Applicability of characterized variance and ecosystem interactions in water quality monitoring

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Academic dissertation in environmental ecology

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CONTENTS

ABSTRACT

Spatial and temporal variation within water bodies causes uncertainties in freshwater monitoring programmes that are surprisingly seldom perceived. This poses a major challenge for the representative sampling and subsequent assessment of water bodies. The sources of variability in lakes are relatively well known. The majority of them produce consistent patterns in water quality that can be statistically described. This information can be used in calibrating the sampling intervals, locations and monitoring methods against the typical variation in a water body as well as the accuracy requirements of monitoring programmes. Similarly, understanding of ecosystem history and functioning in different states can help in contextualizing the collected data. Specifically, studies on abrupt transitions and the interactions involved produce a framework against which recent water quality information can be compared.

This thesis research aimed to facilitate water quality monitoring by examining 1) feasible statistical tools to study spatial and temporal uncertainty associated with sampling efforts, 2) the characteristics of variation and 3) ecosystem interactions in different states. Research was conducted at Lake Vesijärvi, southern Finland. Studies of uncertainty utilized data-rich observations of surface water chlorophyll *a* from flow-through, automated and remote sensing systems. Long-term monitoring information of several trophic levels was used in the analysis of ecosystem interactions. Classical sample size estimates, bootstrap methodology, autocorrelation and spatial standard score analyses were used in spatio-temporal uncertainty analysis. A systematic procedure to identify abrupt ecosystem transitions was applied in order to characterize lake interactions in different states.

The results interlink variability at the study site with information required in sampling design. Sampling effort estimates associated with the spatial and temporal variance were used to derive precision information for summary statistics. The structure of the variance illustrated with an autocorrelation model revealed the low spatial representativeness of discrete sampling in the study area. A generalized autocorrelation model and its parameters from the monitoring area were found applicable in sampling design. Furthermore, areas with constantly higher chlorophyll *a* concentrations, which had an effect on the water quality information derived with remote sensing, were identified from the study area. Characterization of the interactions between the main trophic levels in different ecosystem states revealed the key role of zooplankton in maintaining the current state as well as the resilience of the studied pelagic ecosystem. The results are brought into a broader context by discussing the applicability of presented methods in sampling design of water quality monitoring programmes.

According to this thesis research, sampling design in individual monitoring regimes would benefit from the characterization of variance and subsequent uncertainty analysis of different data sources. This approach allows the calibration of sampling frequency and locations on the observed variance, as well as a quantitative comparison between the abilities of different monitoring methods. The derived precision information also supports the joint use of several monitoring methods. Furthermore, analysis of long-term records can reveal the key elements of freshwater ecosystem functioning and how it has responded to earlier pressures, to which recent monitoring data can be compared. This thesis thus highlights analysis of the variance and history of the monitored system in developing a rationalized and adaptive monitoring programme.

LIST OF ORIGINAL PAPERS

This thesis is based on the following papers, which in the text are referred to by their Roman numerals:

I. Anttila, S., Kairesalo, T., & Pellikka, P. (2008). A feasible method to assess inaccuracy caused by patchiness in water quality monitoring – *Environmental Monitoring and Assessment* 142(1): 11-22.

II. Anttila, S., Ketola, M., Vakkilainen, K., & Kairesalo, T. (2012). Assessing temporal representativeness of water quality monitoring data – *Journal of Environmental Monitoring* 14(2): 589-595.

III. Anttila, S. and Kairesalo, T. (2010). Mean and variance estimations with different pixel sizes: case study in a small water quality monitoring area in southern Finland – *Boreal Environment Research* 15(3): 335-346.

IV. Anttila, S., Ketola, M., Kuoppamäki, K., & Kairesalo, T. (2013). Identification of biomanipulation-driven regime shift in Lake Vesijärvi: implications for lake management – *Freshwater Biology* 58(7): 1494-1502.

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THE AUTHOR'S CONTRIBUTION

SA planned studies I–III with contributions from TK (I–III), MK (III) and KV (III). Study IV was planned with equal contributions from SA, KK (formerly KV), MK and TK. SA was the corresponding author in all the papers. TK supervised all the studies.

I SA was responsible for the field sampling and analysis of the flow-through measurements. SA also performed the data analysis, interpreted the results, prepared the figures and wrote the paper. TK and PP revised the paper.

II SA carried out the temporal representation analysis, its interpretation and prepared all the figures. Data analysis and results related to the calibration of automated monitoring data were handled by MK and KV. The paper was written according to the preceding distribution of work and revised by all the authors.

III SA was responsible for the field sampling and analysis of the flow-through measurements. SA also performed the data analysis, interpreted the results, prepared the figures and wrote the paper. TK revised the paper.

IV SA performed the data analysis and prepared the figures based on the long-term monitoring data archived by KK and collected by the University of Helsinki and local environmental authorities. Zooplankton data were reused from the studies of MK. The results were interpreted by all the authors. SA was responsible for the majority of the text, with significant contributions from MK, KK and TK. All the authors revised the paper.

The thesis also includes unpublished additional material analysed by the author.

ABBREVIATIONS

a.k.a.	also known as
Ca.	circa (approximately)
i.e.	id est (that is)
inter alia	among other things
e.g.	exempli gratia (for example)
cf.	confer (compare)
chl-a	Chlorophyll *a*
chl-a:TP ratio	Ratio between chlorophyll *a* and total phosphorus concentrations
TP	Total phosphorus
RSI	Regime Shift Index
SD	Standard deviation
SE	Standard error
Z-score	Standard score
WFD	Water Framework Directive

1. INTRODUCTION

Freshwater lakes and rivers are fundamental to the maintenance and survival of terrestrial life, although they represent only a small fraction (around 0.009%) of the total volume of water in the biosphere (Wetzel, 2001). For humans, lakes and rivers provide a variety of goods and services including water for domestic, agricultural and industrial use, food production and recreational opportunities, as well as less tangible aesthetic and cultural benefits (Maltby & Ormerod, 2011). Freshwater ecosystems confront well-acknowledged threats that endanger the provision of these services. The degradation of surface waters is often also interlinked with global or regional phenomena including climate change, acidification and eutrophication (Schindler et al., 1996; Carpenter et al., 1999; Blenckner et al., 2010). Considering the ever-growing threats to freshwater resources, precise ecological assessments and appropriate management of freshwater ecosystems are required (Hawkins, 2010; Lindenmayer et al., 2011).

The legislative framework to protect and restore aquatic systems in Europe arose from concern over the status of water bodies, where strong economic interests were often set against the diffuse interests of the general public (Hoornbeek, 2004). The Water Framework Directive (WFD; European community, 2000), which is the main initiative to protect European lakes, aims at conditions with minor or no effects from human actions in surface and coastal waters. It strongly guides freshwater quality monitoring programmes in EU countries. The Directive requires assessment of water bodies based on a variety of biological and chemical water quality elements, where the current status is compared against the assumed pristine conditions. The reference condition for a water body is typically estimated with reference sites, modelling, historical data sets or using expert judgment (Hawkins et al., 2010; Andersen, 2011). The current status, on the other hand, is assessed with water quality monitoring data that are for the time being mainly based on manual *in situ* sampling. The WFD has been praised for its integrative way of measuring ecological quality, with a focus on the hydrological catchment instead of administrative borders, and on the harmonization of classification and monitoring methods across Europe (Hering et al., 2010). However, significant criticism has been directed at the underestimation of the effort and costs for the participating countries (Carstensen, 2007), at issues related to the classification and combination of different quality elements (Moss, 2008) and at the insufficient characterization of uncertainty in monitoring data (Carstensen, 2007; Håkanson, 2007; Hering et al., 2010). One of the main concerns has been the lack of precise guidelines on how the spatial and temporal variation within water bodies should be acknowledged in monitoring and subsequent assessment.

Conventional water quality monitoring data include pooled samples taken across seasons from a variable number of locations to derive annual ecological conditions for the monitoring area (Wright et al., 2000). The level of confidence in these summary statistics is dependent on the number of samples collected (Dixon & Chiswell, 1996). The greater the variation in water quality, the greater is the number of samples needed to obtain a statistically sound estimate that describes parameter behaviour (Strobl & Robilliard, 2008). The collection of data, however, is typically controlled by the available funding for monitoring. Thus, many standard monitoring programmes, for instance related to the Water Framework Directive, and many national monitoring programmes have been criticized for collecting too few samples from too few locations for the sound assessment of ecological status (Knowlton & Jones, 2006; Carstensen, 2007; Erkkilä & Kalliola, 2007; Håkanson, 2007). The consequent error and bias, *inter alia*, in annual mean estimates is in many cases unclear (e.g. Carstensen, 2007; Heffernan et al., 2010). A typical strategy to overcome uncertainty caused by temporal variability has been to perform sampling in specific periods of the growing season to catch certain events in the annual cycle (Barbour et al., 1996; Niemi et al., 2001). On a spatial scale, expert judgment has typically been used in the selection of suitable sampling locations to represent pelagic and littoral areas. Extrapolation based on the bottom area and water masses with varying methods has commonly guided site selection (Carstensen, 2007). These traditional strategies to assess spatial and temporal variation have not been considered sufficient in constantly changing aquatic ecosystems. Criticism clearly originates from the limitations in traditional water sampling, which is still the backbone of most monitoring programs. Several arguments have been presented to show that measurements from discrete locations and a sparse sampling frequency guided by available funding fail to give a synoptic spatial or temporal depiction of water quality and might lead to significant bias in estimations of the water quality status (Håkanson, 2007; Carstensen, 2007; Heffernan et al., 2010). Even though the underlying theoretical concepts to assess uncertainty at temporal and spatial scales are well known among statisticians (e.g. Clarke and Hering, 2006; Carstensen, 2007), these methods have not yet been implemented in water quality monitoring programmes. Strobl and Robilliard (2008) noted that research has been too general or specific to be easily incorporated into large monitoring programmes, given the time and budget constraints. A fundamental problem, however, is typically not in the statistical metholds but the lack of information from variability occurring in monitoring regimes.

1.1 Sources of spatial and temporal variation in lakes

Freshwater ecosystems are under constant change, which occurs at variable spatial and temporal scales. Although this poses a major challenge for water quality monitoring and assessment (Carstensen, 2007; Hawkins et al., 2010; Hering et al., 2010), the sources of variation are relatively well known. Temporal variation in lakes typically follows the main diurnal and seasonal cycles induced by light, temperature and nutrient availability (cf. Wetzel, 2001). Naturally, several factors cause variability in these cycles, including trophic interactions, stochastic (extreme) events driven by climate or human perturbation (Tuvikene et al., 2011). Sources of spatial variation, on the other hand, are associated with run-off from the drainage basin, lake morphology and water movements (e.g. George & Edwards, 1976; George & Heaney, 1978; Chiew & McMahon, 1999; Vuorio et al., 2003; Ekholm & Mitikka, 2006), as well as with biological factors, including the buoyancy properties of different phytoplankton species and movements of zooplankton and fish shoals (Horppila et al., 1998; Moreno-Ostos et al., 2006; Moreno-Ostos et al., 2009).

Horizontal variation in water quality can be dependent on the annual cycle of the ecosystem and is also affected by the climatic conditions. Moreno-Ostos et al. (2006; 2008; 2009) reported differences in spatial variation to be dependent on the dominant algal group and weather conditions. They observed that during the winter, when the studied lake was isothermal and the phytoplankton was dominated by diatoms, there was no significant spatial variation. Conversely, during the summer stratification, when positively buoyant cyanobacteria dominated the phytoplankton community, they found a very strong non-uniform spatial distribution in the phytoplankton. Furthermore, they observed that a favourable growing environment for cyanobacteria can emerge when a calm wind period supports the formation of colonies, but storms and high wind speed periods typically disrupt the patterns in water quality.

Some water quality parameters, such as chlorophyll *a* and inorganic suspended matter can create stationary patterns in the water. This phenomenon has been noted in many studies, and in many monitoring regimes it is considered a typical water quality property (Lindell et al., 1999; Östlund et al., 2001; Dekker et al., 2001; Erkkilä & Kalliola, 2004; Wang & Liu, 2005). For example, rivers carry eroded material from the catchment and create near-shore patterns in lake water quality (e.g. Vuorio et al., 2003). Similarly, runoff from urban areas is another typical point source of pollution that is greatly affected by factors such as the imperviousness of the urban catchment area (Chiew & McMahon, 1999). Localized growing environments for the biological components in the lake can be created by diffuse sources of nutrients and suspended solids arising from surrounding agricultural areas (e.g. Ekholm & Mitikka, 2006) or by bottom topography, which affects the water current speed and sediment resuspension areas (Håkanson, 2004). Wind-induced water movements also create patterns in water quality, which lake morphology can further enhance (George & Edwards, 1976). Schernewski et al. (2000) demonstrated that particles that are driven or resuspended by the wind can be trapped in shallow areas and create localized patterns of water quality.

To summarize, the spatial and temporal variation in lake water quality is a result of many interacting factors. The way these variations are manifested depends on how annual cycle, the lake biota, lake morphology, drainage basin characteristics and variable climatic conditions interact (George & Edwards, 1976; George & Heaney, 1978; Horppila et al., 1998; Schernewski et al., 2000). The majority of variability results from consistent natural and anthropogenic processes typical for the monitoring regime. This encourages that the main features of variability can be statistically characterized.

1.2 Sampling design

Water quality monitoring refers to the acquisition of quantitative and representative information characterizing a water body over time and space (Sanders et al., 1983). This includes the number and spatial distribution of monitoring stations, sampling frequency, the selection of parameters and monitoring methods as well as the mode of data transfer (Strobl & Robillard, 2008). Water quality monitoring can also be seen as a tool that is enforced mainly by the legislative framework to guarantee decisions leading to a healthier environment. For decision making, the complex ecosystem information described with monitoring data needs to be condensed. The key aspects from an otherwise overwhelming amount of information are often isolated with indicators that help policy makers to see the larger patterns of the ecosystem state and determine the appropriate action (Niemeijer, 2002). In the process of condensing data to derive indicators, information is always lost. Therefore, to avoid erroneous decisions, the monitoring data used needs to provide a representative picture of the ecosystem state.

Sampling design, on the other hand, refers to the procedure and criteria for matching the information needs with the requirements for the monitoring data (Strobl & Robillard, 2008). Its ultimate goal is to define the objectives and accuracy criteria for monitoring as completely as possible (Steele, 1987). In practice, however, sampling design is used to provide the required information with sufficient accuracy and with rationalized costs. It is thus a compromise between data collection costs and the ability to cover the different sources of uncertainty that affect the data (Beliaeff & Pelletier, 2011). Therefore, while considering the spatio-temporal representativeness of collected data, the key issue is the understanding of typical variability in monitored areas and the abiotic conditions associated with this variation (Hawkins et al., 2010). Furthermore, understanding of how this variability is captured with available monitoring methods is relevant. In other words, in sampling design the ability of different monitoring methods to measure variation needs to be assessed in relation to the variation typical for the monitored system (Fig. 1).

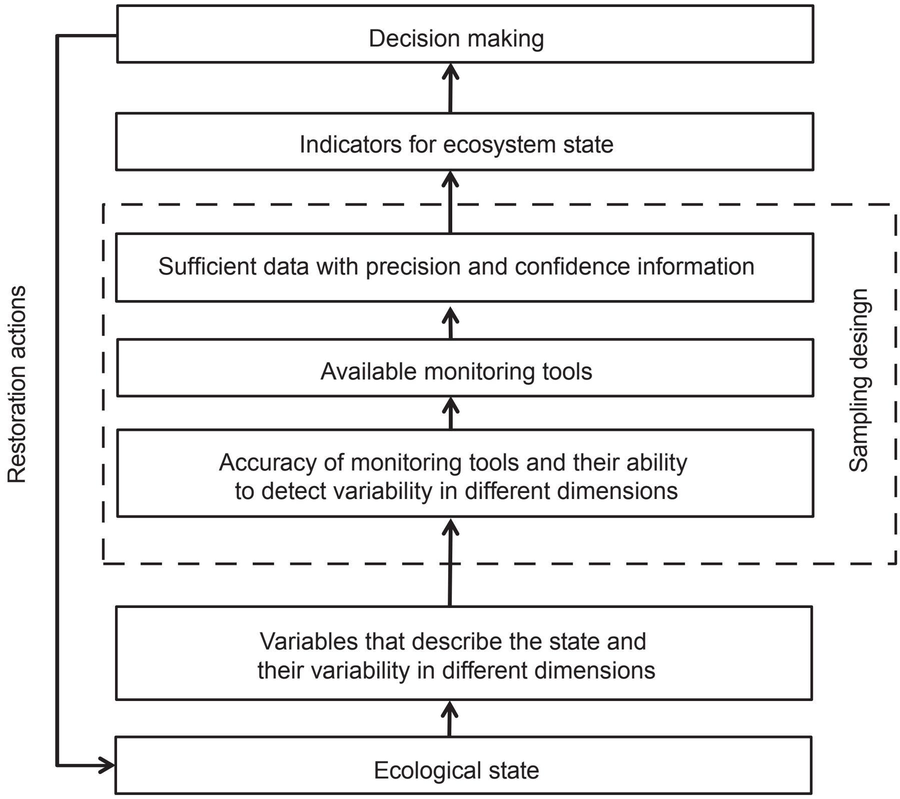

Figure 1. The role of sampling design in deriving representative information on the ecological state of water bodies for decision making.

1.3 Sources of uncertainty in water quality monitoring

The underlying sources of uncertainty in water quality monitoring can be partitioned into analytical error and random sampling error, as well as the uncertainty caused by spatio-temporal variation (Carstensen, 2007; Hawkins et al., 2010). Random sampling error refers to the variation among replicate samples from a single location at the same time, and analytical error includes systematic error in the measurement or prediction of an attribute. These sources of uncertainty are typically considered in monitoring programme guidelines (e.g. Anonymous, 2003). Uncertainty caused by spatial and temporal variation, however, has been neglected in the majority of water quality assessment systems (Hering et al., 2010), and the error caused by a deficient sampling frequency in time and space is often unclear.

The questions of when, where, how often and how many locations to observe have already been noted in early monitoring programmes (Sanders et al., 1983), but have been difficult to address with conventional monitoring methods. Only recently has the importance of these questions in quantitative assessment been raised (cf. Hering et al., 2010). The problem is clearly related to the statistical requirement to obtain a representative sample within an observed system. Essentially, it is a matter of the probability of estimating the true value of a water quality parameter that is affected by different sources of uncertainty. Hawkins et al. (2010) clarified the problem with a diagram showing the effect of different uncertainty sources on a hypothetical ecological index (Fig. 2), where each source of variability increases the uncertainty over observing a true value.

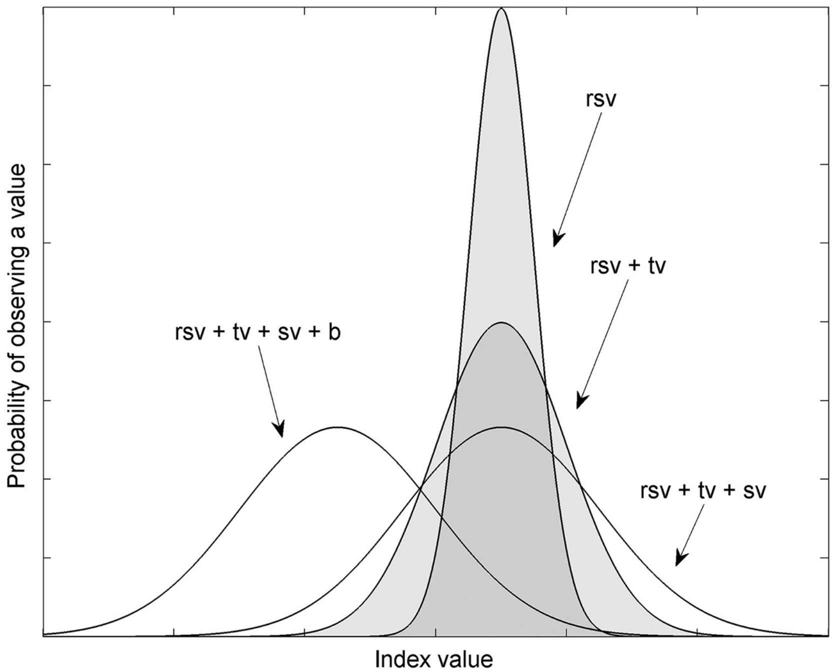

Figure 2. Effect of different uncertainty sources on a hypothetical ecological index. Rsv = random sample variation, tv = temporal variation, sv = spatial variation and b = bias, i.e. analytical or prediction error. Modified from Hawkins et al. (2010) with permission.

Water quality monitoring programmes are still mainly based on traditional manual observations, which benefits from the number of observable parameters, accurate laboratory measurement and the possibility to cover several sampling depths. These discrete measurements, however, lack the potential for synoptic spatial and temporal observations and can be expensive (e.g. Vosa et al., 2003; Le Vu et al., 2011). Therefore, new methodologies, including automated, ship-of-opportunity or flow-through and remote measurements are increasingly being taken in use (Bierman et al., 2011). All of these differ in their ability to measure water quality at spatial and temporal scales. Moored automated monitoring stations, for instance, can cover the whole range of temporal variability (Le Vu et al., 2011), but are limited in the spatial dimension as well as in the number of parameters that can be measured. Ship-of-opportunity or flow-through measurements, on the other hand, can give a more representative picture of spatial variation than discrete measurements (Lindfors et al., 2005; Ruokanen et al., 2007), but their operative application can be expensive, especially in freshwater monitoring areas. Depending on the remote sensing instrument and monitored target, this data source can provide spatially and temporally representative information with varying accuracy from the optically active water quality parameters. Properties of the used instrument such as the spectral, spatial and temporal resolution, as well as the difficulty in making measurements on optically complex waters from large distances, affect the usability of this data source (cf. Bukata, 2005).

While considering the differences between monitoring areas, their surroundings, accessibility, size, water properties, as well as their natural variability, sampling design obviously needs to be adapted to the specific characteristics of the aquatic monitoring area (Håkanson, 2007; Strobl & Robilliard, 2008). Definition of the abilities of different monitoring methods to detect the variance in different dimensions can thus be used as basis for rationalized sampling design. It can essentially allow a quantitative comparison between monitoring data sources and reveals the strengths and weaknesses of different methods in a specific monitoring area. On the other hand, such analysis is also a starting point for data assimilation, where more accurate information can be provided by combining data sources. To allow this, information on the precision of each data source is required (e.g. Pulliainen et al., 2004). Furthermore, since the suitability and costs of different monitoring methods to measure water quality differ between monitoring regimes, the complementary use of several data sources is likely to be beneficial (Vosa et al., 2003; Pomati et al., 2011).

1.4 High-frequency data and their use in representative sampling analysis

One limitation in the characterization of spatio-temporal variability in lakes has probably been the lack of appropriate data from the monitoring area (Hering et al., 2010). Water quality monitoring methods, such as automated, remote sensing or flow-through applications, can provide spatially and temporally extensive information from monitored areas. The significance of these data-rich methods in water quality monitoring programmes is expected to increase, as they can provide a significantly lower cost per measurement ratio than traditional methods. In addition, for the provision of actual data for water quality monitoring programmes, these data sources can be used in characterizing the variability within monitoring areas (e.g. Le Vu et al., 2011; Bierman et al., 2011; Kallio, 2012). Data-rich monitoring methods can give representative estimates of the variance in spatial and temporal dimensions and can be used to assess the uncertainties associated with less frequent or spatially discrete sampling. While these methods are increasingly being taken in use, the maintenance, calibration and management of retrieved data causes expenses that are still in many cases undefined (cf. Huttula et al., 2009). However, data-rich monitoring sources are rightfully claimed to provide new information on the dynamics within an ecosystem that is undetectable with discrete and infrequent sampling.

At its simplest, a representative set of high-frequency data on spatial or temporal dimensions can be used to derive the typical variance for the monitoring regime to be used in the estimation of representative sample sizes. Cochran (1967) presented a basis for determining sample sizes to estimate the sample mean with random sampling and certain margins of error from normally distributed data sets. Regardless of statistical assumptions involved, methods based on this classical approach are still applicable (e.g. Strobl & Robilliard, 2008). Cochran's approach provides a straightforward tool to provide first estimates on sampling requirements when prior information on the variance exists. One step further in the use of high-frequency data is to examine how the variance changes with the distance or time separating observations, i.e. to study and model autocorrelation in data sets (cf. Legendre, 1993). This approach can be used to characterize the spatial or temporal structure in data sets (Bierman et al., 2011). Furthermore, it has applications in calibrating sampling locations to the existing variation by revealing the distance at which observations become statistically independent (Kitsiou et al., 2001; Heffernan et al., 2010). In statistics, bootstrapping refers to the methods where measures of accuracy are assigned to sample estimates (Efron & Tibshirani, 1994). Benefits in different bootstrapping variants include that statistically independent or normally distributed data sets are not required; methods are based on relatively simple computerized calculation and can be based on the actual measured data (Vogel & Shallcross, 1996; Varian, 2005). Several techniques exist to investigate temporal patterns at spatial scales that are also applied in water quality data sets. These are essentially based on the identification of sub-areas within data from different time periods with constantly differing characteristics. Applications range from relatively simple single parameter methods such as standard score analyses, where local means are compared to whole data sets mean (Getis & Ord, 1996), to mathematically more challenging multivariate techniques. Cluster analysis, for instance, is used to measure the similarity in water quality observations between different measurement sites and to group them (e.g. McNeil et al., 2005). Factor and principal component analysis (PCA), on the other hand, are used to describe the relationships between water quality variables and to reduce their numbers by combining them (Singh et al., 2004; Navarro & Ruiz, 2006)

1.5 Long-term records: key to understanding the system

The value of long-term data sets has been strongly emphasized during recent years, and their importance in sustainable management and in mitigation to the presumably increasing ecosystem regime shifts has been highlighted (e.g. Scheffer et al., 2001; Carpenter et al., 2011). Furthermore, Carpenter et al. (2011) underlined the importance of such analysis in contextualising scientific information for decision makers. Analysis of long-term data thus has a direct affiliation with the indicator information derived from environmental monitoring programmes.

Identified interactions in the history of an ecosystem can provide a better understanding of the current ecosystem state and its direction than information based solely on recent monitoring data. Analysis of long-term records before and after an abrupt ecosystem transition (i.e. a regime shift) can reveal features in ecosystems that can be used to contextualize immediate observations. Long-term records and the identification of the interactions between different trophic levels can be used to benchmark ecosystem functioning in different ecological states (Bestelmeyer et al., 2011; Maberly & Elliot, 2012). Information is thus required from the ecosystem components that describe the state (response) and cause the change (drivers), as well as the feedback mechanisms that tend to maintain the present state. This is essential information when interpreting monitoring data, thus providing clear implications for lake monitoring and management. Such analysis obviously requires a representative number of observations from each ecosystem state; in other words, representative long time series are essential (Bestelmeyer et al., 2011).

Ecosystem transitions can be gradual or abrupt, depending on how ecosystem drivers and response mechanisms interact. Complex ecosystems such as lakes include feedback mechanisms that tend to maintain their current state. Slowly increasing pressure caused by climate change or sudden events such as storms or human actions can deteriorate feedback mechanisms (a.k.a. resilience). After crossing a critical level, this can cause a major and abrupt shift in the ecosystem state, the persistence of which depends on the changes occurring in the functional form of the ecosystem (Carpenter et al., 1999; Scheffer et al., 2001; Anderssen et al., 2009; Bestelmeyer et al., 2011). The above-cited authors have identified general types of abrupt transitions, namely linear, threshold and hysteresis. These can be described with the features found in time series of ecosystem driver, response and feedback variables, in their relationships, in the frequency distribution, as well as in the indicative signals for the change, such as temporal variance of the response variable. Bestelmeyer et al. (2011) suggested a systematic approach to the identification of these transition types. They emphasized the benefits of such an approach, for example in the characterization of ecosystem functioning, and its use in pro-active ecosystem management. Thus, deeper understanding of the current state and direction of the ecosystem can be derived by interpreting recent monitoring data against the identified ecosystem interactions and against the potential early warning signals (Contamin & Ellison, 2009).

2. OBJECTIVES OF THE PRESENT STUDY

As the legislation for the protection and restoration of natural waters proceeds, issues concerning representative monitoring have been raised (Carstensen, 2007; Hawkins et al., 2010). The uncertainty associated with temporal and spatial variability in water quality monitoring is one of the major challenges in the next phase of WFD implementation (Hering et al., 2010). On the other hand, the analysis of long-term records is an essential tool in contextualizing and translating scientific information into meaningful policy recommendations and management interventions (Bestelmeyer et al., 2011). Long-term records can reveal the key elements of freshwater ecosystem functioning and responses to earlier pressures. Such analysis is valuable in adaption to and preparation for the threats facing freshwater ecosystems (Contamin & Ellison, 2009; Maberly & Elliot 2012).

This thesis presents tools to characterize spatio-temporal variation and study ecosystem interactions to allow adaptive water quality monitoring. Papers I-III concentrated on the uncertainty associated with the spatial and temporal variability and utilized surface water chl-a as an indicator for water quality. Paper I focuses on the structure of spatial variation in lake water quality, and the results were used to determine the horizontal representativeness of point-source sampling. Paper II concentrates on the temporal representativeness of water quality monitoring at varying intervals and highlights the importance of careful calibration of automated fluorometer measurements. Paper III defines the areas in the study lake (Lake Vesijärvi) with constantly differing water quality and uses this information to assess the representativeness of pixel-type observations of different sizes. Finally, paper IV conceptualizes lake ecosystem interactions and functioning by using long-term monitoring data to derive understanding for the lake management purposes. This thesis combines the key results of the papers and presents a synopsis on the applicability of the results in water quality sampling design (Fig. 3).

The individual objectives were to:

1. Identify feasible tools to assess the spatio-temporal uncertainty associated with water quality monitoring data (I–III);
2. Analyse long-term monitoring records to identify ecosystem interactions in different states for lake management purposes (IV);
3. Discuss how sampling design can benefit from the uncertainty analysis and identified ecosystem interactions (synopsis).

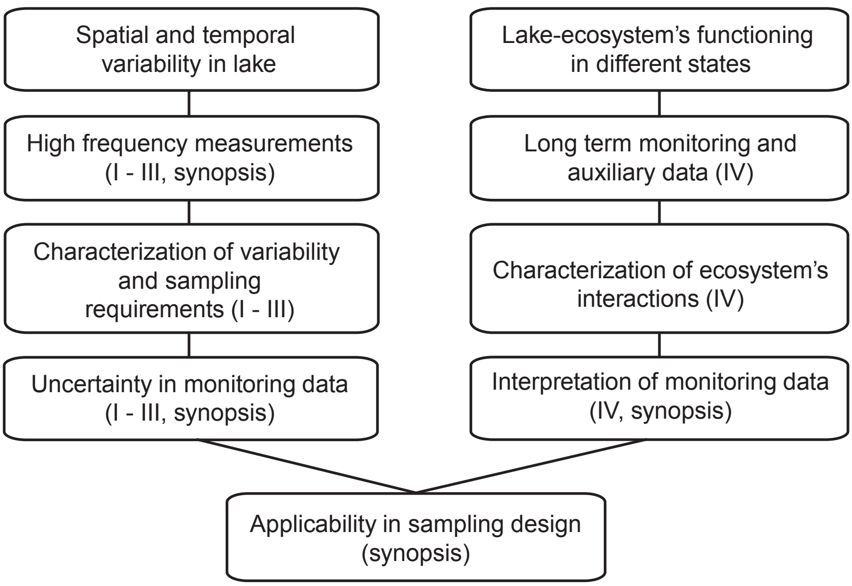

Figure 3. Associations between the main research themes of papers I-IV and synopsis of the thesis.

3. MATERIALS AND METHODS

3.1 Study site

Data sets were collected from the Enonselkä basin of Lake Vesijärvi in Southern Finland (25° 37'24''E 61° 0' 30''N) (Fig. 4). Lake Vesijärvi is relatively large (110 km^2) and shallow (mean depth 6 m). The drainage basin of the lake is relatively small (514 km^2) and the land cover is dominated by forests (ca. 60%) agricultural areas (ca. 23%), wetlands (ca. 9%) and urban areas (ca. 9%). Over 150 000 people live in the vicinity of the lake, the majority in the city of Lahti located around the southern basin of the lake (Fig. 4). The lake was originally oligohumic with highly transparent water, but was polluted by nutrient and organic matter loading from domestic sewage of the city of Lahti, industry, agriculture and timber storage activities (Keto & Sammalkorpi, 1988). It became one of the most eutrophicated lakes in Finland (Kairesalo & Vakkilainen, 2004) and experienced severe cyanobacterial blooms until concern over its status was materialized into restoration ac-

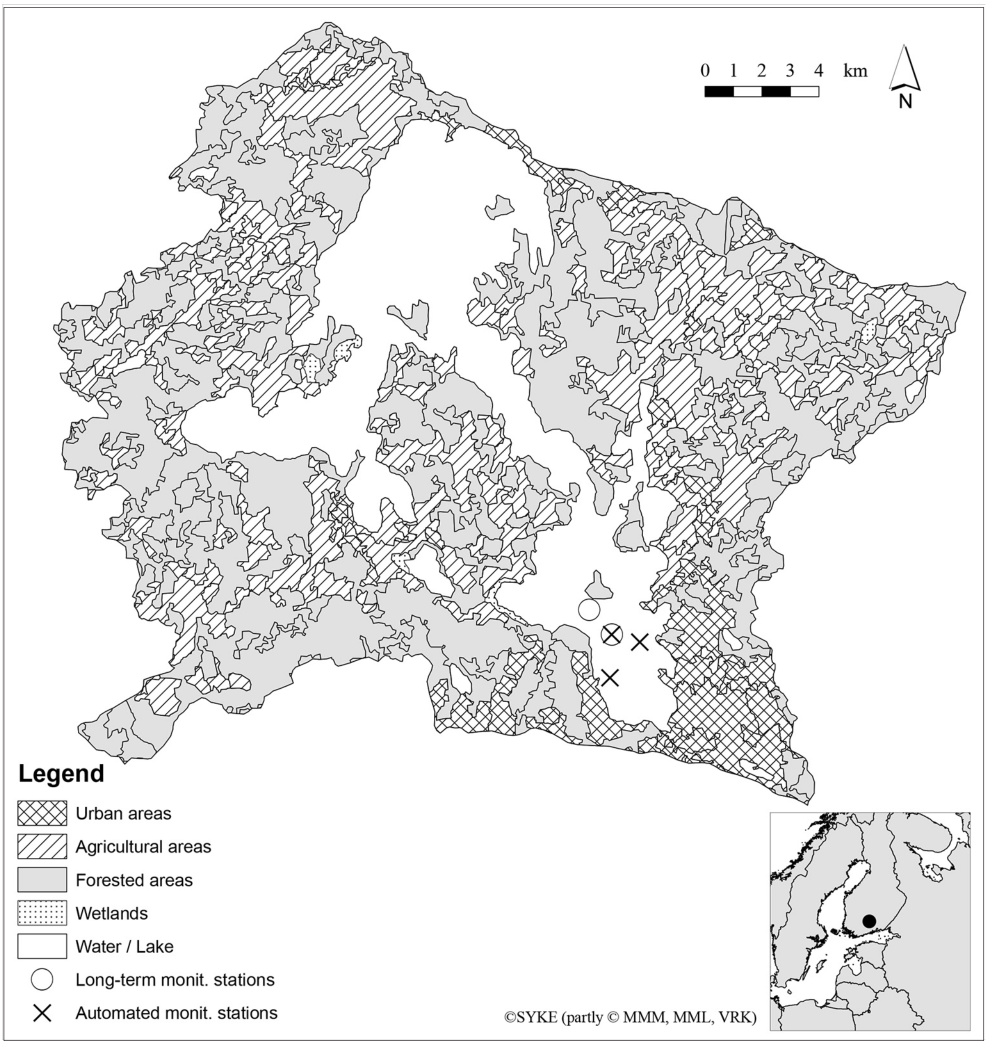

Figure 4. Lake Vesijärvi and land cover information on the drainage basin together with the locations of automated monitoring stations (crosses, II) and longterm sampling sites (circles, IV) in the southern Enonselkä basin.

tions. The municipal sewage load was diverted in 1976 and industrial waste in the 1980s, but the status of the lake remained poor (Keto & Sammalkorpi, 1988) until intensive biomanipulation was performed during 1989–1993 (e.g. Horppila & Peltonen, 1994; Kairesalo et al., 1999). The mass removal of planktivorous fish, which continued with management fishing and the stocking of piscivorous fish, resulted in clearly improved water quality with higher water transparency, lower chlorophyll and nutrient concentrations as well as a collapse in cyanobacterial populations (Horppila *et al.*, 1998, Kairesalo *et al.*, 1999). In the 2000s, however, the condition of the lake showed signs of deterioration and occasional cyanobacterial blooms have also occurred (Kuoppamäki et al., unpublished). In 2009–2010, restoration continued in the Enonselkä basin with large-scale aeration using nine Mixox circulation pumps [Vesi-Eko Oy (Water-Eco Ltd), Kuopio, Finland] that transport and mix oxygen-rich surface water into the hypolimnion. The effects and consequences of this management action for the status of the lake are still unclear.

Short history of monitoring in Lake Vesijärvi

Water quality monitoring data from Lake Vesijärvi and Enonselkä basin extend back to the early 1960s. Monitoring has been conducted in two parallel monitoring programmes by the regional environment authorities and the University of Helsinki. Major limnological parameters, including total nutrients, chlorophyll *a*, Secchi depth, turbidity and conductivity, pH, alkalinity, water colour and micronutrients (Fe and Mg), have been measured and recorded for over 40 years. The number of yearly observations and observed parameters has varied between years, being fewer in the earlier part of the monitoring period, but these have increased since the start of biomanipulation. Manual monitoring has been conducted at several sites. In the Enonselkä basin, the longest and most consistent records have been collected from two monitoring stations located above the deepest points of the basin (Fig. 4). Together with a few shorter monitoring records from other locations, a relatively representative picture of annual variation in the pelagic areas of the lake can be derived. However, as also noted by Horppila et al. (1998), discrete manual sampling is likely to give an insufficient understanding of the within-lake variation.

The first automated water quality monitoring station was installed in 2004 in the Enonselkä basin. At the time of study II, three automated monitoring stations had been installed in the basin, which almost continuously recorded chlorophyll a, phycocyanin, temperature and oxygen concentrations from one to several fixed depths. Although the possibility to measure fine-scale dynamics in water quality and save in expenses was welcomed by researchers and the local authorities, the use of automated measurements has also raised concerns. The amount of total costs from the maintenance, calibration and data management of automated measurements still remain unclear.

The first extensive study concerning the spatial variation of water quality in the lake was conducted by Horppila et al. (1998), who investigated differences in food web components with manual grid sampling in the southern part of Lake Vesijärvi. They concluded that the prediction of water quality development is obscured due to the spatio-temporal variation in the lake, and this sets high requirements for sampling programmes. Other spatial monitoring methods have occasionally been used in Lake Vesijärvi. The usage of flow-through measurements from a moving boat (e.g. Lindfors & Rosenberg, 2011) and interpretation of space-borne remote sensing images (e.g. Vakkilainen et al., 2012) have been conducted in separate research projects over the years. The results have revealed considerable variation in water quality, but the implementation of such data in monitoring programmes has so far been lacking.

3.2 Data sets

Flow-through measurements

Flow-through datasets were collected using a fluorometer system in a moving boat, the position of which was constantly recorded with GPS. The flow-through system allowed spatially extensive measurements in a relatively short period of time (3–4 hours) from the study site. The system pumped water from a depth of 0.4 m into a flow cap that was attached to a SCUFA fluorometer (Turner Design). The fluorometer measured fluorescence (460 nm excitation and 685 nm emission) and turbidity (90º scatter) with a frequency of 1 Hz. Water samples for the calibration of fluorescence values to the chl-a concentration were taken with a Limnos tube sampler from the surface water every 30 minutes. The chlorophyll *a* concentration was spectrometrically analysed after the field campaigns in a laboratory according to standard procedures (SFS 5772). Field surveys were conducted at a constant speed (9–11 km/h) in relatively calm weather conditions. Altogether, nine flow-through measurements campaigns were conducted during the summers of 2005–2007, and are described in more detail in papers I and III.

Automated measurements

Automated monitoring measurements included hourly fluorescence data from three monitoring stations installed in the Enonselkä basin that were collected during two years (2009 and 2010). Each station measured relative chl-a fluorescence (Trios Micro Flu chl sensor, 470 nm excitation and 685 nm emission) and one station also measured the fluorescence of phycocyanin (TriOS Micro Flu blue, 620 nm excitation and 655 nm emission). The relative fluorescence measurements were first transformed to chl-a and cyanobacteria fluorescences by using standard conversion coefficients provided by the manufacturer and the supplier of the instrumentation. Fluorescense of chl-a was then further calibrated with a multiple regression technique as presented, for example, in Seppälä et al. (2007), in which manual water samples taken next to the stations are explained with chl-a and phycocyanin fluorescences. The calibration methodology and the manual sampling are described in detail in paper II. In the subsequent temporal representation analysis, daily mean values of chl-a were used in order to disregard the effect of diurnal variation.

Long-term monitoring data sets

Long-term data sets collected during a 40-year period from the two monitoring stations in the deepest points of the Enonselkä basin (Fig. 4) were combined. Measurements of chl-a, as an ecosystem response variable, and total phosphorous (TP), as the key driver, were harmonized to represent the mean annual conditions (IV). Changes in an important ecosystem trophic component, zooplankton, were described using the length of *Daphnia* (Cladocera) ephippia in lake sediment remains. These data were taken from the detailed study of Nykänen et al. (2010). Results from several earlier studies (Jurvelius & Sammalkorpi, 1995; Peltonen et al., 1999; Ruuhijärvi et al., 2005; Nykänen et al., 2010; unpublished reports) concerning changes in the fish populations in Lake Vesijärvi were used in order to complete the information on different trophic levels during the study period.

Remote sensing estimation

The remote sensing-based interpretation of chl-a presented in this thesis was derived by using Envisat/MERIS satellite data (MEdium Resolution Imaging Spectrometer on board the ENVISAT satellite operated by the European Space Agency [ESA]) and the boreal water quality processor within BEAM software developed for ESA by Brockman Consult. Atmospheric correction was performed according to Doerffer & Schiller (2008a) and chl-a estimation with an inversion algorithm as presented in Doerffer & Schiller (2008b).

3.3 Statistical methods

Classical sample size estimates

Cochran (1977) presented an equation to derive representative sample sizes (n) in order to estimate the mean value from normally distributed data sets with random sampling:

$$n = \left(\frac{t\ s}{d} \right)^2 \qquad (1)$$

where t corresponds the chosen significance level derived from the probability density function of the normal distribution (for instance, 1.96 for 5% acceptable risk for the false estimate), s is the sample standard deviation and d the acceptable margin of error. In paper I, Eq. 1 was applied to the standard deviations derived from the four spatially extensive flow-through measurement campaigns, with a significance level of 5% and the margin of error calculated as the proportional difference from the mean value of each data set (I).

Temporal representativeness of regular sampling

In paper II, a moving block bootstrap method was used in estimating the standard errors of the mean and standard deviation expected with regular sampling at differing intervals. In the moving block bootstrap method, a time series is divided into equal length blocks according to the sample size variant. A random sample is then taken from each block and the sample mean and standard deviation are calculated from these. In paper II, random sampling from each of six time series of chl-a measurements (daily means from three monitoring stations and two years) were iterated 1000 times for each sample size (n), and standard deviations of the resulting means and standard deviations were used to derive the standard errors (SE = $\sigma / \sqrt{n}$) for respective sample sizes. Standard errors derived from the different time series were combined and simple rational functions were fitted. Fitting was performed with Matlab-software (Mathworks Inc.) and utilized the Levenberg–Marquardt algorithm in an iterative minimization process to find the least squares residuals between the model and observations.

Spatial structure analysis

Variogram analysis was used in order to characterize the spatial dependency found in the spatially extensive flow-through measurements and to examine the representativeness of point source samples. The analysis is based on geostatistical methods that were first formalized by Matheron (1971) and are generally explained, for example, in Burrough and McDonnell (1998). The idea is to observe and model the variance between measurements from different locations as a function of the distance that separates them. The assumption is that measurements close to each other are more similar, i.e. have less variance, than measurements separated by larger distances. The dependence of observations in space is also referred to as spatial autocorrelation.

Spatial autocorrelation can be assessed by calculating semivariances for all observation pairs in a data set (Eq. 2):

$$\hat{\gamma}(h) = \frac{1}{2n} \sum_{i=1}^{n} (z(x_i) - z(x_i + h))^2 \qquad (2)$$

where n is the number of observations of parameter z at location x_i, which is separated by distance h from another observation $z(x_i+h)$. Semivariances in large data sets are often further averaged into groups that include observations separated by similar distances. These groups are known as lags. In paper I, semivariances were standardized in order to combine values from different data sets. This was done by dividing semivariances in each lag by the half of variance of all observations in respective lag (a sub-sample from the whole data set). In an empirical variogram (hereafter referred as variogram), the semivariances are plotted as a function of distance and modelled using specific functions. In paper I, a spherical model was chosen, since it described the semivariances in our data sets most suitably (Eq. 3):

$$\begin{aligned}
&\hat{\gamma}(h) = c_0 + c_1\left(\frac{3h}{2a} - \frac{h^3}{2a^3}\right) && \text{for } 0<h<a \\
&\hat{\gamma}(h) = c_0 + c_1 && \text{for } h>=a \qquad (3)\\
&\hat{\gamma}(0) = 0
\end{aligned}$$

where c_0 refers to the nugget parameter, $c_0+ c_1$ is the sill, and a is the range parameter. These parameters define the form of the variogram model. The range parameter defines the maximum distance at which spatial dependence occurs. The nugget parameter accounts for the sampling error and/or spatial dependence occurring at intervals less than the sampling interval. The sill parameter is equal to the variance of a random variable, which means that it represents the maximum semivariance value where spatial dependence still exists. Together with the chosen variogram model, these parameters can be used to define the spatial structure in a data set (Legendre et al., 1989). Anisotropy in the data sets was also studied, but no clear effect on semivariances related to direction was found, so omnidirectional semivariances were used. In paper I, these methods are applied to data from the four spatially extensive sets of flow-through measurements to illustrate their potential in sampling design.

Stationary patterns in water quality

Stationary patterns in water quality were studied by calculating spatial standard scores (z-scores). This analysis can be used to determine whether observations in some locations tend to differ from the mean of the whole data set (Getis & Ord, 1996). The analysis is based on the calculation of z-scores, where local means around each observation are separately compared to the mean of the whole data set and further normalized with the respective standard deviation (Eq. 4).

$$z_n = \frac{\mu_{loc,n} - \mu_{tot}}{\sigma_{tot}} \qquad (4)$$

where $\mu_{loc,n}$ is the local mean around observation n and μ_{tot} and σ_{tot} are the mean and standard deviation of the whole data set, respectively. Local mean was calculated by using an inverse-distance squared method (explained in detail in III). A significant difference from the mean value of the whole data set is reached when the local mean receives a z-score value higher than 1.95 or lower than -1.95.

In paper III, z-scores for each measurement were calculated for nine flow-through field campaigns. These were further interpolated to fine resolution z-score grids with the ordinary kriging method. Kriging is among the geostatistical methods that applies modelled semivariances in spatial interpolation. Variograms defined separately for each data set were used to derive z-score grids. The resulting grids were then classified into binary values [0,1] representing whether they significantly differed from the mean concentration of the whole monitoring regime. Finally, areas where significant difference was observed in more than five occasions were identified.

Ecosystem interactions

In paper IV, a systematic approach suggested by Bestelmeyer et al. (2011) was followed in order to identify abrupt transitions and characterize driver–response interactions in the pelagic ecosystem of Lake Vesijärvi. This approach concentrates on ecosystem driver and response variables and includes the visualization of temporal patterns, analysis of breakpoints in time series, description of the frequency distributions and temporal variance of response variables, and importantly, assessment of the relationships between ecosystem response variable and key driver in different regimes. A method presented in Rodionov (2004) and Rodionov & Overland (2005) was applied to a long time series of water quality parameters (TP and chl-a) and to the length of *Daphnia* ephippia (as an indicator of cladoceran body size) from Lake Vesijärvi to identify breakpoints that separate different regimes. The method sequentially tests whether the next observation in the time series differs from the mean of the previous observations in the same regime. If a significant observation is found (marked with *c* to indicate a potential changing point), the subsequent observations are used to confirm whether the change remains. The significance of a change in the time series is tested with a regime shift index (Eq. 5).

$$RSI_c = \frac{1}{l\sigma_l}\sum_{i=c}^{c+m} x_i^* \qquad (5)$$

where *l* refers to the length of the regimes being tested (cut-off length) and σ_l to the average standard deviation for all one-year intervals in the time series. The number of years from the changing point are marked with $m = 0,...,l-1$ and $\sum_{i=c}^{c+m} x_i^*$ represents the cumulative sum of the normalized difference from the mean level of the hypothetical new regime ($\bar{x}_{new}$). For this regime, the difference from the current regime ($\bar{x}_{cur}$) needs to satisfy the conditions of the Student's t-test (Eq. 6):

$$diff = \bar{x}_{new} - \bar{x}_{cur} >= t\sqrt{2\sigma_l^2 / l} \qquad (6)$$

where *t* refers to the value of the *t*-distribution with 2*l*-2 degrees of freedom at the given probability level *p*. In order to verify the regime shift, the cumulative sum needs to remain positive (in the case of a shift to a greater concentration) or negative (in a shift to a lower concentration) until the cut-off length is reached.

Basically, the minimum interval of detectable regime shifts is determined with the cut-off length (*l*) and probability level (*p*) that affect the sensitivity of the identification. In paper IV, we used a 7-year cut-off length and a 10% significance level to detect major transitions in the time series and respective values of 3 years and 20% to inspect minor changes in the time series. Similar values have also been used elsewhere (e.g. Rodionov & Overland, 2005). After identification of the regimes, the driver–response interaction was examined by fitting linear regression models to study the relationship between TP and chl-a concentrations for the identified regimes. Further details of the methods used are provided in paper IV.

4. RESULTS AND DISCUSSION

4.1 Classical sample size estimates

Environmental assessment of water bodies, which is typically based on summary statistics, requires a certain number of samples in order to be statistically valid. An increase in the number of collected samples evidently reduces the standard error of the mean value. Sample size selection is related to the risk of false estimates (confidence), acceptable margin of error (precision), the variability of the data being sampled and the available funding and time (de Smith, 2011). From the lake manager perspective, funding and time, are typically set by external parties. Therefore the remaining i.e. confidence level, required precision and the variability in data are the factors lake manager need to consider in respect to the information quality to be derived.

Cochran's formula (Eq. 1) provides a starting point for representative sampling analysis if prior knowledge of the data variability exists (Bartlet, Kotrlik & Higgins, 2001). In water quality monitoring, information on variance typically exists from previous observations, research, expert judgment or from similar aquatic ecosystems. In the paper I we concluded that discrete sampling can lead to erroneous mean estimates for the area of interest. We utilized Eq. 1 with measured spatial variance and according to the results, a mean estimate with a margin of error of 20% requires more than 5 random and independent chl-a samples, and the expected error increases rapidly with fewer samples (Fig. 5). Håkanson (1984), who presented one variant of Cochran's equation, claimed that an error larger than 20% carries limited information, since the error bars around the mean will be too large to address questions related to changes in the aquatic system.

This easily incorporated approach can be applied to observed variance in spatial or temporal scales and can provide initial estimates of the expected random sampling error of different

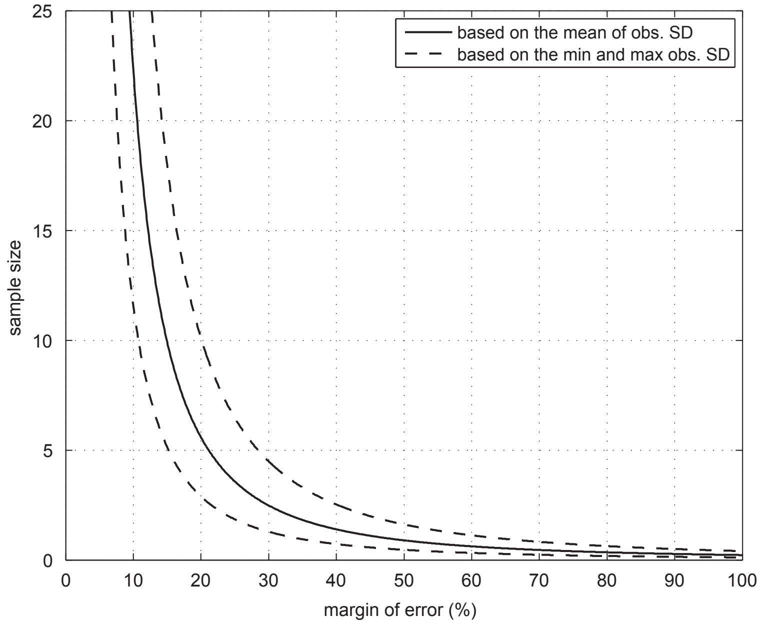

Figure 5. Required sample sizes to estimate the mean chlorophyll a concentration with different margins of error. Estimates are based on standard deviations (SD) observed (obs.) from the four spatially extensive flow-through data sets from Lake Vesijärvi. Modified from study I.

sampling efforts (I). The equation has evolved several variants, all of which are based on the relationship between three elements; two involving risk assessment (significance level and variance) and one involving the size of the effect one is seeking to discover (margin of error) (de Smith, 2011). The usability of the results apparently depends on the prior information on the variance from the observed system. Therefore, the standard deviation used in sampling effort analysis should reflect the variance expected in the specific time period of interest (Hedger et al., 2003). Drawbacks in classical sample size estimates are that they assume random sampling and therefore do not take into consideration the possible dependency between observations or characteristics of variation.

4.2 Temporal representativeness of regular sampling

In paper II, we examined the temporal uncertainty of regular sampling frequencies in estimating the seasonal statistics. The study resulted in standard error models for the mean and standard deviation estimates for different regular sampling intervals (Fig. 6). Based on the measured variance in chl-a, fortnightly sampling would provide reasonable precision in summary statistics (ca. 7% in the mean and 12% in the SD). Loftis and Ward (1980) stated that sample statistics computed from monitoring data can be affected by three general factors: (1) random changes due to storms, rainfall, etc.; (2) seasonal changes; and (3) serial correlation (i.e. autocorrelation). The bootstrap approach used in paper II assumes that the temporal natural variance of a water quality parameter can be described. We used daily time series from two years and three locations to describe the variance. It is likely that these do not comprehensively cover typical inter-annual and spatial variation at the study site, although all chl-a time series showed similar patterns and seasonal succession (Fig. 3 in II). Furthermore, meteorological and anthropogenic perturbations in water quality are partly averaged in the calculation of combined standard errors. The applied method is thus less suitable in water areas where the variation is unpredictable. Benefits in moving block bootstrap method include that it works with dependent data and also allows estimation of the probability of observing high concentrations (Fig. 6 in paper III). Observations of high concentrations are valuable, since they often indicate extreme situations such as algae blooms or rapid water inflows after storms. The risk of not having these observations can therefore lead to ignorance of essential information.

Similar quantitative tools to determine sampling intervals for water quality monitoring is difficult to find in the literature, although the problem is well acknowledged (Strobl & Robilliard, 1998). Ward et al. (1986) stated that establishment of temporal sampling criteria requires appropriate statistical tests with which to obtain the desired information from the collected data. Knowlton and Jones (2006) examined the detection of slow and abrupt rates of change from water quality time series with differing sampling intervals. They concluded that to detect a gradual change (doubling of chl-a over 20 years) would require more than 20 years of observations with monthly or twice-monthly sampling. Furthermore, the abrupt doubling of chl-a in one year required 3 years of weekly sampling in order to reach 75% probability for statistically valid detection. Elsdon and Connel (2009), on the other hand, observed that variation over short time scales of days was large relative to variation at scales of weeks and months. They concluded that monitoring of long-term trends must be mindful of short-term variation and its capacity to confuse interpretations over broader time scales. Temporal representativeness analysis can also include the avoidance of collecting too many samples. Oversampling is rarely a problem in funding-limited manual sampling programmes, but it might be an issue of concern in water quality monitoring by space-borne remote sensing, where even dai-

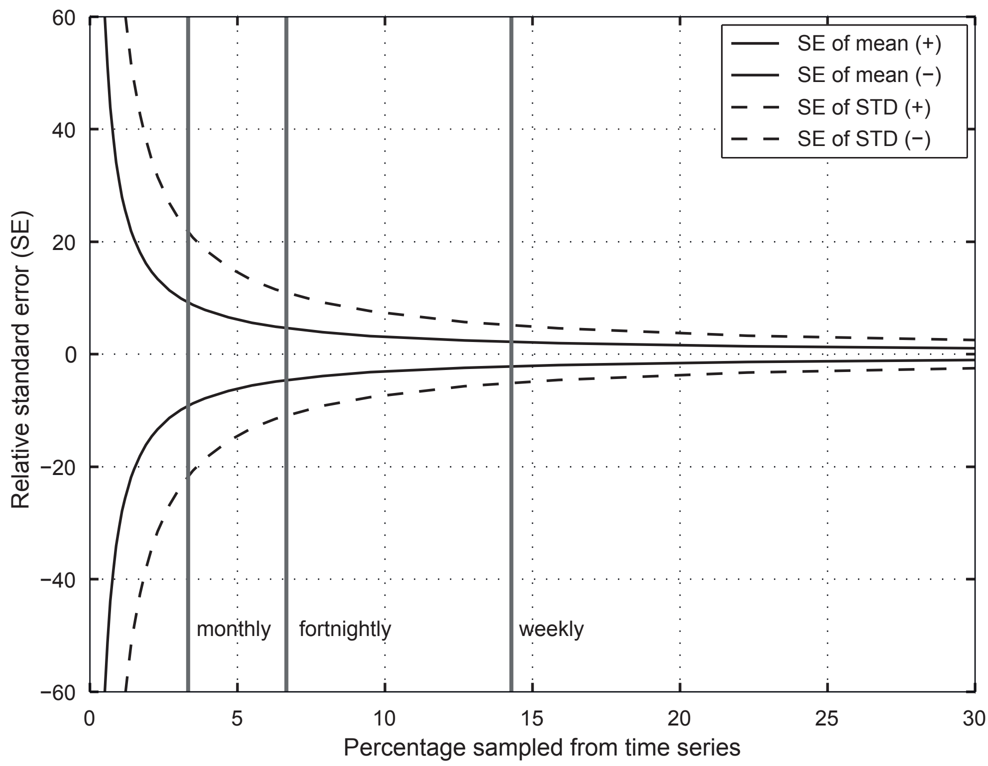

Figure 6. Modelled accuracy limits (± standard error percentages) for the mean and standard deviation estimates of different sampling frequencies from the time series. Vertical lines indicate monthly, fortnightly and weekly sampling intervals (II).

ly observations are typical. As the daily processing of remote sensing data to derive water quality estimates is time consuming, there is a clear need to match the amount of work with the actual information requirements stated by the monitoring programmes.

4.3 Structure of variability

Observations are often dependent either in time or space, and ignoring this can lead to bias in conventional statistical estimates and the significance levels these utilize (Jassby & Powel, 1990; Heffernan et al., 2010). Therefore, further analysis of the structure of variance and its specific characteristics is required in sampling design. High-frequency data accessible with automated measurements, remote sensing or extensive flow-through measurements have been successfully used to reveal within-lake variation (e.g. Pulliainen et al., 2001; Lindfors et al., 2005; Le Vu et al., 2011) and are suitable for characterizing the typical variance for the monitoring area (Curran & Atkinson, 1998; Hedger et al., 2001).

Autocorrelation in data sets reveals the representativeness of discrete water quality measurements as well as the distance between measurements at which they become statistically independent (Bierman et al., 2011). The variogram model in Figure 7 describes the spatial dependency in a combined set of four spatially extensive flow-through measurements. Due to the spatial variation in the monitoring area, semivariances between observations increase rapidly as a function of distance. Consequently the representativeness of discrete measurements decreases. Results from study I thus suggest that due to the patchiness in water

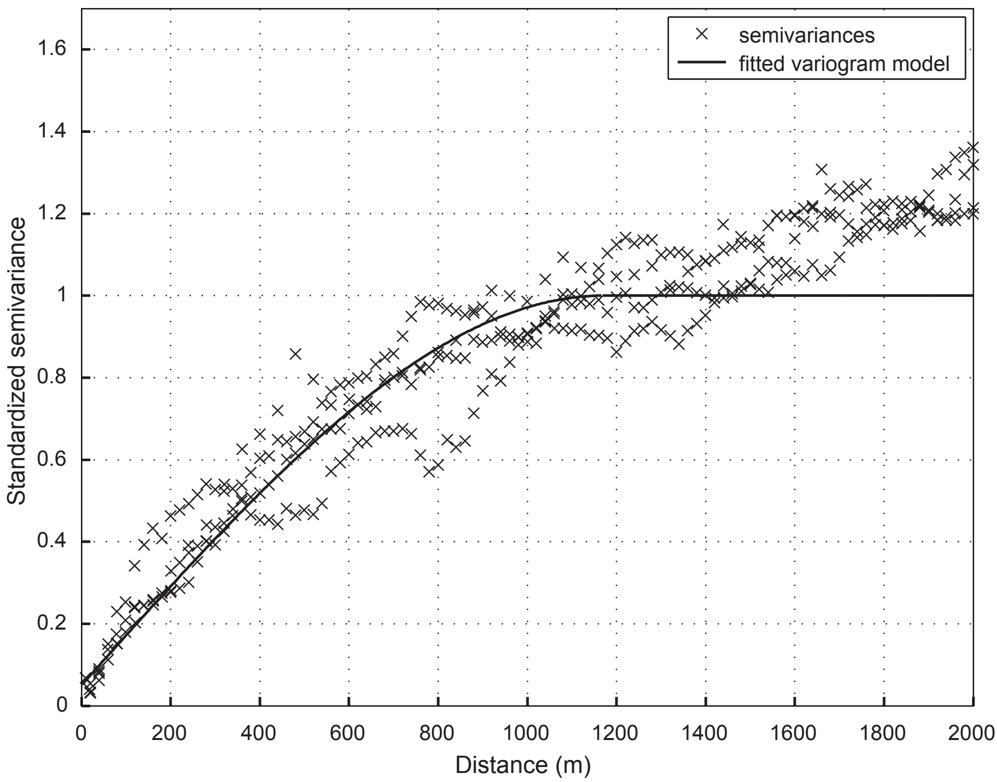

Figure 7. Standardized semivariances and variogram model based on spatially extensive flow-through measurements from the Enonselkä basin. A standardized semivariance value of one represents the respective value for the whole data set (I).

quality, data from a limited number of discrete samples can be very misleading in describing the situation in the monitoring area. In Lake Vesijärvi, for instance, the representativeness of discrete samples decreased to only 50% within a distance of 200 m (Fig. 5 in paper I).

The main outcome from paper I was that a general representation of autocorrelation can be created with certain limitations. Similar conclusions have also reported in spatial dimensions (Kitsiou et al., 2001; Hedger et al., 2001) and in temporal dimensions (Heffernan et al., 2010). The practical implementation of such generalized models in sampling design can be realized through indication of the statistically independent sampling distances (range parameter a in Eq. 3). This is necessary to avoid redundancy in the collected data. The nugget parameter (c_0 in Eq. 3), on the other hand, indicates the random sampling error or variance occurring at smaller distances or time periods than the sampling intervals. This can be valuable in the comparison of different data sources and their sensitivity in detecting small-scale spatial variation. Furthermore, spatial dependency studied across different directions (anisotropy) can indicate that water movements distribute point source pollutants with certain patterns (Wang & Liu, 2005). In this case, the dependency is greater in parallel with the pattern and smaller across it. Furthermore, Kallio et al. (2003) used a similar approach in estimation of the optimal pixel size for remote sensing. Generalized variogram models are also suitable for deriving spatial variance estimates for the point source or transect sampling to be used in data assimilation, as demonstrated in Pulliainen et al. (2004). General models are justified, since the variability is generated by consistent processes and area-specific sources. However, the spatial dynamics can vary during the growing season (Moreno-Ostos et al., 2008) and therefore need to be studied during different periods in the annual cycle and in varying weather conditions (Hedger et al., 2001). A variogram model also assumes that correlation between measurements is not affected by physical boundaries, such as large islands or capes. The analysis thus requires relatively continuous and unbroken water bodies.

4.4 Stationary patterns in water quality and remote sensing in small monitoring areas

If the parameter is known to vary in some kind of structured manner, for example spatially or temporally, then it makes sense to sample less frequently in the less variable phases or zones and more frequently where the variance is greater (de Smith, 2011). Various sources of horizontal variation such as point or diffuse pollution sources and wind-driven patterns in water quality support the formation of stationary patterns, as discussed in the introduction of this thesis. It is noteworthy to recognize that stationary patterns resulting from these sources are typically located close to the shoreline and might also indicate specific pollution sources.

Remote sensing images can provide spatially extensive information from a whole lake in a single image. The example of remote sensing estimation in Figure 8A reveals both the strengths and weaknesses of remote sensing data in small water quality monitoring areas with respect to the spatial resolution. Estimates of the chl-a concentration at a 300-m pixel size with the MERIS instrument cover the whole lake on a cloud-free day, but areas close to land cannot be observed. This is due to the mixed pixel effect from nearby land areas, floating macrophytes and disturbing reflectance from the lake sediments (Koponen et al., 2002). Therefore, water quality information from these areas cannot be reliably derived with remote sensing observations. Spatial variability can thus cause a systematic error in the mean and variance estimations derived with satellite data due to the inability to observe near-shore areas and the averaging of small-scale variance within each pixel (cf. Benson & MacKenzie 1995; Aplin, 2006). The magnitude of this error is dependent on the areal proportion and distribution of areas with differing concentrations as well as the strength of this variability.

In study III, the spatial z-score analysis identified areas where the chl-a concentration typically differed from the mean of the monitoring area (Fig. 8B). These dynamic areas may pinpoint potential pollution sources, but also indicate upcoming changes in water quality as they may also function as a source of nutrients and particulate matter. Thus, if these areas are neglected in the monitoring programs, information on the reasons behind the changes in water quality might be lost (III). When using remote sensing data in small or rugged water areas, this is an issue of special concern. The pixel sizes of the remote sensing data currently used in operative water quality monitoring range from 250 m to 1000 m, and information from the water areas close to land cannot be derived. However, if remote sensing is applicable,

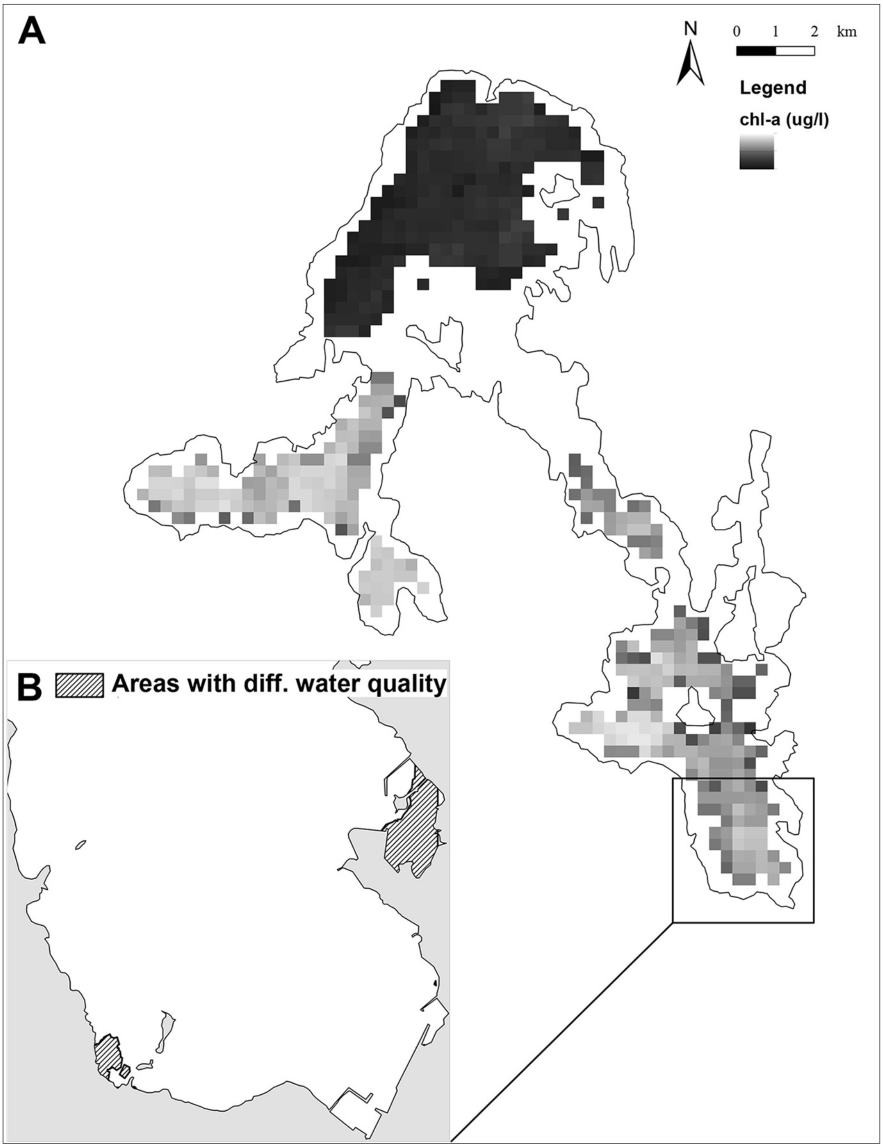

Figure 8. Chlorophyll *a* concentration in Lake Vesijärvi estimated from a MERIS/Envisat satellite image taken on 19.8.2010 (A). Areas with constantly differing water quality in the southernmost Enonselkä basin were detected with z-score analysis (B, modified from III).

pixel observations typically cover a relatively large area of the monitoring regime, even when mixed pixels are disregarded. Therefore, they can give spatially representative mean value estimations from the illuminated water (Fig. 5A in III). However, information from often dynamic near-shore areas is lost and variance estimates are obscured (Fig. 5B in III). Such analysis on scale depended observations can help in evaluating the spatial precision of available remote sensing data for different monitoring areas.

4.5 Ecosystem interactions

Broad understanding of the interactions between water quality variables is useful in solving various water quality related problems (Sanders et al., 1983). Paper IV highlights the importance of long-term data in identifying the ecosystem interactions for lake management purposes. We used a general systematic approach suggested by Bestelmeyer et al. (2011) to identify an abrupt ecosystem transition that occurred during the biomanipulation of Lake Vesijärvi from 1989–1993. Break-point analysis divided the long time series of the key pelagic ecosystem driver (TP), the response variable (chl-a) and the indicator of trophic structure (the size of *Daphnia* ephippia in lake sediment) into two distinct regimes: a eutrophic state before biomanipulation and a mesotrophic state after restoration (Fig. 9). In the eutrophic state, the lake followed a linear tracking response, i.e. the chl-a concentration linearly followed the TP concentration. After the biomanipulation, however, the chl-a concentration remained relatively low and stable, and did not follow the changes in TP (Fig. 10). Thus, the driver–response interaction apparently changed during the biomanipulation, also suggesting a change in ecosystem functioning, which is one of the main indicators of regime shifts (Scheffer et al., 2001; Bestelmeyer et al., 2011). In paper IV, we concluded that the regime shift was initiated by the diminished fish-mediated nutrient transfer from the benthic and littoral habitats to the lake pelagic zone, as reported in earlier studies (Hansson et al., 1998; Horppila et al., 1998; Kairesalo et al., 1999). However, the current mesotrophic state was only reached after an increase in the size of efficiently feeding zooplankton (Fig. 9C). This typical feedback mechanism in biomanipulation, initiated by the mass removal of planktivorous fish and aiming at enhanced ecosystem resilience (Carpenter et al., 1985), was earlier considered less important in Lake Vesijärvi. This was probably due to the inconsistent zooplankton records, a deficiency that was improved by Nykänen et al. (2010) with palaeolimnological data. Another conclusion in paper IV is that the current clearer water regime in Lake Vesijärvi is fragile and the lake could return to a eutrophic state. This is probably because the nutrient concentrations still provide a luxurious growing environment for phytoplankton (Ojala et al., 2003), enhanced feedback grazing is artificially controlled by fishing management and because of the recent observations of deteriorating water quality (Kuoppamäki et al., in preparation).

Indicators of the ecosystem transition in Lake Vesijärvi, i.e. the identified break points (Fig. 9.), the bimodal frequency distribution of the response variable and peaked temporal variance (Figs 3A and B in IV), as well as the altered relationship between driver and response variables (Fig. 10), had similarities with irreversible hysteresis and reversible threshold types of transitions (Bestelmeyer et al., 2011; Carpenter et al., 2011). The change in ecosystem functioning, i.e. enhanced zooplankton grazing, points to a nebulously reversible hysteretic change, but the current fragile state in the pelagic ecosystem of Lake Vesijärvi suggests that the transition could be reversed. The distinction between these two types of regime shifts can be artificial in the case of Lake Vesijärvi, mainly because the lake is still managed, but also because ecosystem responses to several additional drivers, including oxygen deficiency, qualitative changes in phytoplankton communities and zooplankton feeding behaviour, the effects of which can vary between years (Winder & Schindler, 2004; Havens, 2008). It is likely that an alternate stable

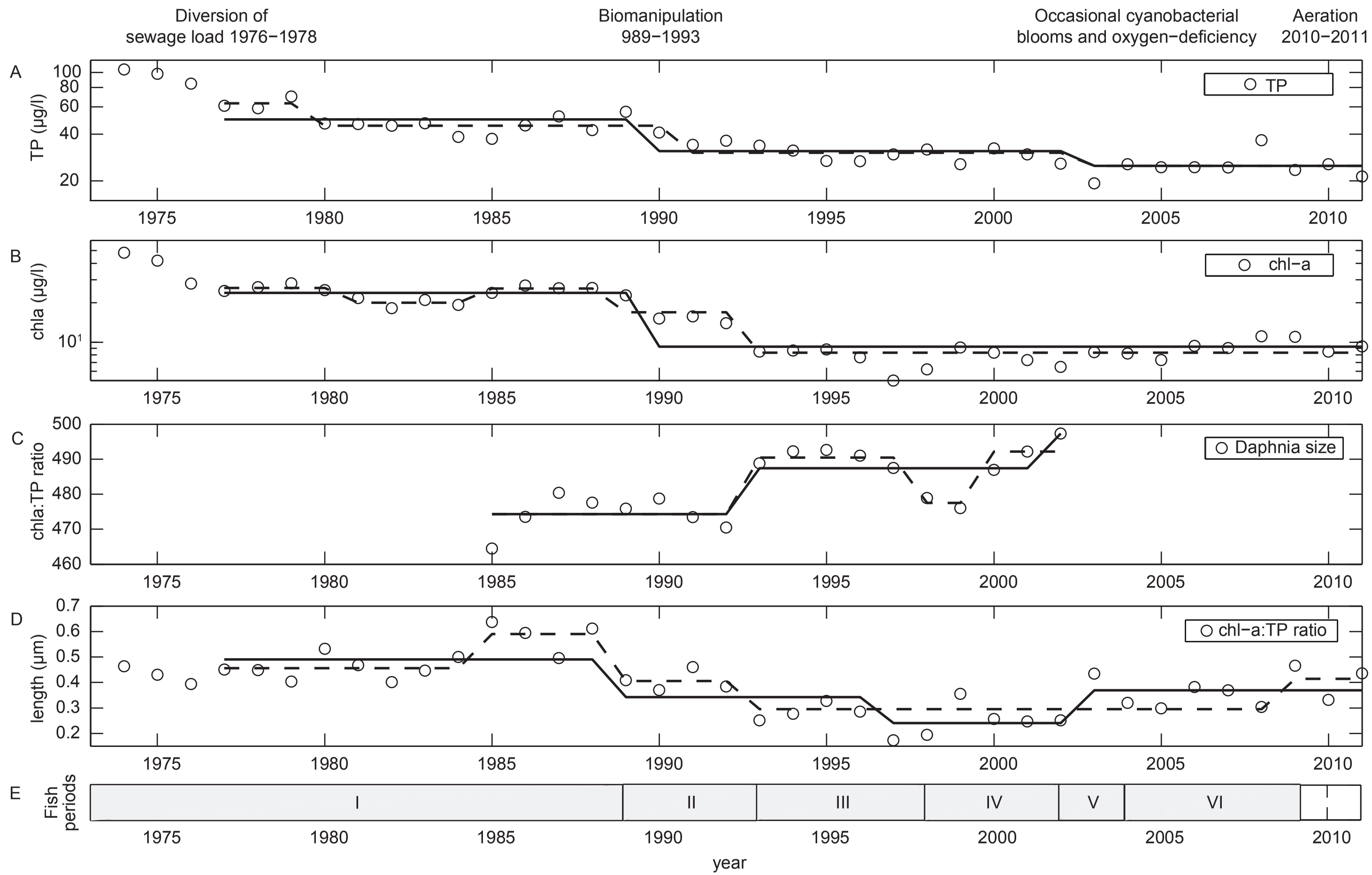

Figure 9. Harmonized time series of the main driver TP (A), response variable chl-a (B), mean length of *Daphnia* ephippia in sediment (C), the chl-a:TP ratio (D) and fish periods (E). Mean values for regimes delineated by breakpoint analysis with cut-off lengths of 7 years (solid line) and 3 years (dashed line) are presented in Figures A–D. Roman numerals in fish periods refer to: I high planktivorous fish density, II fish removal, III a low fish density, IV slightly increasing fish density, V smelt collapse, and VI smelt recovery. Note the logarithmic scales in time series A and B. (IV)

state has not been reached in lake Vesijärvi following the biomanipulation.

The importance of representative data has been highlighted in regime shift analyses, since the power of regime shift indicators declines rapidly with increasing within- and between-year variability in used variables (Contamin & Ellison, 2009; Carpenter et al., 2011). Temporally unrepresentative monitoring can hide the information required, for instance, in the temporal variance, and spatial variation can increase the uncertainty in the collected time series, as considered earlier in this thesis. In study IV, the harmonization of the time series and the use of information from several trophic levels increased the confidence in the analysis of regime shifts and ecosystem interactions. The univariate threshold-testing technique applied to time series from several trophic levels revealed the time lag in the correspondence of variables. This was essential in concluding on the importance of zooplankton grazing as a feedback and resilience mechanism in the pelagic ecosystem of Lake Vesijärvi. The detection of the time lags in ecosystem responses would probably be missed with multivariate techniques such as principal component analysis, which combine information from a variety of variables applied in regime shift detection (cf. Andersen et al., 2009).

4.6 Sampling design

Regardless the direct relationship with the cost of monitoring programmes, quantitative criteria for specifying the sampling effort are surprisingly seldom used in monitoring programmes (Strobl & Robillard, 2008; Hering et al., 2010). It is likely that an all-encompassing schema for sampling design cannot be determined in constantly changing and dynamic aquatic environments. Nonetheless, even less comprehensive datasets and feasible statistical tools increase the rationale in the planning and quotation of monitoring programmes (I, II, III). This was also supported by Carstensen (2007), who stated that sampling requirements should not be interpreted as exact numbers, but as an indication towards more representative and rationalized monitoring to derive the required information.

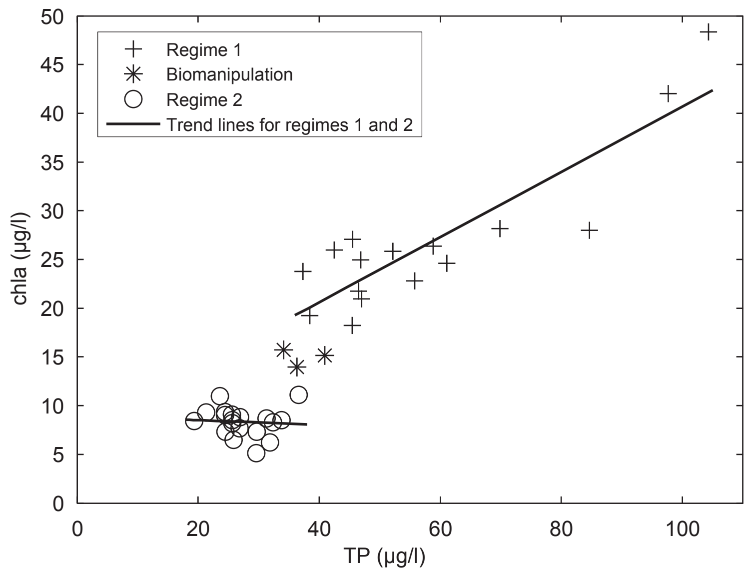

Figure 10. Correlation between chl-a and TP concentrations for the eutrophic regime from 1974 to 1989 (Regime 1; crosses) and the clear-water regime from 1994 to 2011 (Regime 2; circles), together with respective linear regression lines. The years of transition during the biomanipulation (1990–1992) are marked with asterisks. (IV)

Key components in the general schema of water quality monitoring include the determination of the objectives, sampling design, data handling and analysis, as well as information utilization (Sanders et al., 1983; Ward et al., 1986; Allan et al., 2006). Monitoring programs should be directed by the objectives, since they determine the parameters to measure and the requirements for their accuracy (Lovett et al., 2007; Timmerman & Ottens, 2000). The indicators for the ecological state used in the WFD, for instance, set the parameters for the assessment and more generally the required precision[1] and confidence[2] (Anonymous, 2003). The "adequate" and "sufficient" levels of precision and confidence are related to spatial and temporal coverage of conducted sampling, but also to the abilities of the monitoring methods used to measure the existing variation. In this context, sampling design, i.e. where, when and how to monitor, is crucial, since the costs for the monitoring and management of water bodies can be extremely high (Strobl & Robillard, 2008).

A recent strategy for the monitoring of environmental status in Finland (Anonymous, 2011) recommended the use of data-rich monitoring techniques such as remote sensing and automated monitoring to provide spatially and temporally more representative information. However, data-rich monitoring methods do not alone solve the problems related to cost-efficient water quality monitoring. Restrictions caused by specific properties of these monitoring methods and the clear need for calibration and accuracy assessment hinder their use to cover the sampling requirements in itself. Instead, different methods should be considered as complementary (e.g. Pulliainen et al., 2004; Seppälä et al., 2007; Strobl & Robilliard, 2008; Izydorczyk et al., 2009). Description of the typical variance in different dimensions is also a starting point for the rationalized joint use of several monitoring methods by allowing quantitative comparison between the abilities of different methods in a specific monitoring area. Furthermore, defined precision for spatial or temporal dimensions are required in the accuracy assessment of ecological models and in the assimilation of several data sources (e.g. Marsili-Libelli et al., 2003; Pulliainen et al., 2004). In general, high resolution remote sensing on lake water quality could provide a cost-efficient data source for sampling design (eg. Kallio et al., 2008). A set of such data covering the seasonal changes in a monitoring area allows identification of areas with greater concentrations and variance, and can as well be used in estimation of general models for autocorrelation for monitoring areas (Hedger et al., 2001).

Lake Vesijärvi has a long history of research and comprehensive monitoring by the local authorities and the University of Helsinki. The objectives of this monitoring have included the maintenance of the lake's status and thus the direction of restoration actions, but diverse research purposes also exist. The comprehensive automation of measurements in Lake Vesijärvi was aimed at cost savings. High-frequency measurements have undoubtedly revealed fine-scale dynamics in the ecosystems and also raised several new research questions, but the original aim to save in expenses is arguable. The requirement for additional sampling to calibrate automated measurements (II) and the maintenance of the equipment have turned out to be laborious. Based on the results of this thesis research, the characterized within lake variance can be used to rationalize sampling efforts. For instance, the results suggest that remote sensing observations supported by one suitably located and carefully calibrated automated sensor could provide reasonable spatio-temporal precision in deriving average chl-a concentrations to fulfil WFD requirements per se (cf. Vuori et al., 2009). A comprehensive sampling design is, however, clearly more complex and the assessment of costs can be difficult. Assessment of the status of water bodies requires various types of information, and monitoring methods also differ in the number of measurable parameters. Manual sampling, for instance, allows

[1] The discrepancy between the answer (e.g. a mean) given by the monitoring and sampling programme and the true value (Anonymous, 2003).

[2] The probability (expressed as a percentage) that the answer obtained (e.g. by the monitoring programme) does in fact lie within calculated and stated limits, or within the desired or designed precision (Anonymous, 2003).

the simultaneous sampling of a wide range of parameters, although subsequent analyses can be expensive. In papers I–III, only chl-a concentrations were used to represent spatial variability. However, the variance most likely differs between water quality parameters. Some parameters, such as nutrients and chl-a, can be expected to correlate and similar sampling efforts are probably justified. The distribution of dissolved organic matter, on the other hand, can significantly differ from the above parameters (Bracchini et al., 2004), and different sampling efforts might be required. Further investigations should also be conducted on diurnal and vertical variation in lakes that are affected by factors such as light, temperature, stratification or migration of plankton (e.g. Wetzel, 2001). Both of these produce additional uncertainty sources for water quality monitoring.

An efficient monitoring network design should not only be able to successfully track specific substances, but also be effective in helping to understand how various ecosystem components interact and change over the long term (Strobl & Robilliard, 2008). The identification of ecosystem states and interactions between trophic levels provides insights into general ecosystem functioning (Maberly & Elliot, 2012), and thus has practical applicability in lake management (IV). Reviewing recent monitoring data against the information on ecosystem interactions in different states can help lake managers to link the current measurements to ecosystem functions. Furthermore, understanding of the key interactions can also guide monitoring programmes to include relevant water quality parameters (Bestelmeyer et al., 2011). The drawbacks in approaches involving only the key trophic levels is that they simplify ecosystem functioning and neglect several other potential drivers of the ecosystem state. For lake management, however, the definition of the key elements in ecosystem functioning is crucial. It allows the building and maintenance of resilience of a desired ecosystem state and is therefore probably the most pragmatic and effective way to manage ecosystems (Scheffer et al., 2001). The identification of abrupt transitions can also provide indications of the reversibility of regime shifts that have occurred or are in danger to occur (Andersen et al., 2009; Bestelmeyer et al., 2011). Together with the potential early warning signals for threatening transitions (Fig. 3B in IV), this is valuable information in turning the observations into restoration decisions (Contamin & Ellison, 2009).

Strategies to adjust limited sampling resources to the temporal and spatial variance have taken shape during the long history of water quality monitoring. On temporal dimension, conventional strategies such as timing of sampling to certain seasonal events or regular sampling intervals are justified since prior knowledge on the temporal variation usually exists. On spatial dimension commonly used strategy that aims to get representation from pelagic or littoral areas, is closer to the random sampling strategy, because prior information on the spatial variation from these areas is usually limited. The error associated with the different sampling strategies and retrieved data, however, has been in many cases unknown. The rationalization and improvement of the accuracy of water quality monitoring presume the description of the uncertainty sources that affect the accuracy and precision of the data (Hawkins et al., 2010). Commonly considered analytical error can be relatively easily derived for the different monitoring methods, for instance by comparison against the most accurate data source. The assessment of spatial and temporal precision, however, requires studies on the typical variance in each monitoring area and the abilities of different monitoring methods to detect these variations. Essentially, when the variation is more adequately described, it helps to reduce random variation, improve indicator precision and reduce monitoring requirements (Carstensen, 2007). This can be done by calibrating the sampling sites or frequency and selecting a suite of methods to derive the required information with sufficient accuracy (cf. Fig. 1).

When the variability at spatial and temporal scales is described for a specific monitoring regime, a variety of methods, as also presented in this study, can be applied in the design of sampling schemes. It seems evident that sampling design cannot be harmonized over different water bodies, but needs to be calibrated against the typical variance and characteristics of the specific monitored system (Hedger et al., 2001; Håkanson, 2007) as well as to the monitoring methods available. The procedure thus requires determination of the costs, abilities and uncertainty sources, i.e. bias, random sampling, spatial and temporal errors for each applicable monitoring method in the area and the scrutiny of these with respect to the monitoring goals. In other words, sampling design should be seen as a rational procedure where sufficient information is derived using a suite of monitoring methods that minimize the uncertainty sources, costs and time. Sampling design should also be periodically re-assessed due to changing environmental conditions (Strobl & Robilliard, 2008), and the different dynamics in aquatic ecosystems during the growing season should additionally be noted (cf. Moreno-Ostos et al., 2008).

5. CONCLUSIONS AND FUTURE PERSPECTIVES

The implementation of the WFD has been, and still is, a challenge for almost all EU Member States. Considerable time and resources have been spent on developing tools to obtain the required data for the assessment and to prepare management plans (Hering et al., 2010). A well-acknowledged problem in the use of water quality monitoring data in assessment has been the effect of spatial and temporal variation on the precision and confidence of the data (Carstensen, 2007). This variation has been difficult to overcome with traditional monitoring techniques, and the uncertainty that this causes in the monitoring data is still in many cases unclear. In practice, water managers face the problem of deciding whether the error associated with the predicted average value is small enough to detect changes in the actual conditions (Noges et al., 2009). Although statistical methods to assess the uncertainty sources exist, they have not been implemented in monitoring programmes. In order to be feasible in large-scale monitoring programmes, statistical sampling design tools need to be relatively easy to apply and also linked to the information available from the monitored system.

This thesis research aimed to facilitate water quality monitoring by applying feasible statistical tools to assess water quality variability and by characterizing ecosystem interactions in different states.

The work derived following conclusions:

1. The required sampling effort and design are dependent on the specific properties of individual monitoring areas;
2. Ignorance of spatial and temporal variation can lead to erroneous summary statistics, and monitoring methods vary in their ability to detect variation;
3. Data-rich monitoring methods provide an essential tool to estimate the adequate sampling intervals and locations and the characteristics of variance;
4. General statistical representations of the variance within water bodies can be created with certain limitations;
5. Information derived from past transitions provides a powerful insight into ecosystem interactions and responses to pressures that can be used in interpretation of recent observations;
6. Sampling design should be seen as a rational procedure where sufficient information is derived with a suite of monitoring methods that minimize the uncertainty sources, costs and time and acknowledge the properties of the monitored ecosystem;
7. Fundamentally, as understanding of the variance and history of the observed system increases, the requirements for sampling can also be more accurately defined.

The value of water quality monitoring should be evaluated against the consistency of collected data and the ability to answer to explicit scientific questions (Lovett et al, 2007; Erkkilä & Kalliola, 2007). As anthropogenic disturbance of aquatic systems, the depletion of natural resources and climate change proceed, the significance of sound monitoring programmes and long-term records is expected to increase (Lovett et al., 2007; Andersen et al., 2009; Bestelmeyer et al., 2011). In this thesis research, I aimed to contribute to the development of adaptive monitoring programmes that are calibrated to the typical variance within monitoring sites and that aim at maintaining the natural resilience of ecosystems. In the future, assessment of uncertainty sources in water quality monitoring will probably be further emphasized as the rationalization of monitoring programmes continues. Research is still needed in order to develop a feasible tool set for water ecosystem managers to assess the uncertainty sources, to integrate information and to evaluate the risk of misjudgements in relation to the expected costs.

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