

1 Supplementary information (SI) for: Consistent stoichiometric
 2 long-term relationships between nutrients and chlorophyll-a
 3 across lakes

4 Daniel Graeber Mark J. McCarthy Tom Shatwell Dietrich Borchardt
 5 Erik Jeppesen Martin Søndergaard Torben L. Lauridsen
 6 Thomas A. Davidson

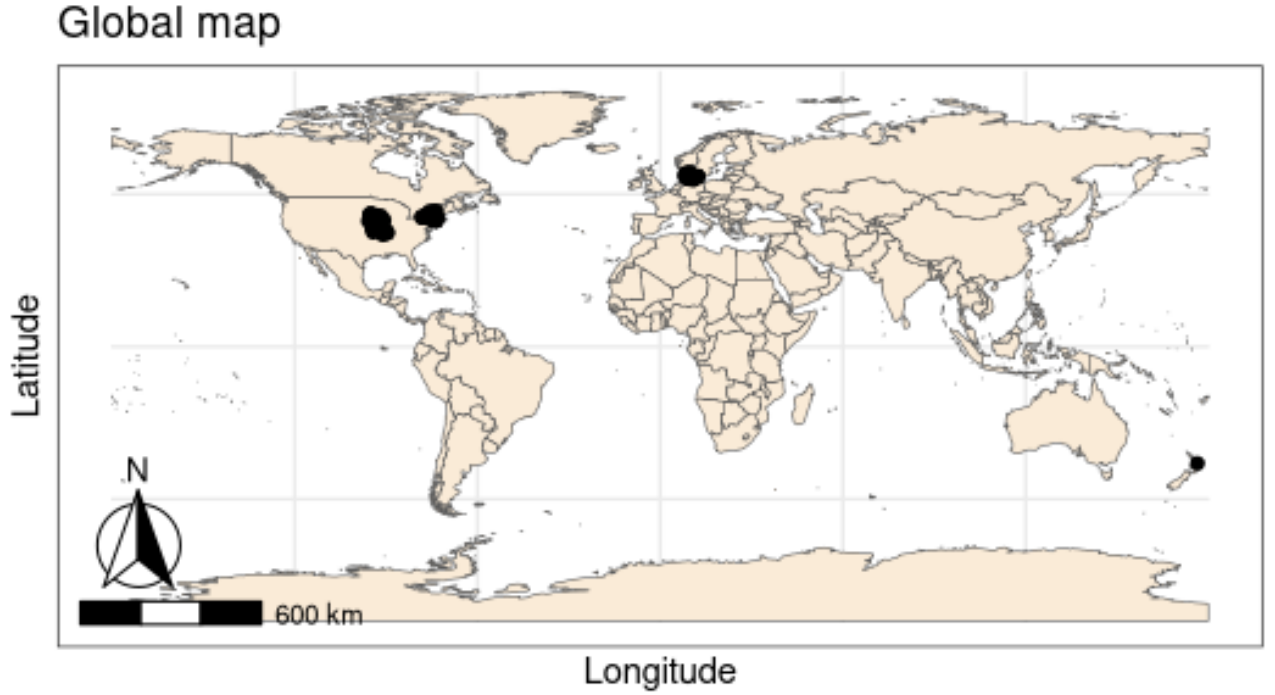
7 **Table of contents**

8	1 Position of study lakes	3
9	2 Description of data-analysis steps	3
10	3 Approach to extract short-term and long-term signals using simple moving aver-	
11	ages	6
12	3.1 Choice of simple moving averages	6
13	3.1.1 How to extract of long-term and short-term signals from time series data using	
14	simple-moving averages	6
15	3.2 Choice of lengths of simple moving averages	6
16	3.3 Approaches to test the usability of simple moving averages and the SAD approach to	
17	assess their ideal length	7
18	3.4 Why we analysed simple moving averages with a hierarchical bootstrap approach . . .	7
19	4 Simulations of the simple-moving average approach	8
20	4.1 Simulation of a long-term signal	8
21	4.1.1 Generating the long-term signal	8
22	4.1.2 Estimating the ideal simple moving average length	8
23	4.1.3 Reconstructing the long-term signal in the relationship between x and y	10
24	4.1.4 Assessing whether we falsely detect a systematic short-term signal	12
25	4.2 Simulation of a short-term signal combined with a long-term signal	12

26	4.2.1	Generating the signals	12
27	4.2.2	Estimating the ideal simple moving average length	13
28	4.2.3	Reconstructing the long-term and short-term signal in the relationship between	
29		x and y	13
30	5	Selecting the best simple-moving average length for the lake data	17
31	6	Selecting the best regression models	18
32	6.1	Choosing the type of regression model	18
33	6.2	Choice of model terms	18
34	7	Separate analyses of the correlation between nutrients and Chl-a for the Danish	
35		dataset and global data	20
36	8	Model intercepts and slopes	22
37	8.1	Slopes, 5-year simple moving averages and residuals	22
38	8.1.1	TN model slopes	22
39	8.1.2	TP model slopes	23
40	8.1.3	Additive model slopes	24
41	8.2	Intercepts, 5-year simple moving averages and residuals	25
42	8.2.1	TN model intercepts	25
43	8.2.2	TP model intercepts	26
44	8.2.3	Additive model intercepts	27
45	9	Random average dataset TN and TP concentrations versus average random dataset	
46		TN:TP	28
47	10	Data and code availability	28
48		References	28

1 Position of study lakes

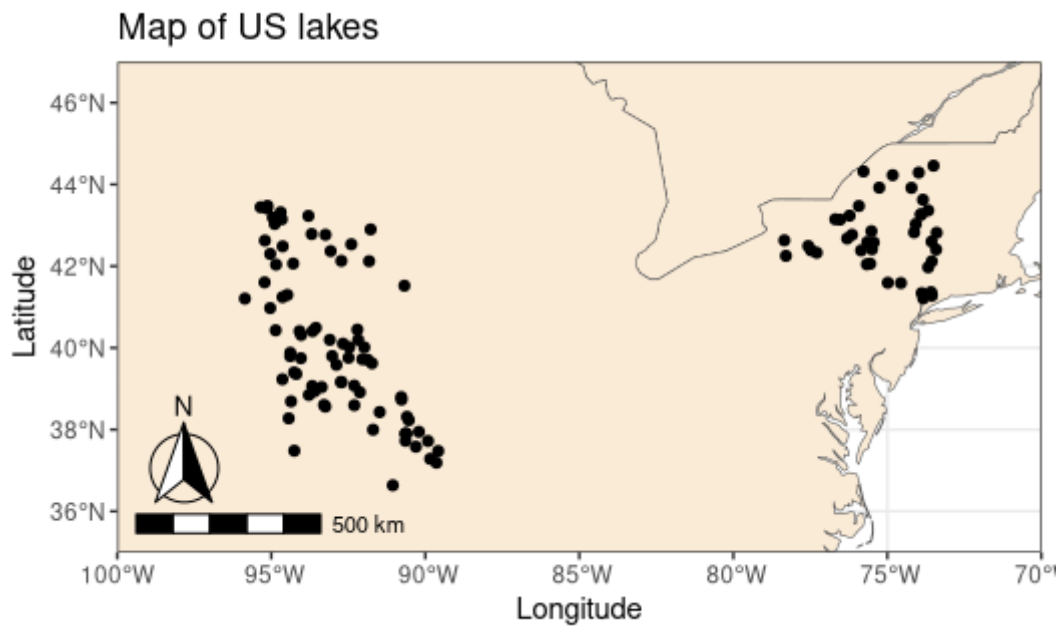
The shallow lakes (avg. depth < 6m) which contained sufficient data (five or more consecutive growing seasons with at least three observations per growing season) to calculate 5-year simple moving averages (SMA) were unevenly distributed globally (SFig. 1), with only one lake in New Zealand, and most lakes in the USA (SFig. 2), and in Denmark (SFig. 3).



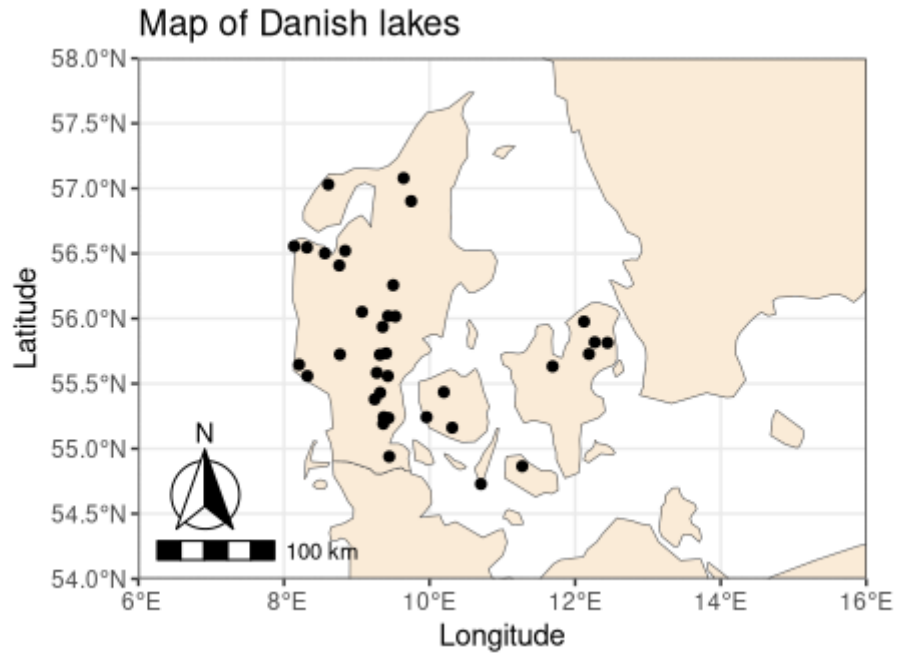
SFig. 1: Global map of lakes with 5-year simple moving average data. Lakes with sufficient data are situated in the US, Denmark and New Zealand.

2 Description of data-analysis steps

Here, we give a short rundown of the data-analysis steps (SFig. 4). In step 1, all possible moving averages are calculated for each lake, in step 2 all moving average data is combined. In step 3, the TN:TP ratio windows are defined with a minimum of \ln molar TN:TP of 0 and a maximum of \ln molar TN:TP of 7, a window width of \ln molar TN:TP of 3 and a step of 0.1 \ln molar TN:TP. The ratio windows are overlapping, hence, each data point can be drafted in multiple windows (step 3). These TN:TP ratio windows are applied to the data in step 4 (in this example a \ln molar TN:TP between 2 and 5). All data filtered in step 4 is then bootstrapped at the lake level (randomly sampled with replacement, step 5a) and one observation for each randomly sampled lake is picked at random (step 5b).



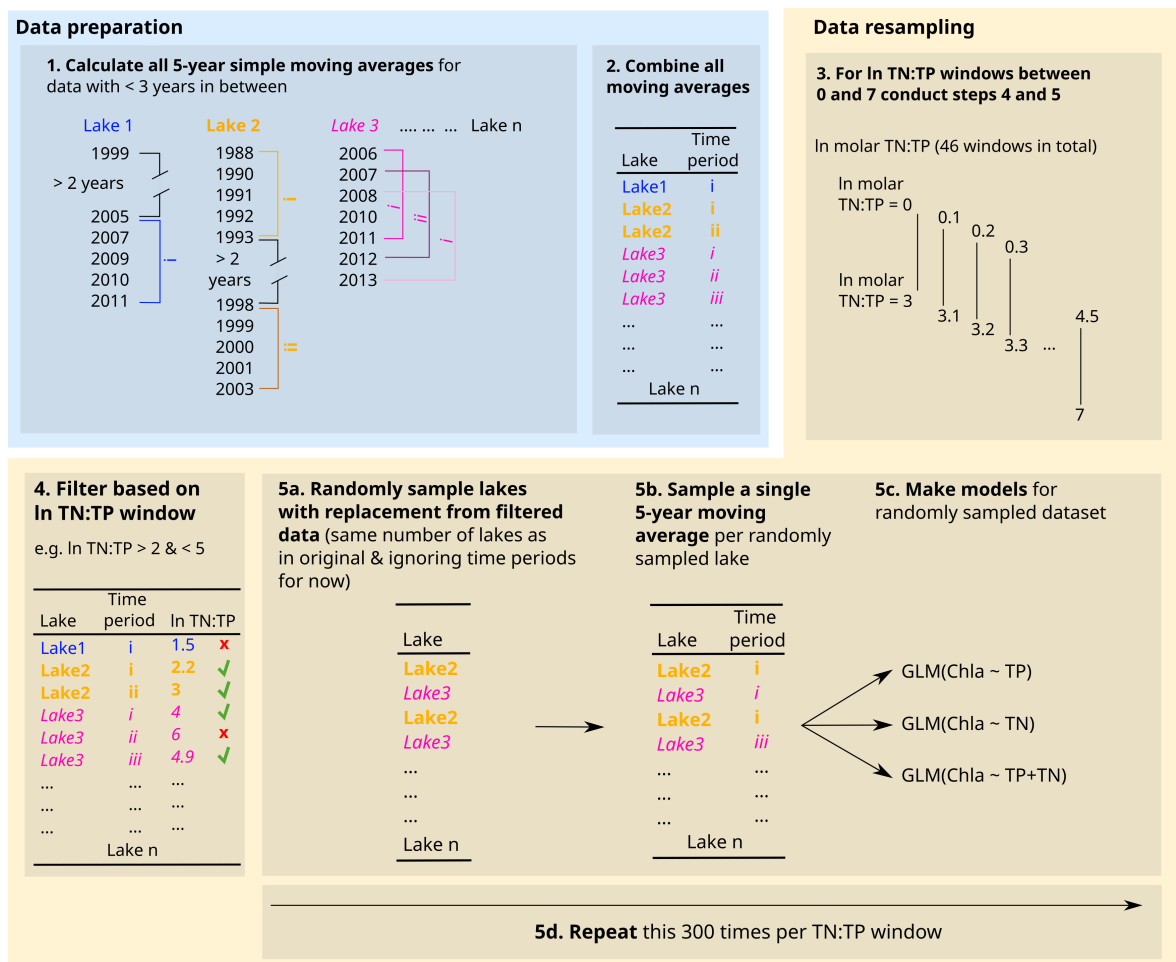
SFig. 2: Map of US lakes with 5-year simple moving average data.



SFig. 3: Map of Danish lakes with 5-year simple moving average data.

64 This hierarchical bootstrap approach is the best way to reflect the structure of the original data. A
65 simple, non-hierarchical bootstrap would favor lakes with more five-year means over lakes with less
66 five-year means, simply because these make up a larger part of the data. Furthermore, sampling
67 without replacement at lake level would result in five-year means from lakes with few data dominating
68 the produced random dataset, as every lake would be sampled every time which then would result in
69 high model leverage of five-year means from lakes with only few data. In contrast, the hierarchical
70 procedure ensures that every lake has the same chance to end up in the randomly sampled bootstrap,
71 in the second step it ensures that for each sampled lake, every five-year mean has the same chance to
72 end up in the random dataset. These notions are in agreement with the findings of an assessment on
73 how to properly resample hierarchical data by non-parametric bootstrap.¹

74 For the generated random sample, three generalized linear models are calculated and kept, if the
75 models converged (step 5c). This is done repeatedly (300 times, step 5d) for the data of each TN:TP
76 ratio window to find all or most of the possible random combinations of lakes, with the aim to calculate
77 the error of the model estimates (pseudo R^2 , AIC, intercept and slopes are used in the study).



SFig. 4: A conceptual depiction of the data-analysis steps conducted within the study.

78 **3 Approach to extract short-term and long-term signals using** 79 **simple moving averages**

80 **3.1 Choice of simple moving averages**

81 We chose to use SMAs to extract the short-term and long-term signals, because these are easy to
82 compute and understand, because this approach compares well to more complex methods for long-
83 term signal prediction.² Finally, we chose SMAs because short-term signals can easily be extracted by
84 using their residuals, which is commonly done in e.g. economics, and has already once been done in
85 limnology.³

86 **3.1.1 How to extract of long-term and short-term signals from time series data using** 87 **simple-moving averages**

88 The SMA should contain the long-term signal and the residuals of the SMA should contain the short
89 term signal. The SMA residuals are calculated as *observation* − *SMA* for a given time point, e.g. an
90 SMA for the years 2010 - 2015 would be positioned in 2013, and this SMA would be subtracted from
91 the original observation of 2013.

92 Please note that only SMAs with odd numbers should be chosen if the SMA residual extraction
93 should work. For even numbers, the time point of the SMA will not be an integer and the short-term
94 observation cannot be aligned correctly (e.g., for a 4-year SMA from 2010 - 2014, the mean of the
95 SMA would be the year 2012.5, which makes alignment of single-year observations impossible).

96 **3.2 Choice of lengths of simple moving averages**

97 Methods to extract different signals for different ranges of time series require to define the length of
98 the signal to be extracted. SMAs are no exception to this rule. Here, an earlier study proposed to use
99 a version of Akaike's information criterion, however, this approach gives one value for each time series,
100 and the authors found the results of their approach highly variable depending on the individual time
101 series.² Furthermore, this approach compares the predictive capability for different simple moving
102 average lengths,² instead we wanted to have the ideal length at which a long-term signal could be
103 extracted if it existed.

104 To detect the ideal simple moving average length, we chose to use the sum of absolute differences
105 (SAD) between single-growing season values and SMAs. The SAD for a time series with a given
106 simple moving average length is calculated as:

$$SAD = \sum_{i=1}^k |SMA_i - \text{growing season observation}_i| \quad (1)$$

Here, i is the year and k is the length of the time series. For each year i , the absolute difference between growing season observation (the mean of all values for a growing season) and value of the simple-moving average for the same year is calculated.

3.3 Approaches to test the usability of simple moving averages and the SAD approach to assess their ideal length

To test the capabilities of our SAD approach to calculate the best length for SMAs, and for SMAs to extract short-term and long-term signals from a time series in which systematic variation and random variation are mixed, we used two simulations and came to the following conclusions:

1. We could find the ideal simple moving average length and reconstruct a systematic long-term signal from a time series with random long-term random noise. Details on the simulation are found below (Section 4.1).
2. If a short-term signal of a correlation between nutrients and chlorophyll a would have been contained in addition to the long-term signal, we also likely would have found it, as we show with a second simulation. Details on the simulation are found below (Section 4.2).

Since the SAD approach worked well with simulated data, we applied it to real time series from our lakes, and show that 5-year SMAs are a good trade-off between simple moving average length and data availability (Section 5).

3.4 Why we analysed simple moving averages with a hierarchical bootstrap approach

SMAs have the drawback that they are a kind of auto-regressive model, where past data points and future data points affect the current value of the simple moving average^[2], potentially affecting results of the regressions between nutrients and Chla. To account for this, we randomized data used for the correlations with the hierarchical bootstrap procedure described in Section 2 and shown conceptually in SFig. 4. Based on this approach, on average, only one observed simple moving average is picked from each lake, and, on average, each lake only appears only once in the dataset, making any effects of SMAs of the same time series interfering with each other impossible (SFig. 4). The same is true for the residuals of the SMAs.

4 Simulations of the simple-moving average approach

4.1 Simulation of a long-term signal

4.1.1 Generating the long-term signal

We mixed two signals, a long-term signal containing a perfect linear correlation between two variables to which we added a short-term signal, with different random noise for the two variables. Ideally we should be able to extract the linear correlation coefficients again from this mix, when using SMAs and the SAD approach.

First we created a long-term signal for a time series with 50 time points (resembling years), a variable x (could be e.g. a nutrient) and a variable y (could be phytoplankton biomass), which is dependent on x .

Here, variable x was created as:

$$x = (\cos(\pi * time_{1,2,...,50}/25) * 2) + 3 \quad (2)$$

where time is an integer from 1 to 50. With that, the long-term signal has a period length of 50, and a simple moving average with a length of 25 should be able to capture it again. The cosine results were multiplied by 5 to which a constant of 3 was added to for better looking positive numbers.

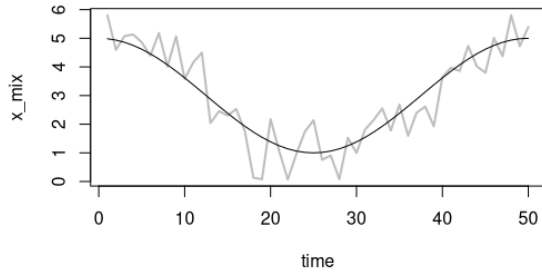
Variable y was then calculated with a linear model:

$$y = 1 + x * 0.5 \quad (3)$$

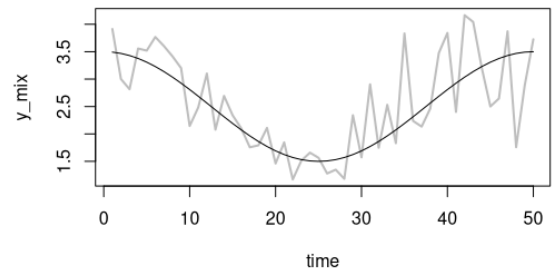
Subsequently, we added random noise from a normal distribution to x and y , using the `rnorm` function with 50 samples in R with a mean = 0 and SD = 0.5 to create two independent random normal distributions, which we added to x and y . The results of the simulation establishment can be seen in SFig. 5. Without the random noise inserted by the normal distributions, $r^2 = 1$, slope = 0.5, and intercept = 1 for the correlation between x and y . By adding the random noise, the r^2 between x and y is lowered to 0.52, and the intercept and slope are changed randomly (intercept = 1.46, slope = 0.37). The scatter plot reveals clear variability around the linear model line (SFig. 5c).

4.1.2 Estimating the ideal simple moving average length

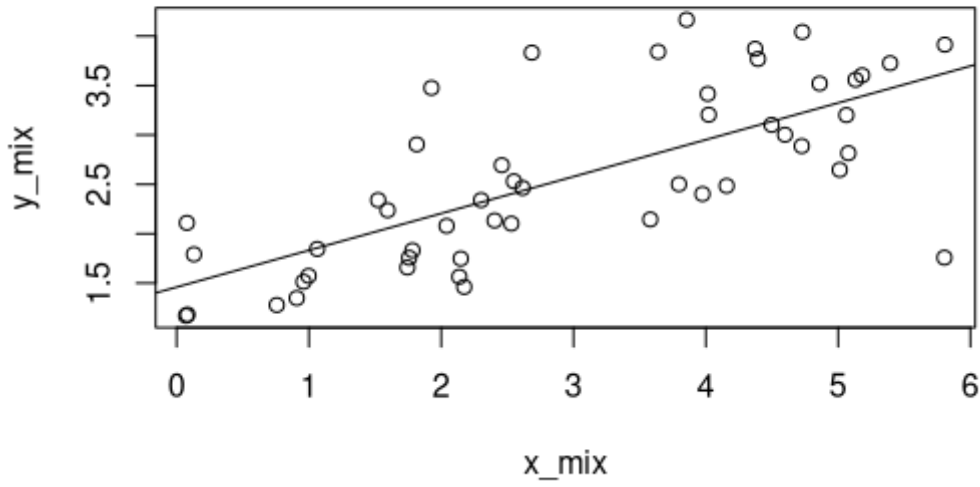
We calculated the SAD for simple-moving average lengths of $k = 2 - 40$ (k equals the number of time steps) for the simulated x and y . In our simulations, we always see the unimodal pattern appearing for the SAD (SFig. 6a, SFig. 6b), where the SMA at the very lower end of the SAD incline capture



(a) x time series



(b) y time series



(c) Linear regression between randomized x and y

SFig. 5: Long-term signal (black line) and long-term plus randomized short-term signal for variable x and y (grey line), and linear regression between randomized variables x and y.

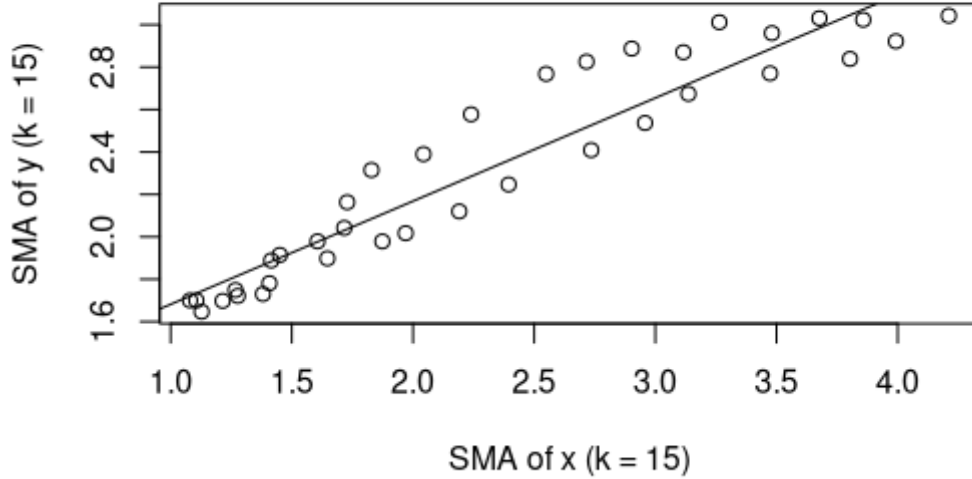
160 still considerable short-term variation, and the SMA shortly before, at or after the SAD peak remove
 161 part of the long term signal (SFig. 6c, SFig. 6d). We, recommend using the SMA in the middle of
 162 the SAD incline, clearly before the SAD peak. In this case we chose the SMA with $k = 15$ (here one
 163 could also use 13 or 17), which largely follows the long-term signal without capturing too much of the
 164 random short term signal (SFig. 6c, SFig. 6d).

165 4.1.3 Reconstructing the long-term signal in the relationship between x and y

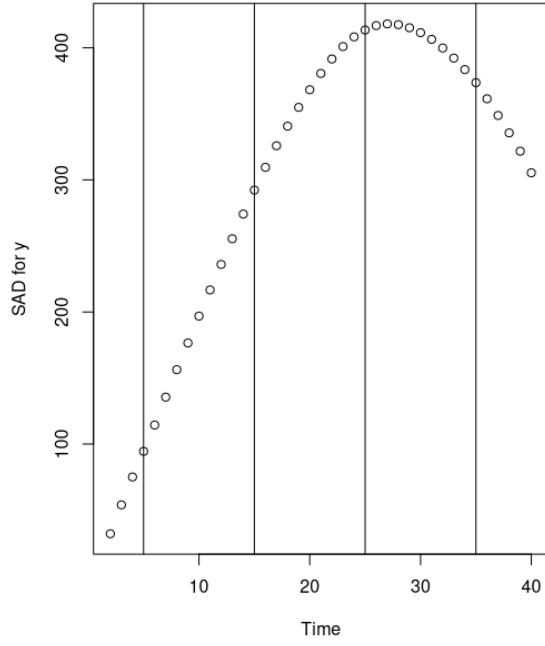
166 We chose SMA with $k = 15$ (SFig. 6c, SFig. 6d) and found that the correlation of the SMA of x and y
 167 improved ($r^2 = 0.9$) (SFig. 7) relative to the correlation of the x and y with random noise ($r^2 = 0.52$)
 168 also reported in Section 4.1.1 (and shown in SFig. 5c).

169 Then, we tested whether we could reconstruct with the SMA data the original slope and intercept of
 170 the linear model for x and y defined in Equation 3. For the linear regression SMA of x and y with $k =$
 171 15, we found a slope = 0.49 and an intercept = 1.19. This was close to the slope = 0.5 and intercept
 172 = 1 of the original linear model (Equation 3), and much closer than the slope = 0.37 and intercept =
 173 1.46 of the regression of x and y with random noise (SFig. 5c).

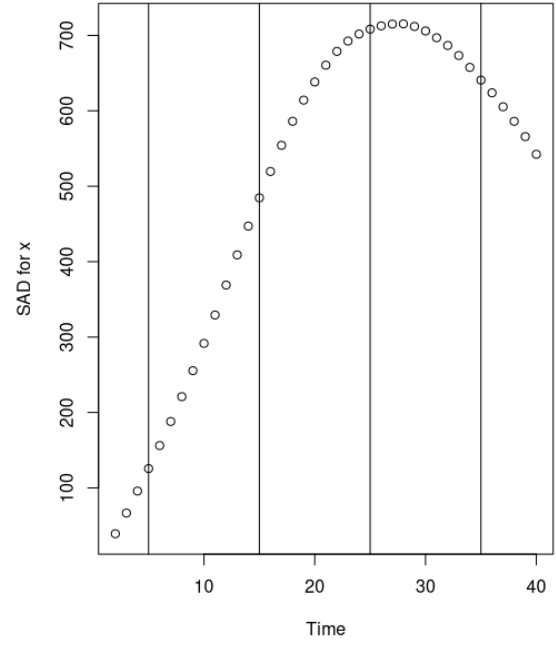
174 We conclude that can find an appropriate SMA length. With that we can successfully reconstruct
 175 long-term signals in the correlation of two variables, such as TN and Chla or TP and Chla.



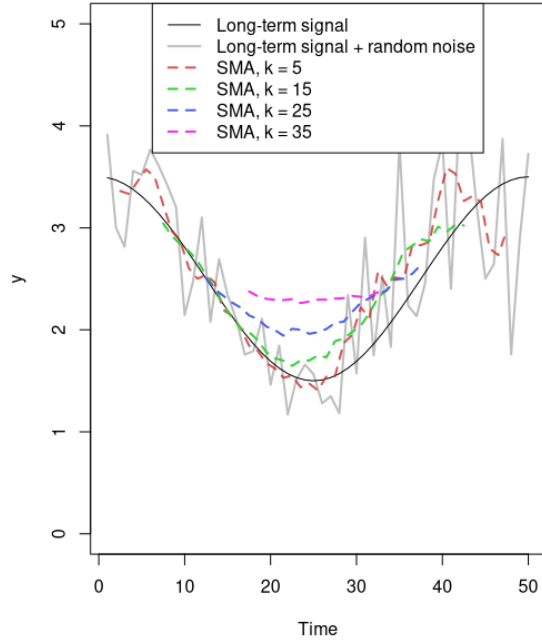
SFig. 7: Linear regression between SMAs with length (k) = 15 of x and y



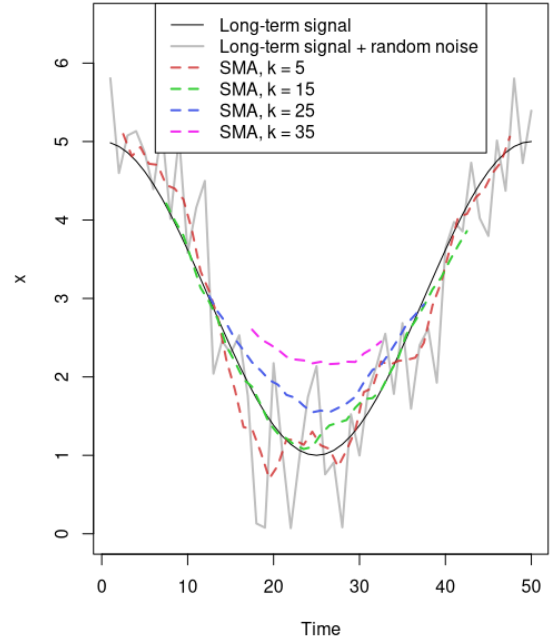
(a) SAD for different SMAs of y (vertical lines)



(b) SAD for different SMAs of x (vertical lines)



(c) y time series with SMA of different length k



(d) x time series with SMA of different length k

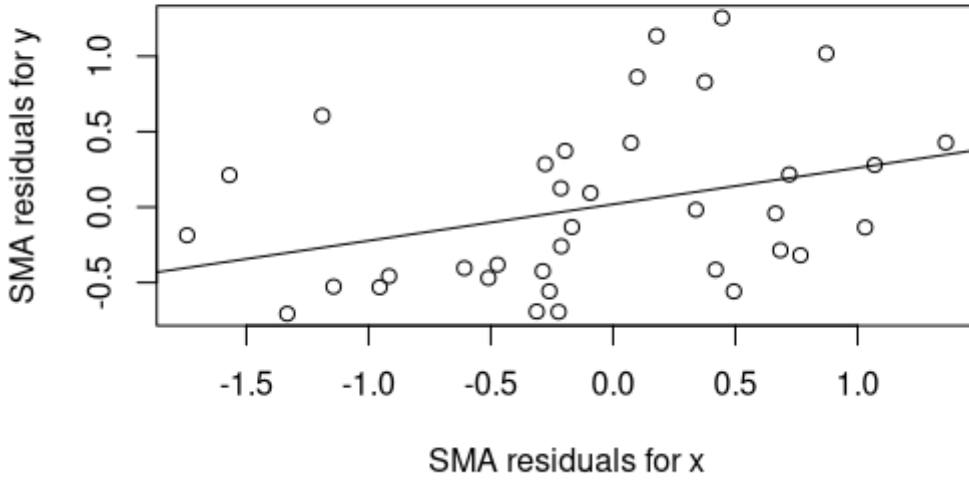
SFig. 6: Sums of absolute differences (SAD) for y and x , as well as plots containing the long-term signal, the randomized long-term signal, and simple moving averages (SMAs) of different lengths (k).

176 4.1.4 Assessing whether we falsely detect a systematic short-term signal

177 Since we only included a random short-term signal, the residuals of SMA with $k = 15$ should only
178 provide random noise for the correlation between x and y . Here, the residuals were calculated as
179 simulated x and y (with random noise) minus the SMA of x and y (see for details)

180 For linear regression of the SMA residuals of x and y , the $r^2 = 0.1141812$, and the scatter plot also
181 indicates no signal of a regression (SFig. 8)

182 This analysis shows that our approach does not falsely detect a short-term signal.



SFig. 8: Scatter plot of x and y residuals, calculated from the simulated x and y minus the SMA ($k = 15$) of x and y

183 4.2 Simulation of a short-term signal combined with a long-term signal

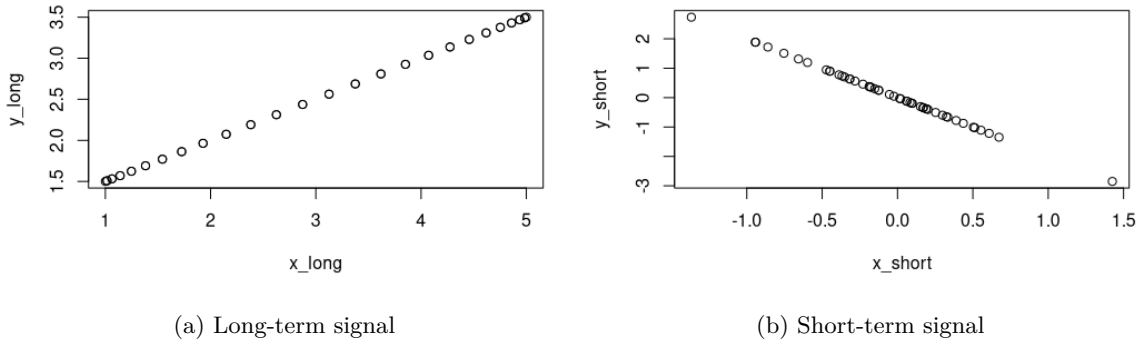
184 Above we show that we can successfully reconstruct a long-term signal and do not falsely detect a
185 short-term signal (Section 4.1).

186 Here, we assess whether we would also detect a short-term signal if it existed in the data using the
187 SMA calculation and residual calculation already described above. Please see our approach descrip-
188 tion above for further details (Section 3) and the long-term simulation for a more detailed example
189 (Section 4.1) of the approach.

190 4.2.1 Generating the signals

191 We again used the long term relationship between x and y as described in Section 4.1.1. Specifically,
192 we calculated the long-term signal (x_{long} and y_{long}) based on Equation 2 and Equation 3 (SFig. 9a).

193 To this, we added a short-term signal for x (x_{short}) and y (y_{short}) based on a regression with a negative
 194 slope. To achieve this, we first created a single normal distribution $N_{short} = N(0, 0.5)$ with 50 values
 195 (one for each time step). Then we calculated $x_{short} = -1 * N_{short}$ and $y_{short} = 2 * N_{short}$, giving an
 196 intercept = 0 and a slope = -2 for the regression between x_{short} and y_{short} (SFig. 9b).
 197 We combined the short-term and long-term signal as $x_{mix} < -x_{short} + x_{long}$ (SFig. 10a) and $y_{mix} <$
 198 $-y_{short} + y_{long}$ (SFig. 10b). The mixed signals x_{mix} and y_{mix} exhibited only a weak relationship
 199 (SFig. 10c).



SFig. 9: Scatter plot of x and y for the long-term and short-term signal

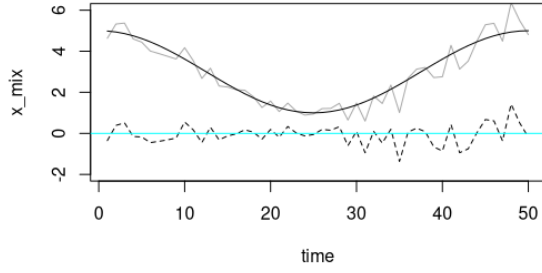
200 4.2.2 Estimating the ideal simple moving average length

201 The ideal SMA length is again approximately $k = 15$, as with longer SMAs, the long-term variation gets
 202 dampened, and shorter SMAs (here $k = 5$) remove less short-term variation (SFig. 11c & SFig. 11d).
 203 On the SAD curve a SMA with $k = 15$ is on the middle of the incline before the SAD peak (SFig. 11a
 204 & SFig. 11b)

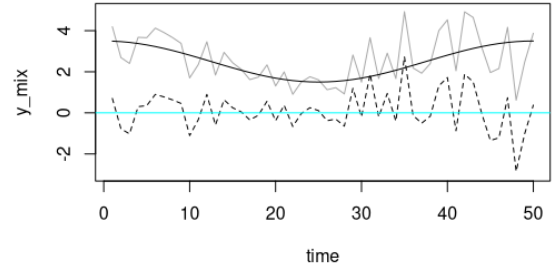
205 4.2.3 Reconstructing the long-term and short-term signal in the relationship between 206 x and y

207 Neither the short nor the long signal was visible in the mixed signal ($r^2 = 0.06$) (SFig. 10c). However,
 208 the long-term signal could be reconstructed to a large extent using SMAs. Here, the SMA with $k =$
 209 15 gave a $r^2 = 0.76$ for the regression between x and y (SFig. 12), and we estimated an intercept =
 210 1.22 and a slope = 0.51, which is close to the actual intercept of 1 and slope = 0.5 of the regression
 211 between x_{long} and y_{long} .

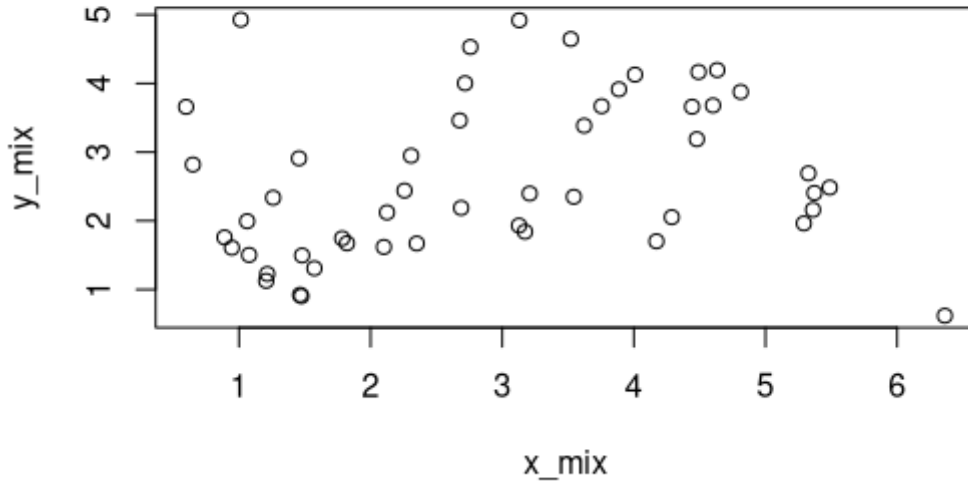
212 We could also reconstruct the short term signal with a $r^2 = 0.83$ (SFig. 13). Here, regressing the SMA
 213 residuals yielded an intercept = -0.22 and slope = -1.88 between x and y , which is reasonably close to
 214 the true slope = -2 and intercept = 0 of x_{short} and y_{short} .



(a) x time series

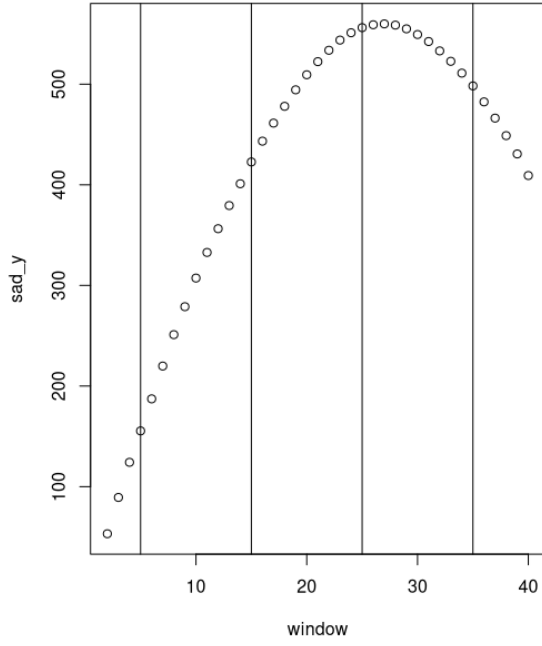


(b) y time series

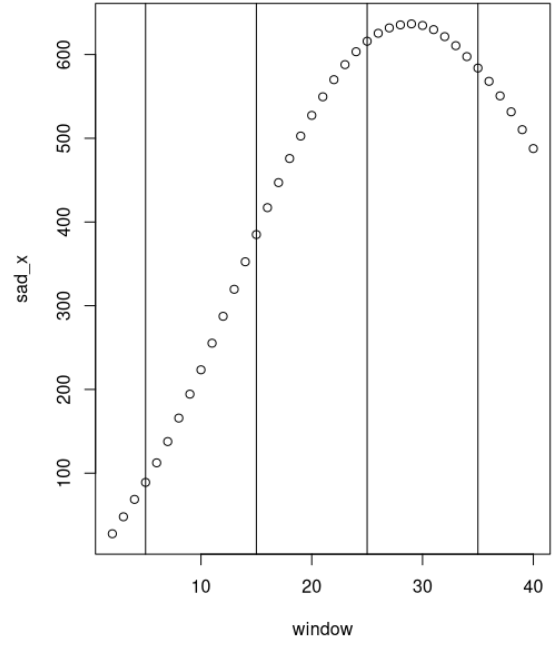


(c) Linear regression between mixed signals of x and y

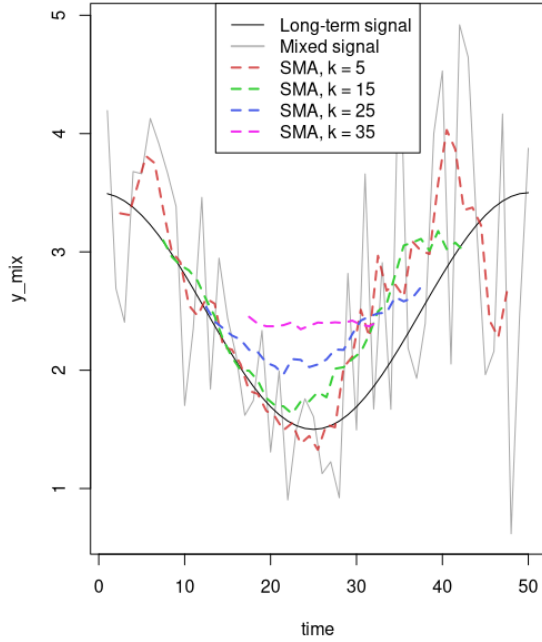
SFig. 10: Long-term signal (black line), short-term signal (black, dashed line) and mixed signal (grey line) for variable over time, and linear regression between mixed signals of x and y.



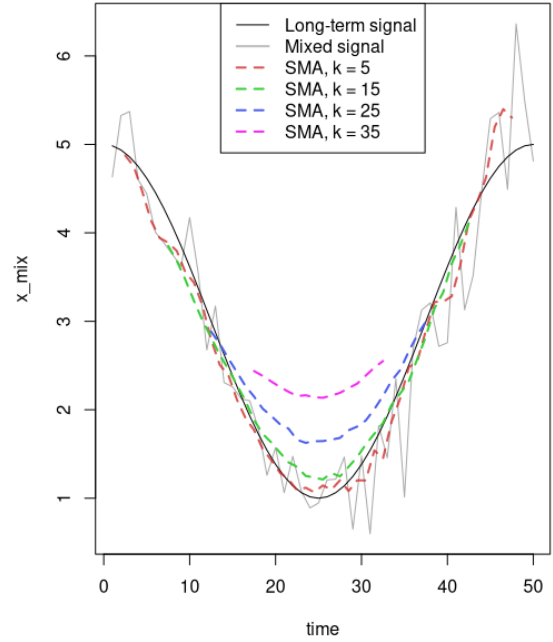
(a) SAD for different SMAs of y (vertical lines)



(b) SAD for different SMAs of x (vertical lines)



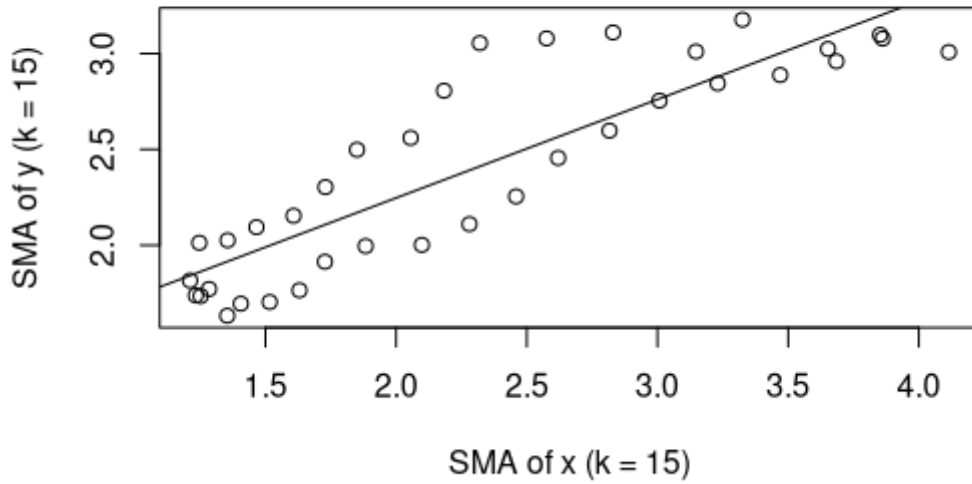
(c) y time series with SMA of different length k



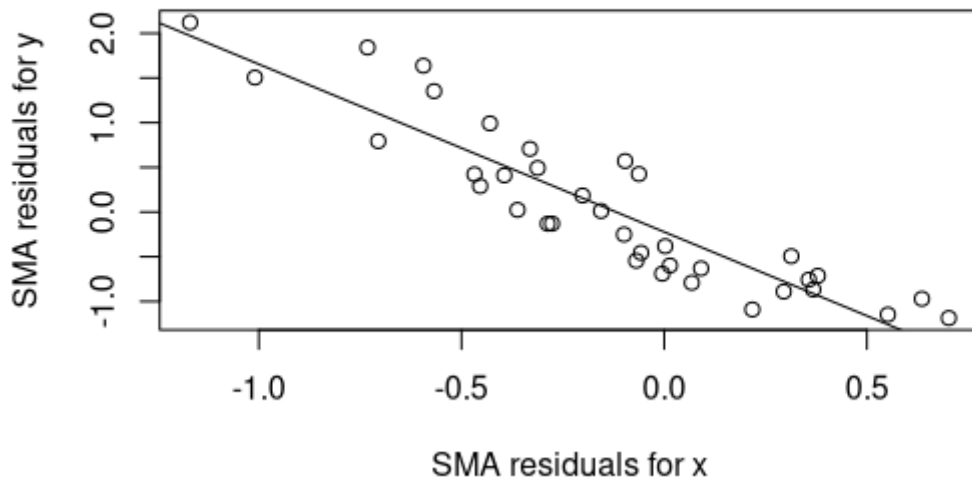
(d) x time series with SMA of different length k

SFig. 11: Sums of absolute differences (SAD) for y and x , as well as plots containing the long-term signal, the randomized long-term signal, and simple moving averages (SMAs) of different lengths (k).

215 We conclude that our approach can reconstruct mixed short-term and long-term signals in the regres-
 216 sion of two variables. This strongly suggests that our approach would have found a short-term signal
 217 of the relationship between nutrients and Chla, if it existed.



SFig. 12: Linear regression between SMAs with length (k) = 15 of x and y

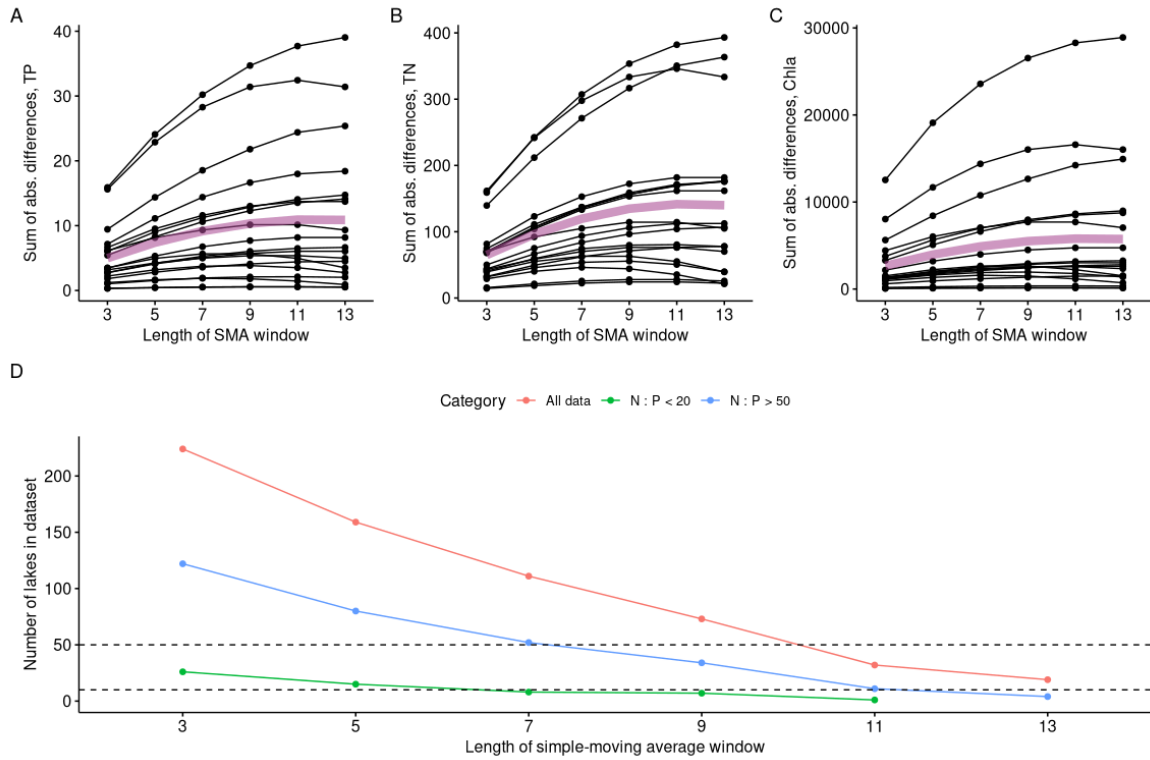


SFig. 13: Scatter plot of x and y SMA residuals, calculated from the simulated x and y minus the SMA ($k = 15$) of x and y

5 Selecting the best simple-moving average length for the lake data

We use the SAD approach described above (Section 3.2) to select the ideal SMA length for the real lake data. As can be seen in the simulations with a only long-term, or a mixed long-term and short-term signal, the ideal SMA length – i.e. the SMA length where the short-term variation is largely removed, but the long-term variation is not dampened – is at the range of SAD before the peak but not at the lower end of the incline (see SMA plots of simulation results in Section 4.1.2 and Section 4.2.2).

The SAD of the real lake data shows exactly the same pattern as the simulated data with an increase, peak and subsequent decrease with longer SMAs. Here the average SAD peak was at an SMA length of 7 to 11 years, but some time series already showed a decline in SAD with SMA lengths of more than 7 years (SFig. 14). We therefore considered a 5-year SMA to be ideal, as this was still on the ascent of the SAD for all time series. A 5-year SMA also allowed us to retain a relatively high number of shallow lakes (SFig. 14).



SFig. 14: Sums of absolute differences (SAD) TP (A), TN (B) and Chla (C), and number of lakes in the dataset dependent on length of SMA for all data, observations with TN : TP < 20, and observations with TN : TP > 50 (D).

6 Selecting the best regression models

6.1 Choosing the type of regression model

We chose generalised linear models with a Gamma link function instead of simple linear models for the 5-year SMAs because Chl-a concentrations best followed a Gamma distribution. In contrast, the residuals of the SMAs best followed a Normal distribution. We assessed this using the `fitdistrplus` package in R,⁴ where we tested how well normal, log-normal and gamma distributions fit the data. We kept the descriptor variables as they were, so we did not apply any data transformations (log or otherwise). In both cases we used the GLM function from the GLM package in Julia, with a Gamma link function for the 5-year SMAs and a Normal link function for the SMA residuals. A Normal link GLM is equivalent to a linear model. However, we used the GLM function in both cases for maximum comparability.

6.2 Choice of model terms

To find the models that parsimoniously explained Chl-a concentrations, we used Akaike's information criterion (AIC)⁵. Here, we compared one-way models with TN or TP concentrations as explanatory variables for Chl-a concentrations with either additive models containing both TN and TP, or with models containing both TN and TP and an interaction term between TN and TP.

Due to the nature of the data, we calculated thousands of AIC values over the range of molar TN:TP ratios. To compare AIC values, we were not interested in their absolute values, but in the reduction of AIC by the models. To assess this, we calculated the delta AIC (ΔAIC) between models, i.e. the change in AIC by adding or removing model terms. To test the improvement in AIC for the additive models, we calculated two ΔAIC for each sample. To compare the TN+TP additive models with the TP only models, we calculated $\Delta AIC_{TP \text{ vs } TN+TP}$ as follows:

$$\Delta AIC_{TP \text{ vs } TN+TP} = AIC_{TP \text{ model}} - AIC_{TN+TP \text{ model}} \quad (4)$$

Similarly, we calculated the $\Delta AIC_{TN \text{ vs } TN+TP}$ as:

$$\Delta AIC_{TN \text{ vs } TN+TP} = AIC_{TN \text{ model}} - AIC_{TN+TP \text{ model}} \quad (5)$$

To compare the additive models (TN + TP) and models with interaction (TN * TP), we also calculated the $\Delta AIC_{TN+TP \text{ vs } TN*TP}$ for each random sample:

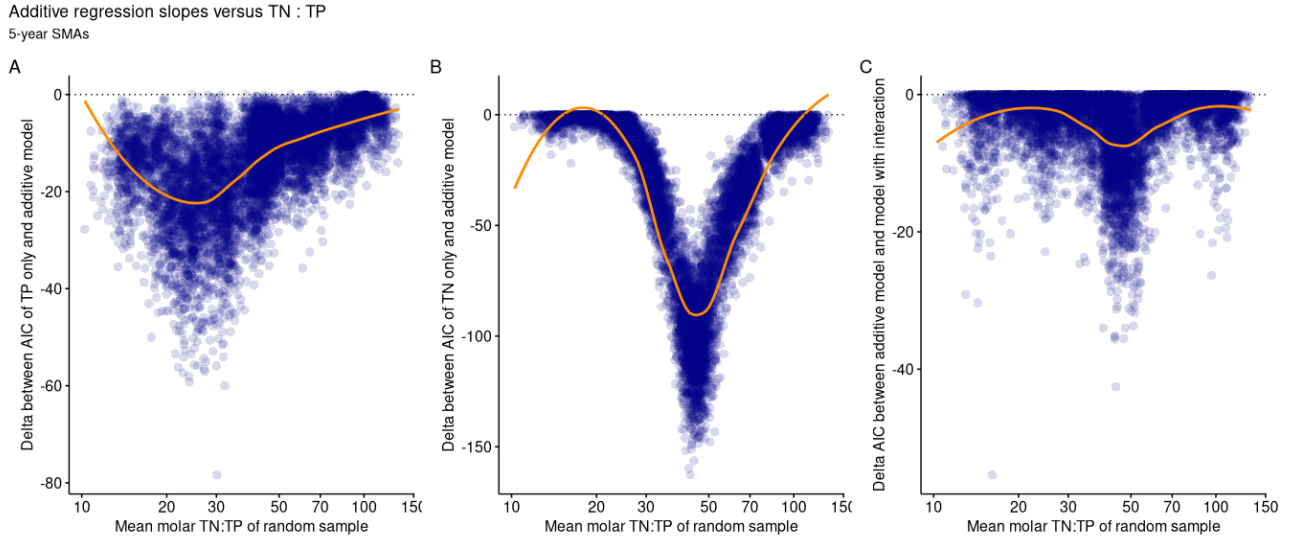
$$\Delta AIC_{TN+TP \text{ vs } TN*TP} = AIC_{TN+TP \text{ model}} - AIC_{TN*TP \text{ model}} \quad (6)$$

Here, a negative ΔAIC indicates a reduction in the AIC, i.e. less information is lost and the model explains the data better while being parsimonious. A ΔAIC at or above zero indicates no improvement in the model.

If we plot the $\Delta AIC_{TP \text{ vs } TN+TP}$ calculated by Equation 4 against the mean molar TN:TP of the random samples for the 5-year SMAs used in the study, we find considerable variation in the response. In particular, for TN:TP < 40, we find that almost all model solutions have a negative $\Delta AIC_{TP \text{ vs } TN+TP}$ (SFig. 15 A). For the $\Delta AIC_{TN \text{ vs } TN+TP}$ calculated by Equation 5, we find a clear negative deviation from zero, around TN : TP = 50 (SFig. 15 B).

The distribution of ΔAIC along the TN : TP axis further supports the idea in the main text that TN and TP affected Chla differently along the TN : TP axis, and that their effects on Chla complement each other in the additive model with TN + TP.

The use of an interaction term did not improve the model quality, as indicated by the lack of deviation of $\Delta AIC_{TN+TP \text{ vs } TN*TP}$ from zero (calculated by Equation 6, SFig. 15 C).

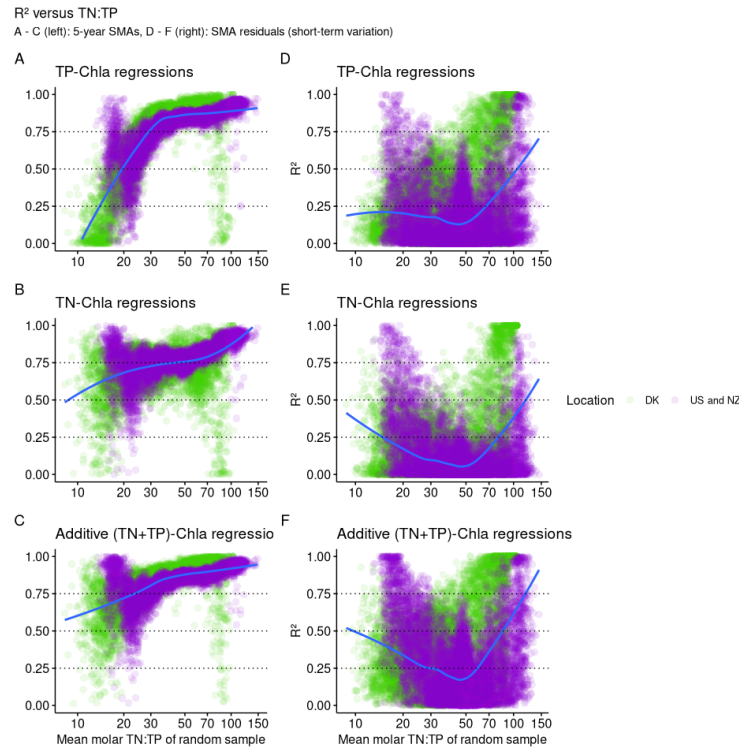


SFig. 15: Results on Delta AIC for TP-only models versus additive models (panel A) or TN-only models versus additive models (panel B), and for the Delta AIC between additive models and models with interaction term between TN and TP (panel C). The models were constructed for the 5-year simple moving averages (SMAs), therefore for lakes with 5 or more years of consecutive data. Positive values indicate an increase of the AIC (hence reduced model quality), negative values indicate a decrease of the AIC (hence increased model quality). See also Section 2 for details on the statistical approach. The darker the points, the more overlapping solutions were found for the R^2 by the bootstrap procedure. The orange line is the average response, based on a LOESS function.

7 Separate analyses of the correlation between nutrients and Chl-a for the Danish dataset and global data

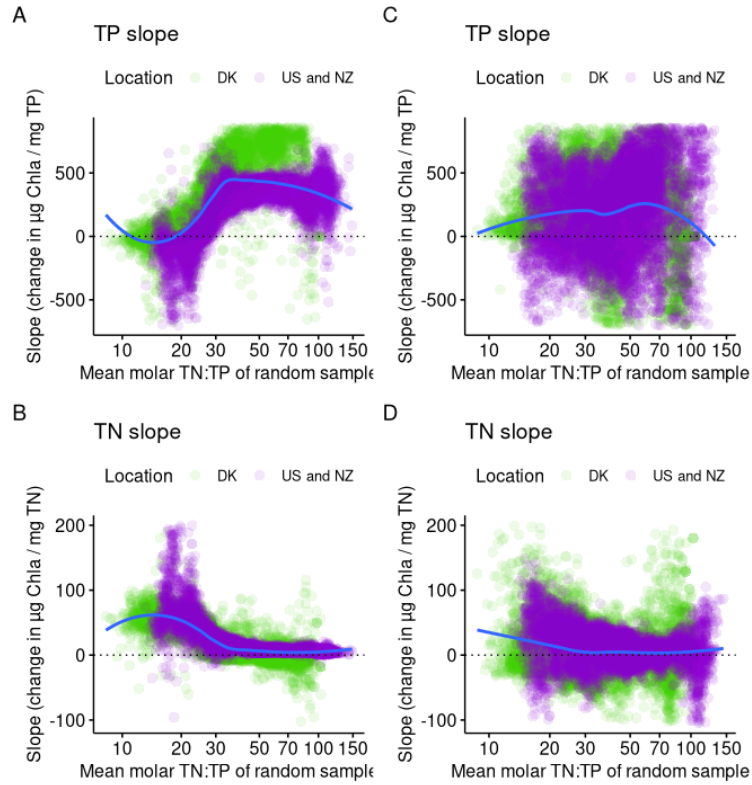
To check whether the Danish dataset (Aarhus University, Danish Centre for Environment, <https://odaforalle.au.dk>) and global dataset⁶ revealed the same response of Chl-a to TN or TP at the same TN:TP ratios, we conducted a separate analysis of the 5-year SMAs for both datasets using exactly the same statistical approach as for the entire dataset. As for the full dataset, the SMAs were randomly combined using the hierarchical bootstrap procedure (Section 2).

The separate analysis reveals two things. Due to the lower number of data within the separate analysis, the patterns are linked to somewhat higher uncertainty, hence higher variability of the model results on the y axis (SFig. 16, SFig. 17). Still the two datasets give the exactly same answer as the full dataset presented in the main text for the pattern of R^2 (SFig. 16) and slope (SFig. 17) along the TN : TP axis.



SFig. 16: Explained variance (R^2) of generalized linear models for the long-term variation based on 5-year simple moving average (SMA) (A - C), and the short-term variation based on the SMA residuals. Shown are results from generalized-linear models with Gamma distributions for 5-year SMAs, and linear models with Normal distribution SMA residuals between total phosphorus (TP, mg / L, panel A) and/or total nitrogen (TN, mg / L, panel B) and chlorophyll a (Chl-a, μg / L). These are plotted against the mean molar TN : TP of each of randomly sampled dataset. The darker the points, the more overlapping solutions were found for the R^2 by the bootstrap procedure (indicating the error of the R^2). The orange line is the average response based on a LOESS function.

Additive model (TN+TP-Chla) slopes versus TN:TP
A & B (left): 5-year SMAs, C & D (right): SMA residuals (short-term variation)

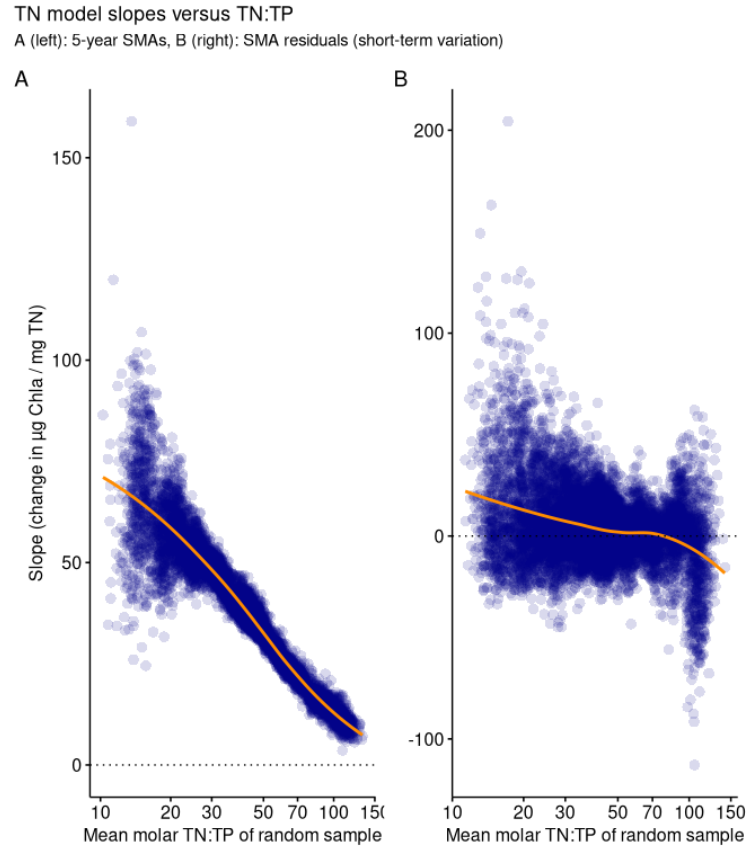


SFig. 17: Slopes of the additive models for long-term variation based on 5-year simple moving averages (SMA) (A & B) or short-term variation contained within SMA residuals (C & D) versus the mean molar TN : TP of each randomly sampled dataset. Shown are slopes from additive models between total phosphorus (TP, mg / L, panel A, C) or total nitrogen (TN, mg / L, panel B, D) and chlorophyll a (Chla, µg / L) versus the mean molar TN : TP of each of randomly sampled dataset. The darker the points, the more overlapping solutions were found for the slopes by the bootstrap procedure (indicating the error of the slopes). The orange line is the average response, based on a LOESS function. For easier comparison, we used the same y-axis range for the TP slopes of the 1-year SMA and SMA residuals, which removed 942 or extreme values for TP slopes of the the SMA residuals (see SI for full plot). Hence, $N = 8252$ iterations or $n = 9142$ for the TN slopes or the TP slopes of the 5-year SMAs, respectively (A & B); and $n = 12858$ or $n = 13800$ iterations for the TP and TN slopes of the SMA residuals, respectively (C & D).

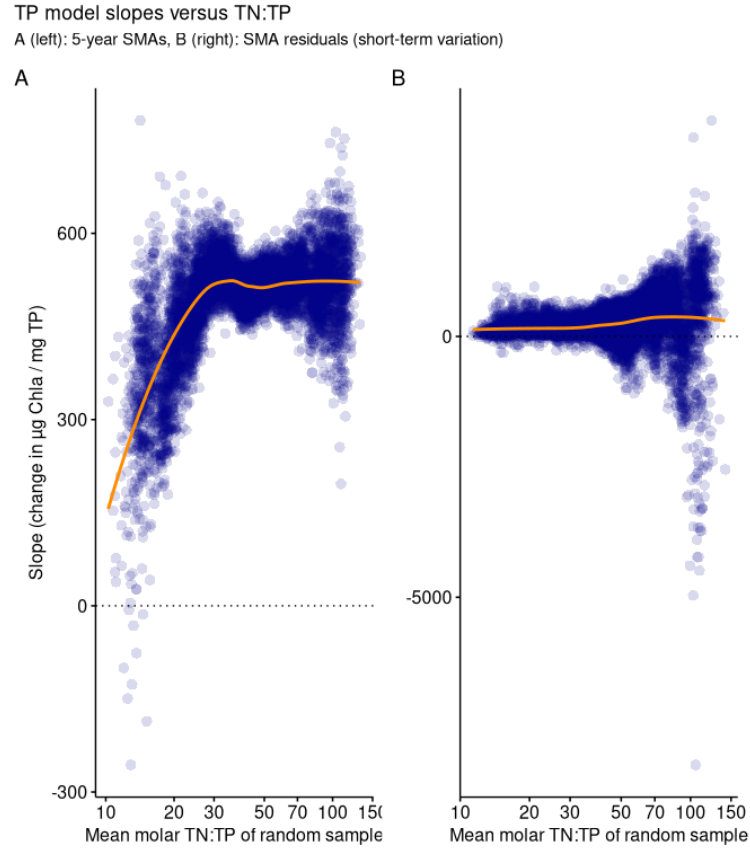
281 8 Model intercepts and slopes

282 8.1 Slopes, 5-year simple moving averages and residuals

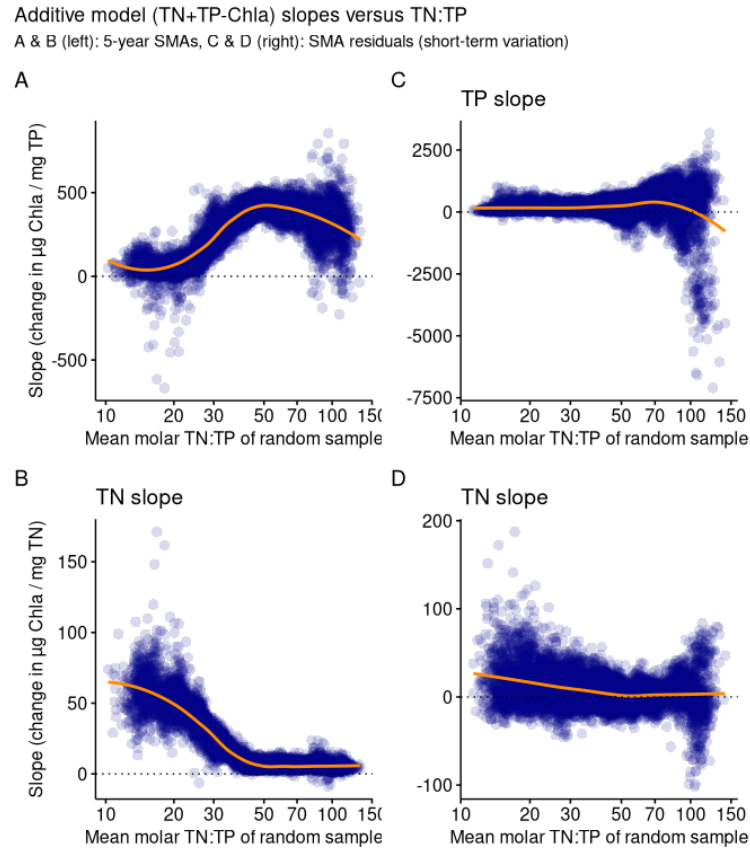
283 8.1.1 TN model slopes



SFig. 18: Slopes of the TN models for long-term variation based on 5-year simple moving averages (SMA) (A) or short-term variation contained within SMA residuals (B) versus the mean molar TN : TP of each randomly sampled dataset. Shown are TN model between total nitrogen (TN, mg / L , panel B, D) and chlorophyll a (Chla, $\mu\text{g} / \text{L}$) versus the mean molar TN : TP of each of randomly sampled dataset. The darker the points, the more overlapping solutions were found for the slopes by the bootstrap procedure (indicating the error of the slopes). The orange line is the average response, based on a LOESS function.



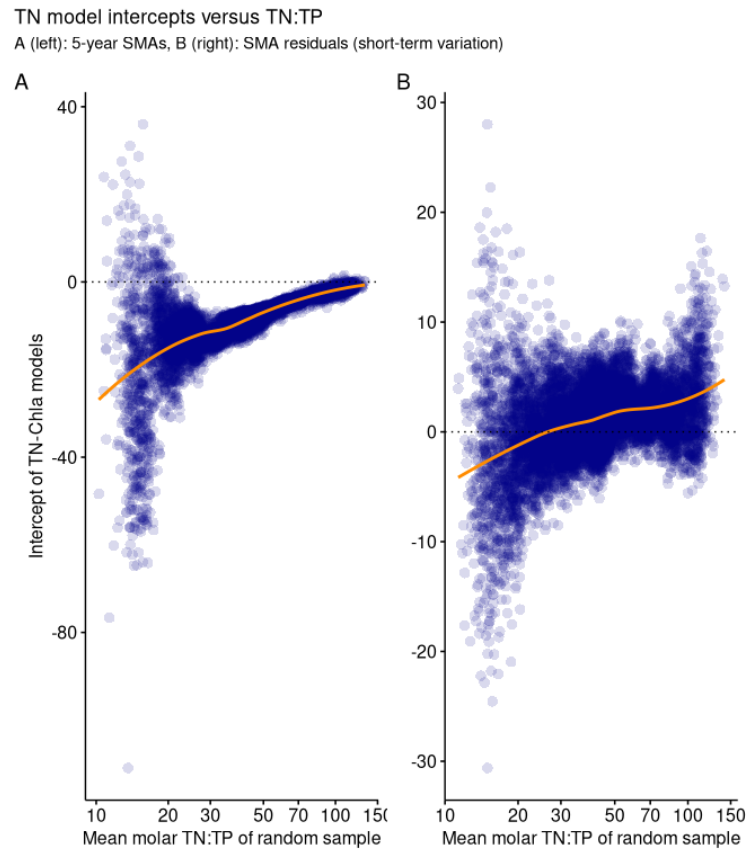
SFig. 19: Slopes of the TP models for long-term variation based on 5-year simple moving averages (SMA) (A) or short-term variation contained within SMA residuals (B) versus the mean molar TN : TP of each randomly sampled dataset. Shown are TP model slopes between total nitrogen (TP, mg / L, panel B, D) and chlorophyll a (Chla, $\mu\text{g} / \text{L}$) versus the mean molar TN : TP of each of randomly sampled dataset. The darker the points, the more overlapping solutions were found for the slopes by the bootstrap procedure (indicating the error of the slopes). The orange line is the average response, based on a LOESS function.



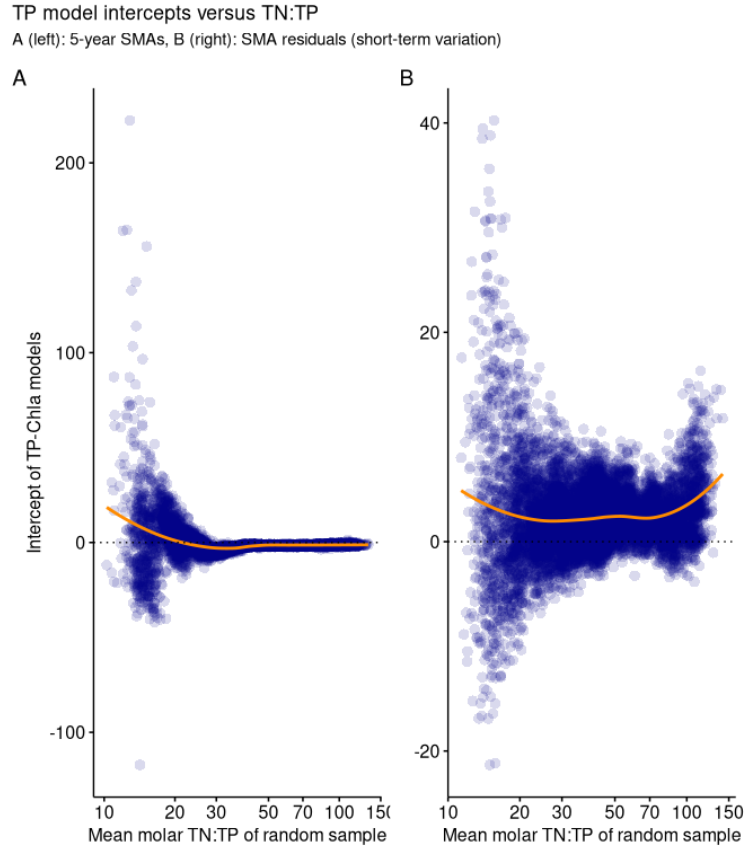
SFig. 20: Slopes of the additive models for long-term variation based on 5-year simple moving averages (SMA) (A & B) or short-term variation contained within SMA residuals (C & D) versus the mean molar TN : TP of each randomly sampled dataset. Shown are slopes from additive models between total phosphorus (TP, mg / L, panel A, C) or total nitrogen (TN, mg / L, panel B, D) and chlorophyll a (Chla, $\mu\text{g} / \text{L}$) versus the mean molar TN : TP of each of randomly sampled dataset. The darker the points, the more overlapping solutions were found for the slopes by the bootstrap procedure (indicating the error of the slopes). The orange line is the average response, based on a LOESS function.

286 8.2 Intercepts, 5-year simple moving averages and residuals

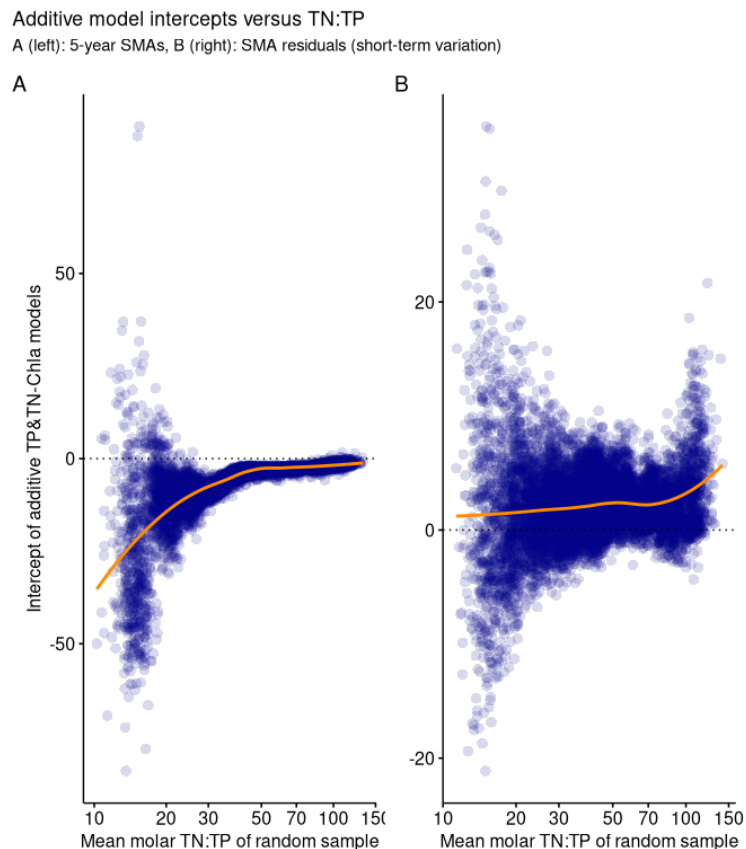
287 8.2.1 TN model intercepts



SFig. 21: Intercepts of the TN models for long-term variation based on 5-year simple moving averages (SMA) (A) or short-term variation contained within SMA residuals (B) versus the mean molar TN : TP of each randomly sampled dataset. Shown are TN model intercepts between total nitrogen (TN, mg / L, panel B, D) and chlorophyll a (Chla, μg / L) versus the mean molar TN : TP of each of randomly sampled dataset. The darker the points, the more overlapping solutions were found for the intercepts by the bootstrap procedure (indicating the error of the intercepts). The orange line is the average response, based on a LOESS function.

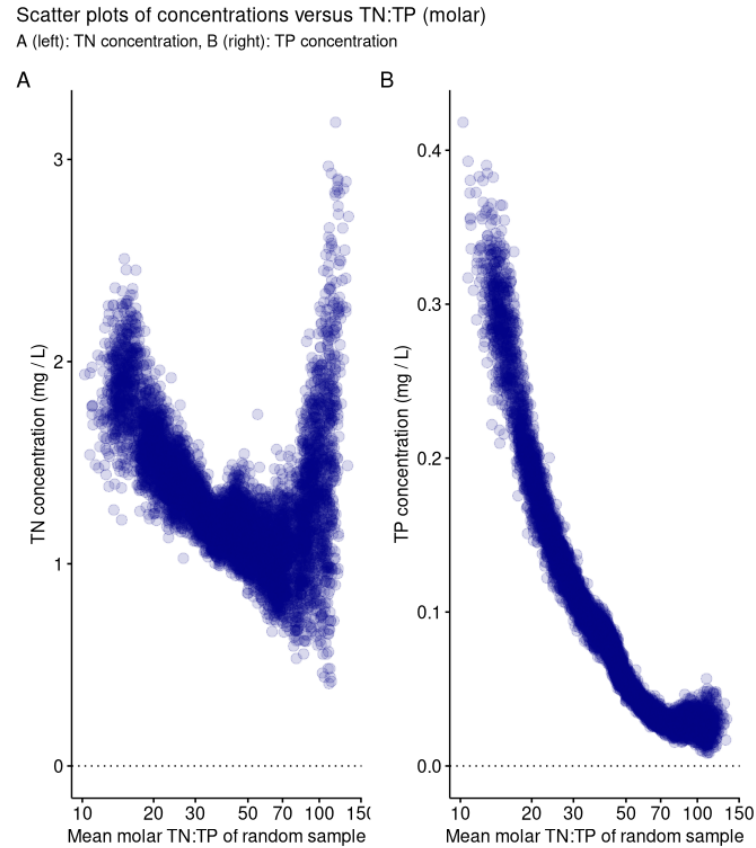


SFig. 22: Intercepts of the TP models for long-term variation based on 5-year simple moving averages (SMA) (A) or short-term variation contained within SMA residuals (B) versus the mean molar TN : TP of each randomly sampled dataset. Shown are TN model intercepts between total nitrogen (TP, mg / L, panel B, D) and chlorophyll a (Chla, μg / L) versus the mean molar TN : TP of each of randomly sampled dataset. The darker the points, the more overlapping solutions were found for the intercepts by the bootstrap procedure (indicating the error of the intercepts). The orange line is the average response, based on a LOESS function.



SFig. 23: Intercepts of the additive models for long-term variation based on 5-year simple moving averages (SMA) (A & B) or short-term variation contained within SMA residuals (C & D) versus the mean molar TN : TP of each randomly sampled dataset. Shown are intercepts from additive models between total phosphorus (TP, mg / L, panel A, C) or total nitrogen (TN, mg / L, panel B, D) and chlorophyll a (Chla, μg / L) versus the mean molar TN : TP of each of randomly sampled dataset. The darker the points, the more overlapping solutions were found for the intercepts by the bootstrap procedure (indicating the error of the intercepts). The orange line is the average response, based on a LOESS function.

9 Random average dataset TN and TP concentrations versus average random dataset TN:TP



SFig. 24: Scatter plots of TN (panel A) and TP (panel B) concentrations versus TN:TP ratios for the 5-year SMA. The less transparent the points, the more overlapping data are displayed.

10 Data and code availability

Links to used open-access software, all code developed for this study, as well as all data used in this study are available here: <https://git.ufz.de/graeber/long-term-nutrient-chla-links-shallow-lakes>. All code developed for this study is published under the BSD-3-Clause License (allowing open access and free software usage with full recognition of the original copyright).

References

1. Ren, S. *et al.* [Nonparametric bootstrapping for hierarchical data](#). *Journal of Applied Statistics* **37**, 1487–1498 (2010).
2. Svetunkov, I. & Petropoulos, F. [Old dog, new tricks: A modelling view of simple moving averages](#). *International Journal of Production Research* **56**, 6034–6047 (2018).

- 302 3. Carpenter, S. R. & Leavitt, P. R. [Temporal Variation in a Paleolimnological Record Arising](#)
303 [from a Trophic Cascade](#). *Ecology* **72**, 277–285 (1991).
- 304 4. Delignette-Muller, M. L. & Dutang, C. [Fitdistrplus: An R Package for Fitting Distributions](#).
305 *Journal of Statistical Software* **64**, 1–34 (2015).
- 306 5. McElreath, R. *Statistical Rethinking: A Bayesian Course with Examples in R and Stan*. (CRC
307 Press, 2018).
- 308 6. Filazzola, A. *et al.* [A database of chlorophyll and water chemistry in freshwater lakes](#). *Scientific*
309 *Data* **7**, 310 (2020).