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Original research article

Assessing temporal scales and patterns in time series: Comparing methods based on redundancy analysis

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ABSTRACT

Time-series modelling techniques are powerful tools for studying temporal scaling structures and dynamics present in ecological and other complex systems and are gaining popularity for assessing resilience quantitatively. Among other methods, canonical ordinations based on redundancy analysis are increasingly used for determining temporal scaling patterns that are inherent in ecological data. However, modelling outcomes and thus inference about ecological dynamics and resilience may vary depending on the approaches used. In this study, we compare the statistical performance, logical consistency and information content of two approaches: (i) asymmetric eigenvector maps (AEM) that account for linear trends and (ii) symmetric distance-based Moran's eigenvector maps (MEM), which requires detrending of raw data to remove linear trends prior to analysis. Our comparison is done using long-term water quality data (25 years) from three Swedish lakes. This data set therefore provides the opportunity for assessing how the modelling approach used affects performance and inference in time series modelling. We found that AEM models had consistently more explanatory power than MEM, and in two out of three lakes AEM extracted one more temporal scale than MEM. The scale-specific patterns detected by AEM and MEM were uncorrelated. Also individual water quality variables explaining these patterns differed between methods, suggesting that inferences about systems dynamics are dependent on modelling approach. These findings suggest that AEM might be more suitable for assessing dynamics in time series analysis compared to MEM when temporal trends are relevant. The AEM approach is logically consistent with temporal autocorrelation where earlier conditions can influence later conditions but not vice versa. The symmetric MEM approach, which ignores the asymmetric nature of time, might be suitable for addressing specific questions about the importance of correlations in fluctuation patterns where there are no confounding elements of linear trends or a need to assess causality.

1. Introduction

Ecological and other complex systems (e.g. urban, economic) are hierarchically structured, meaning that patterns manifest and processes operate at distinct scales of space and time (Allen et al., 2014; Levin, 1992; Nash et al., 2014). This creates complexity that needs to be accounted for to accurately model temporal patterns in time series. Quantitative methods, including detrended fluctuation analysis (Gao et al., 2011, 2012) and nonlinear time series analyses (Kantz and Schreiber, 2004; Kodba et al., 2005), have been used for assessing complexity in time series. Redundancy analysis, a form of canonical ordination (Angeler et al., 2009; Garcia et al., 2012) is also increasingly used in time series modelling. In canonical ordinations, time is modelled in its original form using the principal coordinates of neighbour matrix (PCNM) approach, a form of spectral decomposition of the linear time vector akin to a Fourier transform (Borcard and Legendre, 2002; Borcard et al., 2004). That is, the PCNM method converts the time vector and creates a series of temporal (PCNM) variables with distinct sine-wave properties (Angeler et al., 2009). These PCNM variables can then be used in redundancy analysis to effectively model distinct fluctuation frequencies of response variables that are inherent in the data. Because this method facilitates identification of temporal patterns from seasonal, to decadal to millennial scales, it has gained popularity for assessing hierarchical dynamics and resilience of ecological systems (Angeler et al., 2011; Spanbauer et al., 2014).

Recently the PCNM-based approach has been refined into distance-based Moran's eigenvector maps (MEM; Dray et al.,

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2006), which are more robust at handling correlation structures and increase the proportion of explained variation compared to the original PCNM approach (Dray et al., 2006), and asymmetric eigenvector maps (AEM; Blanchet et al., 2008). The latter has been specifically designed to account for directional processes, which are often central to ecological dynamics, especially in the current period of rapid environmental change (Blanchet et al., 2008). AEM models directional processes more efficiently than MEM. That is, when the AEM analysis converts the time vector, it creates a first variable that is linear, accounting for monotonic trends in response variables. All subsequent variables have sine-wave properties and are suitable for modelling temporal change from slow to progressively shorter fluctuation frequencies (Blanchet et al., 2008, 2011). MEM is similar in this regard, with the exception that no linear variable is created (Legendre and Legendre, 2012). MEM therefore is inappropriate for modelling linear temporal patterns, since it requires detrending of response variables prior to RDA model construction (Blanchet et al., 2011; Legendre and Legendre, 2012).

As researchers are increasingly using redundancy analysis in time series modelling (Angeler et al., 2013a,b; Baho et al., 2014; Kampichler et al., 2014; Matabos et al., 2014), we need to better understand how different methods influence model outcomes and inference, especially when interests are to understand the dynamics and resilience of complex ecological systems. The objective of this paper is to compare the statistical performance, information content and logical structure of time series models based on MEM and AEM. We use water quality data from the Swedish long-term monitoring programme of lakes, covering a 25 year period. This period has been shown to capture environmental change, especially recovery from acidification and decreasing water transparency (Angeler and Johnson, 2012; Evans et al., 2005; Monteith et al., 2007). Previous studies suggested that AEM could outperform MEM, as detrending might reduce explanatory power (Blanchet et al., 2008, 2011; Legendre and Gauthier, 2014). As MEM is purported to be less robust at handling linear trends, we were interested in comparing approaches using a dataset known to have undergone monotonic long-term trends. Specifically, we hypothesize that modelling outcomes based on MEM and AEM will differ with the inclusion of water quality variables showing monotonic change. Modelling results were studied concerning the amount of variance explained and the number and patterns of temporal scales detected by MEM and AEM. We expect important implications for inference regarding the detection of complex patterns in ecological time series and conclusions about the organization and resilience of complex systems deriving from these methods.

2. Materials and methods

2.1. Study area

In the late 1980s, Sweden initiated a long-term monitoring programme of multiple habitats and trophic levels of lakes (Fölster et al., 2014, http://www.slu.se/aquatic-sciences). Three circumneutral headwater lakes (Allgjuttern, Fräcksjön and Stora Skärsjön) were selected for this study, based on the length of their water chemistry time series (25 years). The study lakes are situated in the mixed forest (boreal) ecoregion of southern Sweden and are of a similar size (Table 1). Forests constitute the main land cover in the catchments and forestry is the main source of disturbance. Long-term runoff, water residence times and mean depths are quite different between the three lakes (Table 1).

The lakes presented here are located in an area of historically high acid deposition. The long-term trends in lake sulfate (SO_4) concentrations reflect the declines in acid deposition (Fig. 1a). All lakes had similar sulfate concentrations in 1988, concentrations have declined more rapidly in Fräcksjön than either Allgjuttern or Stora Skärsjön. While all lakes are circumneutral, pH has increased over the study period (Fig. 1b) and alkalinity is increasing slightly in all three lakes (Fig. 1c). The lakes display different temporal patterns in total organic carbon (TOC) concentrations (Fig. 1d), with increases in Fräcksjön, no clear temporal trend in Allgjutern and slight decline in Stora Skärsjön.

2.2. Sampling

Standard sampling and laboratory protocols for water quality variables were used throughout the study period (Fölster et al., 2014). Water quality samples were taken during the ice-free period usually from February to early November, corresponding to spring, summer and autumn seasons. Samples were collected at 0.5 m depth with a Plexiglas® sampler and kept cool during transport to the laboratory for further analysis. Samples were analysed for variables related to acidity (pH, alkalinity, sulfate and chloride concentrations), nutrients (total phosphorus, total nitrogen, organic nitrogen, soluble reactive phosphorus, and silicon), water clarity (Secchi disc depth, water colour, and total organic carbon), ionic strength (electrical conductivity) and temperature. In total, 23 environmental variables were used for time series modelling in this study. All physicochemical analyses were done by SWEDAC certified laboratories (Swedish Board for Accreditation and Conformity Assessment, SWEDAC; http://www.swedac.se/en/) at the Department of Aquatic Sciences and Assessment, Swedish University of Agricultural Sciences, following International (ISO) or European (EU) standards when available (Fölster et al., 2014).

2.3. Statistical analyses

All statistical analyses were carried out in R 3.0.2 (R Development Core Team, 2012) using packages *nlme* (Pinheiro et al., 2008), the 'aem.time' function (AEM package developed by Blanchet and Legendre (2013)) and the 'quick PCNM' function (PCNM package developed by Legendre et al., 2013).

2.3.1. Time series analyses

We compared the outcomes of time series models for each lake based on MEM and AEM. Our approach can be outlined as follows:

(1) AEM and MEM analyses were carried out to extract a set of orthogonal temporal variables that are derived from the time vector comprised of 25 time steps (i.e., 25 sampling points

Table 1
A brief summary of the properties of the three study lakes.

Name	Altitude (masl)	Catchment area (km^2)	Runoff (mm/yr)	Precipitation (mm/yr)	Lake area (km^2)	Mean depth (m)	Water residence time (years)
Allgjuttern	129.8	0.85	250	650	0.16	11.4	7.30
Fräcksjön	62.5	4.26	460	950	0.27	6.0	0.60
Stora Skärsjön	55	2.05	550	1150	0.33	3.8	0.95

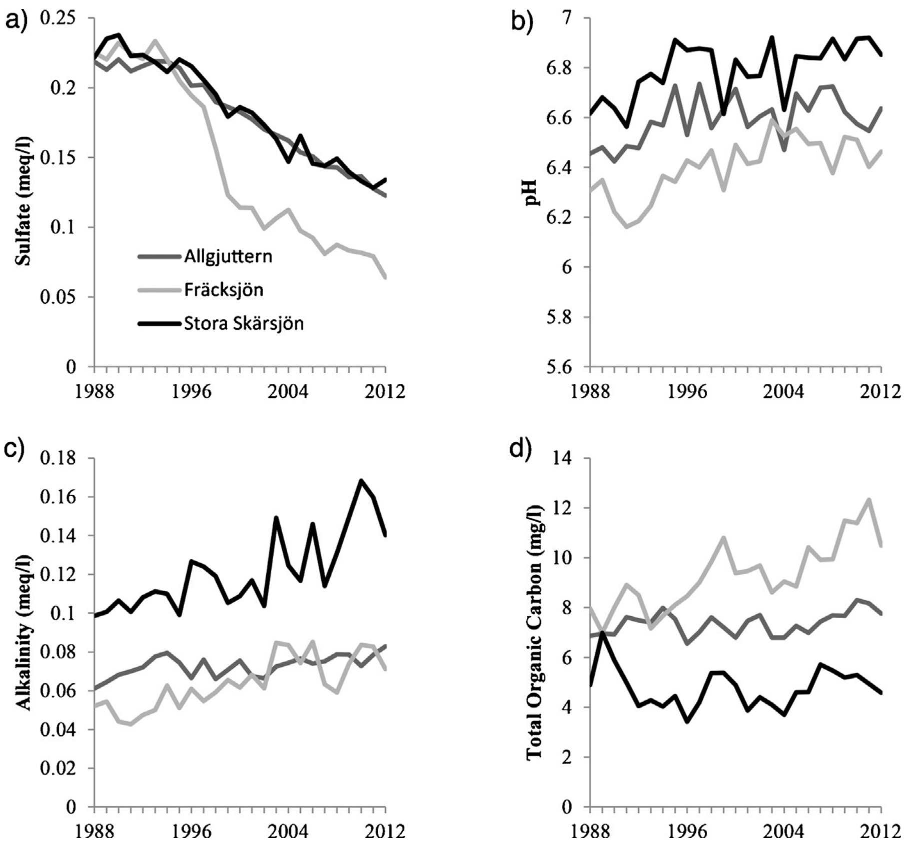

Fig. 1. Temporal pattern of selected water quality variables between 1988 and 2012 for (a) sulfate, (b) pH, (c) alkalinity and (d) total organic carbon. Sulfate shows decreasing trend while alkalinity and pH increase over time across all three lakes. Patterns of total organic carbon were more variable among lakes.

comprising yearly averages between 1988 and 2012) and that can be used as explanatory variables to model temporal relationships in the water quality variables. In the case of AEM, the first variable models linear trends, while in MEM all variables depict sine-wave patterns (Legendre and Legendre, 2012). These extracted temporal variables are then used as explanatory variables in the time series models based on RDA.

(2) Two types of time series models were constructed using redundancy analysis (RDA), one based on MEM and the other on AEM, with the 23 water quality variables as the response variables. In both approaches, RDA selects significant temporal variables (AEMs and MEMs) using forward selection procedures. The selected AEM and MEM variables are linearly combined in the RDA models to extract temporal structures from the water quality variable matrices. The modeled temporal patterns that are extracted from the data are collapsed on significant RDA axes, which are tested through permutation tests. These RDA axes are independent from each other and the number of significant RDA axes can therefore be used to determine the number of temporal scales at which water quality variables fluctuate in the lakes (Angeler et al., 2011). The R software generates linear combination (lc) score plots, which visually present the modelled temporal patterns that are associated with each RDA axis. All water quality variables were scaled, by dividing individual values by their respective root mean square values, prior to the analysis.

The main difference between the two models resides in their characteristic functions (eigenfunctions). The AEM framework produces only positive eigenvalues. The response variables do not require detrending when using AEM, as the produced eigenvalues are not direct measures of temporal correlation and trends are important components of directional processes (Blanchet et al., 2011). In contrast, MEM divides the time vector (25 time steps) into 12 eigenvectors having positive eigenvalues and 12 eigenvector having negative eigenvalues (Legendre and Legendre, 2012). Detrending of response variables is necessary with the MEM approach because trends can force the selection of particular eigenfunctions and their corresponding eigenvalues (Blanchet et al., 2011; Legendre and Legendre, 2012).

2.3.2. Methods comparison

Spearman's rank correlations were used to compare the temporal patterns modelled at each temporal scale (i.e. temporal patterns associated with each RDA axis in the models) between MEM and AEM. This was done using the linear combination (lc) scores for each RDA axis that were obtained by both methods. Similarly, the relationship between individual water quality variables (raw data) with the linear combination (lc) scores extracted from the significant canonical axes of the time series models for each lake were investigated by means of Spearman's rank correlations so as to assess which water quality data explained the temporal patterns identified.

3. Results

3.1. Time-series modelling

The analyses from the time series modelling of water quality variables based on AEM and MEM revealed significant temporal structure for all three lakes between 1988 and 2012. The overall variance explained by AEM models (adjusted R^2 values; Allgjuttern

0.78, Fräcksjön 0.78 and Stora Skärsjön 0.60) for each lake was higher than MEM models (Allgjuttern 0.66, Fräcksjön 0.64 and Stora Skärsjön 0.33) (Table 2). The models revealed fluctuation patterns (Figs. 2–4) at distinct temporal scales of the abiotic lake environment. However, the temporal fluctuation patterns of water quality variables were unique for each lake (Figs. 2–4), and temporal structures modelled by AEM differed from those modelled by MEM. AEM revealed temporal dynamics at: four, five, and three significant temporal scales for Allgjuttern, Fräcksjön and Stora Skärsjön, respectively (Figs. 2–4). MEM showed temporal dynamics at four scales for Allgjuttern, four for Fräcksjön, and two for Stora Skärsjön (Figs. 2–4).

Spearman rank correlation analysis, using the linear combination (lc) scores of modelled temporal patterns for each time scale (RDA axis), showed that the temporal patterns generated by AEM were generally not correlated with those obtained from MEM. A significant, negative correlation between modelling methods was found for the temporal pattern associated with RDA axis 2 in Allgjuttern (Table 3). Spearman rank correlation analysis also revealed that more water quality variables correlated with the significant canonical axes from AEM than from MEM. On average, AEM showed that 17 water variables were correlated with the first RDA axis, compared with three using MEM (Table 4 and see supplementary Table A.1 for correlation analysis between water variables and all significant RDAs).

4. Discussion

Previous studies have suggested that asymmetric eigenvector maps (AEM) outperform distance-based Moran's eigenvector maps (MEM) (Blanchet et al., 2008, 2011; Legendre and Gauthier, 2014) when directional processes are inherent in the data. We tested this conjecture using a dataset comprised of water quality variables from boreal lakes that have been shown to exhibit significant, decadal long environmental change, mainly due to changes in land use, acid deposition and climate (Angeler and Johnson, 2012; Evans et al., 2005; Monteith et al., 2007; Renberg et al., 1993). The temporal patterns identified by each canonical axis using redundancy analysis (RDA) differed between the two methods. However, AEM was found to be superior to MEM, consistently explaining a higher amount of variance than MEM. Our finding suggests that modelling approach affects insights into the temporal structure of environmental relationships has important implications for quantifying and understanding the complexity of temporal dynamics in, and ultimately the resilience of, ecological systems. Using data from three lakes allowed for more general conclusions to be drawn about

Table 2
Comparison of the adjusted variance explained by time series modelling based on RDA, using AEM and MEM approaches. Shown are: the variance explained by the overall model, which are consistently higher in AEM than MEM, and the individual significant canonical (RDA) axes.

Asymmetric eigenvector map						
Lake	Overall variance	Significant RDA				
		1	2	3	4	5
Allgjuttern	**0.78**	0.42	0.10	0.09	0.03	–
Fräcksjön	**0.78**	0.42	0.12	0.06	0.05	0.03
Stora Skärsjön	**0.60**	0.32	0.11	0.06	–	–

Moran's eigenvector maps					
Lake	Overall variance	Significant RDA			
		1	2	3	4
Allgjuttern	**0.66**	0.30	0.13	0.04	0.04
Fräcksjön	**0.64**	0.25	0.10	0.07	0.03
Stora Skärsjön	**0.33**	0.21	0.06	–	–

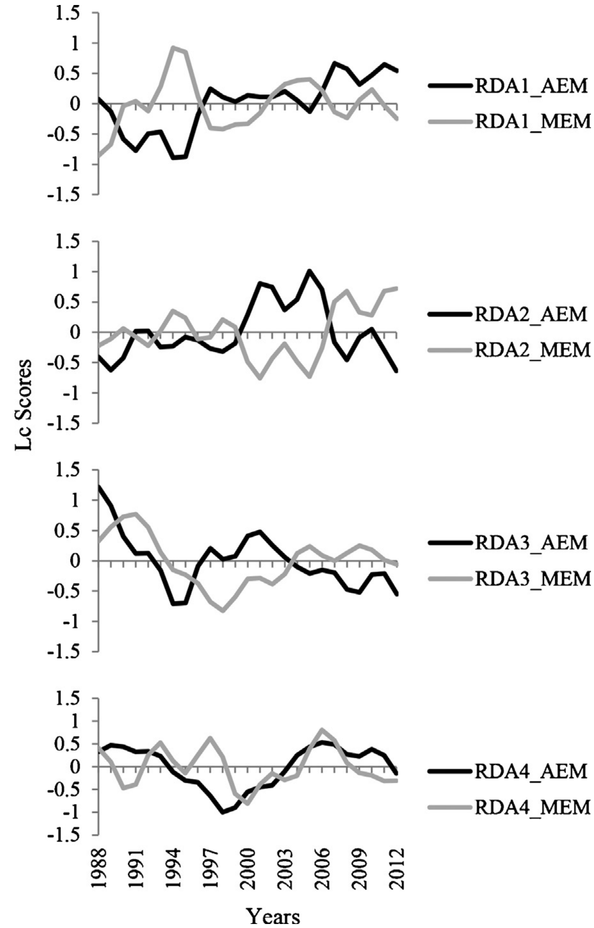

Fig. 2. Time series models showing modelled fluctuation frequencies of water quality variables from Allgjuttern at different temporal scales (RDA axes). Shown are the patterns based on the linear combination (lc) scores of significant AEM variables (black lines) and MEM variables (grey lines), which generally differ from each other.

how detrending affects model outcomes, as well as underpinning conclusions with ecological realism.

In addition to the MEM approach explaining less variance than the AEM approach, we found differences in the temporal pattern modelled. In RDA, the first RDA axis explained the dominant patterns in the data based on the amount of variance explained. The impact of detrending was most apparent on the first significant RDA axes of the MEM models (Tables 2 and 4).

Detrending has been criticized for potentially filtering out key ecological patterns from the analysis (Hill and Gauch, 1980; Wartenberg et al., 1987). Findings from our study suggest that detrending can be especially problematic when assessing complex systems dynamics, because the impacts of environmental change are scale specific (Nash et al., 2014). Regional environmental change is often slow, with ecosystem changes in biotic and abiotic conditions unfolding over decades, centuries or millennia (Renberg et al., 1993; Sheffield et al., 2012). Indeed, Angeler et al. (2013a) have shown that patterns of decreasing acid deposition and water clarity changed monotonically over two decades and that these changes were manifested at a specific scale in lakes. This makes clear that although detrending is needed to satisfy mathematical assumptions of certain modelling techniques, including MEM, it can lead to ecological misinterpretations of the underlying temporal structures (i.e. the number of temporal scales and temporal fluctuation patterns). These misinterpretations can be especially severe when interpreting resilience in ecological

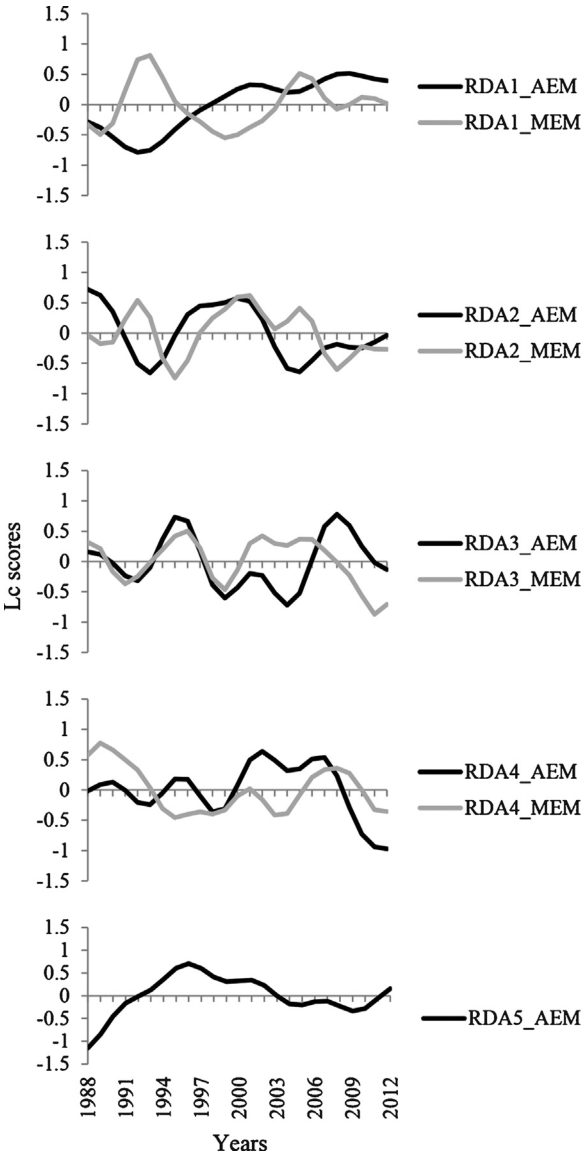

Fig. 3. Time series models showing modelled fluctuation frequencies of water quality variables from Fräcksjön at different temporal scales (RDA axes). Shown are the patterns based on the linear combination (lc) scores of significant AEM variables (black lines) and MEM variables (grey lines), which generally differ from each other.

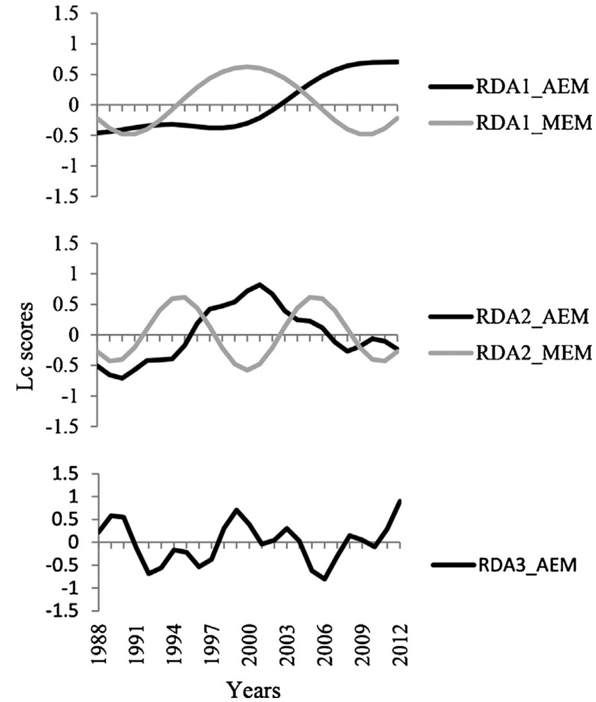

Fig. 4. Time series models showing modelled fluctuation frequencies of water quality variables from Stora Skärsjön at different temporal scales (RDA axes). Shown are the patterns based on the linear combination (lc) scores of significant AEM variables (black lines) and MEM variables (grey lines) which generally differ from each other.

systems where an understanding of scale-specific patterns and processes is crucial (Allen et al., 2014; Nash et al., 2014). Our results also suggest that method choice is crucial for inferring patterns and dynamics when ecosystems undergo significant environmental change.

Perhaps most importantly, MEM fails to represent the causal structure of time series. MEM is a symmetric method where it is assumed the states before and after has equal influence on the current state. This may be appropriate for assessing correlation but is not appropriate for consistency with the causal structure of environmental time series where earlier states can influence later ones but not the other way around. The asymmetric nature of AEM where earlier states can influence later ones but not vice versa is more appropriate for multivariate analysis of time series as it explicitly preserves the temporal structure of causality. AEM is more appropriate to infer causal relationships especially when considering the unidirectional nature of time (which is not as relevant in many spatial contexts), for example if conditions at t_n affects conditions at t_{n+1}, then it seems unlikely that conditions at t_{n+1} influence conditions at t_n (Dowe, 1992; Polk, 1962). MEM, which is a symmetric method, might be able to represent correlation more adequately than causality.

Selecting the right multivariate time-series technique and having a proper understanding of the data set are crucial for successful analysis and inference. In summary, MEM and AEM are valuable tools for modelling temporal structures present in ecological and other complex systems. Available statistical packages and simple codes facilitate an automatic analysis in R, a freely available programme. These modelling tools help researchers objectively define and identify the temporal scaling structure present in ecological and other complex systems. In some cases, where linear trends are of importance AEM might be a better tool than MEM. In others, when linear trends are weak or absent, or

Table 3
Spearman rank correlation analysis showing the correlation between the significant canonical (RDA) axes extracted from AEM and MEM. Significant values are shown in bold.

Lake	Temporal scale	Spearman's correlation coefficient (rho)	*P*-value
Allgjuttern	1	−0.29	0.15
	2	**−0.67**	**<0.001**
	3	0.02	0.91
	4	0.31	0.13
Fräcksjön	1	−0.14	0.52
	2	0.08	0.71
	3	0.15	0.46
	4	0.09	0.65
Stora Skärsjön	1	−0.16	0.45
	2	−0.11	0.61

Table 4
Spearman rank correlation analysis showing the water quality variables correlating with the first significant canonical (RDA) axes from time series analyses using RDA, based on AEM and MEM approaches. Only significant ($P < 0.05$) correlations and the associated correlation coefficients (Spearman rho) are shown.

Water quality variables	Allgjuttern		Fräcksjön		Stora Skärsjön	
	AEM	*MEM*	*AEM*	*MEM*	*AEM*	*MEM*
Alkalinity (meq/L)	–	–	0.71	–	0.72	–
Ca (meq/L)	−0.74	–	−0.94	–	−0.87	–
Cl (meq/L)	−0.66	–	−0.62	0.51	−0.71	–
Electrical conductivity (mS/cm)	−0.83	–	−0.91	–	−0.80	–
K (meq/L)	−0.77	–	–	0.59	−0.51	–
Mg (meq/L)	−0.75	–	−0.86	–	−0.72	–
Na (meq/L)	−0.55	–	−0.75	0.44	−0.61	–
pH	0.43	–	0.68	–	0.50	–
Secchi depth (m)	−0.40	–	−0.81	–	−0.77	–
Silicon (mg/L)	–	–	–	–	0.52	−0.54
Sulfate (meq/L)	−0.83	–	−0.93	–	−0.91	–
Soluble reactive phosphorus (μg/L)	−0.43	0.75	–	0.89	0.67	−0.56
Temperature (°C)	–	–	0.42	–	0.40	–
Total nitrogen (μg/L)	−0.43	–	–	–	–	–
Total organic carbon (mg/L)	0.61	–	0.83	–	–	−0.43
Total phosphorus (μg/L)	−0.95	–	−0.59	–	–	−0.57
Water colour (Abs 420 nm)	0.64	–	0.85	–	0.67	–
Ammonium (μg/L)	−0.64	–	–	–	–	–
Nitrates and nitrile (μg/L)	–	–	–	–	–	−0.65
Organic nitrogen (μg/l)	–	–	–	–	–	–
Total cations	−0.73	–	−0.90	–	−0.76	–
Total anions	−0.83	–	−0.95	–	−0.79	–
Soluble unreactive phosphorus (μg/L)	−0.90	–	−0.42	–	−0.71	–

when specific hypotheses are posed about the importance of fluctuation patterns without confounding elements of linear change or when an assessment of causality is not of interest, MEM may also be useful.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at http://dx.doi.org/10.1016/j.ecocom.2015.04.001.

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