

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

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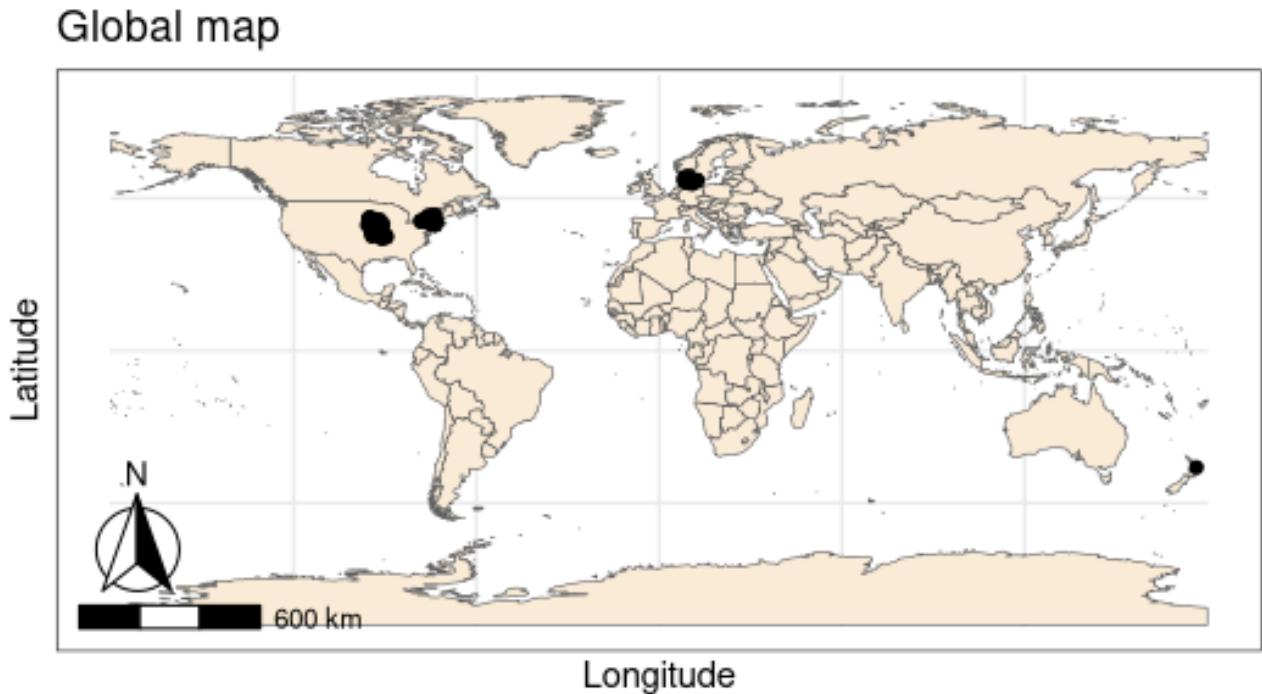
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## 49 1 Position of study lakes

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

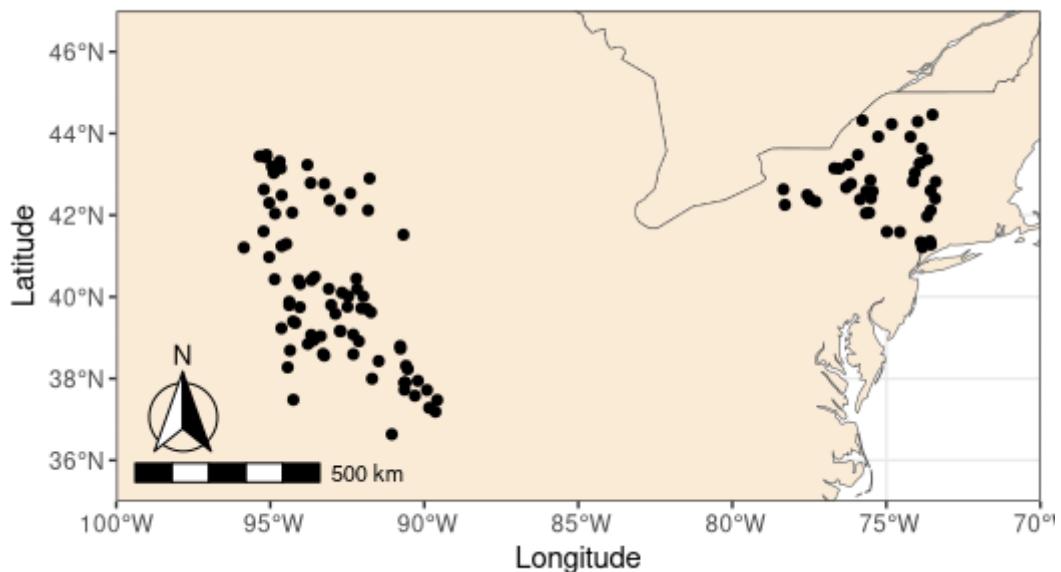


SFig. 1: Global map of lakes with 5-year simple moving average data. Lakes with sufficient data are situated in the US, Denmark and New Zealand.

## 54 2 Description of data-analysis steps

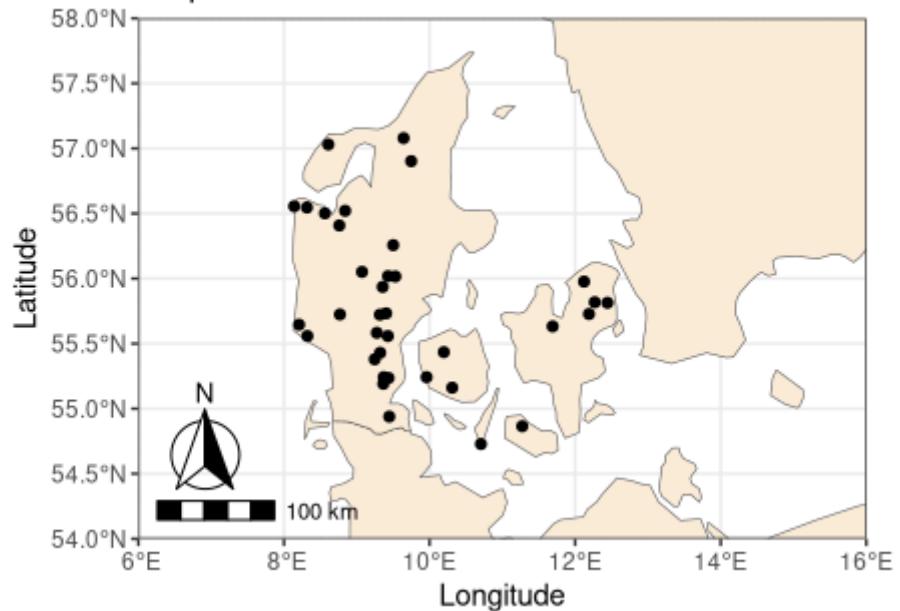
55 Here, we give a short rundown of the data-analysis steps (SFig. 4). In step 1, all possible moving  
56 averages are calculated for each lake, in step 2 all moving average data is combined. In step 3, the  
57 TN:TP ratio windows are defined with a minimum of ln molar TN:TP of 0 and a maximum of ln  
58 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  
59 ratio windows are overlapping, hence, each data point can be drafted in multiple windows (step 3).  
60 These TN:TP ratio windows are applied to the data in step 4 (in this example a ln molar TN:TP  
61 between 2 and 5). All data filtered in step 4 is then bootstrapped at the lake level (randomly sampled  
62 with replacement, step 5a) and one observation for each randomly sampled lake is picked at random  
63 (step 5b).

Map of US lakes



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

Map of Danish lakes



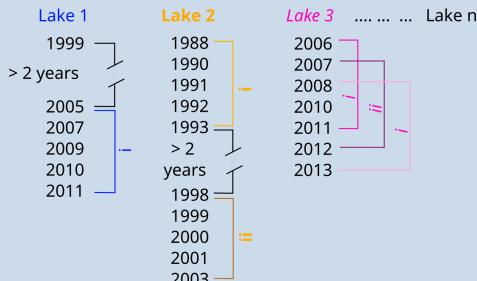
SFig. 3: Map of Danish lakes with 5-year simple moving average data.

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.<sup>1</sup>

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<sup>2</sup>, AIC, intercept and slopes are used in the study).

#### Data preparation

##### 1. Calculate all 5-year simple moving averages for data with < 3 years in between



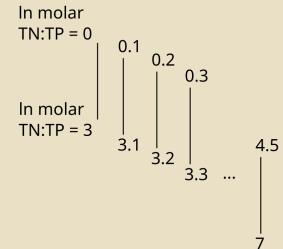
##### 2. Combine all moving averages

Lake	Time period
Lake1	i
Lake2	i
Lake2	ii
Lake3	i
Lake3	ii
Lake3	iii
...	...
...	...
...	...
Lake n	

#### Data resampling

##### 3. For In TN:TP windows between 0 and 7 conduct steps 4 and 5

In molar TN:TP (46 windows in total)



#### 4. Filter based on In TN:TP window

e.g. In TN:TP > 2 & < 5

Lake	Time period	In TN:TP
Lake1	i	1.5 x
Lake2	i	2.2 ✓
Lake2	ii	3 ✓
Lake3	i	4 ✓
Lake3	ii	6 x
Lake3	iii	4.9 ✓
...	...	...
...	...	...
...	...	...
Lake n		

#### 5a. Randomly sample lakes with replacement from filtered data (same number of lakes as in original & ignoring time periods for now)

Lake
Lake2
Lake3
Lake2
Lake3
...
...
...
Lake n

#### 5b. Sample a single 5-year moving average per randomly sampled lake

Lake	Time period
Lake2	i
Lake3	i
Lake2	i
Lake3	iii
...	...
...	...
...	...
Lake n	

#### 5c. Make models for randomly sampled dataset



#### 5d. Repeat this 300 times per TN:TP window

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.<sup>2</sup> 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.<sup>3</sup>

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.<sup>2</sup> Furthermore, this approach compares the predictive capability for different simple moving  
102 average lengths,<sup>2</sup> 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:

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

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

110 **3.3 Approaches to test the usability of simple moving averages and the**  
 111 **SAD approach to assess their ideal length**

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

115 1. We could find the ideal simple moving average length and reconstruct a systematic long-term  
 116 signal from a time series with random long-term random noise. Details on the simulation are  
 117 found below (Section 4.1).

118 2. If a short-term signal of a correlation between nutrients and chlorophyll a would have been  
 119 contained in addition to the long-term signal, we also likely would have found it, as we show  
 120 with a second simulation. Details on the simulation are found below (Section 4.2).

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

124 **3.4 Why we analysed simple moving averages with a hierarchical bootstrap  
 125 approach**

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

134 **4 Simulations of the simple-moving average approach**

135 **4.1 Simulation of a long-term signal**

136 **4.1.1 Generating the long-term signal**

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

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

144 Here, variable x was created as:

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

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

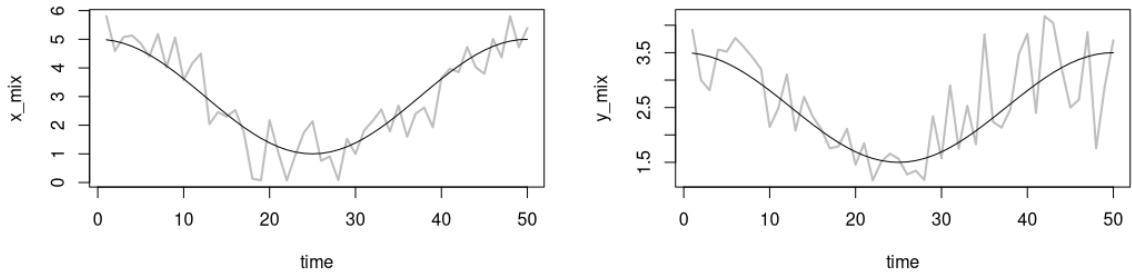
148 Variable y was then calculated with a linear model:

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

149 Subsequently, we added random noise from a normal distribution to x and y, using the rnorm function  
150 with 50 samples in R with a mean = 0 and SD = 0.5 to create two independent random normal  
151 distributions, which we added to x and y. The results of the simulation establishment can be seen  
152 in SFig. 5. Without the random noise inserted by the normal distributions,  $r^2 = 1$ , slope = 0.5, and  
153 intercept = 1 for the correlation between x and y. By adding the random noise, the  $r^2$  between x and  
154 y is lowered to 0.52, and the intercept and slope are changed randomly (intercept = 1.46, slope =  
155 0.37). The scatter plot reveals clear variability around the linear model line (SFig. 5c).

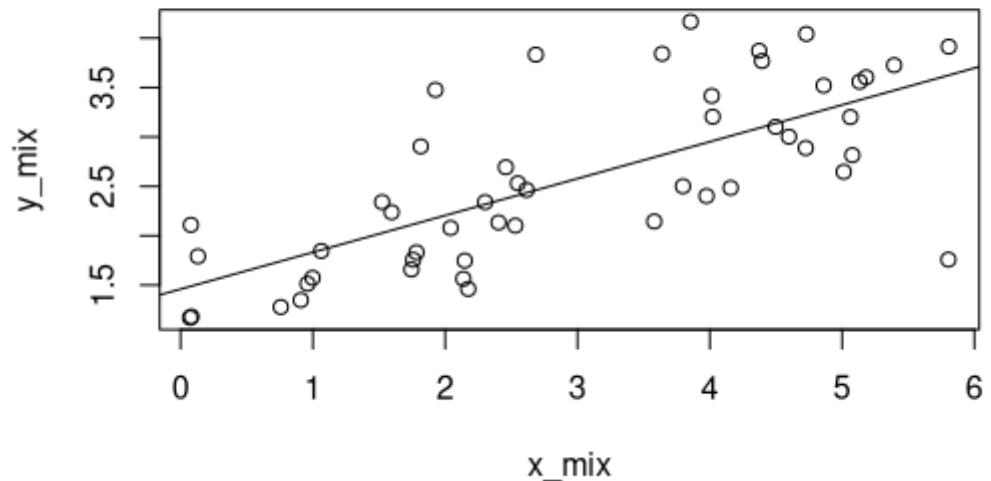
156 **4.1.2 Estimating the ideal simple moving average length**

157 We calculated the SAD for simple-moving average lengths of k = 2 - 40 (k equals the number of time  
158 steps) for the simulated x and y. In our simulations, we always see the unimodal pattern appearing  
159 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.

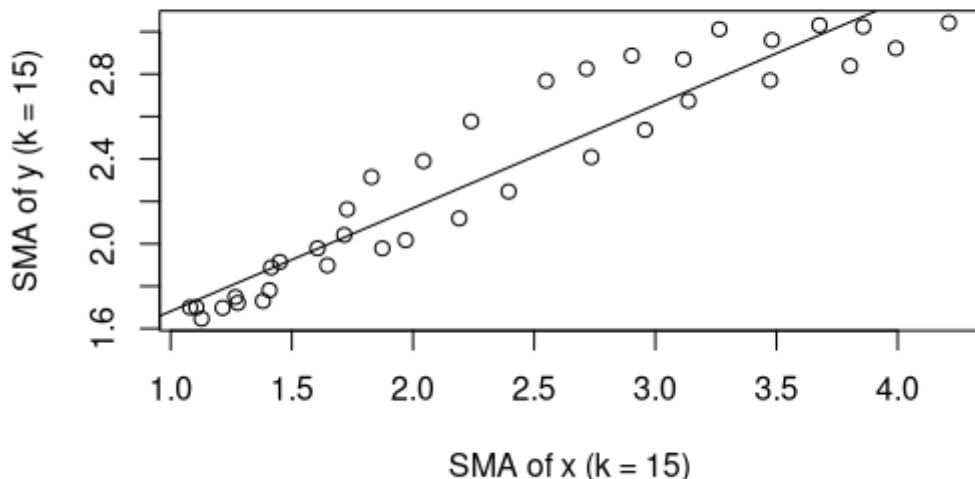
160 still considerable short-term variation, and the SMA shortly before, at or after the SAD peak remove  
 161 part of the long term signal (SFig. 6c, SFig. 6d). We, recommend using the SMA in the middle of  
 162 the SAD incline, clearly before the SAD peak. In this case we chose the SMA with  $k = 15$  (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

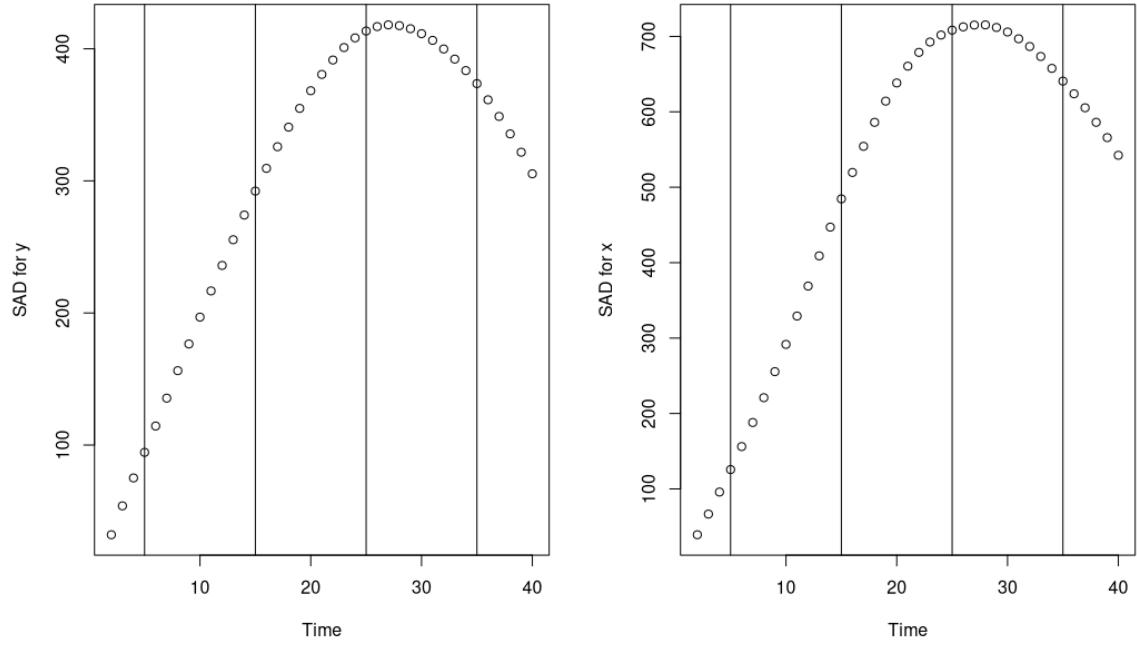
166 We chose SMA with  $k = 15$  (SFig. 6c, SFig. 6d) and found that the correlation of the SMA of x and y  
 167 improved ( $r^2 = 0.9$ ) (SFig. 7) relative to the correlation of the x and y with random noise ( $r^2 = 0.52$ )  
 168 also reported in Section 4.1.1 (and shown in SFig. 5c).

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.

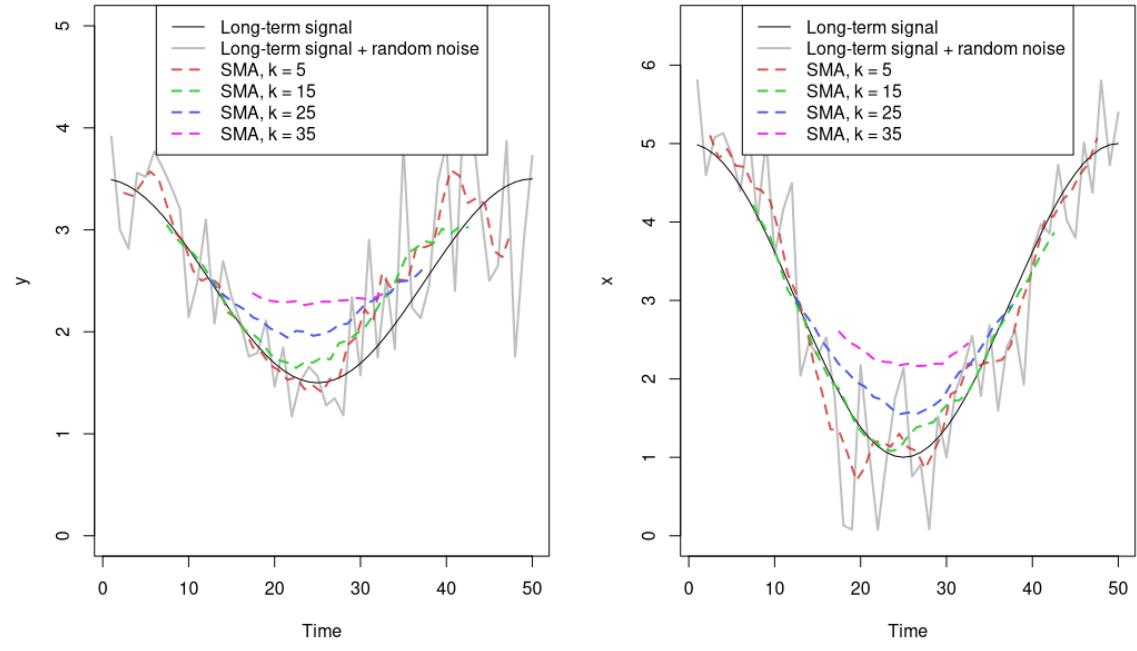


SFig. 7: Linear regression between SMAs with length ( $k$ ) = 15 of x and y



(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  $k$

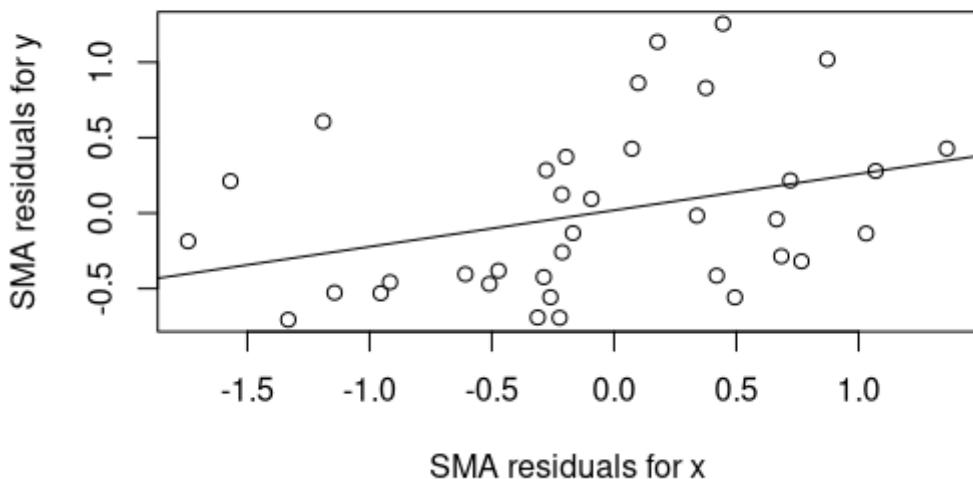
SFig. 6: Sums of absolute differences (SAD) for y and x, as well as plots containing the long-term signal, the randomized long-term signal, and simple moving averages (SMAs) of different lengths ( $k$ ).

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).

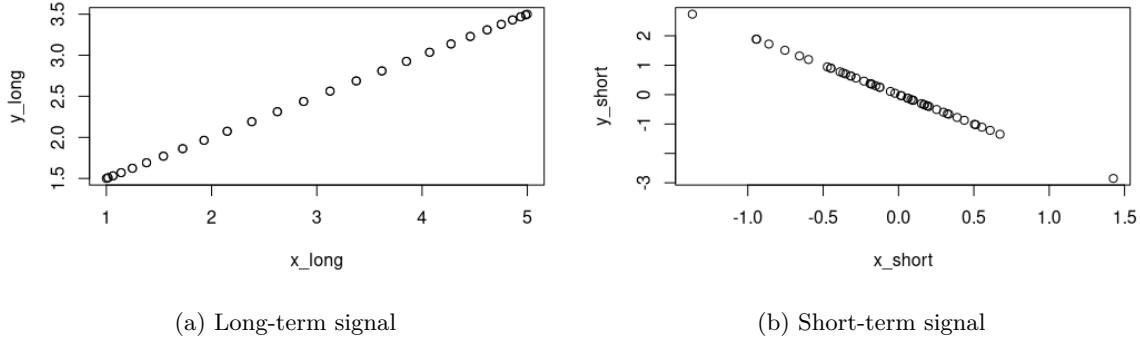
186 Here, we assess whether we would also detect a short-term signal if it existed in the data using the  
187 SMA calculation and residual calculation already described above. Please see our approach descrip-  
188 tion above for further details (Section 3) and the long-term simulation for a more detailed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

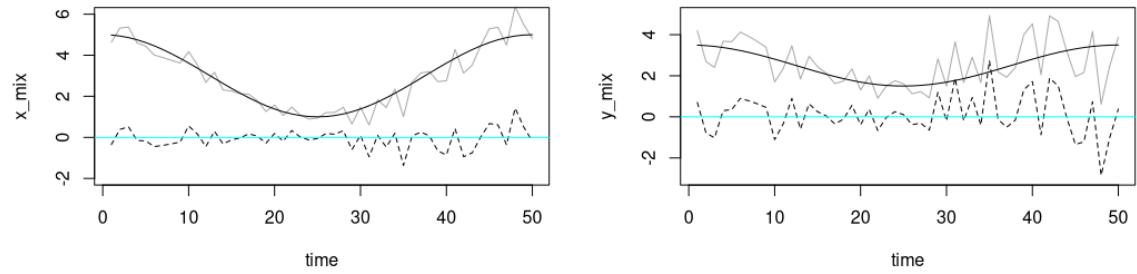
#### 200 4.2.2 Estimating the ideal simple moving average length

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

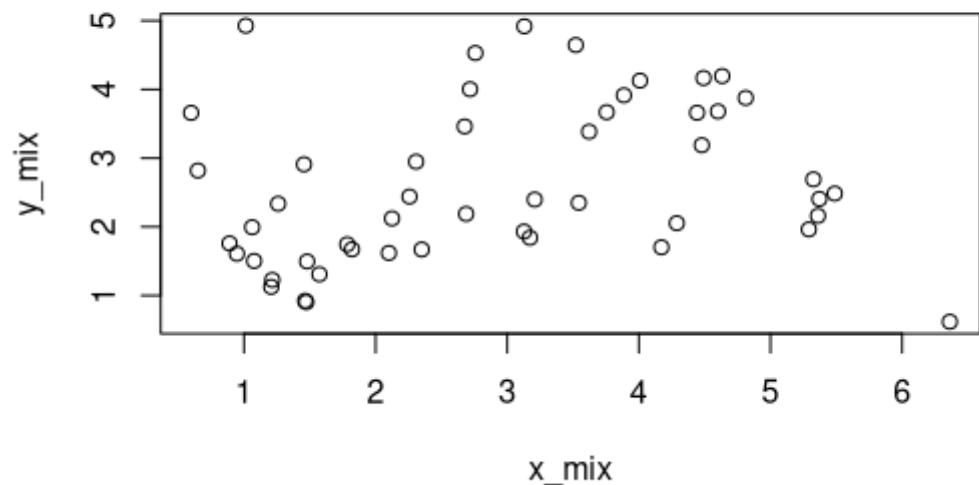
207 Neither the short nor the long signal was visible in the mixed signal ( $r^2 = 0.06$ ) (SFig. 10c). However,  
 208 the long-term signal could be reconstructed to a large extent using SMAs. Here, the SMA with  $k =$   
 209 15 gave a  $r^2 = 0.76$  for the regression between x and y (SFig. 12), and 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  $y_{short}$ .



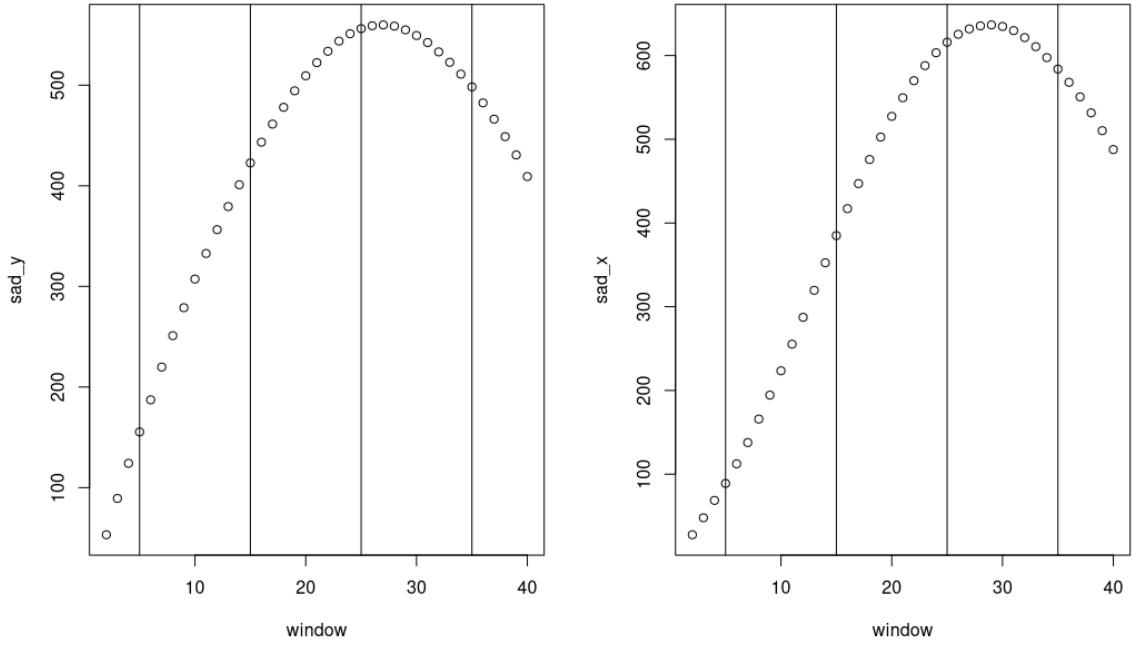
(a) x time series

(b) y time series



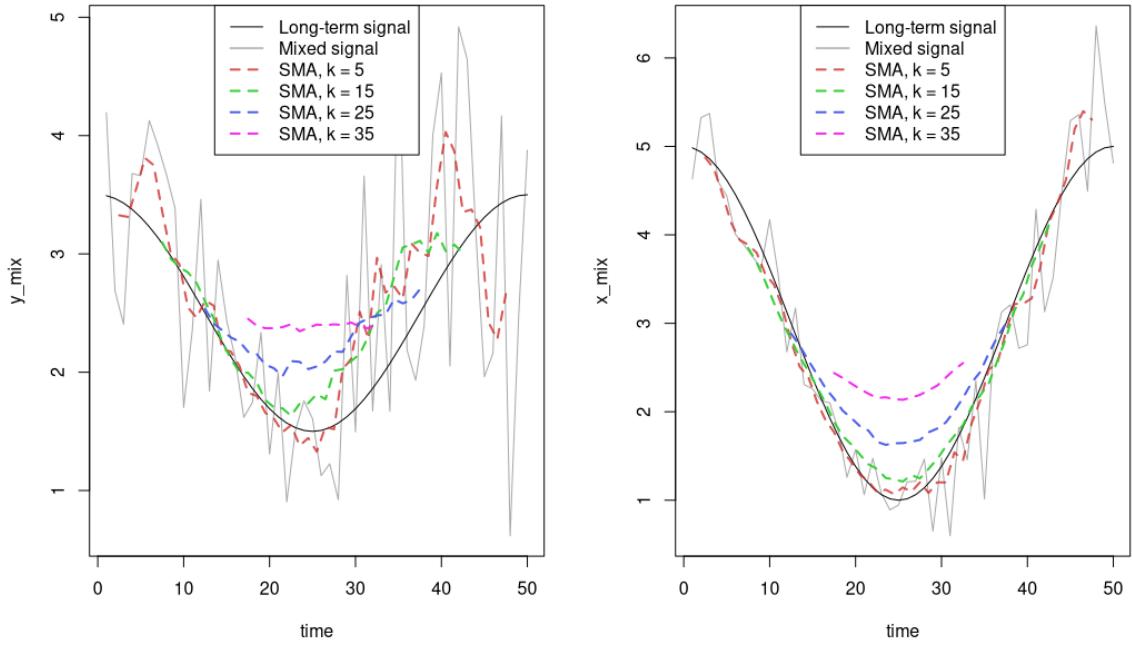
(c) Linear regression between mixed signals of x and y

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)

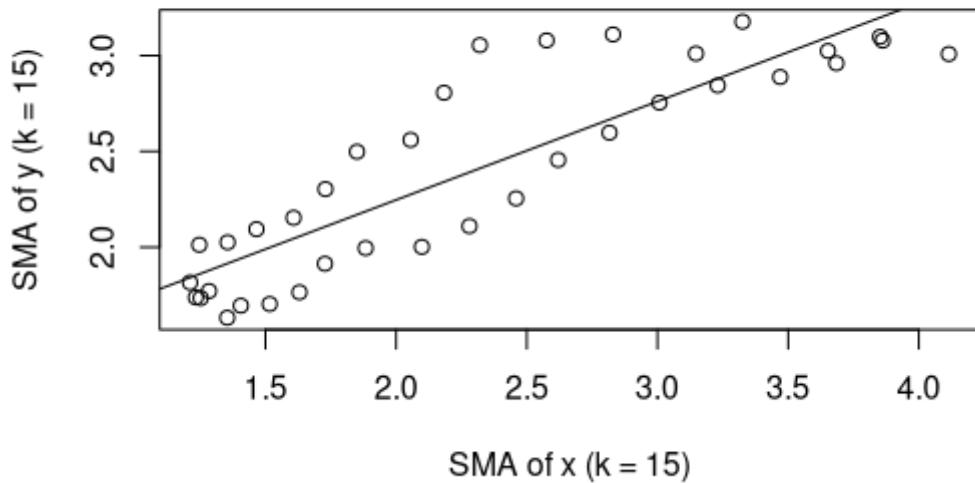


(c) y time series with SMA of different length  $k$

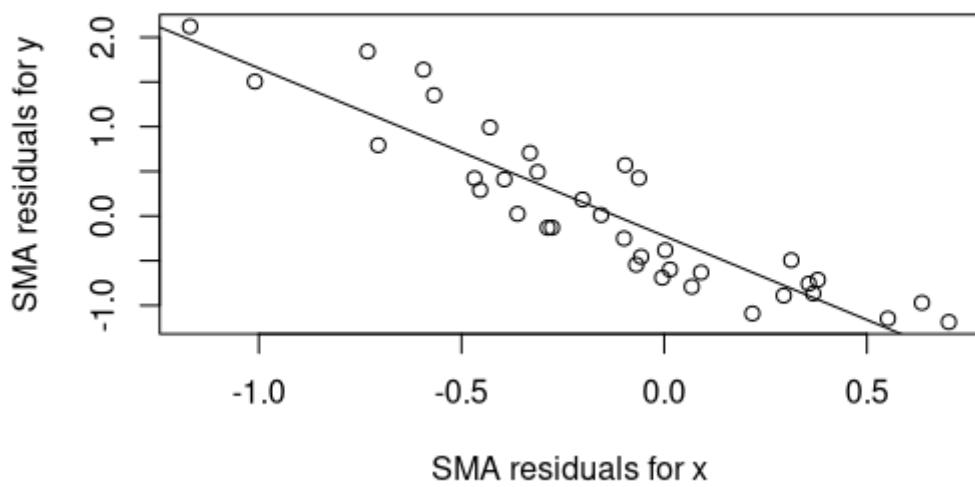
(d) x time series with SMA of different length  $k$

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

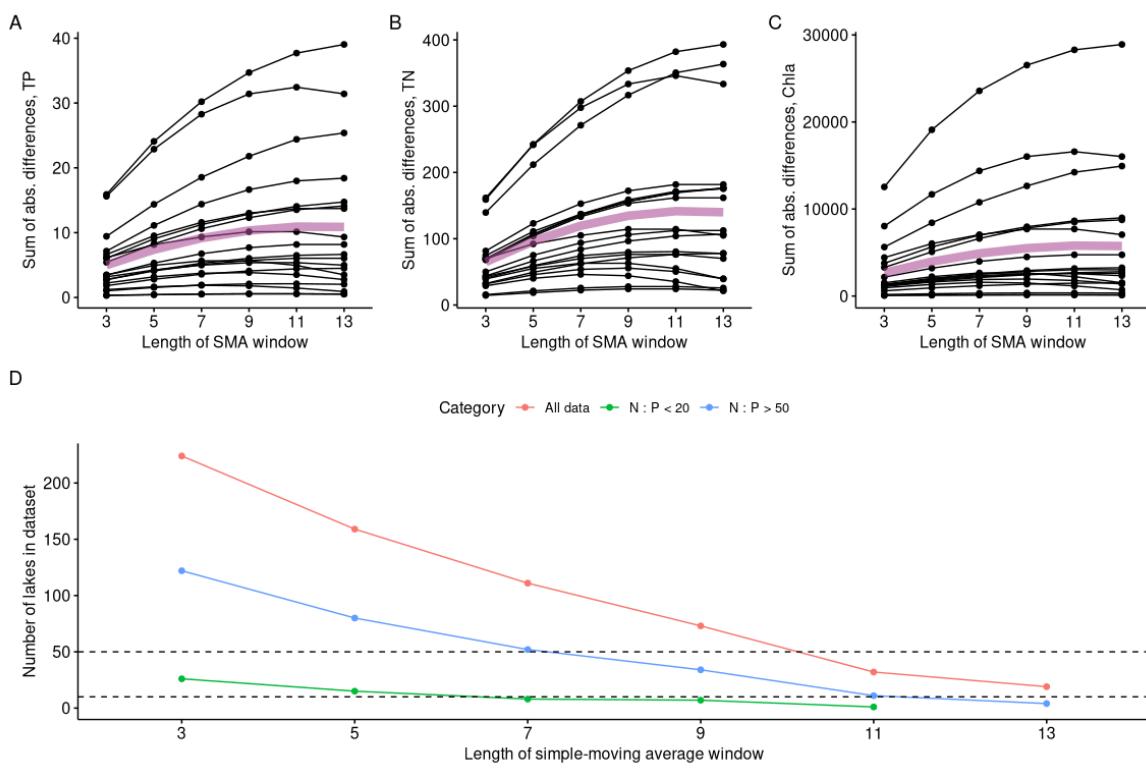


SFig. 13: Scatter plot of x and y SMA residuals, calculated from the simulated x and y minus the SMA (k = 15) of x and y

218 5 Selecting the best simple-moving average length for the lake  
 219 data

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

225 The SAD of the real lake data shows exactly the same pattern as the simulated data with an increase,  
 226 peak and subsequent decrease with longer SMAs. Here the average SAD peak was at an SMA length  
 227 of 7 to 11 years, but some time series already showed a decline in SAD with SMA lengths of more  
 228 than 7 years (SFig. 14). We therefore considered a 5-year SMA to be ideal, as this was still on the  
 229 ascent of the SAD for all time series. A 5-year SMA also allowed us to retain a relatively high number  
 230 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).

231 **6 Selecting the best regression models**

232 **6.1 Choosing the type of regression model**

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

242 **6.2 Choice of model terms**

243 To find the models that parsimoniously explained Chl-a concentrations, we used Akaike's information  
244 criterion (AIC)<sup>5</sup>. Here, we compared one-way models with TN or TP concentrations as explanatory  
245 variables for Chl-a concentrations with either additive models containing both TN and TP, or with  
246 models containing both TN and TP and an interaction term between TN and TP.  
247 Due to the nature of the data, we calculated thousands of AIC values over the range of molar TN:TP  
248 ratios. To compare AIC values, we were not interested in their absolute values, but in the reduction  
249 of AIC by the models. To assess this, we calculated the delta AIC ( $\Delta AIC$ ) between models, i.e. the  
250 change in AIC by adding or removing model terms. To test the improvement in AIC for the additive  
251 models, we calculated two  $\Delta AIC$  for each sample. To compare the TN+TP additive models with the  
252 TP only models, we calculated  $\Delta AIC_{TP \ vs \ TN+TP}$  as follows:

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

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

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

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

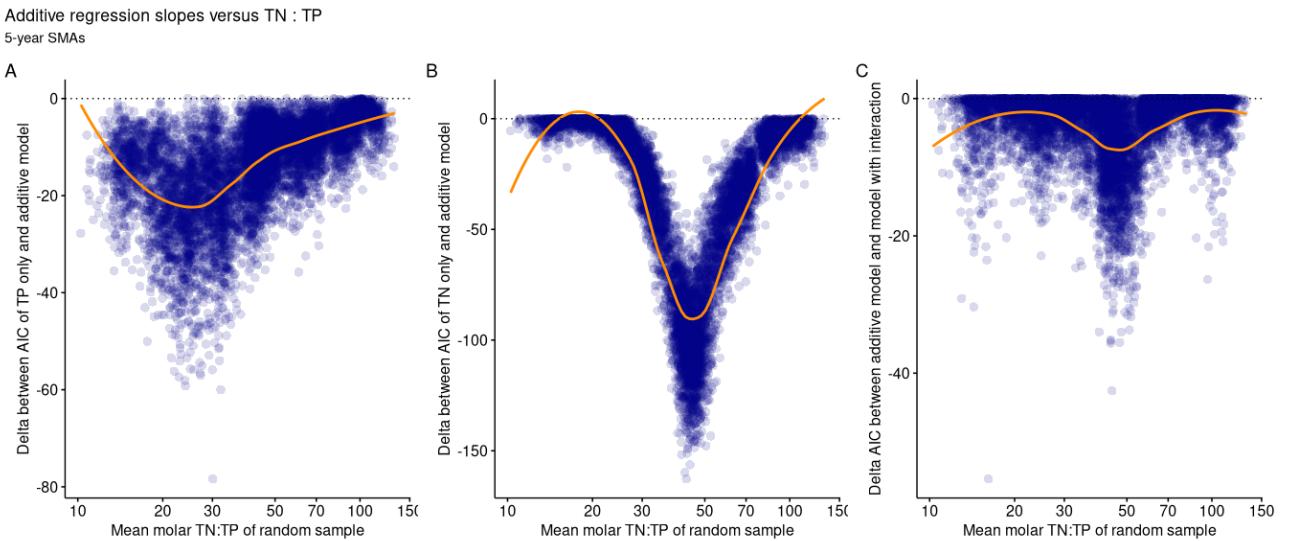
$$\Delta AIC_{TN+TP \text{ vs } TN*TP} = AIC_{TN+TP \text{ model}} - AIC_{TN*TP \text{ model}} \quad (6)$$

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

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

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

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

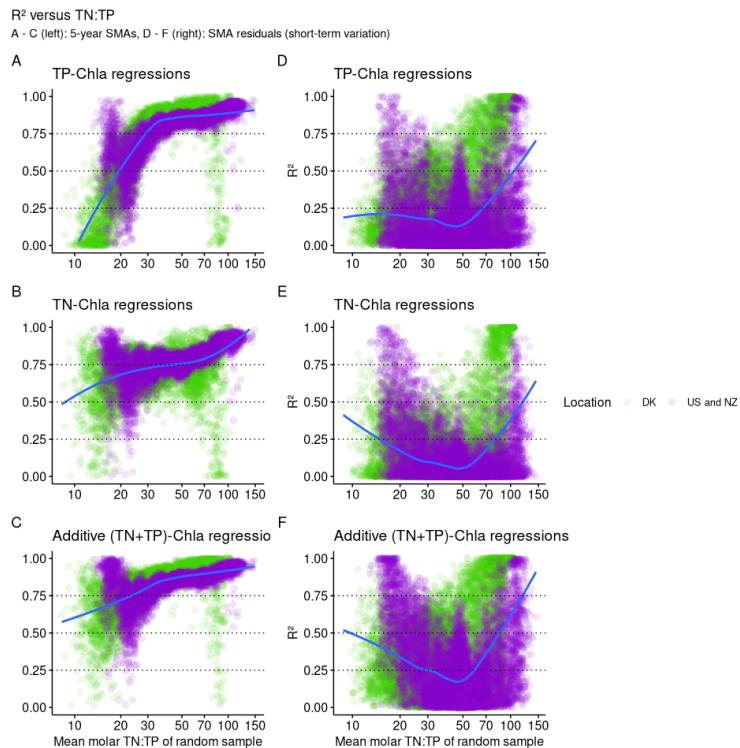


SFig. 15: Results on Delta AIC for TP-only models versus additive models (panel A) or TN-only models versus additive models (panel B), and for the Delta AIC between additive models and models with interaction term between TN and TP (panel C). The models were constructed for the 5-year simple moving averages (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.

269 **7 Separate analyses of the correlation between nutrients and**  
 270 **Chl-a for the Danish dataset and global data**

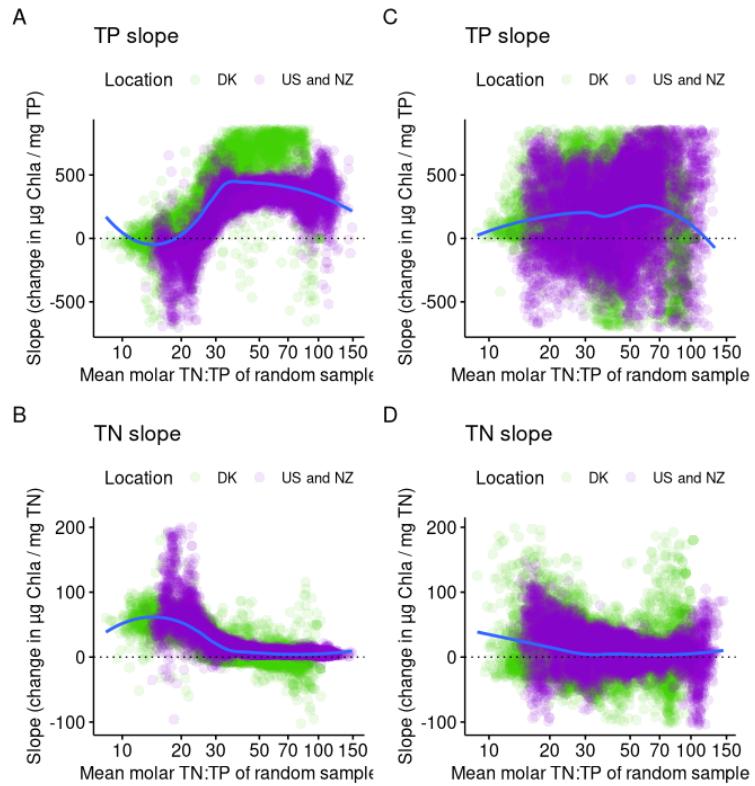
271 To check whether the Danish dataset (Aarhus University, Danish Centre for Environment,  
 272 <https://odaforalle.au.dk>) and global dataset<sup>6</sup> revealed the same response of Chl-a to TN or TP at  
 273 the same TN:TP ratios, we conducted a separate analysis of the 5-year SMAs for both datasets using  
 274 exactly the same statistical approach as for the entire dataset. As for the full dataset, the SMAs  
 275 were randomly combined using the hierarchical bootstrap procedure (Section 2).

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

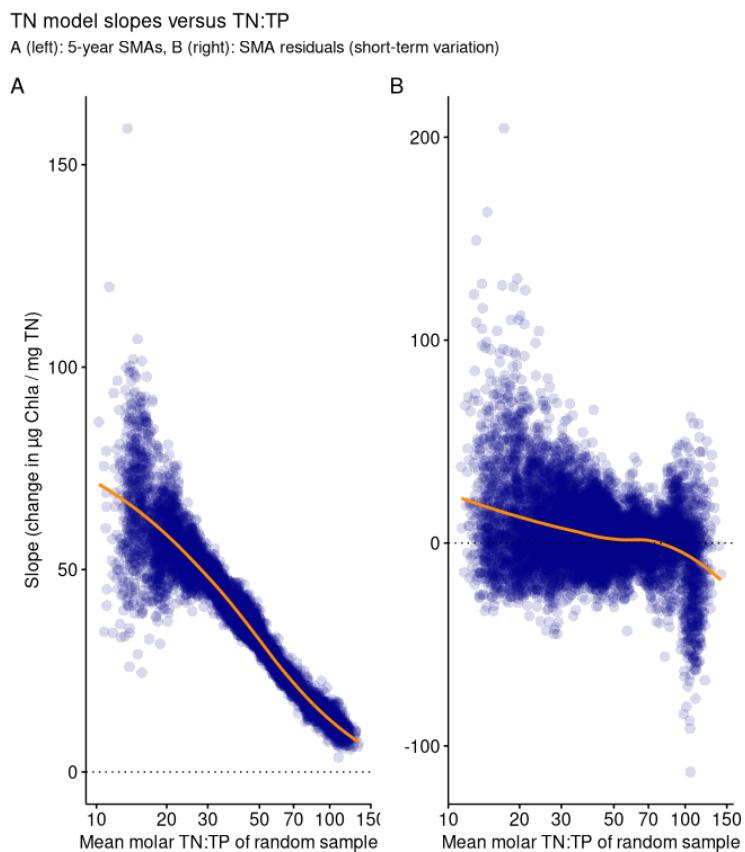


SFig. 17: Slopes of the additive models for long-term variation based on 5-year simple moving averages (SMA) (A & B) or short-term variation contained within SMA residuals (C & D) versus the mean molar TN : TP of each randomly sampled dataset. Shown are slopes from additive models between total phosphorus (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).

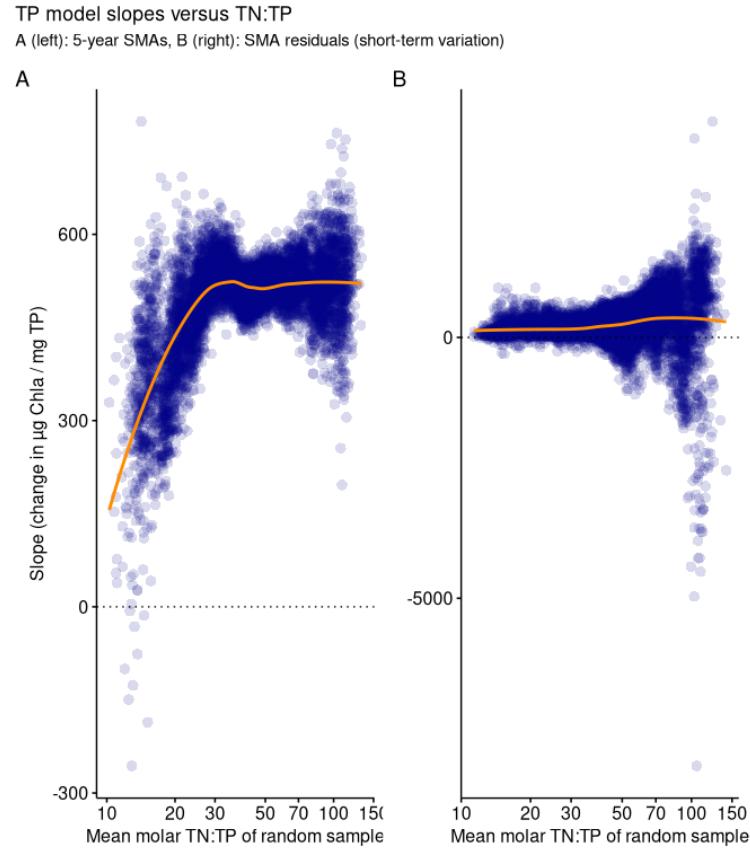
281 8 Model intercepts and slopes

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

283 8.1.1 TN model slopes



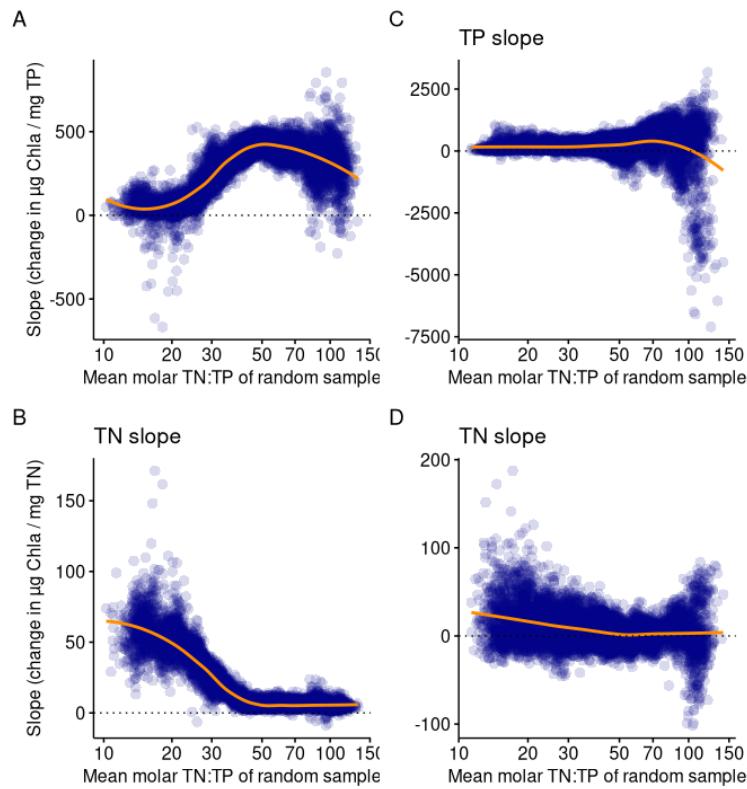
SFig. 18: Slopes of the TN models for long-term variation based on 5-year simple moving averages (SMA) (A) or short-term variation contained within SMA residuals (B) versus the mean molar TN : TP of each randomly sampled dataset. Shown are TN model between total nitrogen (TN, mg / L, panel B, D) and 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.

285 8.1.3 Additive model slopes

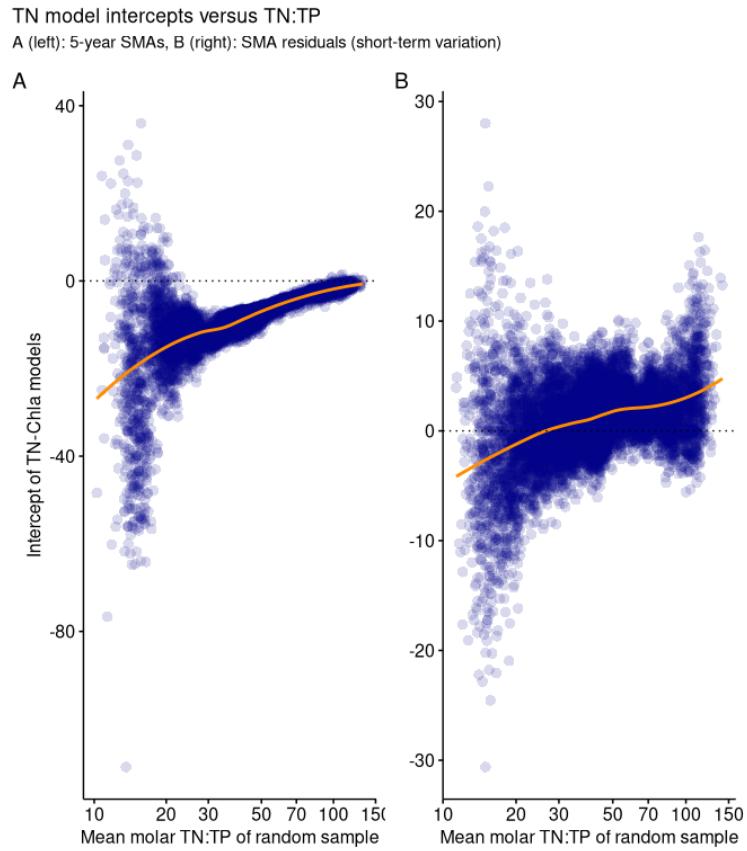
Additive model (TN+TP-Chla) slopes versus TN:TP  
A & B (left): 5-year SMAs, C & D (right): SMA residuals (short-term variation)



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, 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.

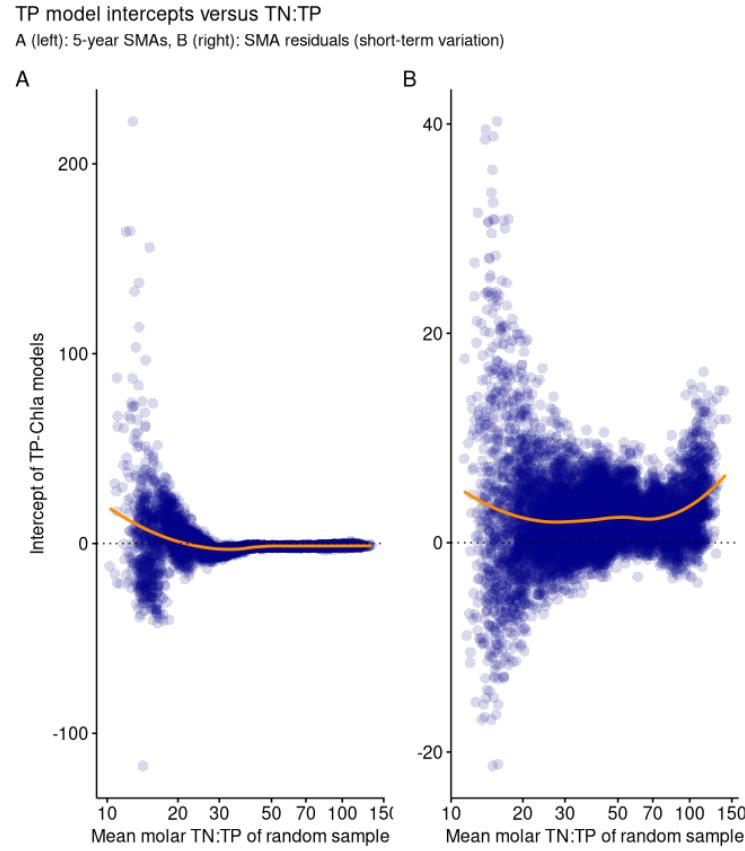
286 8.2 Intercepts, 5-year simple moving averages and residuals

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,  $\mu$ g / 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.

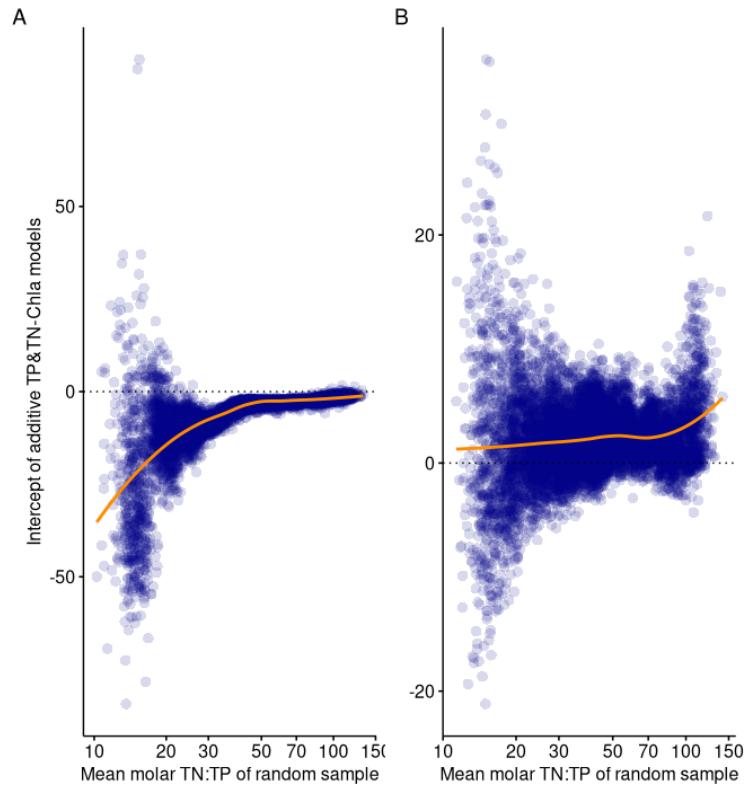
288 8.2.2 TP model intercepts



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,  $\mu$ g / 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.

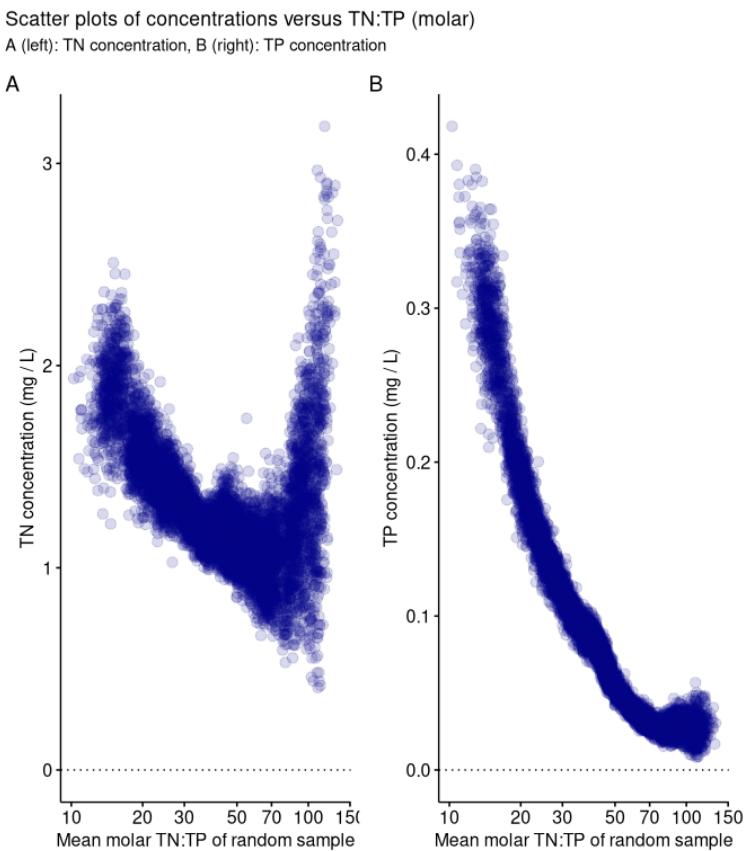
289 8.2.3 Additive model intercepts

Additive model intercepts versus TN:TP  
A (left): 5-year SMAs, B (right): SMA residuals (short-term variation)



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,  $\mu$ g / 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.

290 **9 Random average dataset TN and TP concentrations versus**  
291 **average random dataset TN:TP**



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

292 **10 Data and code availability**

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

297 **References**

298 1. Ren, S. *et al.* Nonparametric bootstrapping for hierarchical data. *Journal of Applied Statistics*  
299 **37**, 1487–1498 (2010).

300 2. Svetunkov, I. & Petropoulos, F. Old dog, new tricks: A modelling view of simple moving  
301 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).