# Spatial statistics of hydrography and water chemistry in a eutrophic boreal lake based on sounding and water samples

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# Abstract

Spatial variability, an essential characteristic of lake ecosystems, has often been neglected in field research and monitoring. In this study, we apply spatial statistical methods for the key physics and chemistry variables and chlorophyll a over eight sampling dates in two consecutive years in a large (area 103 km<sup>2</sup>) eutrophic boreal lake in southern Finland. In the four summer sampling dates, the water body was vertically and horizontally heterogenic except with color and DOC, in the two winter ice-covered dates DO was vertically stratified, while in

the two autumn dates, no significant spatial differences in any of the measured variables were found. Chlorophyll *a* concentration was one order of magnitude lower under the ice cover than in open water. The Moran statistic for spatial correlation was significant for chlorophyll *a* and  $NO_2+NO_3-N$  in all summer situations and for dissolved oxygen and pH in three cases. In summer, the mass centers of the chemicals were within 1.5 km from the geometric center of the lake, and the 2nd moment radius ranged in 3.7–4.1 km respective to 3.9 km for the homogeneous situation. The lateral length scales of the studied variables were 1.5–2.5 km, about 1 km longer in the surface layer. The detected spatial "noise" strongly suggests that besides vertical variation also the horizontal variation in eutrophic lakes, in particular, should be considered when the ecosystems are monitored.

### Keywords

Eutrophic lake Spatial variability Ecosystem response Water quality Lake monitoring

# Introduction

Physical and biogeochemical processes modify the properties of water in its flow from the upper parts of drainage basins to lakes and further downstream. Internal biogeochemical processes are known to be time and depth dependent in lakes. Although an essential property of terrestrial ecosystems, horizontal variability has often been neglected in the pelagic lake ecosystems, ', however, uneven horizontal spatial distribution of chemical constituents and chlorophyll *a* may exist in lakes as well. An uneven distribution may be caused by circulation dynamics and the impact of external, mainly atmospheric and hydrologic drivers (see George & Edwards 1973; George & Heaney 1978; Caron et al. 2008; Van de Bogert et al. 2012). In addition, biogeochemical processes also produce spatial heterogeneity, and positive feedbacks can strengthen the variations in the spatial biogeochemical fields. Horizontal heterogeneity is more evident in larger lakes with more complex physical structures such as semi-isolated sub-basins and areas with high or low external loading (e.g., Anttila & Kairesalo 2010; Weyhenmeyer et al. 2004), upwelling (e.g., Csanady 1977; Kondratyev & Filatov 1999), and intense biological activity (Cloern et al. 1992; Heini et al. 2014) than in small lakes. Turbulence and convective mixing are the main physical factors smoothing vertical and horizontal differences. Consequently, vertical differences in the water chemistry can be pronounced in small lakes (Salonen et al. 1984) with less wind stress and wave power to drive the turbulence (Cloern et al. 1992; Vuorenmaa et al. 2014), and in such deep lakes where vertical mixing does not reach the lower water layers (Wetzel 2001).

Due to the spatial physical and chemical heterogeneity, also the phytoplankton may possess corresponding spatial variability in lakes (e.g., Anttila & Kairesalo 2010; Heini et al. 2014). Feedback loops can strengthen the heterogeneity and lead to short-term patchiness in physical and biogeochemical variables. For example, phytoplankton increases the absorption of solar radiation that increases the temperature and consequently the rate of metabolism. Heterogeneity of the surrounding environment may also influence the metabolism of aquatic ecosystems (Van de Bogert et al. 2012). It has been suggested that in eutrophic lakes, spatial variance and patchiness can be important characteristics of plankton and water chemistry that supports a wide range of organisms living in ostensibly uniform environment (Hutchinson 1967). In oligotrophic lakes, spatial differences in the water chemistry can be more difficult to detect because of low inorganic nutrient concentrations and low metabolic activity of organisms.

Besides the spatial variability, seasonality is an important characteristic of temperate and boreal lakes (Cloern et al. 1992; Salonen and Leppäranta, 2009; Vuorenmaa et al. 2014). Although spatial and temporal variability are closely interconnected, their interplay regarding the ecosystems is still poorly understood. For example, littoral areas can be highly productive in comparison to the pelagic areas (Kairesalo 1980+; Wetzel 2001), and mineralization of organic matter in the bottom sediments may induce differences in the vertical structure of water chemistry. In our study lake, Lake Vanajanselkä, for example, water pH may vary more than 2.5 units between the epilimnion and hypolimnion during the summer stagnation (Heini et al. 2014).

#### AQ1 AQ2

Heterogeneous spatial distributions need to be considered in lake monitoring, from both the theoretical and practical point of view. According to a common tradition, lakes have been mapped based only on one or a few sample sites per lake (Hedger et al. 2001; UN/ECE 2003; Mitikka & Vuori 2009). The samples have been taken mostly from the middle or the deepest point of a lake, and the focus has been on the vertical profile rather than on the horizontal differences. However, the deepest area in a lake can be the most oligotrophic spot because it often situates far from the littoral zones and from the inflows, which bring nutrients and other chemical constituents to the lake from the catchment. Therefore, a careful sampling strategy is needed rather than using one fixed reference sampling point (see Kallio et al. 2003; Anttila et al. 2008; Arst et al. 2008). In modeling the lake ecosystem, it is crucial that spatial variability is accounted for, especially in the period of stratification (Göransson et al. 2004), although shortage of proper field data often limits the validation. Besides, sampling interval is another issue, which has to be taken into consideration in lake monitoring (see, e.g., Anttila et al. 2012; Van de Bogert et al. 2007).

Our previous results from Lake Vanajanselkä (Leppäranta et al. 2012; Heini et al. 2014) have suggested that in summer the spatial variability of chemistry variables is remarkable and shows similar patterns. To look deeper into this question, the key chemical variables have been examined here using spatial statistics methods. The data include eight sampling dates from the years 2009 and 2010 using the same sites in all cases. Two of them are from the early summer (May 31 and June 9), two from the late summer (August 3 and 5), two from the autumn (October 26 and 28), and two from the ice-covered winter period (March 18 and 23). The results show that there were two categories of factors behind the spatial variability. One category includes the external drivers, i.e. weather and hydrological conditions, which cause mixing events and produce the spring runoff peak with large transport of nutrients and other chemicals from the upstream. The other category covers the internal factors and feedback loops, which include sub-basin scale circulation and biogeochemical processes. The results show that spatial variability can be strong and irregular in summer but disappears in autumn.

# Material and methods

## Lake Vanajanselkä

The study was performed in Lake Vanajanselkä, which is the main basin of Lake Vanajavesi water system in southern Finland ( $61^{\circ} 00'-61^{\circ} 20' N \times 24^{\circ} 00'-24^{\circ} 30' E$ , Fig. 1). It is a large and shallow eutrophic lake with annual median total phosphorus (TP) of 28 mg m<sup>-3</sup> (in the period 2000–2009) and August median chlorophyll *a* of 19 mg m<sup>-3</sup> (in the period 2000–2009) (Finnish Environment Institute, Hertta database, http://wwwp2.ymparisto.fi/scripts/hearts/welcome.asp ). The surface area of Lake Vanajanselkä is 103 km<sup>2</sup>, the mean and maximum depths are 7.7 and 24 m, respectively, and the catchment area is 2774 km<sup>2</sup>. The lake belongs to the drainage basin of River Kokemäenjoki, which flows to the Gulf of Bothnia, Baltic Sea. The lake is annually ice-covered, on average from the beginning of December until the beginning of May. Eutrophication of the lake has resulted due to extensive human impact since the early eighteenth century. The water quality was very poor in the 1960s and 1970s (Kansanen & Aho 1981), and thereafter, industrial and municipal loading has markedly decreased improving the water quality (Leppäranta et al. 2012).

#### Fig. 1

Bathymetric map of Lake Vanajanselkä. The sampling sites (1-16) are given as black dots (No1 = lowermost in the Western basin, No16 = uppermost in the Eastern basin). Also, the geometric center of the sampling sites is given. The darker shading in the map means deeper parts in the lake (see scale on the right of the figure)



The weather was somewhat different between the study years. Year 2009 was close to normal, but 2010 is characterized as a year with extremes, cold winter, and very warm summer. In 2009, ice thickness was 38 cm at maximum but as much as 55 cm in the following year. Ice breakup was close to average in both years, April 27 in 2009 and April 21 in 2010. The summer was a little colder than normal in 2009 (mean July temperature 16.8 °C) but exceptionally warm in 2010 (mean July temperature 21.8 °C), with the highest temperatures from mid-July to the beginning of August. The warm weather in 2010 was associated with several thunderstorms. In both summers the precipitation was 10–20% less than normal. In autumn, the weather cooled down, and October air temperature was colder than average in 2009 but close to normal in the following year. In both years, the mean water temperature was close to 6 °C throughout the lake in October. During the summer samplings, the weather was calm and sunny before mid-day, and in the afternoon, the conditions changed to slightly stronger wind and more clouds. In the autumn samplings, the wind conditions were rather similar, but the days were not as sunny and warm. The maximum wind speed never exceeded 5 m  $\rm s^{-1}$  on the

#### sampling days.

Inflow to the lake is dominated by River Lepaanvirta. With its mouth in the southeast, it accounts for about 90% of the total inflow (Jokiniemi 2011). The outflow strait is situated opposite to the inflow, in the northwest. The theoretical residence time of the lake is 450 days. Crossing Lake Vanajanselkä, there is a southeast–northwest underwater esker (sill depth 7 m), which separates the lake into western and eastern sub-basins with almost identical surface areas (see Fig. 1). During the field campaigns in 2009 and 2010, the discharge was low in comparison to the annual average except in May 31, 2010 (Heini et al. 2014). The daily inflow comprised < 1% of the volume of the uppermost 5-m water layer, which represents the photic zone (Leppäranta et al. 2012). At 5-m depth, the area of the horizontal slice is 61% of the total lake area, and the uppermost 5-m water layer accounts for 49% of the total volume of the lake. For more details of this lake research project and the results of phytoplankton and inorganic nutrients, see Heini et al. (2014). Results of winter conditions have been presented by Leppäranta et al. (2012) and Yang et al. (2012).

### Sampling and measurements

During the study period in 2009 and 2010, the data was gathered four times per year on nearly the same dates: ice-covered winter (March 18–23, 2009, and March 23–26, 2010), early summer (May 31, 2009, and June 9, 2010), late summer (August 3, 2009, and August 5, 2010), and autumn (October 26, 2009, and October 28, 2010). The winter data was distributed over several days, but in other cases, the sampling was made in 1 day. In situ measurements and water sampling were started each day at 10:30 a.m. and finished at 4:00 p.m. local time (GMT + 2 h on March, GMT + 3 h at other times), with solar noon at about 10:20 a.m. GMT. During the fieldwork in summer and autumn, three boats were used, each with two persons, which made it possible to take a large number of samples within a relatively short time. In winter, a snow mobile was used for on-ice travel. The samples were collected from 16 different sites, which made up an almost regular grid with 1.5 km spacing between the grid points throughout the main parts of the two sub-basins (Fig. 1).

The surface water samples were taken from the uppermost 1 m layer (in 2009) or at 1 m below the surface (in 2010), and the bottom water samples were taken at

1 m above the sediment. In 2009, the samples were taken with three lifts by a Limnos tube sampler (height 40 cm, volume 2.8 l) and in 2010 by a 100-cm long Limnos tube sampler (volume 7.0 l). The depths at the sampling sites varied from 10 to 21 m. Also, temperature and oxygen profiles were collected with an YSI sounding instrument (0545, 556 MPS and Pro DO, Yellow Spring Instruments).

The laboratory measurements for chemistry of the water samples included inorganic nitrogen (nitrite and nitrate nitrogen NO<sub>2</sub>+NO<sub>3</sub>-N and ammonium nitrogen NH<sub>4</sub>-N), phosphate phosphorus (PO<sub>4</sub>-P), total nitrogen, total phosphorus, dissolved organic carbon (DOC), color, chlorophyll a, pH, and electric conductivity. The standard methods (see Keskitalo & Salonen 1994; Arvola et al. 1996) were applied, and the analyses were carried out by professional laboratory technicians at the water chemistry laboratory of Lammi Biological Station, University of Helsinki. Inorganic nitrogen, phosphate phosphorus, total nitrogen, and total phosphorus concentrations were determined with a flow injection analyzer (QuikChem®8000, Zellweger Analytics Inc., Lachat Instruments Division, Milwaukee, WI, USA) from water samples, which had been filtered through Whatman GF/C filters (inorganic nutrients), or from non-filtered samples (total nutrients). Water pH was measured using an Orion pH meter during the sampling day in the laboratory, immediately after returning to the laboratory, in an open system with stirring the sample water, and chlorophyll *a* was determined after hot ethanol extraction using a Shimadzu UV-visible recording spectrophotometer UV-2100 at the wavelengths of 665 nm and 750 nm. The samples for inorganic nutrient and chlorophyll *a* measurements were filtered during the sampling day and analyzed in the following day or later (when analyzed later, the chlorophyll a samples were kept in a refrigerator or in a deep-freezer).

The spatial structure of the observed physical and biogeochemical variables was examined based on spatial moments, correlations and trend surfaces. The R Statistical Computing Platform was employed in the statistical calculations. The details are given in the Annex. The first view is provided by the spatial moments, which give measures for the mass center and overall spatial variability of any spatial field, while the general spatial correlation is given by the Moran *I* index. (Semi-)variogram presents the variability of any quantity as a function of distance. The use of trend surface analysis enables a further look into the separation of the spatial components into a "regional-trend," "local" component, and random error-

noise. Here, we focus essentially on the regional trend in the data within the relatively small spatial extent of the sample area. Also, a thin plate spline regression (TPS) procedure was employed for the chlorophyll *a* data for the summer data in 2009 and 2010.

# Results

## Seasonal variation and stratification

The characteristics of the lake water beneath the ice cover (in March), during the spring (May/June) and summer (August) as well as during the autumn mixing (October) are shown in Table 1. In winter, chlorophyll *a* concentration was one order of magnitude lower than during the other sampling periods, and in winter, vertical stratification appeared in dissolved oxygen due to the consumption of oxygen at the lake bottom. In summer, despite a relatively small (ca. 5 °C) temperature difference between surface and bottom of the lake, the chemical stratification was strong, except for color and DOC. In contrast, in October, due to the autumnal overturn, the lake was isothermal (spatial standard deviations were 0.1-0.2 °C), and no significant differences in any of the measured chemistry variables were found between the surface and the bottom (*t* test and Mann-Whitney rank sum test; P > 0.1).

#### Table 1

Characteristics of water temperature, chemistry and chlorophyll *a* in the four study sea seasonal mean values, and the differences between the mean surface and bottom values a DO = dissolved oxygen,  $NH_4$ -N = ammonium nitrogen,  $PO_4$ -P = phosphate phosphorus, 1 N = nitrite-nitrate nitrogen, DOC = dissolved organic carbonAQ4

	Mar		May/June		August		Octo	
	Surface	Bottom	Surface	Bottom	Surface	Bottom	Surface	
Temperature (°C)	0.28	2.2	13.0	9.4	20.1	14.3	5.8	
DO (%)	98	62	111	88	114	27	95	
pН	7.32	7.04	7.79	7.27	8.67	6.93	7.59	
Conductivity (mS m <sup>-1</sup> )	131	135	115	122	118	124	121	

Color (mg Pt L <sup>-1</sup> )	64	73	68	67	52	53	38
$\begin{array}{c} \mathrm{NH_4-N}\\ \mathrm{(mg\ m^{-3})} \end{array}$	8	55	15	47	9	35	10
$\begin{array}{c} PO_4 - P \\ (mg m^{-3}) \end{array}$	16	17	2	3	1	19	9
$\frac{\text{NO}_2 + \text{NO}_3 - \text{N}}{(\text{mg m}^{-3})}$	697	555	694	744	326	626	201
DOC (mg m <sup>-3</sup> )	10.5	10.8	9.6	9.2	9.2	9.0	8.5
Chlorophyll $a (mg m^{-3})$	1.4	0.72	14.4	8.0	23.1	3.5	6.0

Due to the intense biogeochemical processes in summer, it was the most interesting season to carry out the spatial distribution statistics, and to compare the spatial distribution of lake water in summer with that in autumn when the lake was well-mixed (Fig. 2). The boxplots displayed a distinct seasonal variation in pH, nitrite-nitrate nitrogen, and water temperature at the 1-m depth during summer. These three variables generally exhibited the least variation within each of the four dates. Whereas chlorophyll *a* concentration displayed similar distribution for the first three sample dates but the level of the August 5, 2010, sample distribution was greater than the others by a factor of 2.

#### Fig. 2

Seasonal boxplots for the eight lake variables showing their distributional properties in the summer experiments. Date 1 = June 2009, date 2 = August 2009, date 3 = May 2010, and date 4 = August 2010 The last sentence ". Date 1 ... August 2010" must be deleted because figure has been slightly modified. (the delete command did not work here?)



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### Spatial central moments and correlations

The geometric center was located near the underwater esker, and therefore, mass center deviations to northeast or southwest went to the eastern or western basin, respectively. The mass centers of these water quality quantities were not far from the geometric center of the grid, and the moments illustrate how the masses were oriented and concentrated with respect to their centers (Fig. 3). Inorganic nitrogen and chlorophyll a showed the largest shifts from the geometric center, and chlorophyll a was spread as a non-homogeneous field. Mostly the deviations of the mass centers were within 1 km from the geometric center and at most the distance was about 1.2 km or the size of a grid cell (Table 2). Also, the 2nd moment radius of the spatial mass did not deviate much from a homogeneous field, mostly less than 100 m, i.e., the masses were not much concentrated or spread compared with the homogeneous case. In our grid, the 2nd moment radius would be 3.85 km for a spatially homogeneous case, and the collected water sample data shows the range from 3.67 to 4.06 km. Smaller values than the homogeneous case refer to more concentrated mass around the lake center while large values tell of more weight closer to the shore areas. Largest variations were observed for the nutrients, both for the mass centers and the 2nd moment radius, which reflects their distributed source area and internal consumption. In summer, only for P-PO<sub>4</sub> the 2nd moment radius was consistently greater than in the homogeneous case.

#### Fig. 3

Vectors presenting the first spatial moments of **a** chlorophyll a, **b** inorganic nitrogen, **c** pH, and **d** DO in the May/June (points 1 and 3) and August (points 2 and 4) data (unit km). The histograms present the deviatoion of the second moment radius from homogeneous case (unit m)

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#### Table 2

Spatial moments of the chlorophyll *a* and chemistry data in June, August and October. Maximum shift refers to maximum deviation of the mass centre from the geometric centre, and the and order radius shift refers to difference of the mass distribution from a

homogeneous usid.	Max shift (n)			Min order manns shift (m)			
	May/June	August	October	May/June	August	October	
Temperature (°C)	76	208	81	- 10, 16	-5,13	- 11, 9	

DO (%)	93	1191	48	-20, 6	-13, 8	0, 9
рН	50	53	18	- 10, 7	- 10, 2	0, 3
Conductivity (mS m <sup>-1</sup> )	61	29	15	- 10, 7	- 10, 4	0, 7
Color (mg Pt L <sup>-1</sup> )	310	208	89	1, 23	- 30, 8	- 20, 26
$NH_4$ -N (mg m <sup>-3</sup> )	808	1239	561	- 140, 58	-180, 29	- 130, 215
$PO_4$ -P (mg m <sup>-3</sup> )	605	400	267	84, 195	0,135	- 90, 70
$\frac{\text{NO}_2 + \text{NO}_3 - \text{N}}{(\text{mg m}^{-3})}$	206	630	90	- 11, 18	-15, 25	2, 55
DOC (mg $L^{-3}$ )	139	188	94	- 19, 79	- 20, 0	- 17, 24
Chlorophyll $a$ (mg m <sup>-3</sup> )	597	583	106	- 70, 18	- 60, 54	5, 58

Table 2 further shows that in May/June, chlorophyll *a* was centered towards northeast in both the surface and the bottom layers. Nutrients mass centers were also relatively far from the geometric center,  $NH_4$ -N southwest and  $PO_4$ -P west. In August, the heterogeneity was stronger, with chlorophyll *a* mass center still towards northeast.  $NH_4$ -N and  $PO_4$ -P were centered south in the surface layer and, respectively, northeast and southwest in the bottom layer. Also, temperature and DO shifted towards west from the geometric center. In October, the spatial distributions were homogeneous, the only exception being the location of  $NH_4$ -N mass center northeast from the geometric center.

The degrees of freedom were rather low in the data to estimate the variogram functions. The estimation consequently covered the range from zero just to 5 km distance, and the outcome is shown for the temperature, DO, pH, NH<sub>4</sub>-N, and chlorophyll *a* in Fig. 4. The first up-crossing of the level  $\gamma = 1$  corresponds to the auto-covariance length scale, which was here 1.5–2.5 km in the surface layer and 1.0–1.5 km in the lower layer. This length scale represents the spatial range of variability or the "spatial memory" of the system. The form of the variogram was sub-linear. In October, the range was at smallest. Beyond the auto-covariance length scale, which scale at smallest. Beyond the auto-covariance length scale, the scaled variograms were above one due to negative auto-

covariance, and the curves did not show asymptotic saturation towards  $\gamma = 1$ , because the number of data was too low to estimate longer range spatial covariance. We do not have data close to the sites to evaluate the nugget effect, but extrapolation suggests that it is non-zero and less than 0.5. Other, independent available data suggests that for the temperature that should be of the order of 0.1 and for the DO much smaller.

#### Fig. 4

Semi-variograms of DO, pH, NH<sub>4</sub>-N, and chlorophyll *a*. The semi-variograms have been scaled by the corresponding variances for clarity. At origin, semi-variogram is zero, but the limit on the right side can be non-zero representing the nugget effect; this uncertainty is illustrated by the rectangles in the 0-1.5-km interval AQ6



The Moran statistic *I*, which illustrates the presence of spatial correlation in the "global" sense (Table 3), were significant for chlorophyll *a* and  $NO_2+NO_3-N$  during all summer samples, for dissolved oxygen (DO) in May/June and in August 2010, and for pH in June 2010 and in August 2009 and 2010. Moran statistic greater than 0.45 was found for DOC,  $NO_2+NO_3-N$  and DO in May 2009, and for pH, DO and  $NO_2+NO_3-N$  in June 2010. The overall summer levels in 2009 were high, as mentioned previously, for chlorophyll *a*,  $NO_2+NO_3-N$  and DO, and additionally for pH in summer 2010. However, the magnitude of Moran I in summer 2010 was not as high as in the previous summer but statistically

significant nevertheless. These patterns indicate a substantial degree of spatial dependence among the variables highlighted ( $P \le 0.01$ ). Only in three cases (e.g., PO<sub>4</sub>-P in June 2009 and August 2010) the Moran statistic was negative, suggesting a chessboard type pattern, but the Moran I values in each of these cases were not statistically significant.

#### Table 3

Moran statistics for the spring/summer samplings to measure the global spatial correlation. Abbreviations, see Table 1

Variables	2009 June 9	2009 August 05	2010 May 31	2010 August 3			
Temperature	0.05	0.18	0.14	0.38*			
DO (%)	0.51*	0.54*	0.47*	0.27			
рН	0.24	0.40*	0.64*	0.42*			
NH <sub>4</sub> -N	0.28	0.15	0.16	- 0.12			
NO <sub>2</sub> +NO <sub>3</sub> -N	0.48*	0.49*	0.50*	0.47*			
PO <sub>4</sub> -P	-0.26	NA	0.2	- 0.17			
DOC	0.53*	0.25	0.08	0.47*			
* $p$ value = 0.01 or less							

### Spatial trend surfaces

The trend surface analysis allowed us to decompose the data into its various spatial components, and each of the nine response (dependent) variables was mapped with the trend surface routine. A lattice configuration (see Fig. 1) with 16 data points at 1-m depth, corresponding to the sample collection network, was used in the analysis, and a special focus was put on the more prominent variables such as chlorophyll a, NO<sub>2</sub>+NO<sub>3</sub>-N, pH, and DO. Since assessment of the regional component is the main interest here and the fact that the sample size is small, the model fitting was confined to 1st and 2nd order surfaces.

In all the sample periods, during the four summer dates and for the four variables (chlorophyll a, NO<sub>2</sub>+NO<sub>3</sub>-N, pH, and DO), except in May 2009, all the surface fits

were statistically significant at the 0.01 level for either the 1st order or 2nd order surfaces and are presented in Table 4. In May 2009, only pH and  $NO_2+NO_3-N$ surface fits were significant.  $NO_2+NO_3-N$  had significant  $R^2$  for all summer cases while chlorophyll *a* and DO were significant in June 2010 and in both August samplings. Water pH had significant fits in summer except in June 2010. In five cases the 1st order fit (plane surface) outperformed the quadratic fit (see the underlined values on Table 4). These results, initially, are very encouraging even with the small sample size. There appears to be a very strong spatial neighborhood effect in the lake chemistry for  $NO_2+NO_3-N$ , pH, chlorophyll *a* and DO in which their spatial distributions can be explained, to a degree, by longitude and latitude. However, noticed too that we are not extrapolating outside the sample network where data were not available.

#### Table 4

Adjusted  $R^2$  for the trend surface analysis showing both the 1st order and 2nd order values for their respective surfaces. Abbreviations, see Table 1

Variables	2009 June 9	2009 August 05	2010 May 31	2010 August 3			
	1st 2nd	1st 2nd	1st 2nd	1st 2nd			
Chl a	0.24, 0.28	0.65*, 0.86*	0.33*, 0.27*	0.43*, 0.48*			
DO	0.28, 0.17	0.67*, 0.71*	0.24*, 0.45*	0.32*, 0.26			
рН	0.31*, 0.24	0.47*, 0.51*	0.0, 0.30	0.66*, 0.63*			
$NO_2 + NO_3 - N$	0.32*, 0.65*	0.57*, 0.73*	0.69*, 0.64*	0.48*, 0.40*			
Italicized, 1st trend surface $R^2$ greater than 2nd order							
p value = 0.01  or less							

The mapped results of the four summer dates for chlorophyll *a* are displayed in Fig. 5. The coefficient of determination,  $R^2$  values for June 9 and August 5, 2009, were 94 and 98%, and for May 31 and August 3, 2010, they were 99 and 63%, with RMSE of 1.5, 0.9, 0.5, and 4.2, respectively. It should be noticed that for August 3, 2010, the magnitude of chlorophyll *a* was a factor of 2 greater than the range of values for the other three dates. This could be a contributing factor, which produced the higher RMSE and lower  $R^2$ . Overall, these results are somewhat

surprising with only longitude and latitude used as the explanatory variables. Even considering the small sample size, we feel these results are partly due to the geometry of the basin and inflow/outflow points, and confined spatial extent of the sample area with its relatively small variance of chlorophyll *a*. This is, certainly, applicable for the summer dates with August 3, 2010, being an exception (see Fig. 2). It is difficult to assess the robustness of the individual prediction surface, however, since no validation data exists.

#### Fig. 5

Second-order fit surfaces of **a** chlorophyll *a*, **b** NO<sub>2</sub>+NO<sub>3</sub>-N, **c** pH, and **d** DO (%) for the early and late summer



### Spatial structures

Chlorophyll *a*, inorganic nutrients, pH and DO had commonly distinct spatial variations in the summer data as the second-order fits to the grid data illustrate (Fig. 5). Chlorophyll *a* concentrations were regularly at highest in the E-NE part of the lake basin while inorganic nitrogen concentrations in May/June were highest and in August lowest in the same region (Fig. 6). The pH values were irregular in May/June but in August chlorophyll *a* concentrations followed closely with the

highest pH values in the eastern basin of the lake. However, the highest and lowest DO concentrations and saturation levels appeared at every sampling in different parts of the lake. The results given in Table 3 show that three of the four described variables were best characterized with first order surfaces except for chlorophyll *a*. In contrast, DOC, water color, electrical conductivity, and water temperature did not vary significantly between the sampling sites both in May/June and in August. In October, the spatial fields of the water chemistry and chlorophyll *a* showed minor, irregular, variability.

#### Fig. 6

The spatial distribution of chlorophyll a at 1 m depth in early and late summer 2009/2010 as an example. The maps are drawn based on the isoplets of the concentrations



If the TPS surfaces are compared to the trend surfaces for chlorophyll *a* concentration, the early summer cases show different spatial patterns. In 2009, there were two maximum values, one on the southeast side and another on the very northeast corner of the sample network, while in 2010, a single maximum concentration occurred. This difference is attributed to the data point for the second sample row on the northeast side. Trend surface analysis cannot handle maximum values correctly due to its smoothing properties, and for these two dates, at least, a more sophisticated model is required. The TPS model, however, incorporates these maximum values into the surface producing a more realistic rendition of the "true" spatial pattern.

# Discussion and conclusions

Our data provide a rarely seen insight into the spatial variability of lake properties and processes even though the sample size was limited to eight snapshots at 16 sampling sites. Therefore, the degrees of freedom to strong conclusions about the spatial variability of water chemistry and chlorophyll *a* remain rather limited, which clearly emphasizes how challenging this kind of a sampling program is in terms of manpower. A few similar studies have been performed before but those have been mainly focused on biology of inland waters (Cloern et al. 1992; Van de Bogert et al. 2012) and especially in the marine environment (Jassby et al. 1997). Also, remote sensing have been applied in studying horizontal distribution of water quality variables (Hedger et al. 2001), but in spite of its good spatial resolution remote sensing can only cover the near-surface layer of the water column.

In winter under ice the lake had an inverse thermal stratification accompanied with weak vertical differences in DO and pH, both indicating intense microbial activity of the bottom sediment. At that time, physical forcing was mainly caused by release of heat from bottom sediment and consequent weak thermohaline circulation (Leppäranta et al. 2012). In autumn, the entire water body was homogeneous due to intense horizontal and vertical mixing.

In summer, the top water layer concentrations of inorganic nitrogen and phosphate phosphorus varied considerably between the different parts of the basin, and parallel with these variables also chlorophyll *a*, DO, as well as pH varied in a

rather wide range. Chlorophyll *a* was abundant, in particularly, in the eastern basin while nutrient distributions varied in different months due to net external flux and consumption (Heini et al. 2014). In contrast, DOC and color did not show any significant horizontal or vertical variation.

The question to which degree the spatial, i.e., horizontal and vertical, structures in Lake Vanajanselkä were caused by the external and/or internal factors, our results suggest that both are important in summer but in fall the spatial structures disappear. In our previous paper (Heini et al. 2014), we have tackled the issue to some extent by showing that chlorophyll a and the inorganic nutrient concentrations were closely inter-connected. That was the case especially in late summer when cyanobacterial biomass (predominantly *Microcystis* genus) was high (e.g., in August 2009 it contributed to 31% of the total phytoplankton biomass, which was on average 6 mg  $m^{-3}$ , wet weight) and the cells formed a dense surface 'bloom' into the uppermost water column. At that time the interplay between phytoplankton, including cyanobacteria, and the inorganic nutrients was especially strong (Heini et al. 2014). Water pH and DO concentration followed spatially the variation in chlorophyll a concentration, suggesting that pH and DO reflected the metabolic activity of phytoplankton, a well-known phenomenon in lakes (Verduin 1957; Van de Bogert et al. 2007; Staehr et al. 2012). pH levels above 9.0 in the epilimnion clearly indicate a very high photosynthetic rate especially when the pH levels were at the same time in the hypolimnion below 7.0. Actually, the low pH values in the hypolimnion are in good agreement with our previous observations showing that in winter, under ice, the water pH near the lake bottom decreased in the course of time, suggesting that microbial decomposition (mineralization) of organic matter had a key role in determining water pH near the bottom sediment (Leppäranta et al. 2012). Degassing of CO<sub>2</sub> during the measurements may have slightly elevated pH in a few samples with lower pH but obviously not in most of the samples because of their higher pH and alkalinity.

Although external factors, first of all solar radiation and wind stress, are the primary drivers causing temporal and spatial variation in lake ecosystems, the inlake factors such as basin characteristics (especially bathymetry) and metabolic processes also influence the variability of water chemistry and organisms in time and space (Wetzel 2001; Stauffer et al. 2014). Because of the close interaction between the external and internal factors, it may be difficult to conclude which one is the key driver at a certain time and place. This is especially true because one key factor may be replaced by another in time scales less than 1 day, as our previous results of Lake Vanajanselkä suggest (Heini et al. 2014). For example, pH values above 9 implied that carbon dioxide became a limiting factor for photosynthesis that might support the growth of cyanobacteria, because these are capable to utilize bicarbonate and carbonate instead of  $CO_2$  (Reynolds 1984; Badger & Price 2003). In addition, since many cyanobacteria are able to utilize N<sub>2</sub> instead of nitrate-N and ammonium-N, their growth should not be limited by the inorganic nitrogen concentrations close to the detection limit. Consequently, it can be foreseen that there are several drivers influencing simultaneously on the physical, chemical, and biological processes with varying power as well as with their characteristic temporal and spatial extent.

#### AQ7

In theory, the interplay between the physical, chemical, and biological drivers may result in the situation, which was found in the study lake: high spatial and temporal variability in pH and DO together with varying chlorophyll a concentrations and low inorganic nutrient concentrations. However, the primary reason for the spatial variability of inorganic nutrients and chlorophyll *a* is a question, which cannot be answered with the present data. One factor, which should not be ignored, is the inflow of nutrients from the catchment. The main inflow, River Lepaanvirta, contributes 90% of the annual inflow to Lake Vanajanselkä (Jokiniemi 2011, see also Heini et al. 2014), and it drains into the southeastern part of the lake. The river inflow is highly peaked in April–June, has a minimum in late summer and another weaker minimum in mid-winter (Jokiniemi 2011). The peak level is about three times the summer minimum. We have earlier shown (Leppäranta et al. 2012; Heini et al. 2014) that the eastern part of the lake basin usually has higher nutrient concentrations than the western part, and as a consequence the phytoplankton biomass and chlorophyll a concentrations are higher in the eastern area relative to the western area.

In summer, the discharge of River Lepaanvirta is usually low and its impact on the water chemistry of Vanajanselkä basin is smaller than in spring and autumn. Also, the low spatial variation in color and DOC, both known to be rather stable relative to the biogeochemical processes and which originate mostly from the catchment (Leppäranta et al. 2012), suggests that the external loading had a minor influence

on the results. The same indicates the hydrological residence time, which is 1.5 years. Altogether, the results indicate that in summer the in-lake processes had a strong influence on the water chemistry and the spatial variation of different variables while in autumn the external drivers caused complete mixing with homogenous water quality.

In conclusion, the observed spatial "structure" of chlorophyll a and other water chemistry variables showed that the lake is sensitive to changes in the internal and external drivers, and the horizontal variation of water quality variables should be taken into account in the monitoring sampling protocols of eutrophic lakes, in particular. This was also reported earlier by Göransson et al. (2004). Neglecting lateral variations would lead to introduction of variations that erroneously could be interpreted as temporal variation. However, monitoring programs tend to have a limited, often decreasing funding. For a cost-efficient monitoring program, a strategy can be developed on the basis of a preparatory study to locate the critical points, which would show the evolution of the state of the whole lake. This is crucial in summer stratification, but in autumn well-mixed conditions, lakes have become homogeneous and one sampling site is needed. Also, by taking integrated samples from several points at the lake and perform the analysis on composite samples, random variations would decrease and any trends would be much easier to detect with only slightly increasing sampling costs. Results based only on one sampling point should be interpreted with special care and need to be confirmed by spatially distributed sampling and/or model examinations.

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# Annex. Spatial statistical methods

Spatial moments. Consider a spatial field f = f(x, y), e.g., concentration of a chemical constituent, and set the origin of the coordinate system in the geometric centre of the lake. The first moment  $\mathbf{R}_1$  (vector) of f gives the deviation of the mass centre of f from the geometric centre, while the second moment  $\mathbf{M}_2$  (matrix) measures the covariance of f around the mass centre as well as deviations from isotropy. These moments are defined by

$$\boldsymbol{R}_{1} = \int_{S} f(\boldsymbol{r}) \, \boldsymbol{r} dS, \, \boldsymbol{M}_{2} = \int_{S} f(\boldsymbol{r} - \boldsymbol{R}_{1}) \, (\boldsymbol{r} - \boldsymbol{R}_{1})^{2} dS$$
 A1

where S is the lake area and **r** is the radius vector from the geometric centre of the lake. In case of homogeneous field,  $\mathbf{R}_1 = 0$ . For a homogeneous  $1 \times 1$  square lake,  $M_{2,xx} = M_{2,yy} = \frac{1}{12}$  and  $M_{2,xy} = M_{2,xy} = 0$ , and the radius of deviation is  $\sqrt{M_{2,xx}^2 + M_{2,yy}^2} = \sqrt{\frac{1}{6}} \approx 0.408$ . A detailed look into the spatial variation is provided by the semi-variogram, which is defined by

$$\gamma(h) = \frac{1}{2} Var \left[ f \left( x + h_x, y + h_y \right) - f \left( x, y \right) \right], h = \sqrt{h_x^2 + h_y^2}$$
 A2

where  $h_x$  and  $h_y$  are the x- and y-distances from the point (x, y) and *Var* stands for the variance operator. It is seen that  $\gamma(0) = 0$  and  $\gamma(h) \rightarrow \gamma_{0+} \ge 0$  as  $h \rightarrow 0$ ; the quantity  $\gamma_{0+}$ , the nugget effect, is the loss of correlation when stepping a side from a given point. As  $h \rightarrow \infty$ , the limit is  $\gamma(h) \rightarrow Var(Z)$ .

*Moran I index*. In spatial data, the covariance structure is defined by the neighborhood association. Moran *I* index provides a general measure of the spatial correlation/dependence of the data. It is given by

$$I = \frac{\sum_{i,j} w_{ij} \left(f_i - \bar{f}\right) \left(f_j - \bar{f}\right)}{\frac{1}{N} \sum_{i,j} w_{ij} \sum_i \left(f_i - \bar{f}\right)^2}$$
A3

where *N* is the number of data points or regions and  $w_{ij}$ 's are spatial weights between data points *i* and *j*. With equal weights, the usual correlation coefficient is obtained. To determine whether the index *I* deviates from zero (random distribution) and its expectation E(I) is statistically significant, a test is used that relies on the asymptotic distribution of *I*, which is Gaussian, with mean  $E(I) = -\frac{1}{N-1}$  and variance  $\sigma_I^2$ . The hypothesis of no spatial autocorrelation is rejected at  $\alpha \times 100\%$  significance level if the statistic  $|Z_{obs}| = \frac{1-E(I)}{\sigma_T}| > Z_{\alpha/2}|$ , where  $Z_{\alpha/2}$  the cutoff of the standard Gaussian distribution. Values greater than E(I) indicate positive spatial correlation with the size indicating the strength of the correlation (Schabenberger & Gotway 2005). However, we were concerned using this test with a sample size less than 25, so we ran the statistical test on a Monte Carlo procedure. The Monte Carlo test is a permutation bootstrap test in which the observed values are randomly assigned to the various sample points and the test statistic is computed *n* number of times (Bivand et al. 2013). The results were the same in each case.

*Trend surface analysis* technique provides the separation of the spatial components into a "regional-trend," "local" component and random error-noise. Geographical (spatial) coordinates of latitude and longitude, as the exploratory (independent, i.e., covariate) variables, are regressed against the attribute or response variable. Trend surface analysis uses all the points that are available in the data set thus it is considered a "global" approach. Spatial data are fitted with a polynomial equation of different degrees from linear, quadratic, and cubic to higher surfaces. A general polynomial trend surface equation of order p is as follows:

$$f(x, y) = \sum_{r+s \le p} \beta_{rs} x^r y^s$$
 A4

where x and y are longitude and latitude,  $\beta_{rs}$ 's are regression coefficients, and r and s are the surface exponents. There are a series of statistical concerns when using a

trend surface model. First, for small samples, very high correlation values are required to be statistically significant; also, the power of the test decreases substantially with small sample size increasing the probability of committing a type II error. Therefore, in our modeling, all correlations were set at least to a threshold of 0.01 level to be considered significant. Secondly, the edge effects on map boundaries can be problematic, and so we confined the interpolation to the lake data point boundaries. Thirdly, the order of the polynomial equation, which determines the degrees of freedom, is limited by the number of sample points in order to have adequate degrees of freedom for testing of statistical significance. We kept the trend surface fitting to an order of 2 or quadratic surface, which confined our analysis to the overall trend or the regional component of the spatial domain (Davis 2002).

A positive advantage of trend surface analysis is that it offers an easy way to understand the spatial structure whereby regional features can be modeled by low order equations with the basic trends in the data more apparent (Burroughs & McDonnell 1998). Another advantage particular to our analysis, is due to the uniform/lattice configuration of the sample points, that add increased robustness to the trend surface modeling. Since the sample size is relatively small, the adjusted value of the coefficient of determination,  $R^2$  was used to assess the strength of the regression model as a measure of the explained variance or the "goodness of fit." The adjusted  $R^2$  was computed as the sum-of-squares of the residuals from the regression line or curve having *N*-*K* degrees of freedom, where *N* is the number of data points and K is the number of parameters fit by the regression equation. The adjusted  $R^2$  was further used to estimate the expected shrinkage in  $R^2$  that would not generalize to the population because the regression solution is over-fitted to the data set by including too many independent variables in the form of higher order surfaces. The "gstat" package in R Statistical Computing Platform was used in fitting the polynomial trend surface (R Core Team 2015).

*Thin plate spline regression (TPS)* provides a more complete characterization of a continuous statistical surface. The thin plate spline is a two-dimensional variation of the cubic spline. Given a set of data points, a weighted combination of thin plate splines centerd about each data point gives the interpolation function that passes through the points exactly while minimizing the so-called bending energy or tension. Bending energy is defined here as the integral over domain of the squares

of the second derivatives which acts as a smoothing function (Rupert et al. 2009). As with the trend surface analysis, longitude and latitude are used as the spatial coordinates for the explanatory variables in the regression model. Also, the adjusted  $R^2$  is used to indicate the strength of the fit. The TPS function in the 'fields' package within the R platform was used to fit the TPS regression surfaces to the data. The reason we chose TPS was because of distinct advantages that TPS offers with relatively small sample size data sets, and there is no need to specify the number of terms in the model so initial modeling strategies are precluded (Wood 2003). In addition, TPS modeling does not require the prior estimation of the spatial covariance structure, which can be problematic with a small sample size, and non-stationary data does not pose a problem.

AQ8

#### AQ9

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**AQ10** 

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