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Ecological Thresholds and Regime Shifts: from theory to operation

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1   **Abstract**

2   There is an apparent gap between the prominence of present theoretical frameworks involving

3   ecological thresholds and regime shifts, and the paucity of efforts to conduct simple tests and

4   quantitative inferences on the actual appearance of such phenomena in ecological data. There

5   is a wide range of statistical methods and analytical techniques now available that render

6   these questions tractable, some of them even dating half a century back. Yet, their application

7   has been sparse and confined within a narrow subset of cases of ecological regime shifts. Our

8   objective is to raise awareness on the range of techniques available, and to their principles and

9   limitations, in order to promote a more operational approach to the analysis of ecological

10   thresholds and regime shifts.

Regime Shifts in Ecology

The observation that managed ecosystems often fail to respond smoothly to changing pressures has generated perplexity and eventually lead researchers to draw parallels between the behaviour of ecological systems and other complex systems with non-linear dynamics, such as the global climate, the human immune system, and the world economy (cf. [1] for a popular account). Initial reports of kelp forest disturbance and recovery [2], freshwater ecosystem shifts engineered by beavers [3], and vegetation shifts affected by fire [4] have lead on to an ever-growing research effort on ECOLOGICAL THRESHOLDS and REGIME SHIFTS (see Glossary), whose underlying theoretical framework [5, 6] (Box 1) has been shown to be applicable to a broad range of ecosystems from coral reefs to forests and lakes [7,8]. These concepts are now also making their way into the minds and discussions of policy makers and might soon be translated into legislative frameworks [9].

Ecological regime shifts can be defined as abrupt changes on several trophic levels [10], leading to rapid ecosystem reconfiguration between alternative states. These shifts are generally thought to be driven by external perturbations (e.g. climatic fluctuations, overexploitation, eutrophication, and invasive species), but the exact mechanism is often unclear. The subject has become a fast growing scientific discipline, manifested by a 12-fold increase in publications between 1991 and 2006, twice as fast as the growth rate of research effort in ecology as a whole (7.7 % year^{-1}, ISI Web of Science). Most of the reported cases of ecological regime shifts are inferred from time series of monitoring data, while direct evidence by controlled experiments of the existence of alternative states is difficult to find [11]. Surprisingly, the general techniques available to test for regime shifts and thresholds have only to a limited extent been applied to these data sets. As formal tests of regime shifts have a long history in the context of climate change research (e.g. [12]) it is not surprising

1 that formal statistical tests for ecological regime shifts have mostly been restricted to the

2 effects of climate change on marine communities [13]. These observations suggest that there

3 is a need to increase the awareness of ecologists on the availability and diversity of

4 approaches allowing inferential analyses of ecological regime shifts and thresholds, helping

5 this important research field to move to a more operational phase.

6

7 Here, after exploring research efforts in several fields we provide a review of methods for

8 regime shift and threshold detection relevant to ecosystems, including both informal

9 EXPLORATORY DATA ANALYSIS and formal HYPOTHESIS TESTING approaches, with the aim of

10 encouraging a more quantitative approach to the study of these phenomena. Finally, we

11 provide an operational summary of available software that can be useful for investigating

12 abrupt changes in ecological data sets. As some of the terms are used differently among

13 different research traditions, a glossary is provided.

14

15 **Detecting thresholds and regime shifts in ecological data**

16 Figure 1 shows that there are at least three ways by which an ecological system might exhibit

17 abrupt changes over time; two which are reversible in response to changes in environmental

18 drivers, while a third (Figure 1C) and most undesirable one is not [14]. Thus the existence of

19 an abrupt CHANGE-POINT is a necessary but not sufficient condition for demonstrating

20 BISTABILITY and HYSTERESIS (Box 1), as it might actually derive from sudden changes in the

21 main drivers of the systems. It should also be kept in mind that while most ecological regime

22 shifts are inferred from abrupt changes over time, time itself is never the actual underlying

23 driver. Identification of the environmental driver(s) is complicated by the general

24 interrelatedness of different social and environmental factors, and often also by the lack of

25 data. Identification of a change-point in time is therefore the natural first step towards

1 identifying a potential driver, which again is the first step towards identifying a regime shift

2 mechanism that might eventually be relevant for policy-making.

3

4 There is an abundance of methods for identifying abrupt changes in time series, most of them

5 developed in scientific fields other than ecology. The basic change-point problem, i.e.

6 detecting a step change in the mean value in a sequence of random variables, has a long

7 history in statistical inference (Box 2). The general scientific literature contains a bewildering

8 diversity of methods that in a widest sense correspond to change-point detection, either in

9 time or space (Box 3). In this review we contend that terms like regime shift [10,14], abrupt

10 change [15], break- or change-point [16], STRUCTURAL CHANGE [17], ecological threshold

11 [18], tipping point [19], and observational inhomogeneity [20], basically address the same

12 problem and that methods developed for their analysis should have general relevance for the

13 study of ecological regime shifts. The rapid growth of this literature already makes it hard to

14 maintain an overview, and increases risk of unnecessary reinvention. For example, one of the

15 threshold detection methods proposed in Ref. [21] is basically a rediscovery of the basic

16 change-point problem presented a half a century earlier in Ref. [22] (Box 2).

17

18 **Exploratory data analysis**

19 A substantial part of the literature on ecological thresholds and regime shifts follows an

20 explorative approach where data are pre-processed in various ways that render the presence of

21 thresholds or jumps more evident to heuristic inspection, but usually without any statistical

22 significance tests. The AVERAGE STANDARD DEVIATES (ASD) compositing method [23] is a

23 rather popular representative based on simple heuristics rather than an underlying statistical

24 model. The ASD was for example used to propose the occurrence of regime shifts in the

25 North-Pacific in 1977 and 1989 [24] (Box 4). It has however been demonstrated that the ASD

1   method is prone to false positives for AUTOCORRELATED time series, that is, to detect a regime

2   shift when in fact there is none [25]. We recommend therefore that ASD, despite its

3   popularity, is replaced by methods presented below for inference on regime shifts in ecology.

4

5   PRINCIPAL COMPONENT ANALYSIS (PCA) and related techniques are known under a variety of

6   names (EMPIRICAL ORTHOGONAL FUNCTIONS (EOF), SINGULAR SPECTRUM ANALYSIS (SSA),

7   etc.). PCA is used to compress, by linear combinations, a large number of correlated time

8   series into a small number of uncorrelated ones that contain as much as possible of the

9   original total variance [26, 27]. The presence of threshold phenomena in the reduced set could

10   become more evident to visual inspection, but further processing and statistical testing is

11   recommended. Applications to regime shift detection include the reduction of 100 climatic

12   and ecological time-series from the North-Pacific into just two variables [24] (Box 4) or the

13   combination of different climatic indices related to Pacific fisheries into a single one [28].

14   The conclusions drawn from a PCA can be strengthened by combining it with other

15   independent approaches to multivariate time series analysis, such as CHRONOLOGICAL

16   CLUSTERING [29,30] (Box 4). For example, PCA and chronological clustering were found to

17   yield comparable regime shift patterns in 78 time series from the North and Wadden Seas

18   [31].

19

20   PCA methods have well known limitations [27], such as the inability to capture relationships

21   that are not linear, and the possibility of the reduced variables being distorted by the

22   requirement of linear independence. Variants of non-linear dimensionality reduction [32] have

23   been developed independently and also partly based on very different underlying concepts, in

24   for example cognitive psychology [33] and oceanography [34]. The ARTIFICIAL NEURAL

25   NETWORK-based approach [34] is claimed to be able to reveal multimodality, which in

1 principle would be very relevant for detecting regime shift mechanisms related to bistability

2 and hysteresis loops. Unfortunately, it has also been shown that this approach [34] is prone to

3 false positives, as it is reported to find multimodality even in data sets generated from a

4 multivariate normal distribution [35], which, by definition, cannot be MULTIMODAL. Our

5 opinion of the current state of this field is that non-linear dimensionality reduction methods

6 should primarily be used if simpler methods such as PCA and chronological clustering have

7 been documented to be incapable of capturing important variations in a data set. Conclusions

8 will also in this case be strengthened if there is a general agreement between several

9 independent methods.

10

11 **Inferential statistics and hypothesis testing**

12 In the search for ecological regime shifts there is always a risk for thresholds being detected

13 in what is actually just random fluctuation. Statistical hypothesis testing aims at limiting this

14 possibility to a predetermined fixed value, typically a significance level of 5%. If the time of

15 the threshold event is known (e.g. introduction of an invasive species, change in management

16 practice, deforestation event) the significance probability of the regime shift under a null

17 hypothesis of no change can be analyzed using intervention methods from standard statistical

18 textbooks [36]. While originally aimed at testing for a shift in a time series following a

19 particular action, INTERVENTION ANALYSIS has also been applied to data where the change-

20 point was not known a priori, but hypothesized following exploratory data analysis [37].

21 Classical intervention analysis cannot be used for situations with the change-point occurring

22 at an a priori unknown time. This calls for sequential tests where the existence of a regime

23 shift is tested for at every point in time, and which must be characterized by higher critical

24 values of the test statistic than in classical statistical methods (cf. Box 2) due to the so-called

25 type I error (false positive) inflation in multiple tests. The underlying principle of the

1 sequential methods is to compare a test statistic with its distribution under the null hypothesis.

2 Critical values at different significance levels are tabularized for regularly observed data

3 points, typically time series [38], whereas critical values for irregularly spaced observations

4 must be calculated case-by-case and therefore can be computationally costly, but the

5 continuous increase in computing power has greatly alleviated this constraint. Sequential test

6 methods have mainly been developed for univariate time series, particularly within

7 econometrics [17, 39] (Box 3) and climate research [40, 41] (Box 3).

8

9 The most commonly investigated regime shift hypothesis is a step change in mean level using

10 parametric [40, 42, 43] or non-parametric [44] methods. Regime shift detection methods

11 involving changing variance, shift in the frequencies of fluctuations, or even simultaneous

12 interrelated shifts in several ecosystem components at a particular point have also been

13 proposed [45], but their application to practical data analysis has so far been limited. The

14 computational burden increases exponentially with the number of change-points in the data

15 set [17]. While methods intended for identifying only single thresholds can also be employed

16 to the individual subsets separated by a significant change-point in a hierarchical fashion [46],

17 this will normally be less efficient than a DYNAMIC PROGRAMMING approach [39]. As the

18 goodness of fit will generally increase with the number of change-points, model selection

19 procedures involving penalties for the number of model parameters are to be recommended

20 [47].

21

22 One problem associated with the classical statistical framework for investigating regime shifts

23 against a null hypothesis with no regime shift is the lack of STATISTICAL TEST POWER for

24 robust inferences. Ecological time series displaying regime shifts are generally much shorter

25 (typically 20-40 time steps, usually years) than the typical time series that has driven the

1   development of threshold detection methods in econometrics and climate research (often >

2   100 time steps). As change-points occurring at the extremes of a time series do not lend much

3   power to hypothesis testing, it is only those change-points located near the middle of the time

4   series that can be detected with confidence. Moreover, since ecological data are typically also

5   noisier than climatic or economic data, a null hypothesis of no change-point is unlikely to be

6   rejected within a classical statistical testing framework.

7

8   Testing the existence of hysteresis poses a statistical challenge even greater than threshold

9   identification, because modelling hysteresis requires a memory effect to be included into the

10   model formulation such that the present regime becomes dependent on previous states.

11   Statistical inference must therefore be based on comparing the observations with the output of

12   a dynamical model. In THRESHOLD AUTOREGRESSIVE (TAR) models the dynamics can switch

13   between different linear autoregressive models depending on a linear function of the previous

14   state relative to a threshold value [48]. The classical Canadian lynx population data could be

15   modelled with a TAR model having two regimes, representing the increasing and declining

16   phases of the lynx population cycle [49]. Otherwise, quantitative statistical studies of regime

17   shifts with hysteresis in ecology are remarkably few. Needless to say, data requirements are

18   high, as several transitions are needed to identify hysteresis effects (e.g. typically >10

19   transitions in the Canadian lynx data sets [49]). Additional complications caused by to

20   missing values, measurement errors, and non-stationarity could also contribute to the paucity

21   of applications of these analyses.

22

23   Although most of the threshold testing procedures described in the literature are univariate,

24   they can naturally be expanded to include multiple variables. The advantage of multivariate

25   analyses is that the power of testing increases provided that all variables show similar trends

1   and have interactions that can be accounted for in the analysis. However, if only a subset of

2   the variables shows a threshold response, the power of the test decreases and the outcome can

3   become less clear. Simultaneous estimation of changes in the community interaction matrix

4   (i.e. the density-dependent effects of a population both on itself and on other populations) has

5   been suggested [50], but this approach will usually inflate the number of parameters such that

6   the data requirements will be beyond what is realistic for ecological time series.

7   Consequently, parsimonious consideration of the variables to be included in a multivariate

8   test is recommended.

9

10   **Available software for analysing regime shifts**

11   Most of the statistical methods discussed in this review are implemented in available software

12   packages (Table 1). Table 1 is not an exhaustive list of relevant software, but rather a

13   selection of possible starting points for scientists interested exploring different approaches to

14   quantitative regime shift detection. The list contains both tools requiring little background

15   knowledge, such as standalone products or Excel add-ins, as well as toolboxes or packages for

16   some of the major statistical computing environments such as R, Matlab, and O-matrix. The

17   emphasis in Table 1 is on inferential tools for hypothesis testing, but some of the software

18   listed also implements exploratory analysis methods.

19

20   **Conclusions and future perspectives**

21   The remarkable paucity of inferential analyses of ecological regime shifts and thresholds in

22   the literature is at odds with the vigorous growth of this research direction, and could be

23   attributable to the perception that these techniques are so data-demanding that only

24   exceptionally few long-term ecological data sets would meet the requirements. However, the

25   impressive impetus to the development and implementation of observational platforms across

1   a broad range of ecosystems over the past two decades (e.g. the US NSF Long term ecological

2   research (LTER) network and the EU Water framework directive (WFD) monitoring system)

3   has already and will continue to deliver a wealth of data sets that could meet the requirements

4   of even the more demanding of the techniques available. Lack of awareness on available

5   techniques or misperceived data requirements should not keep ecologists from applying

6   statistical techniques for threshold detection.

7

8   As human pressures on ecosystems continue to increase worldwide, the need for analytical

9   approaches allowing the detection of ecological thresholds and regime shifts becomes a

10   matter of urgency. Particularly, the impacts of climate change on biodiversity and ecosystems

11   are currently assumed to be smooth, involving a continuous increase in impacts and

12   extinctions as global temperature rises [51]. Well-documented fisheries statistics have shown

13   that even relatively smooth climatic changes might lead to strong regime shifts in ocean

14   ecosystems [13], increasing the likelihood of more prevalent and abrupt regime shifts as the

15   planet warms beyond ecological thresholds for a growing fraction of species and ecosystems.

16   Ecologists should increasingly contribute quantitative evidence of ecological thresholds for

17   the future environmental policy making.

18

19   This review has documented a diversity of approaches, differing in complexity, power and

20   requirements, which we hope will stimulate the transition from a phenomenological

21   assessment of ecological regime shifts and thresholds to an operational one. All of the

22   exploratory and inferential techniques covered here require that the threshold has to be

23   crossed in order to be detected, which means that they cannot directly be used to prevent

24   abrupt changes in ecosystems [1]. However, the accumulation of a broad empirical basis on

25   the presence of ecological threshold and regime shifts in response to key pressures, such as

1   increased nutrient inputs, ecosystem fragmentation or climate change, will certainly help

2   develop a predictive framework to be used to anticipate and avoid changes associated with

3   loss of essential ecosystem functionality. The accumulating knowledge base of ecological

4   thresholds across different ecosystems should be accompanied by developing quantitative

5   methods that allow confident extrapolation of thresholds for ecosystems that have not yet

6   experienced, in particular irreversible, regime shifts.

7

8   **Acknowledgements**

1   **Glossary**

2   **Artificial neural network:** a mathematical model where input signals are processed through

3   one or more layers of interconnected computational nodes resembling biological neurons

4   **Autocorrelation:** the smoothness of a time series expressed as the correlation between its

5   successive values

6   **Autoregressive model:** a linear regression model that uses past values to predict the present

7   value of a time series variable

8   **Average standard deviates (ASD):** a regime shift detection method for multiple time series

9   where the individual variables are forced to have the same sign on the same side of a

10   change-point; known to have unacceptable false positive rate on autocorrelated data

11   **Bifurcation:** a qualitative change in the behaviour of a dynamical system resulting from a

12   small change in a system parameter

13   **Bistability:** the existence of more than one locally stable stationary state in a dynamical

14   system

15   **Brownian bridge**: a Brownian motion (random walk) where both ends are clamped to zero

16   **Change-point:** a step change in the mean value, or more generally, the distribution of a time

17   series variable

18   **Chronological clustering:** a hierarchical grouping of successive steps in a multivariate time

19   series according to a dissimilarity measure, also called constrained or stratigraphic

20   clustering

21   **CUSUM:** cumulative sum of scaled deviations from a target value, such as the mean of a time

22   series

23   **Dissimilarity measure:** a single numerical value expressing a distance between two

24   multivariate objects, such that identical objects have 0 dissimilarity

Dynamic programming: a computationally efficient method for solving sequential decision problems by recursion

Ecological regime shift: a sudden shift in ecosystem status caused by passing a threshold where core ecosystem functions, structures, and processes of are fundamentally changed

Ecological threshold: the critical value of an environmental driver for which small changes can produce an ecological regime shift

Ecotone: a transitional area between two adjacent ecological communities

Empirical orthogonal function (EOF): a principal component decomposition of a multivariate time series

Exploratory data analysis: the analysis of data for the purpose of formulating hypotheses worth testing, thus complementing the conventional statistical tools for hypothesis testing

Hypothesis testing: making statistical decisions about data by asking a hypothetical question formulated as a null hypothesis

Hysteresis: a property of systems that can follow different paths when increasing and when relaxing a perturbation

Intervention analysis: a test of the hypothesis that an event at a known time caused a change in an autoregressive time series model

Likelihood ratio: the relative probabilities of an observed data set under two alternative hypotheses

Matrix decomposition: expressing a matrix as a product of (usually) simpler matrices

**Multimodal distribution:** a probability distribution with more than one peak

Principal component analysis (PCA): an orthogonal MATRIX DECOMPOSITION of the covariance or correlation matrix of a multivariate data set to reduce the dimensionality of interrelated variables

Recursive processing: a computational method for processing new data incrementally as they arrive, instead of processing them all in a single batch

Singular spectrum analysis (SSA): a technique for estimating the frequency components of a time series through a principal component decomposition of its autocorrelation matrix

Statistical test power: the probability that a statistical test will reject a false null hypothesis; the sensitivity of the test

Structural change: a change-point with a step change in the parameters of the generating model for a time series

Threshold autoregressive model: a time series model that can change structurally depending on the past values of the series (rather than at a particular change-point in time)

1   **Box 1: Theoretical and mechanistic approaches to regime shifts**

2   An abrupt jump in a system indicator when changing continuously a driver is an example of

3   the class of phenomena known as bifurcations. In general, a BIFURCATION is a qualitative

4   change in system state, including appearance and disappearance of available regimes or

5   alteration of their stability, as drivers exceed specific threshold values. Bifurcation theory [52]

6   is the branch of mathematics which studies them, identifying a broad catalogue of possible

7   types of transitions: from steady to cyclic regimes, to irregular (chaotic) fluctuations, etc.

8   Ecological analyses have been restricted mainly to transitions between two steady states. In

9   the typical case there is a range of driver values for which two steady stable states are possible

10   (for example high and low internal phosphorus (P) loading in a lake at the same rate of

11   external P supply [53], as illustrated in panel A). This phenomenon, known as bistability,

12   makes the actual system state depend on a hysteresis loop of past history (panel B; see also

13   Figure 1, column C).

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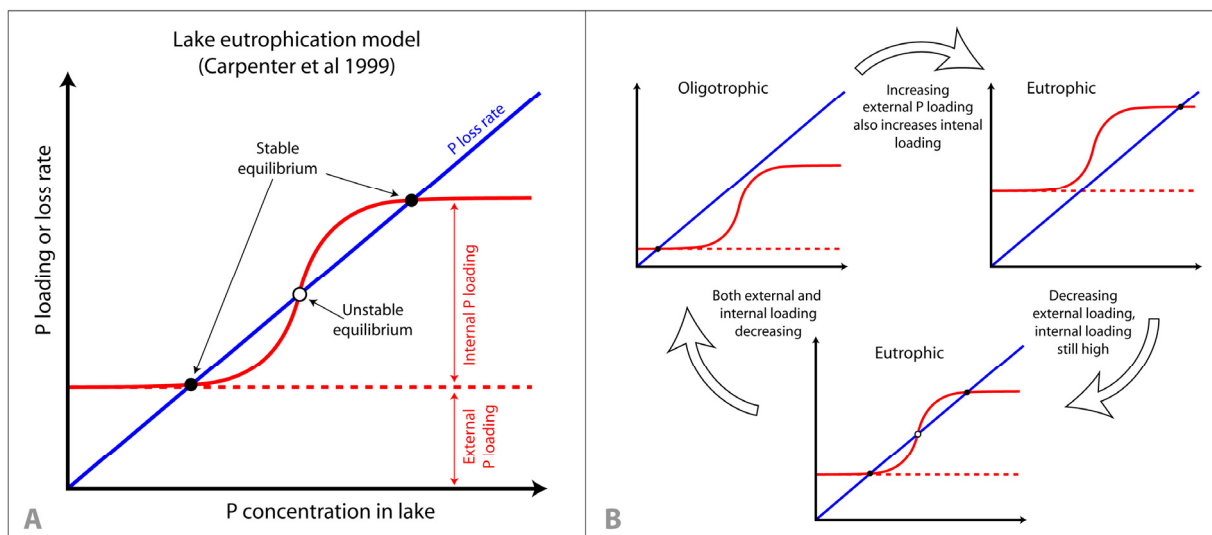
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16

17   Regime shifts and bifurcations occur even in rather simple ecosystems; for example, models

18   of food chains with only 3 trophic levels can display virtually any of the known bifurcation

19   types [54]. Attaining reliable predictive power from realistic complex models, however, faces

1   the difficulty of constraining model parameters from the relatively short and noisy time series

2   typically available in ecology. As a consequence mechanistic models can rarely be used to

3   predict accurately non-linear phenomena in ecological systems, but they can still give

4   qualitative predictions that could be useful to interpret observations. For example, simplified

5   models of grazing interactions [5] or of desertification [7] allow understanding the availability

6   of multiple stable states for ecosystems in terms of the classical image of a marble rolling

7   down a rugged landscape [5], for which the final rest state varies with the initial condition.

8   They also reveal that system indicators will tend to change more slowly when approaching a

9   regime change (this is called "critical slowing down" [52]). This and other features have led

10   to propose indicators that should in principle enable detection of an approaching threshold

11   before crossing it: rising variance [55], spectrum reddening (i.e. the relative increase of

12   fluctuations of low frequency) [56], increasing return time from perturbations [57, 58],

13   growing skewness [59]. Unfortunately, all these methods are very data demanding, and thus

14   of restricted applicability to the analysis of real ecological time series.

15

1   **Box 2: The basic change-point problem**

2   The simplest case of threshold detection is identical to what statisticians have called the

3   change-point problem: to estimate the change-point $i=k$ in a sequence $\{x_i\}$ of independent

4   random variables with constant variance, such that the expectation of x_i is μ if $i \leq k$ and $\mu + \alpha$

5   otherwise. Quandt [22] showed already in 1958 that the change-point can be estimated by

6   finding the index value k that maximizes a LIKELIHOOD RATIO, which in the case of normally

7   distributed variables corresponds to the ratio of the residual sum of squares for the alternative

8   hypothesis (a change-point at k with $\alpha \neq 0$) to that of the null hypothesis (no change-point, α

9    $= 0$). As this likelihood ratio would be F-distributed in the normal case, Quandt's test statistic

10   would be the maximum or supremum of F (sup(F)). Still, it was evident that a test for the

11   existence of a change-point could not be made from critical values of the F statistic, due to the

12   well-known inflation of p-values in multiple tests (n-1 in this case, since an F value can in

13   theory be computed for every $1 \leq k < n$). The asymptotic distribution of Sup(F) under the null

14   hypothesis of $\alpha = 0$ was not worked out until 16 years later when MacNeill [60] showed that

15   it could be constructed from moments of a BROWNIAN BRIDGE process. Extensions of these

16   results are used for computation of confidence limits of Sup(F) and for general change-point

17   hypothesis testing in software products such as the strucchange package for R [39] (Table 1).
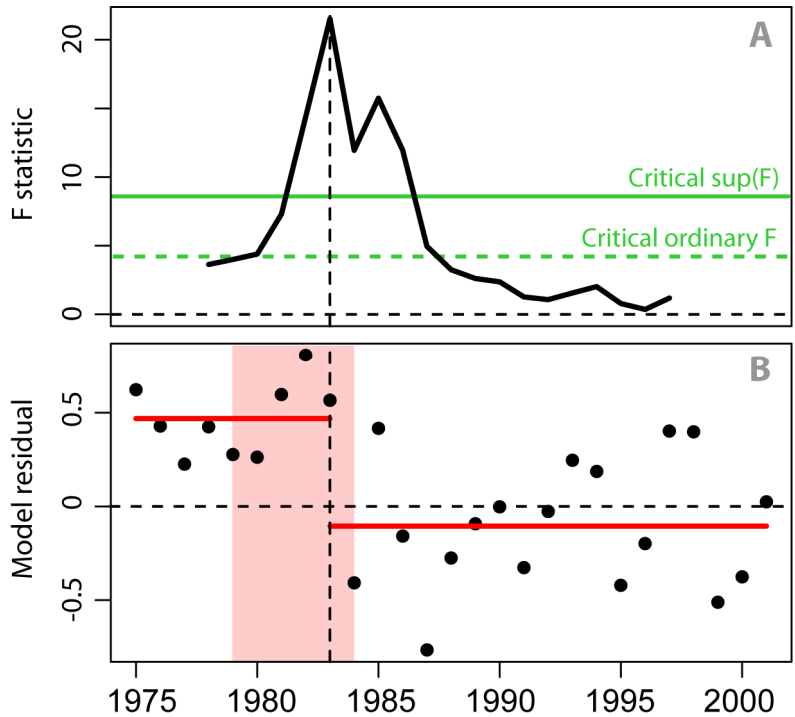
We illustrate the use of this method on a data set [61] where a temporal pattern suggestive of

a change point was found in the residuals of a multiple regression model for bottom-water

oxygen concentrations in the Danish straits (panel B). The change-point F statistic (A) shows

a distinct peak in 1983 and a smaller one in 1985, both higher than the 95% probability level

for the sup(F) statistic under the null hypothesis (green line). Notice that the critical level for

the sup(F) statistic is about twice that of the corresponding ordinary 2-sample F test (dashed

green line). The fitted linear model (B; red line) indicates a 0.5 mg O_2 L^{-1} drop in the model

residuals after 1983, although the 95% confidence interval for the change-point runs from

1979 to 1984 (red shaded area). This step change was interpreted as a consequence of the first

major hypoxia event in the region, leading to a major restructuring of the zoobenthos

community with repercussions on the system's susceptibility to new hypoxia events [61].

Box 3: What can be learned from other scientific disciplines?

The literature is enriched with a diversity of statistical methods for detecting thresholds, originating from other disciplines than ecology. Ecologists should adopt these methods rather than re-inventing new ways for analysing regime shifts.

The goal of statistical process control, dating back to the 1930s [62], is to detect systematic deviations in the mean value of a time series of some quality measure, for example the yield of an industrial process. Parameter estimates of the process or specific statistic, such as the cumulative sums of scaled residuals (CUSUM), are updated, in a RECURSIVE fashion, as new observations arrive. These tools could be applied to ecosystem monitoring programs as early warning indicators of a potential regime shift.

Econometry deals with time series that can be rich in abrupt changes due to both external interventions (e.g. policy options) and internal dynamics (e.g. consumer behaviour or different phases of economic cycles). Econometricians have developed a range of tools for detecting step changes in linear time series models, typically called structural changes or breaks in the econometric literature (see [63] for a recent review). These methods could be readily employed in ecology to obtain statistical evidence of regime shifts.

Climatologists also have a long tradition of investigating regime shift phenomena [12, 40, 41], however, with the concern that some sudden step changes in climate time series might be artefacts of the measurement system, for example due to a change in the measurement method or a relocation of a meteorological station. Therefore, climatologists have developed so-called homogenization methods to account for measurement artefacts [20, 64], and embedded this approach into general procedures for simultaneous detection of climate change and

1   observational bias [65]. Techniques developed in climatology appear particularly suitable for

2   ecological research, due to the similarities in both the studied phenomena and in the

3   observational problems.

4

5   Vegetation ecologists have a range of methods for detecting change-points or discontinuities

6   in the spatial extent of plant communities (reviewed in [66] and [67], among others). Such

7   spatial discontinuities, called ECOTONES, are detected in multivariate data ordered in one

8   dimension through comparisons of DISSIMILARITY MEASURES computed between the two

9   halves of all sequential groups of samples [68]. The vegetation analysis approach is inherently

10 multivariate, but otherwise displays similarities to the sliding window methods used for

11 univariate time series by e.g. econometricians and climatologists. The potential of these

12 methods for detecting regime shifts in multivariate ecological time series [69] deserves to be

13 explored further.

Box 4. Regime shift detection in practice

Here we illustrate the analysis of a particular data set with some of the methods described in the main text. Hare and Mantua [24] (hereafter HM) compiled 100 time series from the North Pacific Ocean and the Bering Sea, covering a 33-year period from 1965 to 1997 (http://www.iphc.washington.edu/Staff/hare/html/decadal/post1977/100ts.xls). 31 of the time series were indicators of atmospheric and oceanic processes while the remaining were biological data, mostly catch and recruitment from commercially important fish stocks, but also some from lower trophic levels. As a first exploratory approach, we perform a Principal Component decomposition of the data set. Several of the time series have missing data which are filled with the mean of the series. The first 2 principal components (PC) of the HM data set contain about 35% of the total variance. As pointed out in the original publication [24], visual inspection of PC1 and PC2 (see figure) suggests abrupt changes around 1976-77 and 1988-89. While HM further analyzed the series with the ASD method, we show instead the use of two different methodologies: First, following within the exploratory approach, we perform chronological clustering [29] of the same 100 time series data, using Ward's linkage method on an Euclidean distance matrix (similar dendrograms are produced by other methods like complete or average linkage). The temporal grouping of three main regimes is consistent with the visual impression of the first two PCs.

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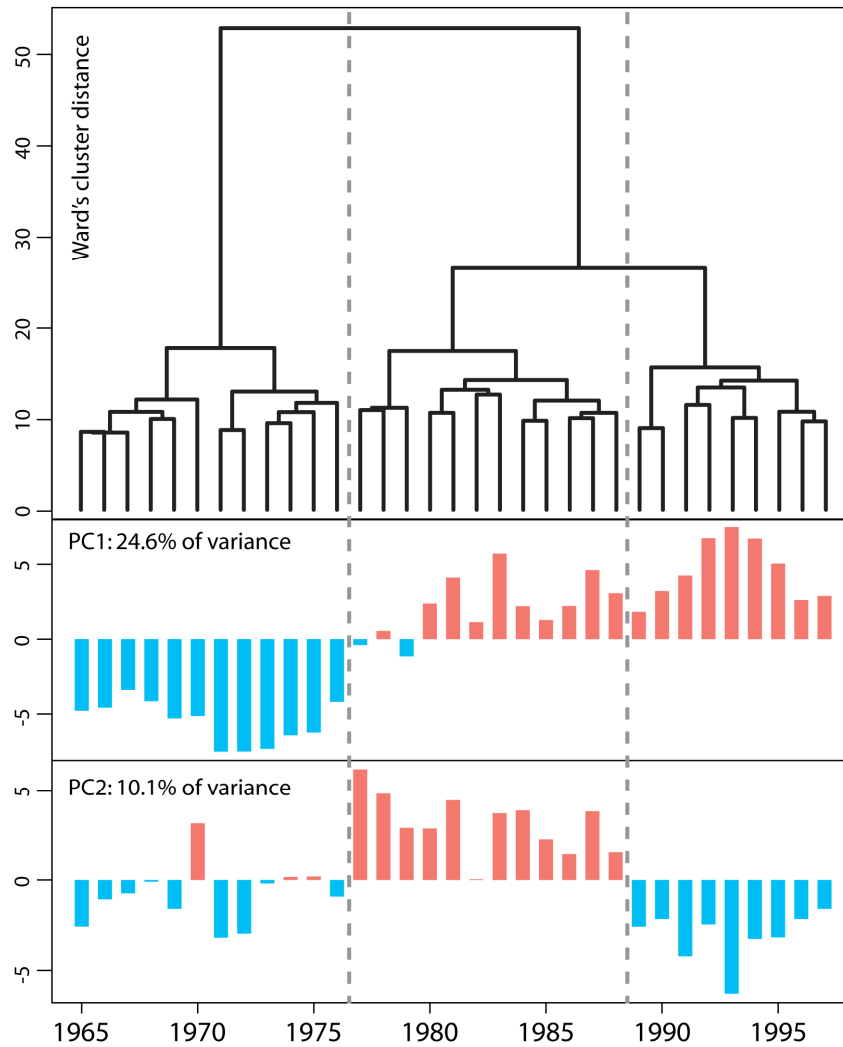
3   Altogether, two reasonably independent exploratory methods both indicate regime shifts in

4   1976-77 and 1988-89 in the area covered by the HM data set. We now move to the inferential

5   methodology by using the sup(F) statistic described in Box 2 to show that the existence of

6   change-points in the 2 first PCs is statistically well supported. Nevertheless the magnitudes of

7   the F statistics indicate that the statistical support for the 1976-77 change-point is stronger

8   than for the 1988-89 one. It has been proposed [24] that the different change-points in the two

9   PCs could be interpreted as the regime shift in 1988-89 not just being a flip back to pre 1977

10   conditions, but rather a transition to an altogether new regime.

11

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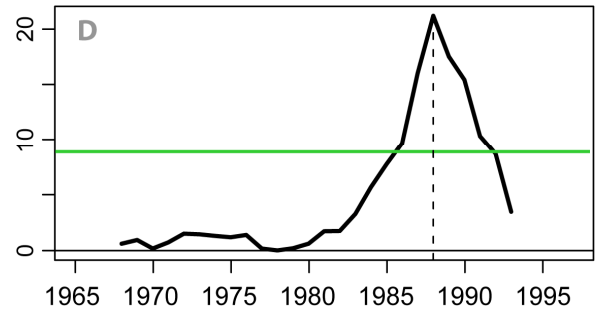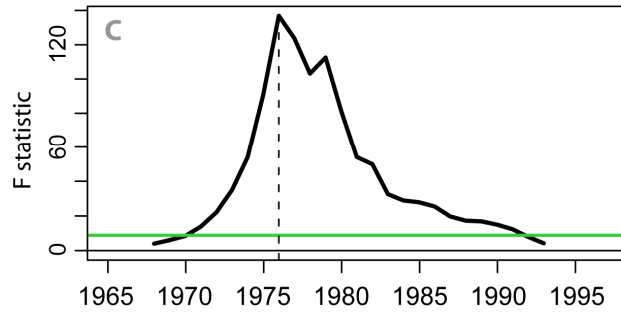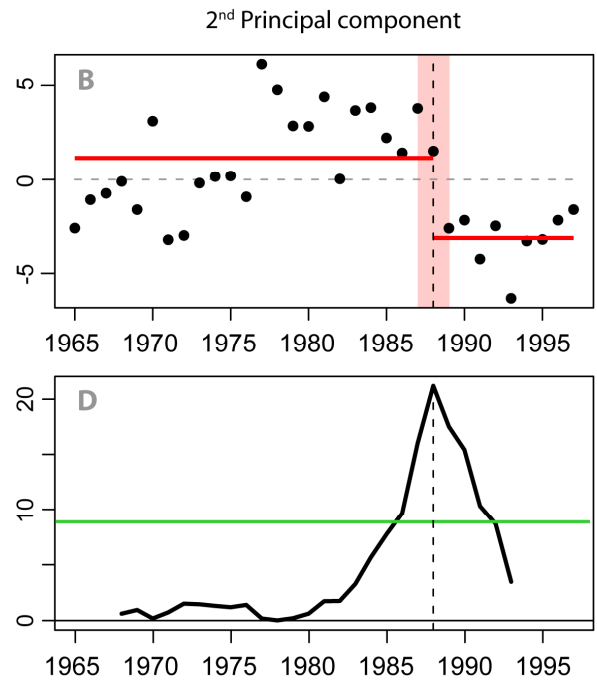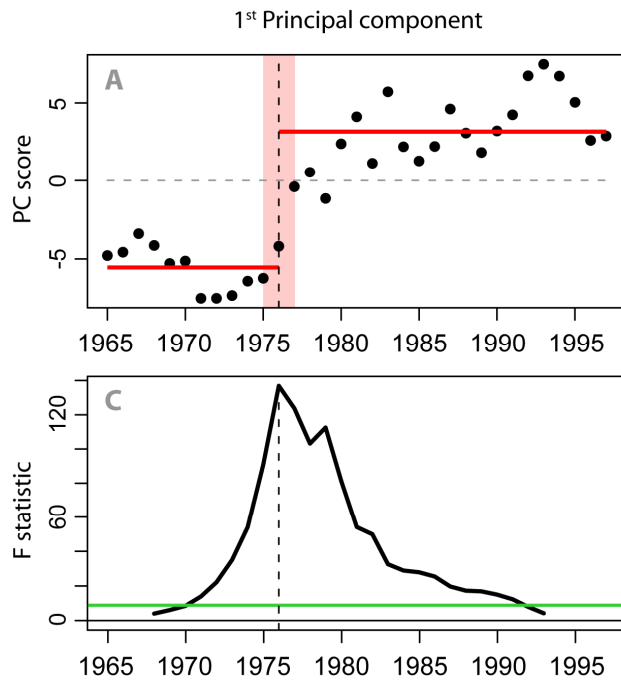
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1 **Table 1. Software for regime shift detection**
2 A selection of available software products with relevance to detection of thresholds and regime shifts in ecological data sets
3
4

Program	Methods	Approach	Availability	Authors	URL
Brodgar	Chronological clustering, dynamical factor analysis, min/max autocorrelation factor analysis, etc.	Inferential	Commercial, standalone with R interface, Windows	A. F. Zuur [30]	www.brodgar.com/brodgar.htm
Change Point Analyzer	CUSUM charts, bootstrap tests	Inferential	Shareware, standalone + Excel add-in, Windows	W. Taylor	www.variation.com/cpa/
Caterpillar-SSA	Singular spectrum analysis, structural change detection	Exploratory	Commercial, standalone, Windows	N. Golyandina, V. Nekrutkin, A. Zhigljavsky [34]	www.gistatgroup.com/cat/index.html
DCPC	Detection of changes using a penalized contrast	Inferential	Freeware, Matlab scripts, multiple OS	M. Lavielle	www.math.u-psud.fr/~lavielle/programs/
Dimensionality Reduction toolbox	Linear (PCA, etc) and non-linear dimensionality reduction methods	Exploratory	Freeware, Matlab scripts, multiple OS	L. van der Maarten [32]	http://www.cs.unimaas.nl/l.vandermaaten/Laurens_van_der_Maaten/Matlab_Toolbox_for_Dimensionality_Reduction.html
Palaeo	Chronological clustering	Exploratory	Freeware, R package, multiple OS	S. Juggins	http://www.campus.ncl.ac.uk/staff/Stephen.Juggins/analysis.htm
Regime Shift Detection	Sequential t-tests, pre-whitening option for auto-correlated data	Inferential	Freeware, Excel add-in, Windows	S. Rodionov [42]	www.beringclimate.noaa.gov/regimes/
STSA - Time Series Analysis Toolbox	Dynamical linear models, TAR models, Singular spectrum analysis, etc.	Inferential	Commercial, O-matrix toolbox, Windows	D. D. Thomakos	www.omatrix.com/stsa.html
Strucchange	Multiple change-points, F-tests, empirical fluctuation processes, etc.	Inferential	Freeware, R package, multiple OS	A. Zeileis, F. Leisch, B. Hansen, K. Hornik, C. Kleiber [39]	cran.r-project.org/src/contrib/Descriptions/strucchange.html
ThEnhancer	Nonlinear diffusion filtering	Exploratory	Freeware, standalone, multiple OS	A. Jacobo, P. Colet, E. Hernandez-Garcia	ifisc.uib.es/ThEnhancer/

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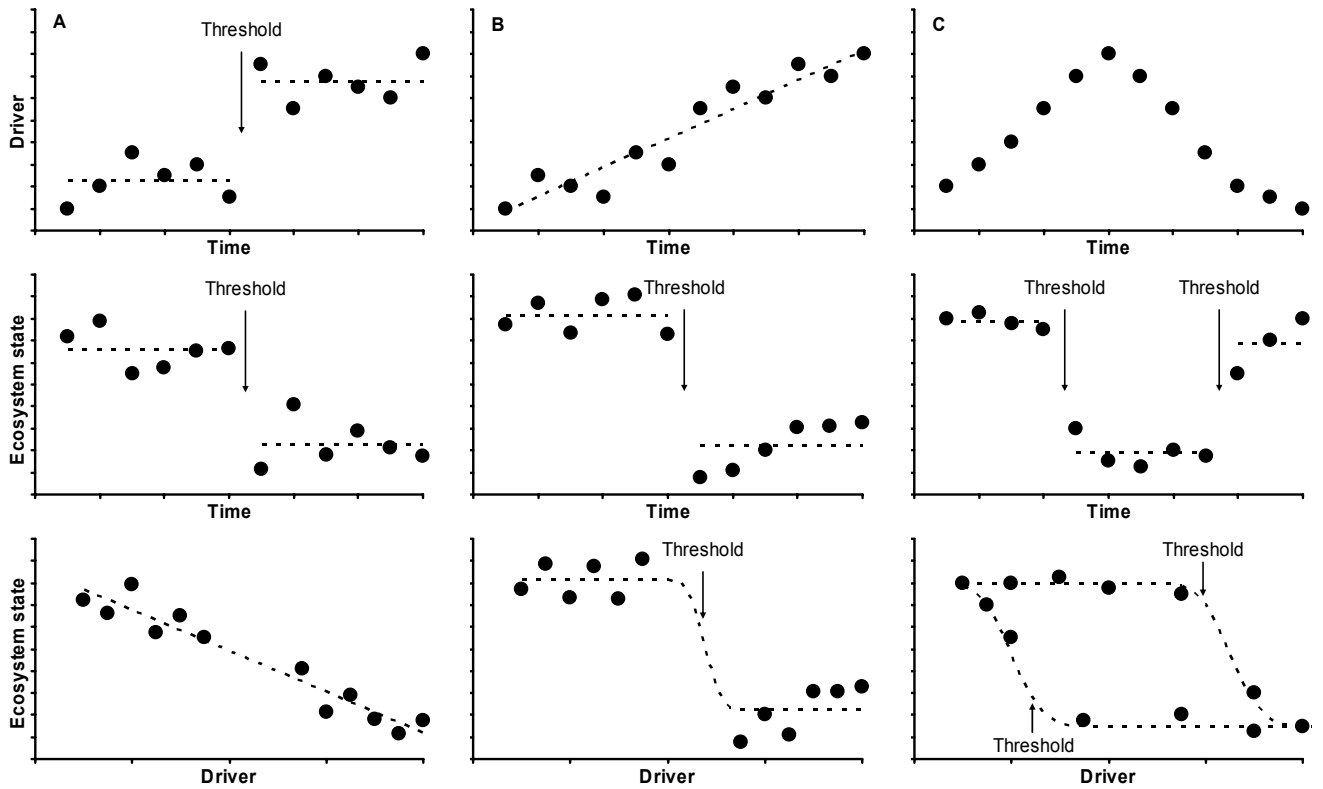
3
4
5 **Figure 1. Three scenarios for regime shifts:** Illustration of differences between regime

6 shifts resulting from smooth pressure-status relationships, threshold-like responses, and

7 bistable systems with hysteresis. The two top rows of graphs show time series of driver (e.g.

8 nutrient inputs) and ecosystem state (e.g. phytoplankton biomass), and the lower row of

9 graphs show the relationship between the driver and ecosystem state. Column A) Regime shift

10 in driver linearly mediated to the ecosystem state. Jumps appear only in the time series.

11 Column B) Regime shift in ecosystem state after driver exceeds a threshold. This is

12 manifested through a jump in the time series of the ecosystem state. Column C) The

13 hysteresis loop linking the ecosystem state to the environmental driver results in jumps

14 between two alternative states when the driver is first slowly increased and then decreased

15 again. Figure inspired by [70].

16