature. A minimum of 300 valves was counted for each sample using a Leitz Dialux 22 microscope with 1000× magnification and phase-contrast. The zonation of the diatom stratigraphic data was carried out on percentage data using optimal sum of squares partitioning (Birks and Gordon, 1985), as implemented in the program ZONE (Lotter and Juggins, 1991). The significant number of diatom assemblage zones was assessed by comparison with a broken-stick model (Bennett, 1996). The differences of spring-overturn TP and the onset of the mixture of the water column between the years dominated by *Stephanodiscus parvus* Stoermer and Håkansson, were tested by a Student's *t*-test.

2.5. Application and evaluation of the initial and screened training-sets

The diatom-inference models (PLS, WAtol and WA-PLS) for log TP of the initial and the screened training-set were applied to the square-root-transformed fossil diatom assemblages of the Greifensee varves using the program CALIBRATE (version 0.82; Juggins and ter Braak, unpublished program). For WA-PLS, error-bars were calculated using the program WAPLS (version 1.1; Juggins and ter Braak, unpublished program) and for WAtol and PLS, the root mean square error of estimation was used (Juggins, personal communication). The inferred log TP concentrations using the initial and the screened training-set of the PLS, WAtol and WA-PLS models were compared with the measured overturn log TP concentrations from Greifensee (1954–1994, unpublished data EAWAG). The root mean square error of evaluation (RMSEE) was calculated and a linear regression between measured and inferred log TP were established using the program SYSTAT (version 4.0).

3. Results

3.1. Environment-species relationship before screening the training-set

The forward selection procedure in CANOCO selected and ranked the environmental variables of the

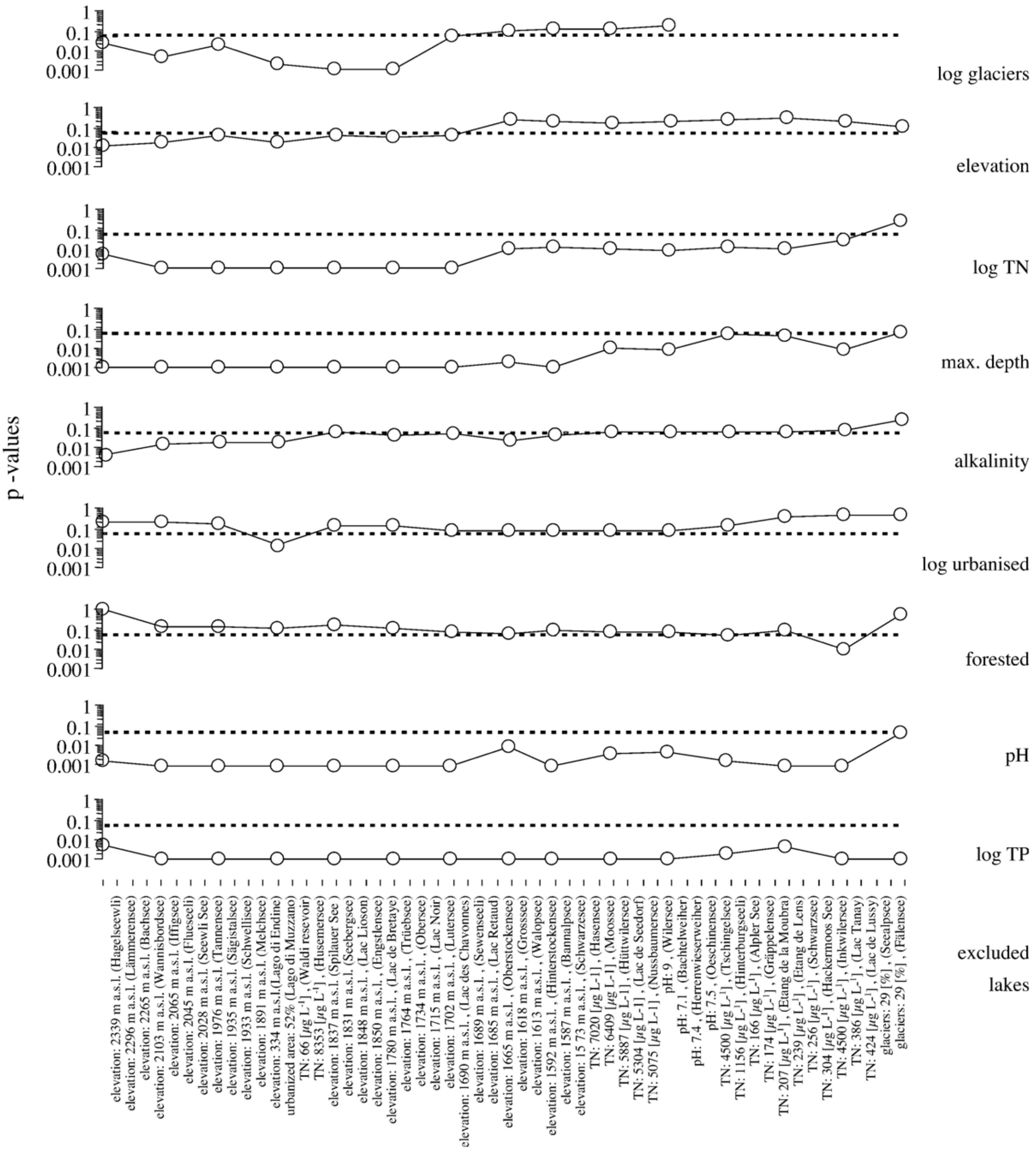

Fig. 3. Results of Monte Carlo Permutation tests for the significance between the distribution of diatom taxa and each individual environmental variable, with the other variables as covariables (conditional effect). Stop criterion for the elimination of lakes was p-value below 0.05 (indicated as dashed line) for the secondary gradient. The labels of the x-axis indicates the name of the eliminated lakes and the reason for its exclusion.

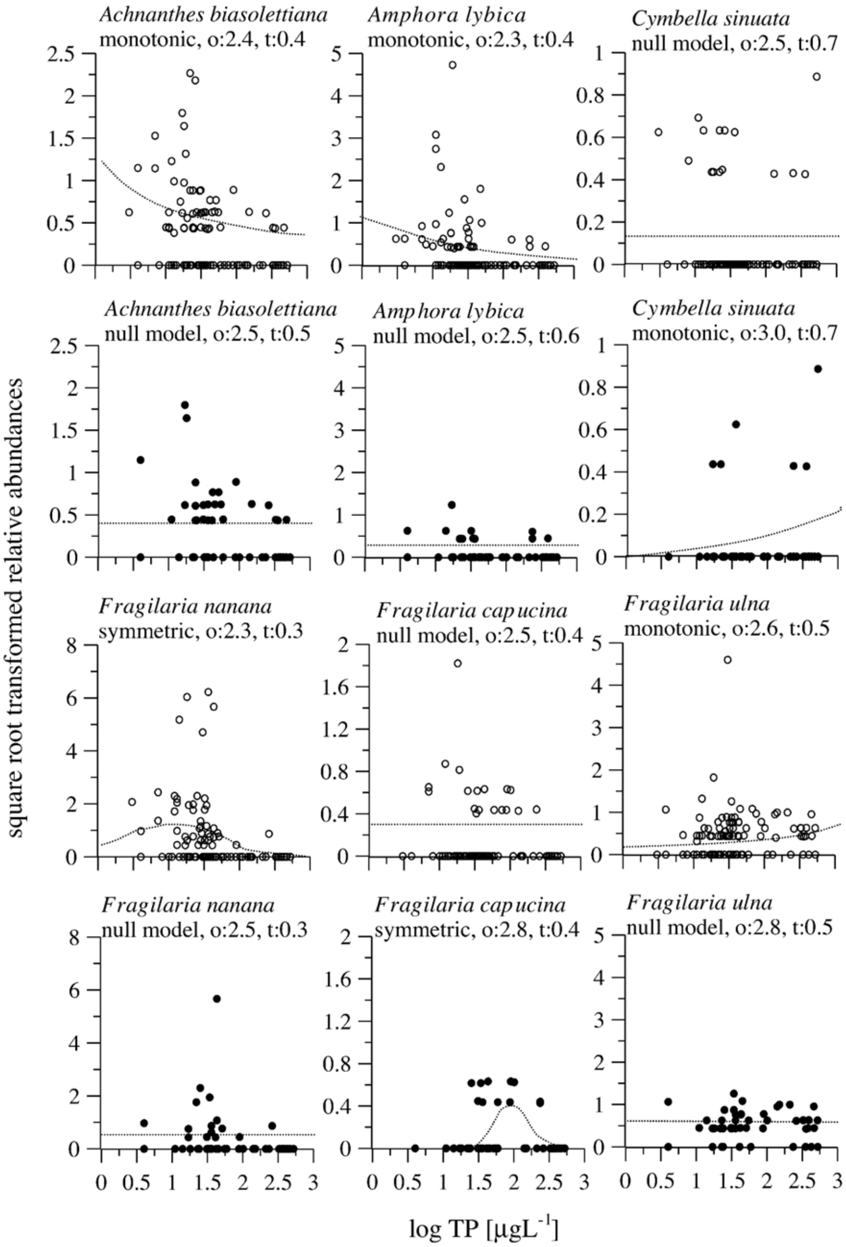

Fig. 4. Distribution and species response curves for log TP obtained using the program HOF for selected taxa of the fossil record. Samples from the initial training-set are represented by hollow circles and from the screened training-set by solid circles. Optima (*o*) and tolerances (*t*) were estimated by weighted averaging.

initial training-set in terms of their importance for explaining in the following order: Elevation, log total phosphorus (log TP), log total nitrogen (log TN), maximum lake depth, pH, log percentage of glaciers in the catchment, alkalinity, percentage of forested, and log percentage of urbanised area in the catchment (Table 1). The correlations between log TP and log urbanised catchment area ($r = -0.03$), pH ($r = -0.05$), forested area ($r = -0.18$) and alkalinity ($r = 0.38$) were lower. However, the correlations between log TP and elevation ($r = -0.57$, $n = 105$, $p < 0.001$), maximum lake depth ($r = 0.47$, $n = 105$, $p < 0.001$) and log catchment area covered with glaciers ($r = -0.45$, $n = 105$, $p < 0.001$) were high. It is important to note that lakes having TP concentrations below 50 μg L^{-1}, elevation, total nitrogen, forest cover and impact of glaciers had a higher variance (Fig. 1). The higher elevation sites have generally lower nutrient contents. The lakes with TP values above 50 μg L^{-1} ($n=29$) are all located below 675 m a.s.l., with the exception of two lakes at 1036 and 1780 m a.s.l. (Fig. 1). The elevation of the sites ranges from 334 to 2339 m a.s.l. (Table 1), with 50% of the lakes located above 887 m a.s.l. (Fig. 1, Table 1).

The CCA (Fig. 2a) demonstrates that the first axis is most correlated with elevation ($r=-0.80$), followed by log TP ($r=0.77$). The environmental variable of interest, log TP, was like log TN, elevation of the sites, the percentage of log catchment covered with glaciers, alkalinity and maximum depth of the lakes significantly related to the distribution and abundance of diatoms, as tested by a Monte Carlo permutation test (999 permutations) of a partial CCA where all other environmental variables initially selected by forward selection were partialled out (Table 1; Fig. 3).

3.2. Environment–species relationship after screening the training-set

The absolute correlation between log TP and the first axis of a CCA (Fig. 2b) increased from |.77| ($n=105$, total inertia$=5.22$) to |.83| ($n=50$, total inertia$=3.42$), whereas the correlation between the first CCA axis and elevation decreased from |.80| ($n=105$, total inertia$=5.22$) to |.63| ($n=50$, total inertia$=3.42$). In order to obtain a calibration set where the distribution and abundance of diatoms were not statistically significantly related to the conditional effects with respect to covariables of the background variables, 52% of the lakes from the initial training-set ($n=105$) were excluded from the inference model for log TP (Fig. 3). These sites are mainly high-elevation lakes having a large influence of catchment glaciers, as well a disproportionate concentration of low log TN or low pH values, compared to the variance of log TN of the other lakes covering the higher end of the log TP gradient (Fig. 1). The TP range of the screened training-set was nearly identical to that of the initial training-set (new TP range: 4 to 522 μg L^{-1}), because the eliminated lakes with unusual combinations of environmental variables were mainly oligo-mesotrophic sites, which were overrepresented in the initial training-set (median 31 μg TP L^{-1}, range: 3–533 μg TP L^{-1}). Nevertheless, the elevational range was narrowed from a range of 334–2339 to 374–1543 m, TN from 67–8353 to 162–4221 μg L^{-1} and pH from 5.7–9 to 7.6–8.9 units (Table 1). Due to the reduction of secondary gradients by eliminating lakes mainly with high impact from glaciers (Fig. 1), the conditional effect with respect to covariables of log TP increased from 2.6% to 4.9%, the marginal effect (without covariables) from 5.0% to 7.6%, and the total inertia of the CCA decreased from 5.22 to 3.42. The background variables had still a marginal effect, when judged alone, on the distribution and abundance of diatoms.

3.3. Diatom-inference model for total phosphorus

The number of taxa, which occurred at least five times, decreased from 164 to 83 due to the exclusion of mainly high-elevation lakes. Not only taxa which had, according to HOF, no significant responses towards log TP (35%), also taxa which had symmetric (25%) and monotonic (32%) responses towards log TP were no longer present in the screened training-set (Table 2). The reduction of secondary gradients changed the estimated species response models from symmetric unimodal to null model for 7 taxa, e.g., *Fragilaria nanana* Lange-Bertalot, and from a null response to symmetric responses for 5 taxa, e.g., *Fragilaria capucina* var. *mesolepta* (Rabenhorst) Rabenhorst (Fig. 4). The percentage of taxa having symmetric unimodal responses to log TP decreased from 30% to 29% and the percent-

Table 3

Apparent and jackknifed error statistics of the diatom-inference log TP models before and after screening using partial least squares with one (PLS 1 comp.) and two (PLS 2 comp.) components, weighted averaging partial least squares with one and two components (WA-PLS 1 comp., WA-PLS 2. comp.) and weighted-averaging with downweighting of tolerance (WA tol)

		RMSE	r^2	Max-bias
Apparent				
Initial	PLS 1 comp.	0.32	0.60	0.60
Screened	PLS 1 comp.	0.25	0.79	0.30
Initial	PLS 2 comp.	0.23	0.80	0.38
Screened	PLS 2 comp.	0.16	0.92	0.15
Initial	WA-PLS 1 comp.	0.24	0.78	0.39
Screened	WA-PLS 1 comp.	0.22	0.85	0.22
Initial	WA-PLS 2 comp.	0.23	0.80	0.38
Screened	WA-PLS 2 comp.	0.16	0.92	0.15
Initial	WAtol	0.28	0.69	0.63
Screened	WAtol	0.25	0.79	0.30
Jackknifed				
Initial	PLS 1 comp.	0.36	0.49	0.74
Screened	PLS 1 comp.	0.38	0.56	1.02
Initial	PLS 2 comp.	0.36	0.53	0.58
Screened	PLS 2 comp.	0.38	0.55	1.10
Initial	WA-PLS 1 comp.	0.29	0.68	0.60
Screened	WA-PLS 1 comp.	0.30	0.62	0.85
Initial	WA-PLS 2 comp.	0.33	0.59	0.60
Screened	WA-PLS 2 comp.	0.35	0.60	0.83
Initial	WA tol	0.36	0.52	0.71
Screened	WA tol	0.48	0.27	1.55

age of diatom taxa which were indifferent to log TP increased from 34% to 37% (Table 2). The performance in terms of root mean square error of prediction and the maximum bias deteriorated for all models and the r^2 decreased for WA-PLS with one component and WAtol (Table 3, Fig. 5). Some taxa that also occurred in the fossil samples had a higher optimum for log TP, as estimated by weighted averaging (Fig. 6a). Taxa that had an estimated optimum for log TP of around 2.5 μg L^{-1}, using the initial training-set, showed a higher range of estimated optima (Fig. 6a). The screening also increased the variance of the estimated tolerance for log TP (Fig. 6b).

3.4. Diatom stratigraphy of Greifensee

The diatom biostratigraphy of Greifensee (Fig. 7) is dominated by planktonic taxa. Their distribution can be divided into two significant diatom assemblage zones (DAZ), because after two divisions the proportion of the variance accounted for the broken stick model was greater than for the observed data. DAZ 1 (1916–1933) was characterised by high abundances of *Cyclotella comensis*, together with *Fragilaria crotonensis*. *Cyclotella distinguenda* var. *unipunctata* Husted and *Fragilaria ulna* Lange-Bertalot, became less common towards DAZ 2. *Asterionella formosa* occurred togeth-

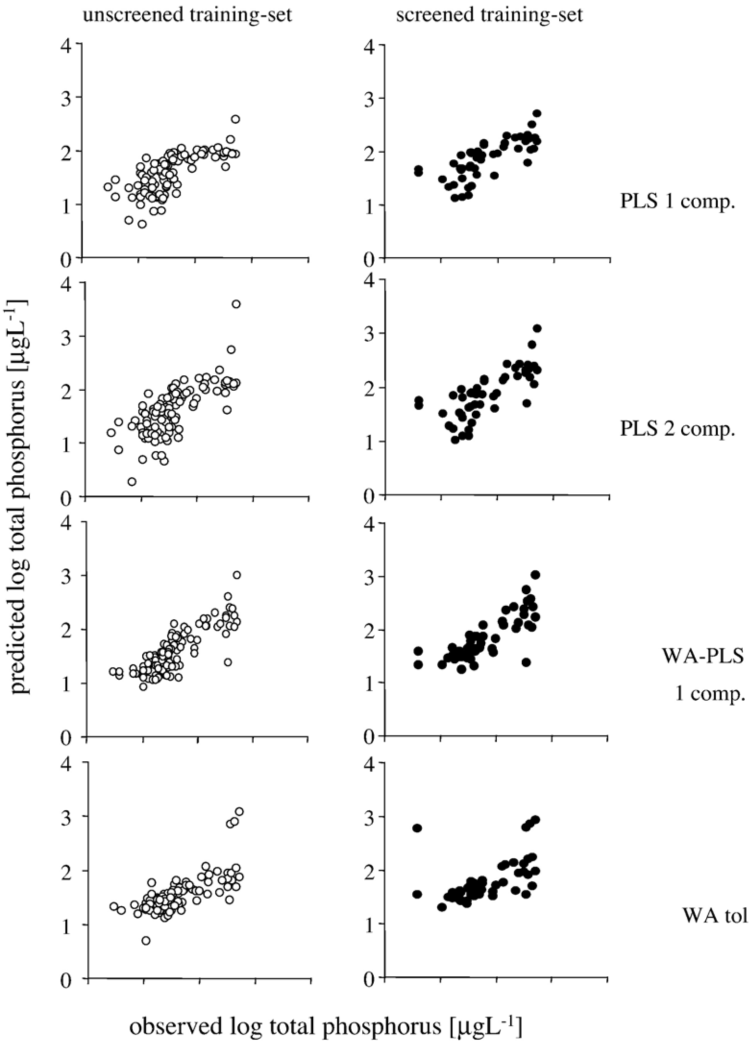

Fig. 5. Plots of observed log TP against jack-knife predicted log TP for diatom-inference models using partial least squares with one and two components (PLS 1 comp., PLS 2 comp.), weighted-averaging with down-weighting of tolerances (WAtol), and the weighted averaging partial least squares with one component (WA-PLS 1 comp.). Samples of the initial training-set are represented by hollow circles and samples of the screened training-set are indicated as solid circles.

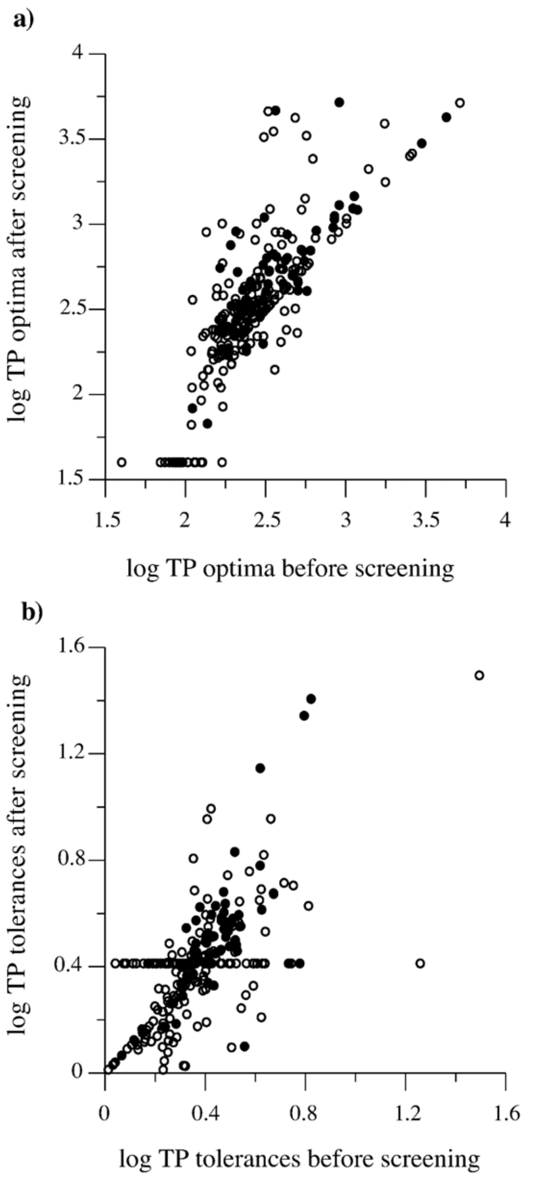

Fig. 6. Relationship of (a) optima and (b) tolerances of all diatom taxa before and after screening of the training-set. Taxa that occurred in the fossil set are indicated as solid circles.

er with *Aulacoseira granulata* Ehrenberg. The transition between DAZ 1 and DAZ 2 was characterized by high abundances of *Tabellaria fenestrata* (Lyngbye) Kützing.

DAZ 2 (1933–1995) is characterized by alternations between *F. crotonensis* and *S. parvus* abundances. According to the accumulation rates, *S. parvus* was dominant in the years 1954, 1967, 1971, 1977 and 1987 and was almost absent in the years 1951, 1956, 1973, 1979 and 1991. This alternation could not be explained by a fluctuation in total phosphorus (Student's *t*-test, $p=0.489$), where the difference in TP concentrations was tested. However, in the years dominated by *S. parvus* the lake seem to have overturned earlier in the season (Student's *t*-test, $p=0.045$), as tested by the differences in the onset of homothermic conditions. Between 1975 and 1985, *Cyclotella praetermissa* increased and in 1990, *T. fenestrata* re-occurred, which had dominated at the transition between DAZ 1 and DAZ 2. *C. comensis*, which was deposited at the beginning of the varve formation, had not yet become re-established at the time of coring.

3.5. Application and evaluation of the two diatom-inference models for nutrients

The general picture of the reconstructions was that since 1916 the inferred TP concentrations in Greifensee were above 50 μg L^{-1} TP, showed low concentration at 1928 and increased from 1930 to 1960 to hypereutrophic conditions, where TP reached a first maximum above 300 μg L^{-1} (Fig. 8). The temporary decline in TP concentrations in 1961 was observed with all models. From 1973 onwards, the measured TP declined gradually in contrast to the inferred TP. The PLS, WAtol and WA-PLS models, developed from both the initial and the screened training-set, were applied to the fossil diatom assemblages of the varved sediment record of Greifensee (Fig. 8). In the apparent error statistic the RMSE of the model performance decreased and the r^2 of reconstructed and measured log TP concentrations in Greifensee increased for all models after the reduction of background variables (Table 4), although the RMSEP and the maximum bias increased when model performance was tested with jackknifing (Table 3). Generally, the inferred log TP using the initial model was lower, which could be explained by the over representation of oligotrophic lakes. However, not only the distribution of lakes contributes to a more accurate reconstruction as the inferred log TP using the initial training-set was less correlated to the observed log TP than the inferred log TP using the screened training-set (Table 4).

For the initial training set the inclusion of a second component could be considered for the PLS model because the jackknifed r^2 was reduced by 13% and the max. bias was reduced by 28% when including an additional component. Therefore, to explore the influence of reducing background variables the reconstructions resulting of the PLS model with one component using the screened training set should be compared with

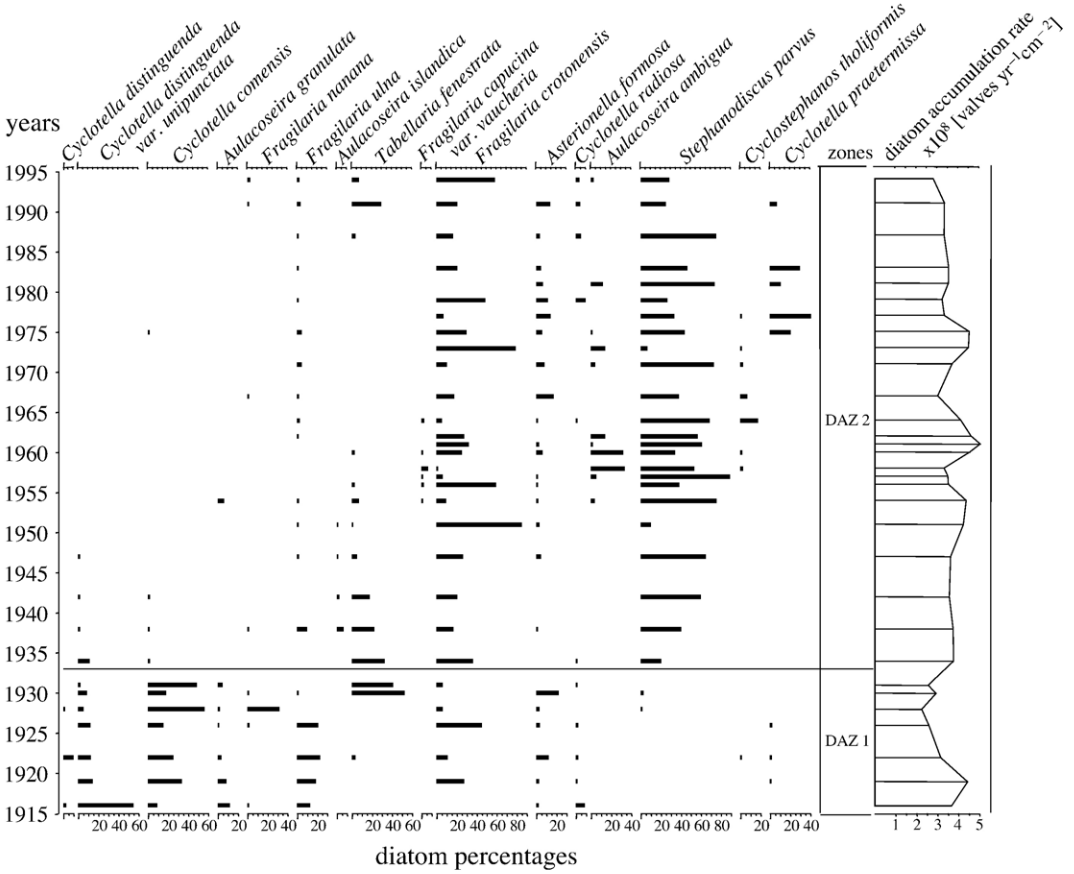

Fig. 7. Stratigraphy of most abundant diatom taxa (relative abundance > 5%) and diatom accumulation-rate for Greifensee.

the PLS model with two components using the initial training set. The slope between observed and inferred was closer to one using the initial set with two components but the RMSEE was lower using the screened set with one component. For the initial training-set the model performance using a PLS model with two components (Fig. 8b) was more accurate than those with only one component (Fig. 8a), because PLS with two components uses secondary gradients to improve estimates of taxon parameters.

Reducing the influence of background variables improved the error statistics of application, using the WA-PLS model with one component only slightly (Table 4).

WAtol, using the initial training-set, (Fig. 8d) overestimated the highest log TP concentrations between 1960 and 1970 and underestimated TP concentrations during the recovery period from 1980 to 1995. The slope between observed and inferred log TP was 2.25. However, the slope between observed and inferred log TP, using the screened training-set, was only 1.62.

4. Discussion

4.1. Reduction of the influence of background variables

Climate was considered a background variable for a diatom-inference model for log TP, thus mainly high elevated lakes were excluded from the inference model for log TP. Elevation and log TP can be considered as confounding variables, because they are highly correlated to CCA axis one and they are significantly correlated to each other ($r = -0.57$). Confounding variables are problematic, because in the training-set we see only the joint effect of both. The impact of climate and nutrients on the diatom communities of Greifensee changed individually. Since a high frequency climate signal, alternation of *F. crotonensis* and *S. parvus*, occurred during a period of hypertrophication which stretched over decades. If past impacts of confounding variables changed individually, resulting reconstructions could lead to misinterpretation of the variable that actually stayed constant (Anderson, 2000). With our present approach, we attempted to reduce the in-

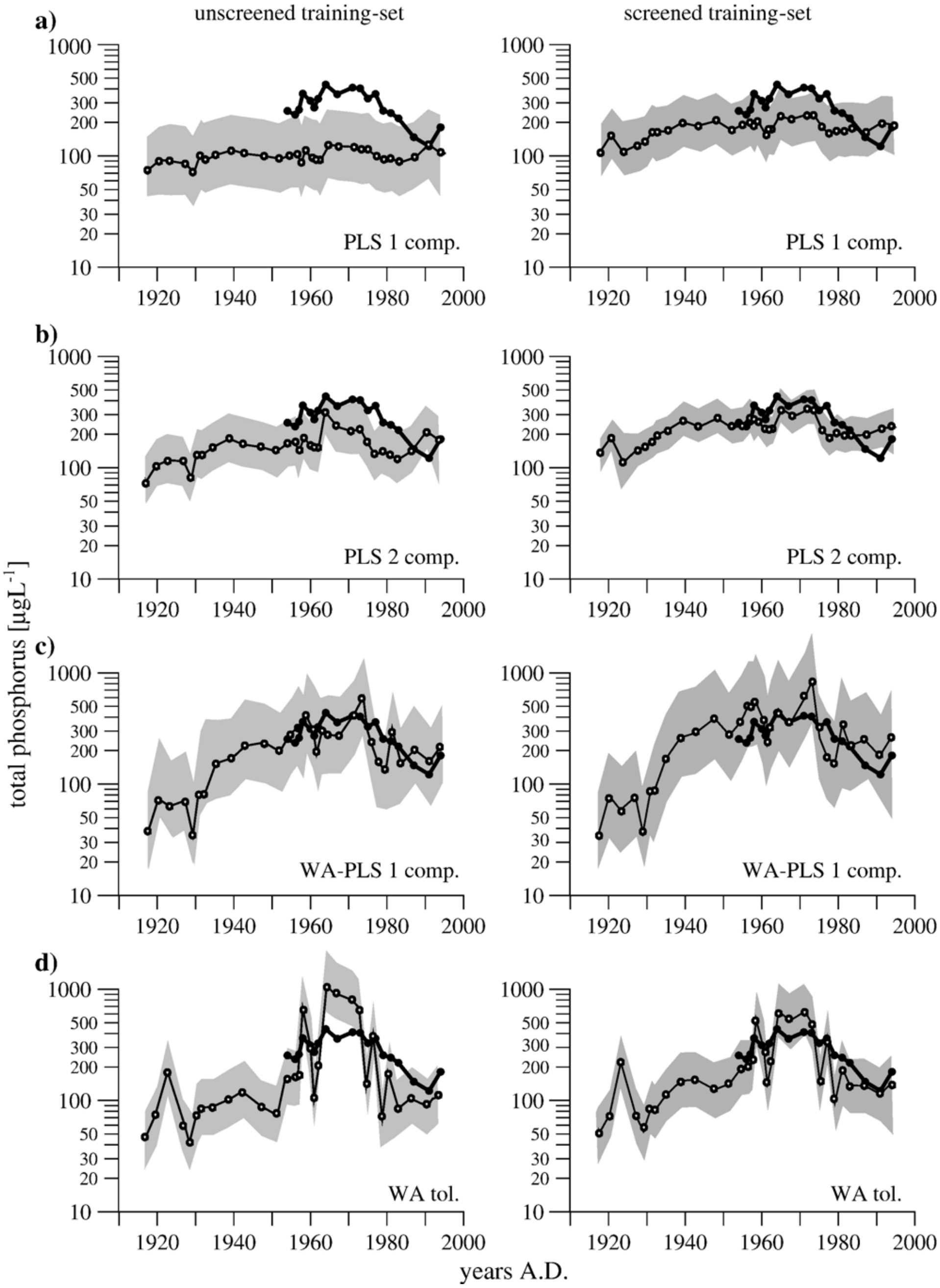

Fig. 8. Diatom-inferred total phosphorus with error bars, using the unscreened (left side) and the screened training-set (right side), using (a)+(b) partial least squares with one and two components (PLS 1 comp., PLS 2 comp.), (c) weighted averaging partial least squares with one component (WA-PLS 1 comp.) and (d) weighted-averaging with down-weighting of tolerances (WA tol.). Measured total phosphorus concentrations are indicated with filled circles.

fluence of this confounding variable. However, although elevation has no conditional effect with respect to covariables on the distribution of diatoms in the screened dataset the marginal effect (no covariables) and the correlation between elevation and log TP remained. Thus the modern distribution of diatoms is still influenced by elevation. One option to be tested could be the elimination of lakes until the marginal effect (no covariables) becomes insignificant. However, by applying the species–environment relation to a slices from a sediment core no guarantee exists that in the new context other environmental variables did not

Table 4
Evaluation of the performance of the screened and non-screened log TP models by comparison with measured data using partial least squares with one and two components (PLS 1 comp., PLS 2 comp.), weighted-averaging with down-weighting of tolerances (WAtol), and the weighted averaging partial least squares with one component (WA-PLS 1 comp.)

		RMSEE	$r^2_{\text{obs–inferred}}$	$\text{Slope}_{\text{obs–inferred}}$
Initial	PLS 1 comp.	0.47	0.03	0.06
Screened	PLS 1 comp.	0.22	0.14	0.15
Initial	PLS 2 comp.	0.28	0.15	0.29
Screened	PLS 2 comp.	0.14	0.30	0.32
Initial	WA-PLS 1 comp.	0.16	0.27	0.59
Screened	WA-PLS 1 comp.	0.18	0.29	0.67
Initial	WA tol	0.35	0.61	2.25
Screened	WA tol	0.22	0.63	1.62

Log TP inferences on varved sediments from Greifensee were compared with measured TP concentrations (1954–1994) by root mean square error of evaluation (RMSEE), r^2 and slope of the regression between observed and inferred TP.

change even more wildly than in your original training set. Past climate change could still result in spurious TP reconstructions.

Secondary gradients are not per se a problem because PLS and WA-PLS with several components can use secondary gradients to update species optima, with the restriction that they are orthogonal and hence uncorrelated to earlier PLS components (ter Braak et al., 1993). The elimination of lakes reduced the numbers of components which should be included in the model (Table 3). The PLS 2 comp. reconstruction using the initial training-set outperformed the PLS 1 comp reconstruction using the screened training-set in our case study. Nevertheless, the additional effect of elevation might not have been fully compensated by the inclusion of further components into the inference model, because it was not orthogonal to log TP. This could be one reason why the reduction of background variables had, next to the inclusion of additional components, an additional positive effect on the application of the log TP inference model (Table 4, Fig. 8). The log TP reconstructions using the screened training-set, where the influence of background variables was reduced, are better correlated with measured log TP when using weighted averaging with down-weighting of tolerances (Table 4).

Periphytic taxa become more important than planktonic taxa in lakes above 1000–1500 m a.s.l. (Lotter et al., 1997b). This change in life-form could be the reason that, after excluding lakes above 1543 m a.s.l., the conditional effect with respect to covariables of elevation was no longer significantly related to the distribution of taxa in our data-set. The initial training-set had 128 more diatom taxa than the screened training-set. These diatoms occurred only in the lakes at high elevation and low TP concentrations. Estimated TP optima of these 128 taxa are confounded by colder climate. Consequently, changes of fossil abundance of these taxa due to climatic cooling, would influence the TP reconstruction, although past trophic conditions might have changed independently of climate. As the screened data-set using WAtol reconstructed past trophic state in Greifensee better, it seems that the new estimated species responses (Figs. 4 and 6) towards log TP are less biased by background variables. One possible explanation that the exclusion of lakes only at the low end of the log TP gradient resulted in higher estimates for most optima for log TP (Fig. 6a) might be that the distribution of lakes along the log TP gradient changed. Weighted averaging is known to be sensitive to the distribution of the environmental variable in the training-set (ter Braak and Looman, 1986). However, the reconstructions using the screened data-set were not only higher, but also more closely correlated with the measured data, indicating that changing lake distribution was not the only reason why the screened model performed better in the reconstruction.

It was unexpected that the screened training-set, which performed better than the unscreened data-set when applied to fossil diatom assemblages of Greifensee would have a worse jackknifed error statistics. However, the improvement of the error statistics was not the main goal when the influence of background variables was reduced. This is the main difference to screening for outliers. While the removal of individual outliers can strengthen the established model, however reducing the influence of background variables changes the whole structure of the environmental variables, which thus results in a different inference model. The proportion of taxa with significant symmetric unimodal responses to log TP did not increase due to screening, which would improve the error statistics (Racca et al., 2003). The RMSEP and the jackknifed maximum bias increased for all models by the reduction of background variables. The ratio between RMSE and RMSEP is an indicator for the robustness of a training-set (Racca et al., 2003). According to the improvements of only the apparent error statistics, it seems that after the reduction of number of lakes the screened model is less robust. Therefore, it could be assumed that the reduction of the range of background variables reduced the applicability of the training-set. However, in varved sediments of the subalpine Seebergsee (1830 m a.s.l.) where a 300 year-long dominance of *S. parvus* was recorded (Hausmann et al., 2002), the log TP reconstructions using the initial and the screened training-set were unexpectedly highly correlated ($r = 0.98$) using a WA-PLS model with one component (S. Hausmann, unpublished data).

According to our results, it is advantageous to pay, next to the error-statistics, attention to the multivariate statistics of the training-set. In order to avoid overriding effect from pH, only lakes on calcareous bedrock were selected for the training-set. In addition to pH, climate is also an important background variable for a diatom-inference model for log TP and could have been considered for the selection of the sites to be sampled. The sampling of high-elevation lakes did not improve the log TP reconstruction of Seebergsee (1830 m a.s.l.) or Greifensee (435 m a.s.l.). If this is not possible a priori, because the training-set was designed for modeling several variables, then the approach presented here can be used to design a variable-specific calibration subset.

4.2. Diatom-inferred total phosphorus reconstructions and historical data from Greifensee (1916–1995)

We assume that the climatic signal recorded in Greifensee influenced the log TP reconstructions, since *S. parvus* had a lower estimated log TP optimum than *F. crotonensis* and climate explained the high frequency alternation between *S. parvus* and *F. crotonensis* better than the change of trophic state. The influence of climate on the diatom-inferred log TP seems to have been stronger before screening because the difference of estimated log TP optima of *S. parvus* and *F. crotonensis* was reduced by 50% due to the reduction of the influence of background variables. Our results showing that *S. parvus* seems to dominate in years with earlier spring overturn confirm the findings of Bradbury (1988), who noted a dominance of *Stephanodiscus* taxa from sediment traps with early spring overturn, and the results of Kilham et al. (1996), who described them as a low-light species. The varved sediments of Greifensee also were used to infer climate by δ^{18}O isotopes (McKenzie and Hollander, 1993). However, due to the superimposed eutrophication signal, McKenzie (1985) postulated that the isotope cycle could be influenced by the trophic state.

In 1916, at the beginning of varve formation in Greifensee, TP concentrations above 50 μg L^{-1} were inferred (Fig. 8). It can be assumed that the lake had lower TP concentrations before the formation of varves which were formed due to anoxic conditions. Analyses of sediment samples from the unlaminated earlier sediments are needed in order to estimate the natural conditions of Greifensee.

The increase of diatom-inferred log TP since 1930 (Fig. 8) coincides with increased concentrations of carotenoids in the sediments (Züllig, 1982) and could be explained by the increasing number of inhabitants within the catchment area (Pleisch, 1970).

The momentarily decrease of log TP in 1960, inferred with all models (Fig. 8), followed the beginning of phosphate precipitation in the sewage plant at 1959 in Uster, the biggest community in the lake catchment. However, in 1970 Greifensee was ranked as the most polluted lake in Europe. The diatom-inferred log TP decreased since 1975, which coincides with the decrease of carotenoids analysed from the sediments from 2.1 to 1.4 μg cm^{-2} between 1974 and 1977 (Züllig, 1982). This decrease of log TP and carotenoids coincides with the beginning of intensive fishstocking with whitefish. This first re-oligotrophication most likely reflects the loss of biomass in the lake by intensive harvesting (Niederer, Administration for Fishery and Hunting Zurich, personal communication). From 1977 onwards, the use of phosphates was restricted, which led to a reduced nutrient input in Greifensee.

At the time of coring, the rehabilitation of Greifensee was not yet complete, because in 2001, spring overturn TP concentrations were still around 80 μg L^{-1}, the lower 7 m of the water column were still anoxic and whitefish still did not reproduce in Greifensee (R. Buergi, EAWAG; personal communication). Another high resolution study of varved sediments, Seebergsee in the Swiss Alps, demonstrated that it took 88 years after the discharge of nutrients ceased before the lake recovered from its phosphorus load (Hausmann et al., 2002).

5. Conclusions

The reduction of the influence of background variables improved the reconstruction of log TP at Greifensee mainly for the method using weighted averaging with down-weighting of tolerances. The results of this case study could be used as a guideline for the design of further training-sets, by careful selection of lakes under the code of practice: Lakes should be placed equidistantly and cover a large range of the gradient of interest and a minimum range of other variables. The way data are collected should ideally be determined by the research objectives. A good sampling design can help in reducing costs and time (Jongman et al., 1987). It would be interesting to apply this approach of reducing the variation of background variables to other more complex training-sets, which have resulted from merging regional training-sets for TP, such as European Diatom

Database (EDDI), which includes Scandinavian lakes with higher DOC levels than the Alps. The approach may also be of potential interest for large merged datasets with marine samples which derive from very heterogeneous environments (De Vernal et al., 2001).

For the definition of background conditions and the progress of re-oligotrophication in Greifensee, sediments representing the undisturbed lake are needed. The analysed sediment core did not entirely cover that period. However, according to oxygen and fish data, trophic state prior to 1916 was not yet reached at the time of coring.

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