

## **Prediction of a complex system with few data: Evaluation of the effect of model structure and amount of data with dynamic bayesian network models**

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1 Prediction of a complex system with few data:  
2 Evaluation of the effect of model structure and amount  
3 of data with dynamic Bayesian network models

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13 **Abstract**

14 A major challenge in environmental modeling is to identify structural changes  
15 in the ecosystem across time, i.e., changes in the underlying process that gen-  
16 erates the data. In this paper, we analyze the Baltic Sea food web in order to  
17 1) examine potential unobserved processes that could affect the ecosystem and  
18 2) make predictions on some variables of interest. To do so, dynamic Bayesian  
19 networks with different setups of hidden variables (HVs) were built and vali-  
20 dated applying two techniques: rolling-origin and rolling-window. Moreover,  
21 two statistical inference approaches were compared at regime shift detection:  
22 fully Bayesian and Maximum Likelihood Estimation. Our results confirm that,  
23 from the predictive accuracy point of view, more data help to improve the pre-  
24 dictions whereas the different setups of HVs did not make a critical difference  
25 in the predictions. Finally, the different HVs picked up patterns in the data,  
26 which revealed changes in different parts of the ecosystem.

27 *Keywords:* Baltic Sea, ecosystem model, model comparison, regime shift,  
28 structural change, hidden variable

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29 **1. Introduction**

30

31

32 Ecosystems are constantly changing in response to both gradual and abrupt  
33 natural and human-induced changes, such as changes in climate, land-use, or  
34 new species arrival. In some cases, these major changes can lead to abrupt  
35 shifts, i.e., regime shifts, affecting the structure and function of ecosystem dy-  
36 namics [1, 2] that are often costly and hard to reverse [3]. For instance, the  
37 Central Baltic Sea has undergone at least two regime shifts. One was induced  
38 by constant nutrient loading from land, causing a change from an oligotrophic  
39 to a eutrophic state in the 1960s, resulting in harmful algal blooms and anoxic  
40 bottoms [4]. Another regime shift occurred in the late 1980s [5, 6] and was in-  
41 duced by overfishing of cod (*Gadus morhua*) and climate, causing a shift toward  
42 a sprat (*Sprattus sprattus*) dominated state [6], which affected the magnitude  
43 of food web processes [7]. The latter regime shift shows a clear indication of  
44 a hysteresis effect as, even after the reduction of cod fishing, the cod biomass  
45 could not be recovered [8, 9]. Such non-stationary changes in ecosystem dy-  
46 namics pose a challenge to ecosystem modelers and data analysts, since it may  
47 be that the functional forms describing the relationships between the variables  
48 change.

49 Bayesian networks (BNs), which belong to the probabilistic graphical mod-  
50 els, are compact representations of the joint probability distribution over a set  
51 of variables whose independence relations are encoded by the structure of an un-  
52 derlying directed acyclic graph [10]. Since BNs do not explicitly model changes  
53 over time, a dynamic approach could represent more realistic modeling [11].  
54 Dynamic BNs extend the concept of BN by explicitly modeling change over  
55 time, i.e., they allow the representation of the relationship between variables at  
56 successive time steps [12]. It is normally assumed that the model structure is  
57 the same in each time step and the parameters over time do not change, i.e., the  
58 model is assumed to be time-invariant. However, it is possible to add hidden

59 nodes to represent non-stationary processes [13]. Hidden variables are unob-  
60 served variables that might represent relevant processes in the system that can  
61 help explain some observed variables of interest [14]. Generally speaking, the  
62 observed variables are not the only ones that affect the system, i.e., there are  
63 a number of unobserved variables and processes that could have an effect but  
64 have not been identified, or no data are available [15]. The value of the HVs can  
65 be inferred from the observed variables linked to them so that a change in the  
66 HV pattern reflects a change in the system. Therefore, dynamic models with  
67 hidden variables are one way of trying to find the signal of change amongst the  
68 multiple ecosystem variables and their interactions [16, 15].

69 The work by [15] evaluated the potential of DBNs with hidden variables in  
70 the regime shift analysis on the Baltic Sea food web by linking different config-  
71 urations of hidden variables to the core structure of the DBN. In their study,  
72 they built three versions of the model, which differed in the hidden variable  
73 setup, with the core structure being the same, in order to analyze the pattern of  
74 the different HVs. This work allowed to investigate whether or not the pattern  
75 of the HVs reflecting specific parts of the system (such as the fish dynamics)  
76 could be separated from the global ecosystem dynamic. They found out that  
77 the different model setups showed the same general patterns. They discussed  
78 the relative scarcity of data but did not assess how much data is needed in  
79 order to implement this kind of model, or whether some setup of HVs performs  
80 better predictions than others. Our new study extends this work by answering  
81 the aforementioned questions and considering new configurations of hidden vari-  
82 ables. On the one hand, we analyzed the amount of data needed to discover the  
83 HV pattern by fitting the models multiple times with an increasing amount of  
84 data. In addition, we compared the ability of two different statistical inference  
85 approaches to detect changes in the ecosystem: Bayesian and Maximum Likeli-  
86 hood Estimation. On the other hand, we explored the predictive power of our  
87 expert-based structure models and compared the results with the ones obtained  
88 by a fixed structure model. Moreover, we examined the model's predictive per-  
89 formance across time by i) increasing the sample size, in order to detect if any

90 of the models constantly outperforms the others, and ii) discarding old data as  
 91 new information is available, in order to determine either if the variations in the  
 92 model’s performance are due to the amount of data available or if some parts  
 93 of the time series are easier to predict than others.

## 94 2. Material and Methods

### 95 2.1. Bayesian networks and dynamic Bayesian networks

96 A Bayesian network (BN) is a statistical multivariate model for a set of  
 97 variables  $\mathbf{X} = \{X_1, \dots, X_n\}$ , which is defined in terms of two components:

- 98 • Qualitative component: A directed acyclic graph (DAG) where each vertex  
 99 represents one of the variables in the model, and so that the presence of an  
 100 edge linking two variables indicates the existence of statistical dependence  
 101 between them.
- 102 • Quantitative component: A conditional distribution  $p(x_i|pa(x_i))$  for each  
 103 variable  $X_i, i = 1, \dots, n$  given its parents in the graph, denoted as  $pa(X_i)$ .

104 The joint distribution of the variables in the network is therefore represented  
 105 in a factorized way as

$$p(X) = \prod_{i=1}^n p(x_i|pa(x_i)), \quad \forall x_1, \dots, x_n \in \Omega_{X_1, \dots, X_n}, \quad (1)$$

106 where  $X = x_1, \dots, x_n$ ,  $\Omega_{X_i}$  represents the set of all possible values of variable  
 107  $x_i$  and  $pa(x_i)$  denotes an instantiation of the parents of  $X_i$ . [Figure 1](#) shows an  
 108 example of a DAG and its joint probability distribution.

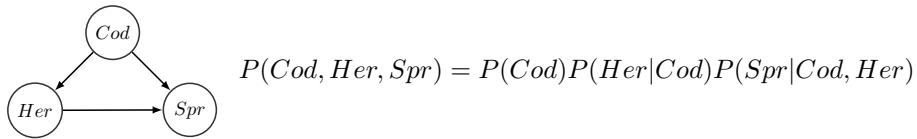


Figure 1: Example of Bayesian network: DAG (left) and joint probability distribution (right).

109 Dynamic Bayesian networks (DBN) extend the concept of BNs by relating  
 110 variables across time. DBNs are defined as a pair  $(B_1, B_{2T})$  [17], where  $B_1$  is

111 a classical BN representing the first time slice ( $t = 0$ ) and  $B_{2T}$  represents the  
 112 transition model, i.e, a two-slice DBN for  $t > 0$ . Therefore, the joint probability  
 113 distribution of  $t = 0$  is the same as Equation (1), whereas the joint probability  
 114 distribution of the following time slices ( $t > 0$ ) is

$$p(X^{(t)}|X^{(t-1)}) = \prod_{i=1}^n p(x_i^{(t)}|pa(x_i^{(t)})), \quad (2)$$

115 where  $x_i^{(t)}$  is the  $i^{th}$  node at time  $t$  and  $pa(x_i^{(t)})$  are the parents of  $x_i^{(t)}$  in the  
 116 graph.

117 The parents ( $pa(x_i^{(t)})$ ) of a node ( $x_i^{(t)}$ ) can either be in the same time slice  
 118 or in the previous one, assuming a first-order Markov process. We are making  
 119 two other assumptions: 1)  $X^{(t-1)} \perp X^{(t+1)}|X^{(t)}$ , the Markov property, i.e,  
 120 the future is independent of the past given the present; and 2) the transition  
 121 processes are time-invariant, i.e. the transition functions are the same for all  
 122 time slices. Figure 2 shows an example of unrolled DBN.

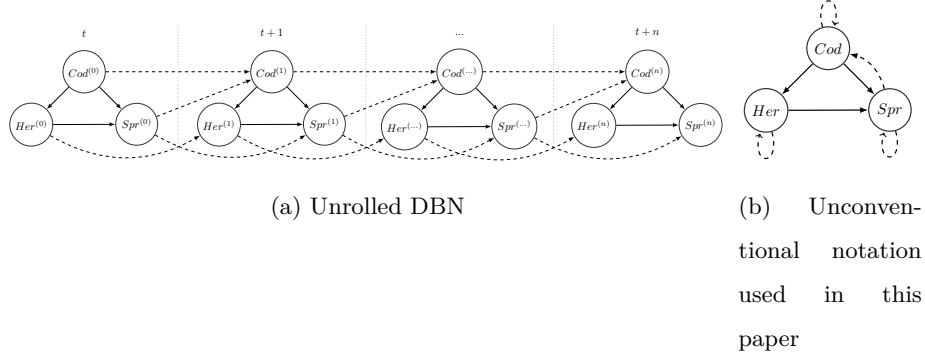


Figure 2: Example of DAG of a DBN. Dependencies within a time slice are represented by solid edges whereas dependencies between time slices are represented by dashed edges. The joint probability distribution of the transition model for this DAG can be written as  $P(Cod^t, Her^t, Spr^t|Cod^{t-1}, Her^{t-1}, Spr^{t-1}) = P(Cod^t|Cod^{t-1}, Spr^{t-1})P(Her^t|Cod^t, Her^{t-1})P(Spr^t|Cod^t, Her^t, Spr^{t-1})$ .

123

124

## 125 *2.2. Parameter learning*

126 The dataset used in this paper contains only continuous variables, which  
127 were parameterized using linear Gaussian distributions. Parameters can be  
128 learned from data using the Expectation-Maximization (EM) algorithm [18].  
129 The goal of the EM algorithm is to find the maximum likelihood estimate of  
130 the model parameters when the data have missing values. The EM algorithm  
131 iteratively finds (E-step) and maximizes (M-step) a current approximation to  
132 the log-likelihood function of the parameters of a model [19]. The algorithm  
133 must be initialized with an initial value of the parameters. In this work, the  
134 initial random values of the parameters were drawn from the standard normal  
135 distribution,  $N(0,1)$ . Then, the E-step computes the expected sufficient statis-  
136 tics (mean and variance) using the current parameter values and the observed  
137 data. Afterward, the M-step maximizes the log-likelihood of the parameters  
138 given the sufficient statistics, obtaining an updated value of the parameter esti-  
139 mate. These two steps iterate until convergence; in our case, until the difference  
140 between consecutive log-likelihoods was small enough. Since the EM algorithm  
141 can get stuck in a local optimum, it was run 100 times for each model, retaining  
142 the model with the highest log-likelihood value for further analyses.

## 143 *2.3. The Baltic Sea food web model*

### 144 *2.3.1. Data description*

145 The data originate from the Gotland Basin in the central Baltic Sea ([Fig-](#)  
146 [ure 3](#)), covering the 38-year period from 1975 to 2012 ([Table 1](#)). They were  
147 obtained from different sources: the fish data are derived from the fish stock  
148 assessment model called Virtual Population Analysis [20], tuned using the Ex-  
149 tended Survival Analysis (XSA) method [21]. This model uses both fish catch  
150 and fish survey data from multiple years as input data and fits an age-structured  
151 fish stock model that accounts for the amount and mean weight of fish in each  
152 year class. It estimates the total biomass of the spawning stock as well as the  
153 number of fish in the next year class (recruitment). The reproductive volume of  
154 cod, i.e., the volume of water in which the environmental factors (in particular,

155 salinity and oxygen concentration) are such that cod eggs survive, is based on a  
 156 spatial interpolation model [22]. Water temperature, zooplankton, and chloro-  
 157 phyll variables are based on direct measurements taken during field sampling  
 158 campaigns. The data are highly variable, both temporally and spatially, and  
 159 therefore the data tend to be noisy, as the observation may vary considerably  
 160 depending on the sampling date and the exact location of the sampling. In order  
 161 to avoid numerical instability, the data were log-transformed and standardized  
 162 to mean 0 and standard deviation 1.

Table 1: Summary of the observed variables used to build the models.

Variable	Description (units)
FCod <sup>a</sup>	Fishing-Induce mortality of cod (instantaneous fishing mortality)
Cod2y <sup>a</sup>	Abundance of juvenile cod, age 2 (number of individuals, in thousands)
SSBCod <sup>a</sup>	Spawning stock biomass of cod (metric tonnes)
FHer <sup>a</sup>	Fishing-Induce mortality of herring (instantaneous fishing mortality)
Her1y <sup>a</sup>	Abundance of juvenile herring, age 1 (number of individuals, in thousands)
SSBHer <sup>a</sup>	Spawning stock biomass of herring (metric tonnes)
FSpr <sup>a</sup>	Fishing-Induce mortality of sprat (instantaneous fishing mortality)
Spr1y <sup>a</sup>	Abundance of juvenile sprat, age 1 (number of individuals, in thousands)
SSBSpr <sup>a</sup>	Spawning stock biomass of sprat (metric tonnes)
Ac <sup>b</sup>	Biomass of zooplankton genus <i>Acartia</i> , measured in spring ( $mg/m^3$ )
Tem <sup>b</sup>	Biomass of zooplankton genus <i>Temora</i> , measured in spring ( $mg/m^3$ )
Ps <sup>b</sup>	Biomass of zooplankton genus <i>Pseudocalanus</i> , measured in summer ( $mg/m^3$ )
Chla <sup>c</sup>	Chlorophyll <i>a</i> concentration in water, measured in spring ( $mg/m^3$ )
Tspring <sup>d</sup>	Sea surface temperature in spring ( $^{\circ}C$ )
Tsum <sup>d</sup>	Sea surface temperature in summer ( $^{\circ}C$ )
RV <sup>e</sup>	Reproductive volume of cod, i.e., volume of water in which the cod eggs can survive ( $km^3$ )

Data source: <sup>a</sup> ICES stock assessment, XSA model [23]; <sup>b</sup> Quantitative Juday net sampling from 0-100 m water layer; <sup>c</sup> Quantitative measurement from water sample 0-10 m water layer; <sup>d</sup> Measurement from water sample; <sup>e</sup> Spatial interpolation model [22].



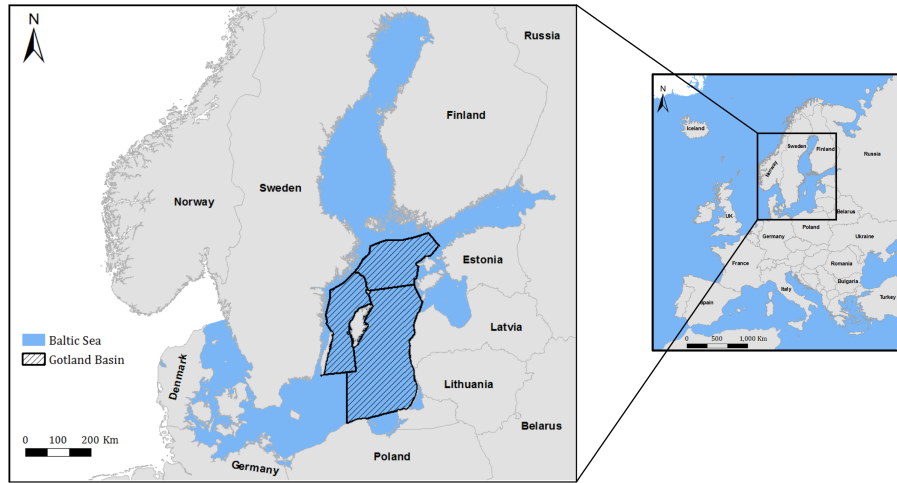


Figure 3: Location of the study area, the Gotland basin (central Baltic Sea, Europe). Source: Map created from layers ‘Europe’ (downloaded from <http://tapiquen-sig.jimdo.com>) and ‘HELCOM subbasins with coastal and offshore division 2018’ (downloaded from <https://maps.helcom.fi>), using the ArcGis software by Esri.

163 *2.3.2. Expert knowledge-based structure*

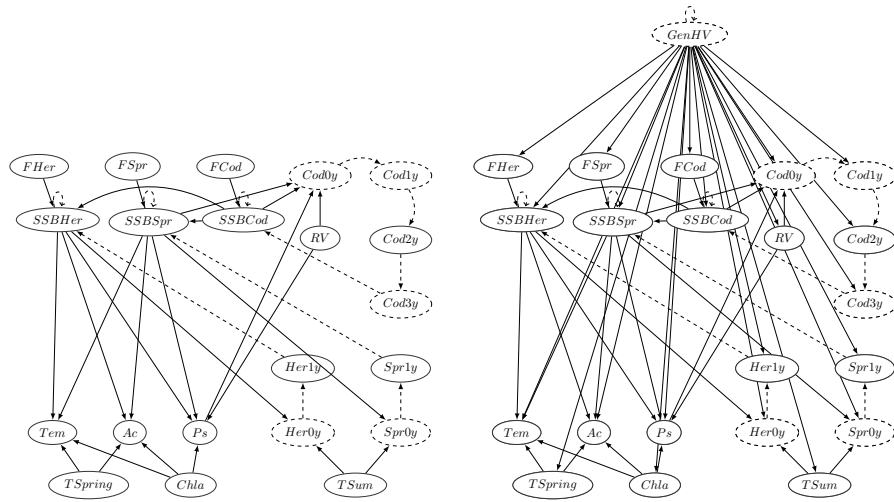
164 BNs can be used to encode expert knowledge over a domain [24, 25]. The  
 165 graphical representation provided by BNs makes them a transparent tool, which  
 166 is especially useful when expert elicitation is required [26, 27]. A Gotland Basin  
 167 food web model structure was built based on expert elicitation (Figure 4a),  
 168 including the key components of the food web and their interactions. Some of  
 169 the variables in this model are only linked to variables in the contiguous time  
 170 slices, which is essential to transmit the temporal dynamic. Five non-observed  
 171 variables, representing juvenile fish stages, were included to act as placeholders  
 172 of the fish stage from birth to maturation. These unobserved variables include 0-  
 173 year old herring, sprat and cod and one-year old and three-year old cod. Herring  
 174 and sprat mature and join the spawning stock at the age two and cod at age  
 175 four [28].

176 The dynamic model is defined in one-year time steps. The fish related  
 177 variables have temporal dependencies across time steps: the spawning stock

178 sizes (SSB) of the three fish species are autoregressive, as they consist of in-  
 179 dividual fish that live for multiple years and therefore their value in one time-  
 180 slice depends on their value in the previous one. The juvenile fish are mod-  
 181 eled separately: they exhibit temporal dependency so that the  $k$ -year old fish  
 182 ( $k = \{0, \dots, 3\}$  for cod and  $k = \{0, 1\}$  for herring and sprat) are  $k+1$  years old  
 183 in the following time slice until they reach maturation and join the spawning  
 184 stock (SSB). The remaining variables are assumed not to directly depend on  
 185 variables in the preceding year, though they may have temporal autocorrelation  
 186 due to the fact that variables affecting them are temporally autocorrelated.

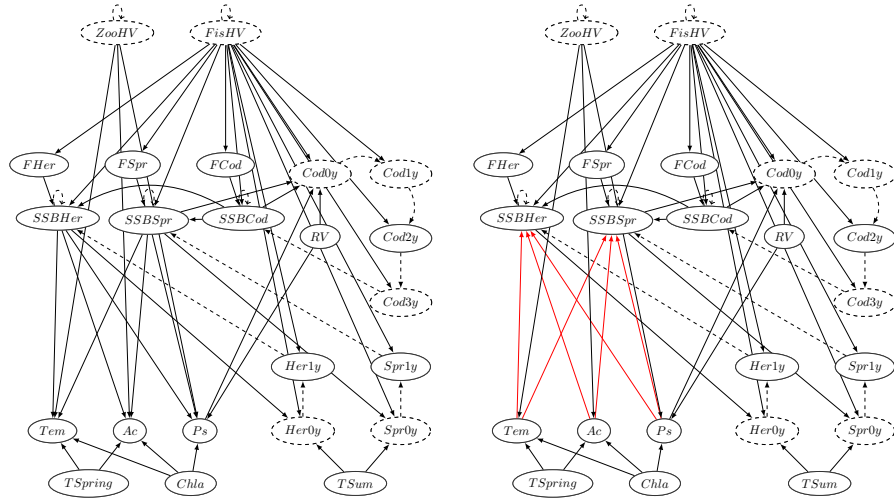
187 The variables described above form the core structure of the expert knowledge-  
 188 based model structure (Figure 4a). However, it is clear that there are other  
 189 variables and processes that could affect the ecosystem dynamics but have not  
 190 been identified or no data are available. For this reason, models with different  
 191 configurations of generic hidden variables (HVs) were built:

- 192 • a model with no general HVs (M0, Figure 4a);
- 193 • a model with one HV (M1, *GenHV*), linked to all other variables in each  
 194 time slice and to itself in the consecutive time slices (Figure 4b);
- 195 • a model with two semi-generic HVs (M2): one linked to all fish-related  
 196 variables (*FisHV*) and another linked to all zooplankton-related variables  
 197 (*ZooHV*) in each time slice and to themselves in the consecutive time slices  
 198 (Figure 4c); and
- 199 • a model (M2r) including *FisHV* and *ZooHV* (Figure 4d), as in M2 but  
 200 reversing the links between the variables *SSBHer* and *SSBSpr* and the  
 201 zooplankton variables. This was done for food web reasons (energy flows  
 202 from phytoplankton to zooplankton to fish) and for computer science rea-  
 203 sons (in model M2, variables *SSBHer* and *SSBSpr* and hidden variable  
 204 *ZooHV* are conditionally dependent given the zooplankton variables, due  
 205 to the v-structure; by reversing the links, they are conditionally indepen-  
 206 dent given the zooplankton variables).



(a) Model M0: no HV.

(b) Model M1: 1 generic HV (*GenHV*).



(c) Model M2: 2 HVs (*FisHV* and *ZooHV*).

(d) Model M2r: 2 HVs (*FisHV* and *ZooHV*).

Figure 4: Expert knowledge-based model structure showing different configurations of HVs. Solid nodes represent observed variables whereas dashed nodes indicate unobserved variables. Solid edges represent direct dependencies between variables within a time slice whereas dashed edges represent direct dependencies between two time slices. *SSBHer*, *SSBSpr*, *SSBCod*, *GenHV*, *ZooHV* and *FisHV* are autoregressive variables.

207 *2.3.3. Naive Bayes structure*

208 In order to explore how well a simple approach would perform, we built a  
 209 Naive Bayes model with a HV as the class. Naive Bayes (NB) is a BN with a  
 210 fixed structure in which one variable, the class  $C$ , is the parent of all remaining  
 211 variables,  $X_1, \dots, X_n$ , which are independent to each other given  $C$ . The strong  
 212 assumption of independence behind NB models is somehow compensated by the  
 213 reduction on the number of parameters to be estimated from data, since in this  
 214 case, it holds that

$$p(c|x_1, \dots, x_n) \propto p(c) \prod_{i=1}^n p(x_i|c) , \quad (3)$$

215 which means that, instead of one  $n$ -dimensional conditional density,  $n$  one-  
 216 dimensional conditional densities have to be estimated.

217 Variables included in [Table 1](#) as well as a generic hidden variable (*GenHV*)  
 218 were used to build the model. The HV takes the place of the class, which is the  
 219 only autoregressive variable in the model ([Figure 5](#)). The dynamic model is de-  
 220 fined in one-year time steps, where the links between time slices only correspond  
 221 to the autoregressive hidden variable, *GenHV*.

222 In what follows we derive the explicit equation of the expected value of the  
 223 HV for model NB. The equations for the rest of the models are derived in a  
 224 similar way. For short, let's denote the variables in model NB (see [Figure 5](#))  
 225 as  $C=GenHV$ ,  $X_1=FHer$ ,  $X_2=FSpr$ ,  $X_3=FCod$ ,  $X_4=SSBHer$ ,  $X_5=SSBSpr$ ,  
 226  $X_6=SSBCod$ ,  $X_7=Her1y$ ,  $X_8=Spr1y$ ,  $X_9=Cod2y$ ,  $X_{10}=Tem$ ,  $X_{11}=Ac$ ,  $X_{12}=Ps$ ,  
 227  $X_{13}=RV$ ,  $X_{14}=TSpring$ ,  $X_{15}=Chla$ ,  $X_{16}=Tsum$ . Let  $\mathbf{X}^{(t)} = (X_1^{(t)}, \dots, X_{16}^{(t)})$   
 228 denote the observed variables at time step  $t$ . Let  $\mathbf{x}^{(t)} = (x_1^{(t)}, \dots, x_{16}^{(t)})$  be any  
 229 of the possible configurations of the observed variables at time step  $t$ . Our goal  
 230 is to model the expected value of the hidden variable at time step  $t$  given all  
 231 the previous observations, i.e.

$$E[C^{(t)}|\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)}] = \int c^{(t)} p(c^{(t)}|\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)}) dc^{(t)}, \quad (4)$$

232 where

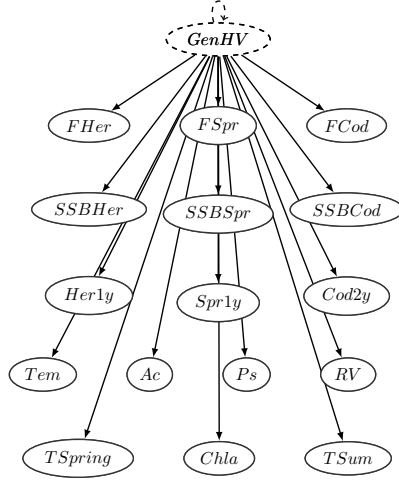


Figure 5: Naive Bayes model. Solid nodes represent observed variables whereas dashed nodes indicate unobserved variables. Solid edges represent direct dependencies between variables within a time slice whereas dashed edges represent direct dependencies between two time slices. *GenHV* is the only autoregressive variable.

$$\begin{aligned}
p(c^{(t)}|\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)}) &= \int p(c^{(1)}, \dots, c^{(t)}|\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)}) dc^{(1)} \dots dc^{(t-1)} \\
&= \frac{1}{Z} \int p(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)}|c^{(1)}, \dots, c^{(t)}) p(c^{(1)}, \dots, c^{(t)}) dc^{(1)} \dots dc^{(t-1)} \\
&= \frac{1}{Z} \int p(c^{(1)}) \prod_{i=1}^t \left( p(\mathbf{x}^{(i)}|c^{(i)}) p(c^{(i)}|c^{(i-1)}) \right) dc^{(1)} \dots dc^{(t-1)} \quad (5) \\
&= \frac{1}{Z} \int p(c^{(1)}) \prod_{i=1}^t \left( p(c^{(i)}|c^{(i-1)}) \prod_{j=1}^{16} p(x_j^{(i)}|c^{(i)}) \right) dc^{(1)} \dots dc^{(t-1)},
\end{aligned}$$

233 with  $Z$  being a normalization constant equal to  $p(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)})$ . Each density  
234  $p(c^{(i)}|c^{(i-1)})$  is a Gaussian density for  $c^{(i)}$  with mean equal to a linear function  
235 of  $c^{(i-1)}$ , and each  $p(x_j^{(i)}|c^{(i)})$  is a Gaussian density for  $x_j^{(i)}$  with a linear function  
236 of  $c^{(i)}$  as mean.

#### 237 2.4. Approach comparison of regime shift detection

238 As an alternative to the already proposed method to detect unobserved pro-  
239 cesses, we also followed a fully Bayesian approach, i.e., including the parameters

240 as random variables and then updating the model by making probabilistic infer-  
241 ence (belief update) for each record in the dataset. The goal of this comparison  
242 was to explore the ability of these two approaches at detecting changes in the  
243 ecosystem. In order to build a fully Bayesian model, we used the Naive Bayes  
244 concept drift detector (NBCD) algorithm [29] from the R package `ramidst`,  
245 which is an R interface to the AMIDST toolbox [30] written in Java. The NBCD  
246 relies on the variational Bayes framework (a class of approximation methods) for  
247 the inference and learning tasks, and uses the NB structure as the base model,  
248 with a variable of interest being the class and the remaining being predictive  
249 variables. Then, a hidden variable ( $H$ ) is added and linked to the predictive  
250 variables in the model. The specific inference method used in our experiments  
251 was the streaming variational Bayes (SVB) algorithm [31].

252 On the other hand, we built a model with the same DAG structure as the  
253 NBCD, but using the EM algorithm to learn the parameters, as implemented in  
254 the `learn_params_dbn_em` function of the Bayes Net Toolbox in MATLAB. Since  
255 we are interested in six variables (SSBCod, SSBSpr, SSBHer, Cod2y, Spr1y and  
256 Her1y), we built six models using the NBCD algorithm and six using the EM  
257 algorithm. Figure 6 shows the DAG used to build the model with Her1y as the  
258 class variable. Note that the DAG is analogous for the remaining variables of  
259 interest. We will analyze the hidden variable  $H$  for each model. For the sake of  
260 clarity, we will refer to this hidden variable as  $H_{EM}$  if it was learned using the  
261 EM algorithm or  $H_B$  if it was learned following the Bayesian approach. In the  
262 case of no ambiguity or no need to distinguish between them,  $H$  will be used  
263 instead.

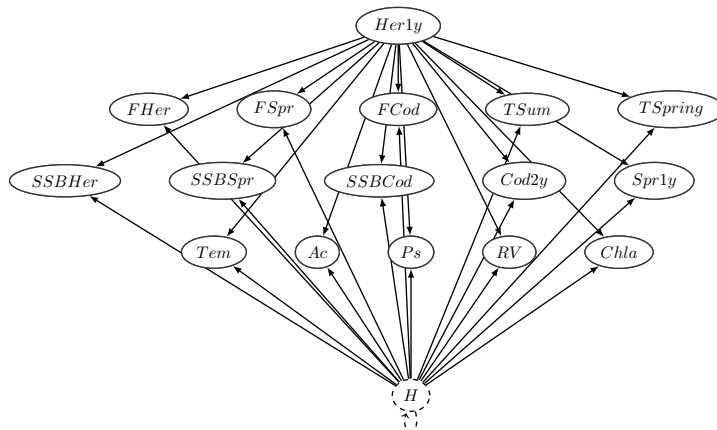


Figure 6: Naive Bayes model with one hidden variable and Her1y being the class. Solid nodes represent observed variables whereas dashed nodes indicate unobserved variables. Solid edges represent direct dependencies between variables within a time slice whereas dashed edges represent direct dependencies between two time slices.

264 In all the models described here and in the previous sections, the autocor-  
 265 related hidden variables try to capture the evolution of the model uncertainty  
 266 over time. Furthermore, the Bayesian approach used in model NBCD takes  
 267 into account the possible lack of independence in the data to some extent by  
 268 updating the parameters each time a new data item arrives. In other words,  
 269 the posterior distribution in a time step becomes the prior distribution in the  
 270 next time step. Notice, however, that we only consider discrete time steps, as  
 271 can be seen in Equation (4). Finer granularity can be achieved by adopting a  
 272 continuous time approach [32] in which time becomes a variable into the model  
 273 equations.

## 274 2.5. Model validation

275 In order to validate the predictive performance of the aforementioned mod-  
 276 els, five-step ahead predictions were carried out. Two cross-validation (CV)  
 277 techniques to train and test the models were used: rolling-origin and rolling-  
 278 window [33]. In the first one, the sample size increases in each fold with respect  
 279 to the origin (last observation of the training set) (Figure 7a), i.e., the data from

280 the test set move to the train set sequentially and the model is recalibrated. In  
281 the second one, the sample size is kept constant in each fold (except for the first  
282 one due to the total amount of data), moving the training set as a window across  
283 time (Figure 7b), i.e., data from the beginning of the time series are discarded  
284 as new data are available.

285 The reason for doing this was to explore whether the variation in the model’s  
286 performance across time is due to the amount of data available or because some  
287 parts of the time series are easier to predict than others. The goodness of the  
288 predictions was evaluated using the log-likelihood of the observations given the  
289 predicted values. We compared the log-likelihoods of the pairs rolling-origin,  
290 rolling-window of each model version using the Wilcoxon Signed Rank test.

291 Moreover, for the rolling-origin case, the log-likelihoods of the five-year pre-  
292 diction of different sets of models (M0, M1, M2, M2r, NB) were compared us-  
293 ing either Wilcoxon Signed Rank Test (for two groups) or Friedman Test with  
294 maxT statistic [34] (for more than two groups). In the case of applying Fried-  
295 man Test, in those cases where significant differences were found, we deployed  
296 Wilcoxon–Nemenyi–McDonald–Thompson’s post-hoc test [35].

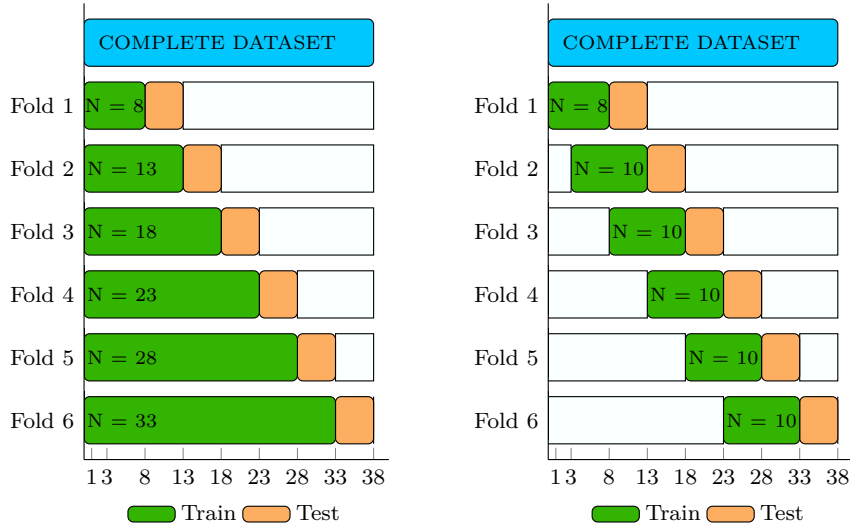
### 297 3. Results

#### 298 3.1. Regime shift detection

299 Models with different configurations of HVs were built in order to detect  
300 processes that could affect different parts of the system. In particular, three HVs  
301 were explored: a *general* HV (GenHV), a *fish* HV (FisHV) and a *zooplankton*  
302 HV (ZooHV). To analyze the HV patterns, we fit the models following the  
303 rolling-origin approach as shown in Figure 7a with the difference that, for each  
304 fold, both train and test sets were used to learn the models. Figure 8 shows the  
305 evolution of the expected value of the HVs in each model (M1, M2, M2r and  
306 NB) for each fold, computed as explained in Equation (4).

307 The three HVs (GenHV, FisHV, ZooHV) showed different patterns among  
308 them and similar to themselves (except for ZooHV) in the other models, i.e.,





(a) Rolling-origin, increasing  $N_{train}$  by 5.

(b) Rolling-window.

Figure 7: Sample size ( $N$ ) used to train and test the models.  $N_{test} = 5$ .

309 GenHV shows similar behavior in models M1 and NB, and so does FisHV in  
 310 models M2 and M2r. Regarding the last Fold, in which the complete dataset is  
 311 used to fit the models, GenHV shows a decrease at the very beginning of the  
 312 time series in both models (M1 and NB), followed by an increase from the period  
 313 1981-1991, point at which they stabilize till the end of the time series, when they  
 314 start decreasing again. On the other hand, FisHV decreases at the beginning  
 315 of the time series, then increases from 1978 to 1998 and finally decreases to its  
 316 first values.

317 Of special interest is variable ZooHV, which shows a different pattern in  
 318 models M2 and M2r, with the former having a zigzag trend and higher variance  
 319 and the latter showing two stable periods separated by an abrupt increase from  
 320 the mid-1980s till 1990s. The difference between ZooHV-M2 and ZooHV-M2r  
 321 is a consequence of reversing the links between the zooplankton variables (Tem,  
 322 Ac and Ps, which will be referred to as  $\mathbf{Z}$ ) and the SSBHer and SSBSpr variables  
 323 (which will be referred to as  $\mathbf{S}$ ). By inverting these links, we transformed the v-  
 324 structure involving these variables (i.e.,  $\mathbf{S} \rightarrow \mathbf{Z} \leftarrow \text{ZooHV}$ ) to a serial connection

325 (i.e.,  $\mathbf{S} \leftarrow \mathbf{Z} \leftarrow \text{ZooHV}$ ), so that the  $\mathbf{S}$  variables and ZooHV are conditionally  
326 independent given  $\mathbf{Z}$ . In other words, given  $\mathbf{Z}$ , new information about  $\mathbf{S}$  does  
327 not influence the ZooHV variable. On the other hand, variables TSpring and  
328 Chla are also involved in the v-structure, therefore given any of the variables in  
329  $\mathbf{Z}$  is observed, TSpring, Chla and ZooHV become conditionally dependent, in  
330 both M2 and M2r models.

331 Since the size of the training set is increased by five in each fold, it is not  
332 surprising that the first and last folds show very different patterns. The fold  
333 at which the pattern of the HV is revealed depends on the specific HV. For  
334 instance, the abrupt increase of variable ZooHV (model M2r) can be seen from  
335 Fold 2 onwards (i. e., with sample size  $N = 13$ ) whereas the stabilization phase  
336 can be observed from Fold 3. On the other hand, variable GenHV (model M1  
337 and NB) takes a bit longer to reveal its final pattern, which can be seen from  
338 Fold 5 onwards. Finally, variable FisHV has a similar pattern to GenHV until  
339 Fold 5. Unlike GenHV, variable FisHV experiments a drastic decrease from  
340 Fold 5 to 6. It appears that variable GenHV could be capturing both FisHV  
341 and ZooHV trends, combining them in a smoother pattern.

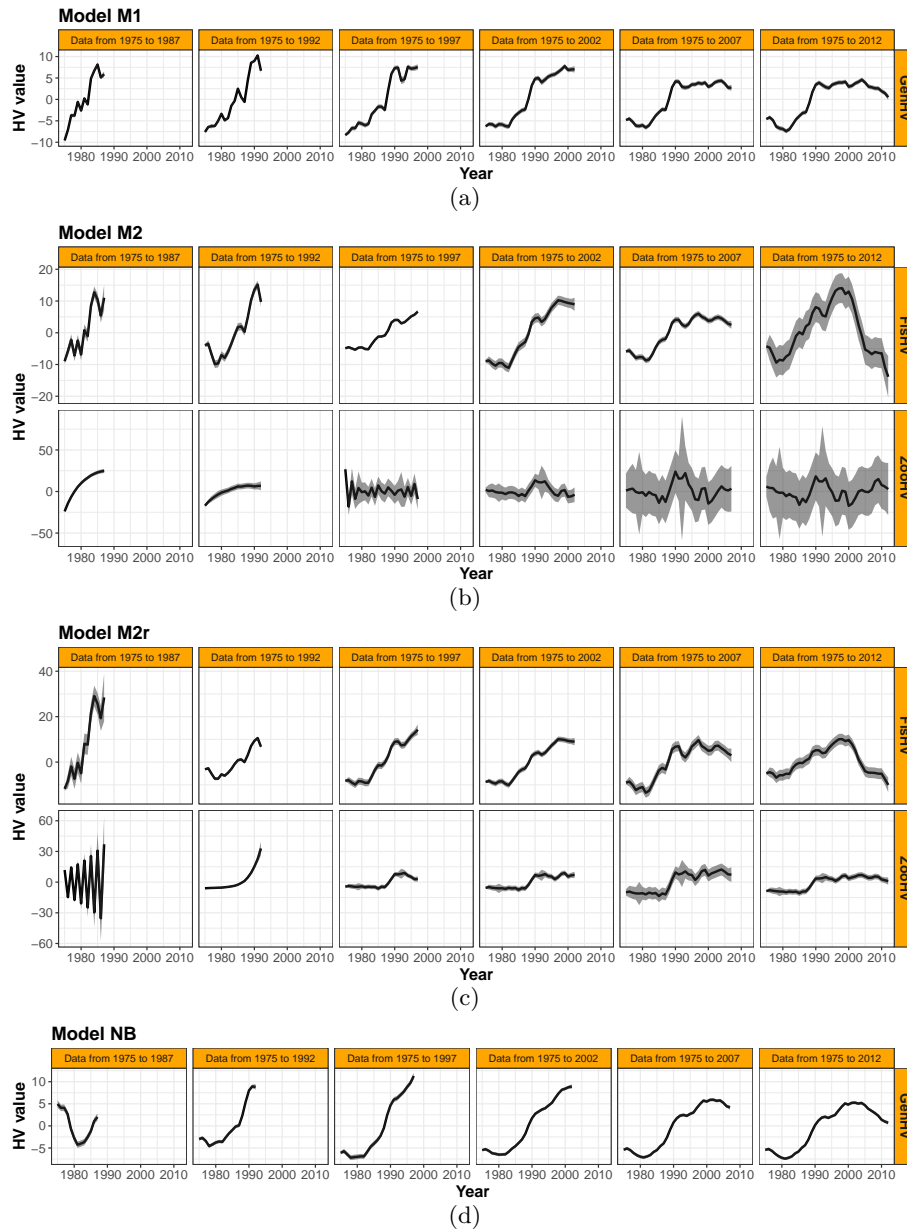


Figure 8: Evolution of the expected value of the hidden variables, increasing the size of the training set by five. Fold 1: *Data from 1975 to 1987*; Fold 2: *Data from 1975 to 1992*; Fold 3: *Data from 1975 to 1997*; Fold 4: *Data from 1975 to 2002*; Fold 5: *Data from 1975 to 2007*; Fold 6: *Data from 1975 to 2012*.

342 *3.1.1. Approach comparison of regime shift*

343 The comparison of regime shift detection between the EM algorithm and the  
344 fully Bayesian approach can be seen in [Figure 9](#). Each individual plot shows  
345 the observed variable of interest (i.e., the *class* variable in the model) and the  
346 expected value of the hidden variable  $H$  following the EM ( $H_{EM}$ ) and Bayesian  
347 ( $H_B$ ) approaches.

348 In general, the Bayesian approach picks up the changes in the observed vari-  
349 ables at the end of the time series. The main reason for this peculiar performance  
350 is the lack of data (it should be kept in mind that our dataset consists of only  
351 38 data points), i.e., what we see at the beginning of the time series is the flat  
352 prior, which rules out the data likelihood until sufficient data is explored. On  
353 the other hand, the EM approach captures the trend of the observed variables  
354 earlier than the Bayesian. It can be seen that  $H_{EM}$  picks up the pattern of the  
355 observed variable acting as the *class*, even when they are noisy, as in the case  
356 of Spr1y and Her1y.

357 In both approaches, a change can be seen near the year 2000 in all models,  
358 which coincides to the abrupt change seen in variable FisHV in models M2 and  
359 M2r ([Figures 8b](#) and [8c](#)) when the entire dataset is used to train the models (fold  
360 6). Moreover, for models where Spr1y and Her1y are the *class* variable,  $H_{EM}$   
361 shows a change near the year 1980, which coincides to the first drift identified  
362 in variable GenHV in models M1 and NB ([Figures 8a](#) and [8d](#)) when the entire  
363 dataset is used to train the models (Fold 6).

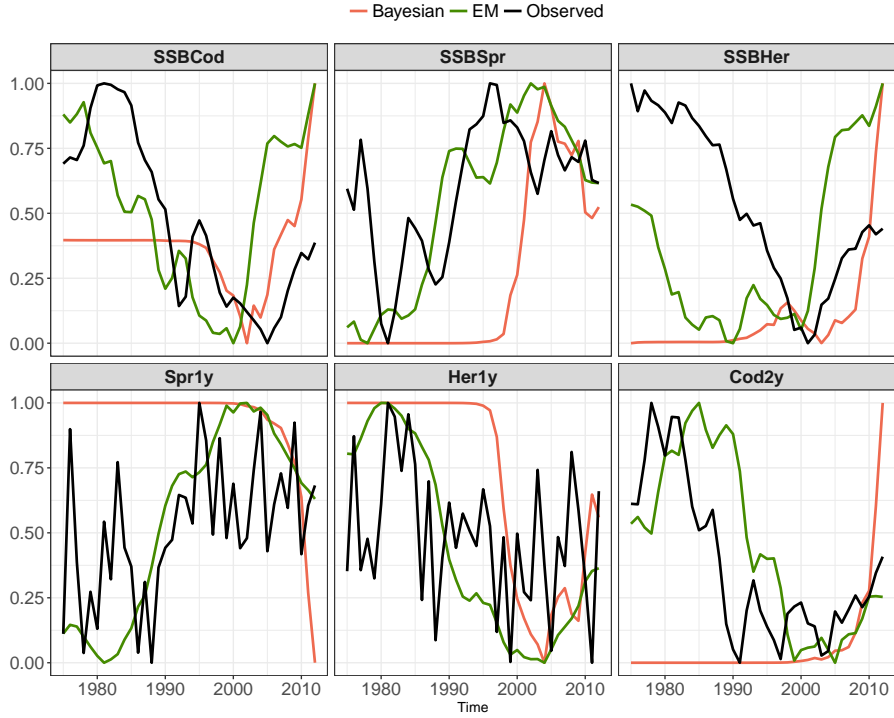


Figure 9: Evolution of the expected value of the hidden variable  $H$  for each model obtained as indicated in Section 2.5. The black line shows the observed data. For visual purposes, the data have been rescaled to interval  $[0,1]$ .

364 *3.2. Predictive performance*

365 The time series of the observed and predicted values for each variable of  
 366 interest, model and Fold of both cross-validation techniques are shown in Fig-  
 367 ures 14a to 14f in Appendix A. From these predictions, we computed the per-  
 368 formance of each model for each variable of interest in terms of its log-likelihood  
 369 (Figure 10b). Furthermore, for the rolling-origin case only, we performed some  
 370 hypothesis testing, which will be further discussed in the upcoming sections.

371 *3.2.1. Does the increase of data improve the performance of the models?*

372 In order to detect whether or not more data help to predict the variables of  
 373 interest, two cross-validation techniques were used to build the models: rolling-  
 374 origin (RO) and rolling-window (RW). Figure 10b shows the performance of

375 each model for each variable of interest in terms of log-likelihood. The results  
 376 show that most variables get improvements in their predictions when more data  
 377 are available to fit the models (p-value <0.05), i.e., when the rolling-origin tech-  
 378 nique is used. [Table 2](#) shows an overview of the hypothesis testing results. In  
 379 particular, variable SSBCod ([Figure 14a](#)) showed significant differences in all  
 380 models except the M2 model, with RO performing better than RW in all sig-  
 381 nificant cases; variable SSBSpr ([Figure 14b](#)) showed significant differences in 3  
 382 out of 5 models, with RO performing better than RW in models M0 and NB  
 383 and RW performing better in model M2r; variable SSBHer ([Figure 14c](#)) showed  
 384 significant differences in all models except the M0 model, with RO performing  
 385 better than RW in 3 out of the 4 significant cases (RW performed better in the  
 386 M2r model); variable Spr1y ([Figure 14d](#)) showed significant differences only in  
 387 the Naive Bayes (NB) model, with RO performing better than RW; variable  
 388 Her1y ([Figure 14e](#)) did not show significant differences in any model; and vari-  
 389 able Cod2y ([Figure 14f](#)) showed significant differences in all models except the  
 390 NB, with RO performing better than RW in all significant cases.

Table 2: An overview of the results of the hypothesis testing of the difference between the  
 rolling-origin (RO) and rolling-window (RW) cross-validation techniques. For each variable of  
 interest, the number of models that present 1) no statistically significant difference in terms  
 of log-likelihood, 2) improvements when more data are available (RO), or 3) improvements  
 when old data are dropped (RW), is shown.

	No differences	RO better	RW better
SSBCod	1	4	0
SSBSpr	2	2	1
SSBHer	1	3	1
Spr1y	4	1	0
Her1y	5	0	0
Cod2y	1	4	0

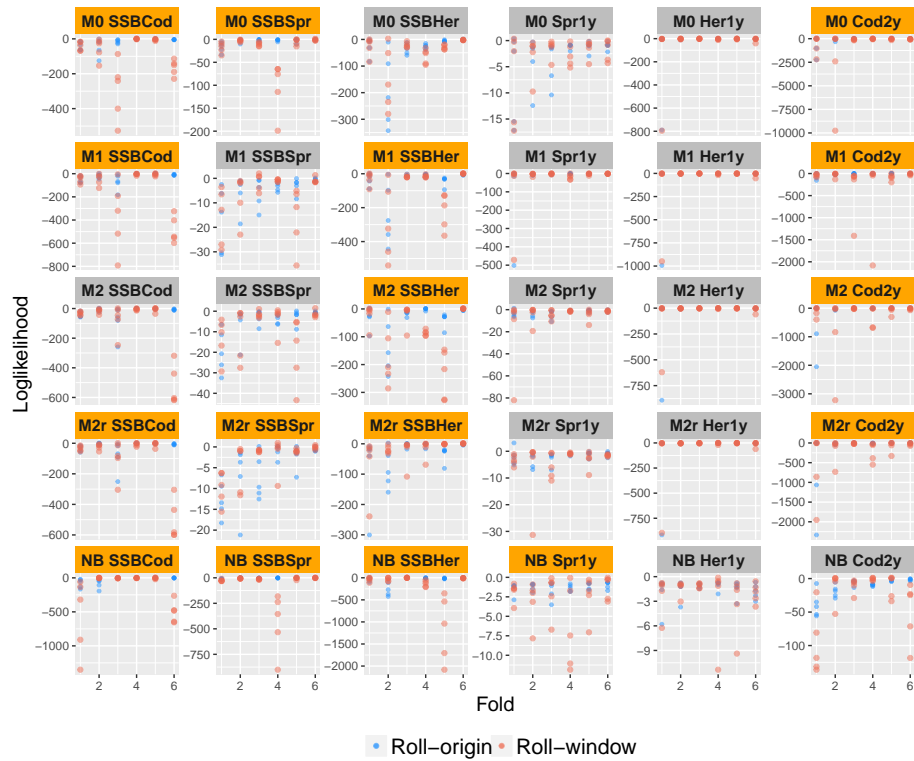
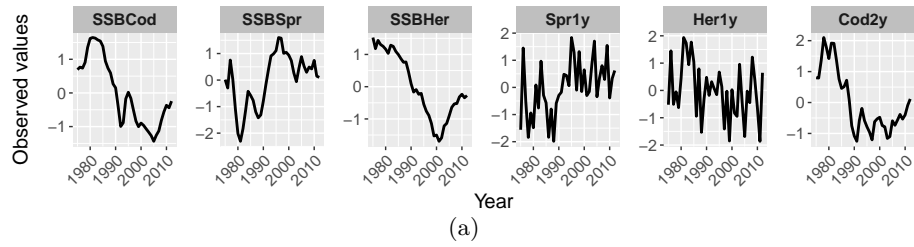


Figure 10: Log-transformed values of the observed variables of interest (a) and log-likelihoods of the predictions obtained from the rolling-origin and rolling-window validation techniques (b). The pairs rolling-origin - rolling-window of each variable and model version were compared using the Wilcoxon signed rank test. Orange labels indicate that the hypothesis test detected significant differences ( $p\text{-value} < 0.05$ ). Figure 10b is arranged so that the five models described in Sections 2.4.2 and 2.4.3 correspond to rows and the six different variables of interest correspond to columns.

391 *3.2.2. Does the introduction of HVs improve the performance of the models?*

392 In order to find out whether or not the introduction of hidden variables  
 393 improves the predictive performance, we compared the loglikelihood of the pre-  
 394 dictions of models M0, M1 and M2, with M0 being the model without hidden  
 395 variables; M1 the model with one generic hidden variable; and M2 the model  
 396 with two hidden variables. We used the Friedman Test to carry out the compar-  
 397 ison. Figure 11 shows the boxplot of the differences between pairs of models.  
 398 Boxplots outlined with color orange indicate that significant differences were  
 399 found between the corresponding pair of models. The results of the tests show  
 400 significant differences only for variables SSBHer and Cod2y, with models M1  
 401 and M2 outperforming model M0 in the case of Cod2y, whereas model M2  
 402 outperformed model M1 in the case of SSBHer.

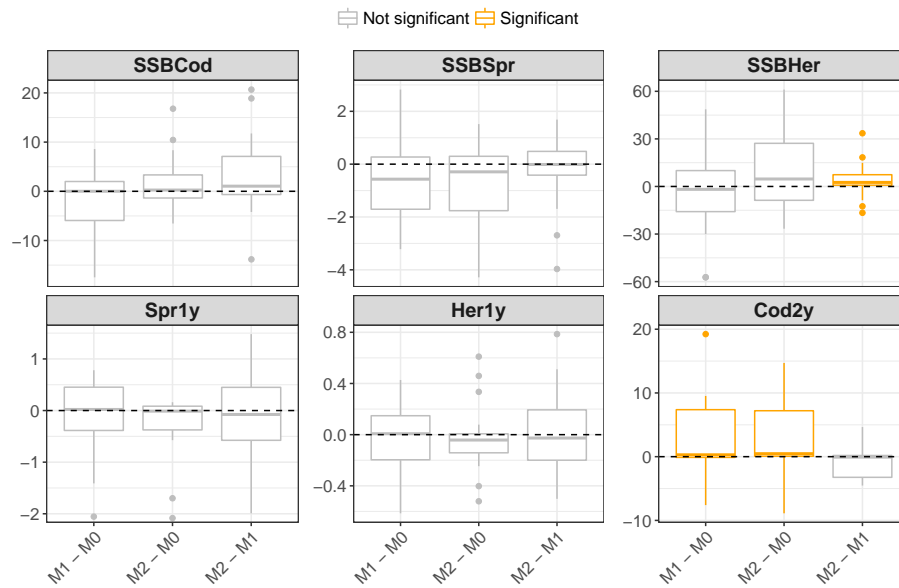


Figure 11: Boxplots of the differences in model performance. Orange outlined boxes indicates that the post-hoc analysis carried out after Friedman test detected statistical significant differences ( $p$ -value  $< 0.05$ ) between the corresponding models. Note that extreme outliers have been removed from the plot.



403 *3.2.3. Does reversing some links improve the performance of the models?*

404 In order to test whether or not reversing the links between variables SSBHer  
 405 and SSBSpr and the zooplankton variables would make any difference in the  
 406 models' prediction, we compared the loglikelihoods of the predictions of models  
 407 M2 and M2r using the Wilcoxon Signed Rank test. Figure 12 shows the boxplots  
 408 of the differences between the pairs of models, for each variable of interest. The  
 409 results of the tests show significant differences only for variables SSBHer and  
 410 Spr1y, with model M2r outperforming model M2 in both cases.

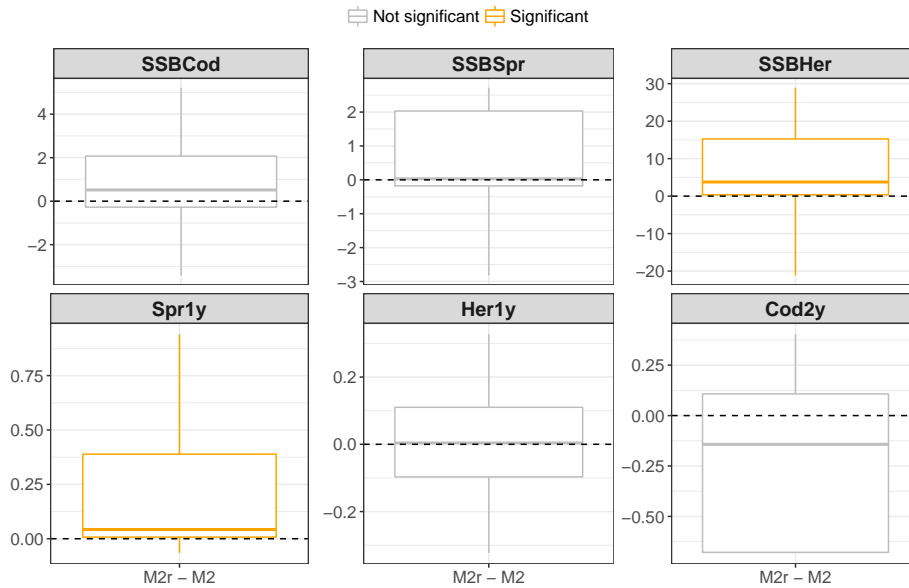


Figure 12: Boxplots of the differences in model performance. Orange outlined boxes indicates that the Wilcoxon Signed Rank test detected statistical significant differences ( $p$ -value  $< 0.05$ ) between the corresponding models. Note that extreme outliers have been removed from the plot.

411 *3.2.4. Does the use of expert-based structures improve the performance of the*  
 412 *models?*

413 In order to test whether or not expert-based structures outperform simpler  
 414 models, such as Naive Bayes, we compared each expert-based model (M0, M1,  
 415 M2, and M2r) with the Naive Bayes (NB) model using the Wilcoxon Signed

416 Rank test. Figure 13 shows the boxplots of the differences between the pairs of  
 417 models, for each variable of interest. The results of the tests show significant  
 418 differences for models SSBSpr, Spr1y, Her1y and Cod2y. In most cases, NB  
 419 outperformed the expert-based models. On the other hand, for variable Cod2y,  
 420 the expert-based models outperformed the NB model, except in the case of the  
 421 pair M0-NB, where no significant differences were found.

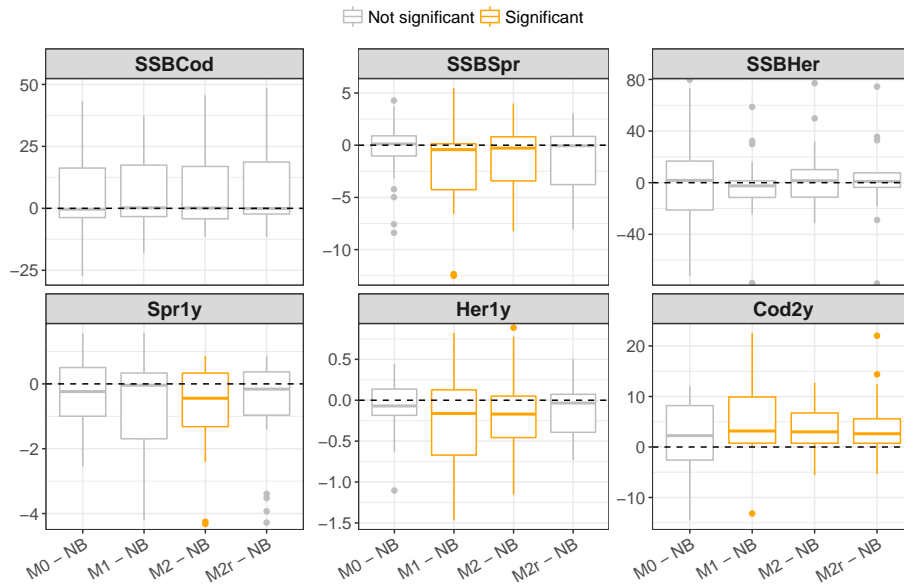


Figure 13: Boxplots of the differences in model performance. Orange outlined boxes indicates that the Wilcoxon Signed Rank test detected statistical significant differences ( $p$ -value  $< 0.05$ ) between the corresponding models. Note that extreme outliers have been removed from the plot.

#### 422 4. Discussion

423 In this paper we have analyzed the Baltic Sea food web aiming at 1) detecting  
 424 changes in its pattern and 2) making reliable predictions on some variables of  
 425 interest. The hidden variables called GenHV and FisHV (models M1, M2, M2r  
 426 and NB) showed a clear increase near the year 1980, with the former occurring  
 427 slightly later. Variable ZooHV (model M2r) shows an abrupt jump, which is

428 delayed in comparison to the increase of the two other HVs.

429       Former studies have found that the Baltic Sea has undergone several periods  
430 of change, with one of them being described in the 1980s [36]. Many publications  
431 have also described a regime shift in the North Sea in the late 80s [37, 38, 39, 40],  
432 which is connected to the Baltic Sea through the Danish Straits, where water  
433 exchange between the two areas occurs. According to the suggestion of some  
434 authors, this regime shift may have been partly caused as a response to a change  
435 of the North Atlantic Oscillation (NAO) in winter [5], which led to an increase in  
436 the winter and early spring air and water temperature. NAO-induced changes,  
437 along with overfishing of cod, triggered a regime shift [36], leading to a period  
438 dominated by clupeids, i.e., sprat and herring [4], after 1990.

439       The regime shift described in the literature coincides with the changes ob-  
440 served in variable ZooHV (in model M2r). This is in line with the research  
441 by [5], where they describe that the abundance of zooplankton varied in accor-  
442 dance with the variations in the NAO. Therefore, it seems reasonable that the  
443 model reflects these variations in the NAO. On the other hand, variable FisHV  
444 (in model M2 and M2r) shows an increase from the beginning of the 1980s till  
445 the beginning of the 2000s, when its tendency drastically changes, towards a  
446 decreasing trend. This hidden variable is linked to 14 fish-related variables;  
447 therefore the hidden variable is trying to capture the global trend of all these  
448 variables. The FisHV could be partly reflecting the indirect change of zooplank-  
449 ton (as they partly predate on those) and partly the change in the large anoxic  
450 area [41] along with the clupeid-dominated period. Variable GenHV (models  
451 M1 and NB) shows a gradual increase from the beginning of the 1980s till 1990,  
452 where a constant period begins. The behavior of this hidden variable could be  
453 reflecting the underlying dynamic of the zooplankton and fish variables, as a  
454 whole, but more research is needed.

455       From the predictive accuracy point of view, significant differences among  
456 the models were scarcely found. In particular, the similar results for the expert-  
457 based models could be regarded as a positive finding in the sense that as long  
458 as the model structure is coherent, the details will not make a critical difference

459 in the predictions. When significant differences are found, our results suggest  
460 that models with a higher number of hidden variables are not outperformed  
461 (Section 3.2.2). Moreover, reversing some links increased the predictive accu-  
462 racy of two variables only, with the remaining variables not showing statistically  
463 significant differences (Section 3.2.3). Finally, the use of simple models, such  
464 as the Naive Bayes, helped with the prediction of some variables, compared  
465 to more complex models based on expert elicitation (Section 3.2.4). The rea-  
466 son for that is that simple models need to estimate fewer parameters, which is  
467 very convenient when few data are available. On the other hand, improvements  
468 were found rather often when comparing the rolling-origin and rolling-window  
469 approaches. In most of the significant cases, having more data improved the  
470 prediction of the outcomes.

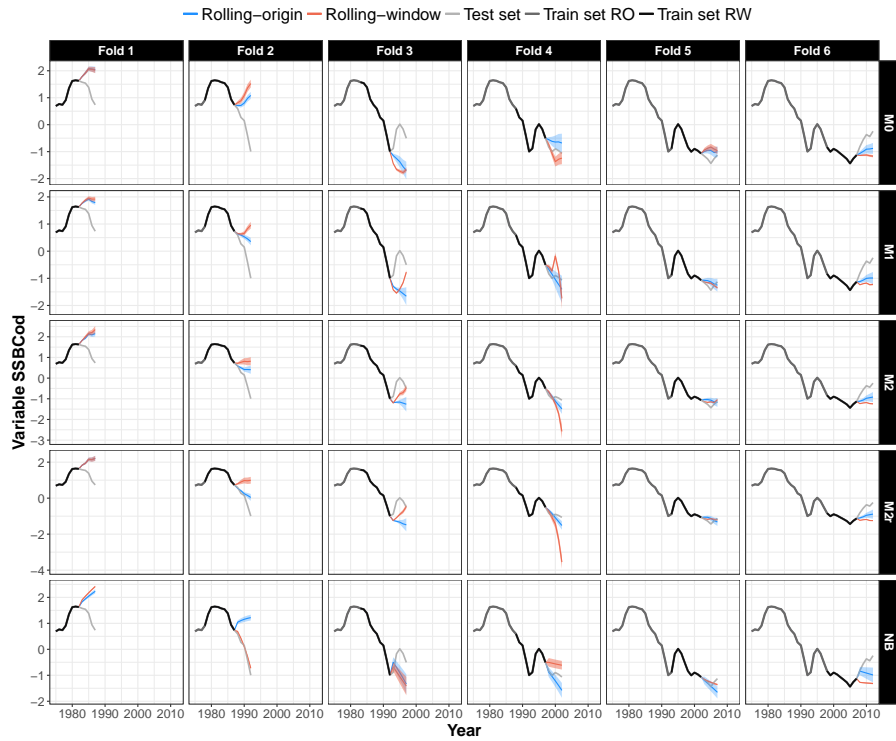
## 471 5. Conclusions

472 The methodology proposed in this paper managed to identify a major regime  
473 shift that occurred in the Baltic Sea during the 1980s. The DBN methodology  
474 can identify changes in ecosystems where only limited data are available, which  
475 is an additional difficulty to cope with. Not surprisingly, the increase in data  
476 size improved the models' predictions. Some systems understanding is needed  
477 to construct the model structure, but the present experiments show that the  
478 exact model setup does not make a critical difference to the results, from the  
479 predictive accuracy point of view. However, the use of different HV setups  
480 helped reveal changes in the different parts of the ecosystem. Therefore, the  
481 presented approach can be a highly useful tool in the study of potentially critical  
482 changes in complex ecological interactions.

## 483 Appendix A Model predictions

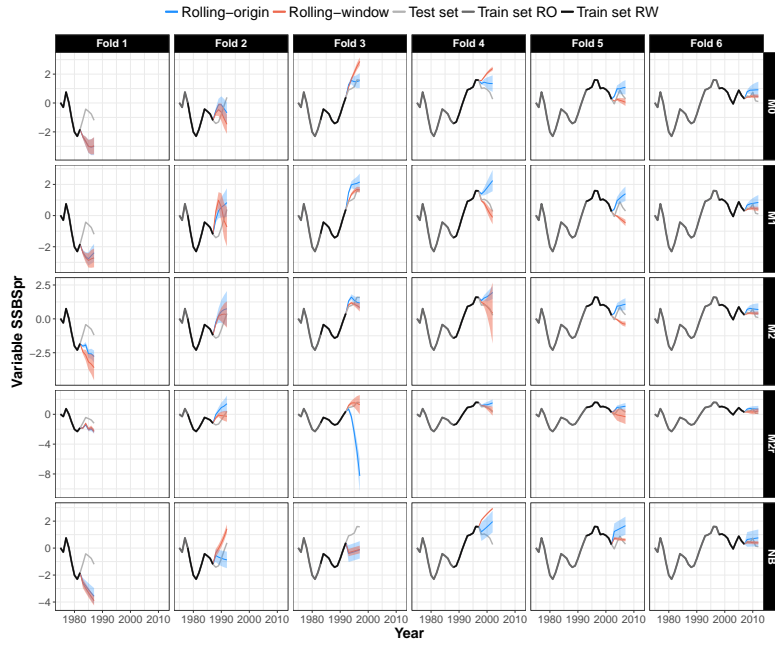
484 The time series of the observed and predicted values for each variable of  
485 interest, model and Fold of both cross-validation techniques are shown in Fig-  
486 ures 14a to 14f. From these predictions, we computed the performance of each

487 model (in terms of log-likelihood) for each variable of interest (Figure 10b). Fur-  
 488 thermore, for the rolling-origin case only, we performed some hypothesis testing  
 489 to compare the predictive performance of the different models (Figures 11 to 13).

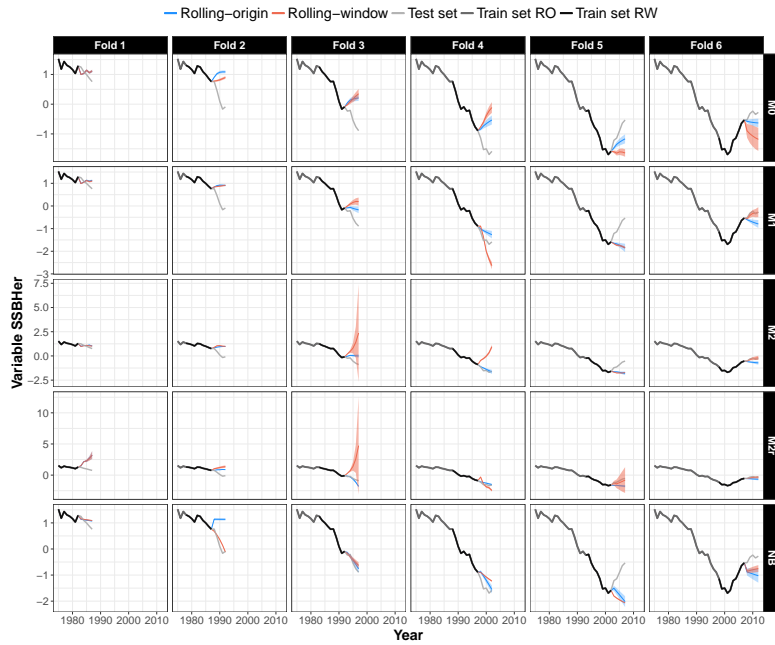


(a) Model predictions for variable SSBCod.

Figure 14: Model predictions (expected value) and observed values used to fit the models, following the rolling-origin (RO) and rolling-window (RW) cross-validation techniques as shown in Figure 7. Black, dark gray and light gray lines correspond to data belonging to the train set of the RW approach, train set of the RO approach and test set, respectively. Red and blue lines correspond to the predictions obtained following the RW and RO techniques, respectively. The shaded bands correspond to the standard deviation.

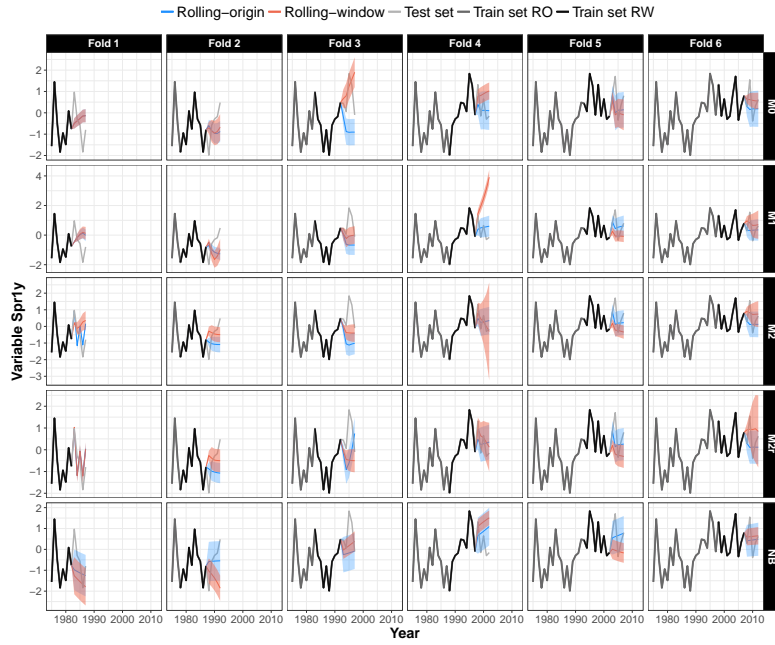


(b) Model predictions for variable SSBSpr.

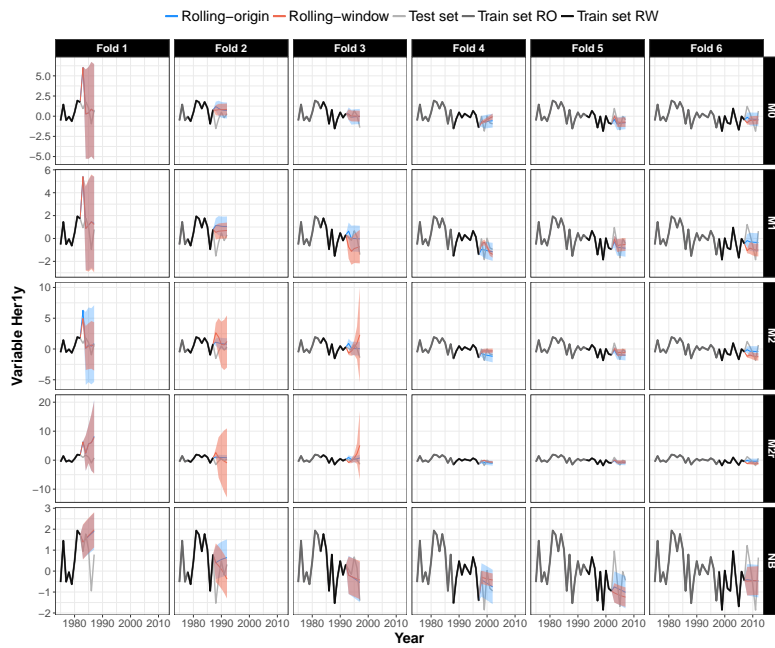


(c) Model predictions for variable SSBHer.

Figure 14: (Cont.) Model predictions and observed values.

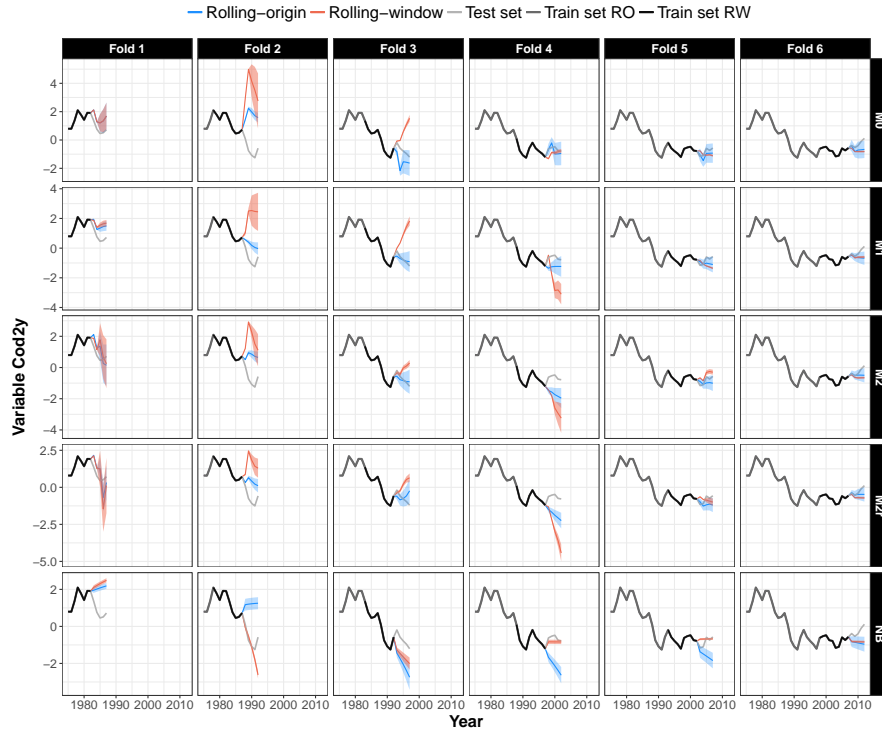


(d) Model predictions for variable Spr1y.



(e) Model predictions for variable Herfy.

Figure 14: (Cont.) Model predictions and observed values.



(f) Model predictions for variable Cod2y.

Figure 14: (Cont.) Model predictions and observed values.

## 490 Appendix B Code

491 The code necessary to run the experiments is available as *Supplementary*  
 492 *material*. In particular, *Supplementary material* contains two `.m` files with the  
 493 MATLAB code, one `.tar.gz` file with the `ramidst` R package, and four files con-  
 494 taining simulated data (three `.csv` and one `.arff`). As the real dataset used in  
 495 this work is protected and cannot be published, we provide simulated data to  
 496 run the code.

497 Most of the experiments carried out in this work were performed using the  
 498 Bayes Net Toolbox (BNT) package in MATLAB. We have created a wrapper  
 499 function, `DBN_foodWebModel`, to reproduce our experiments. We provide some  
 500 examples of how to use this function for the simulated dataset. The results of



501 running this function are stored in .txt files. On the one hand, the expected  
502 value of the hidden variables can be obtained by running the following piece of  
503 code:

```
504 %% ARGUMENTS OF THE DBN_foodWeb FUNCTION:
505 % 1. the csv file
506 % 2. the number of HVs
507 % 3. the goal: 'learning' or 'inference'
508 % 4. the core structure: 'normal', 'reverse', 'NB'
509 % 5. the model version: 'M0', 'M1', 'M2', 'M2r'.
510 % 6. the number of years we want to predict
511 % OPTIONAL ARGUMENTS
512 % CV. Type of cross-validation: 'rol-wind' or 'rol-org'
513
514 %% COMPUTE EXPECTED VALUE OF HIDDEN VARIABLES
515 % Model M1
516 DBN_foodWeb('simulated.csv', 1, 'learning','normal', 'M1', 0, ...
517             'CV','rol-org');
518
519 % Model M2
520 DBN_foodWeb('simulated.csv', 2, 'learning','normal', 'M2', 0, ...
521             'CV','rol-org');
522
523 % Model M2r
524 DBN_foodWeb('simulated_rev.csv', 2, 'learning','reverse', 'M2r', 0, ...
525             'CV','rol-org');
526
527 % Model NB
528 DBN_foodWeb('simulated_NB.csv', 1, 'learning','NB', 'M1', 0, ...
529             'CV','rol-org');
```

530 On the other hand, the predictions of the target variables can be obtained  
531 running the following piece of code:

```
532 %% RUN PREDICTIONS
```

```

533 % Rolling-origin
534 % Model M0
535 DBN_foodWeb('simulated.csv', 0, 'inference', 'normal', 'M0', 5, ...
536             'CV', 'rol-org');
537
538 % Model M1
539 DBN_foodWeb('simulated.csv', 1, 'inference', 'normal', 'M1', 5, ...
540             'CV', 'rol-org');
541
542 %Model M2
543 DBN_foodWeb('simulated.csv', 2, 'inference', 'normal', 'M2', 5, ...
544             'CV', 'rol-org');
545
546 % Model M2r
547 DBN_foodWeb('simulated_rev.csv', 2, 'inference', 'reverse', 'M2r', 5, ...
548             'CV', 'rol-org');
549
550 % Model NB
551 DBN_foodWeb('simulated_NB.csv', 1, 'inference', 'NB', 'M1', 5, ...
552             'CV', 'rol-org');

```

553 Note that the given examples provide the predictions for the rolling-origin case;
554 to obtain the results for the rolling-window approach, the argument 'CV' must
555 be changed from 'rol-org' to 'rol-wind'. Also, note that it is not necessary to spec-
556 ify which are the target variables since the function is specifically programmed
557 to return the values of these variables. Nevertheless, this function can be easily
558 adapted to other datasets and model structures.

559 To compare the variational Bayes and the EM algorithms (for the regime
560 shift detection), we used the `ramidst` R package and the `BNT` MATLAB package.
561 We have created another wrapper function, `NBCDD`, for the experiments carried
562 out in `MATLAB`. An example of how to use this function is provided. To illustrate
563 the example, variable `Cod2y` is used as the class variable. Note that we computed
564 the expected value of the hidden variable (H) for 6 different models, i. e., using

565 6 different class variables.

```
566 %% ARGUMENTS OF THE NBCDD FUNCTION:
567 % 1. the class variable: 'SSBCod', 'SSBSpr', 'SSBHer',
568 %   'Spr1y', 'Her1y', 'Cod2y'
569 % 2. the csv file
570 % 3. the first row to read in the dataset
571 % 4. the last row to read in the dataset
572
573 % An example is given for variable 'Cod2y'
574 NBCDD('Cod2y', 'simulated_NB.csv', 1, 38)
```

575 An example of how to use the `nb_concept_drift_detector_from_stream`  
576 function of `ramidst` R package is also provided.

```
577 # Import dataset in .arff format
578 df <- amidst_data_stream("simulated_NB.arff")
579
580 # Specify the window size and position of the class variable
581 # in the dataset (starting from 0).
582 # For instance, variable Cod2y is the variable in position 15.
583 w_size = 1L
584 class_var = 15L
585 results <- nb_concept_drift_detector_from_stream(df,
586         class_index = class_var,
587         window_size = w_size)
588
589 # 'results' is a list containing the expected value of the hidden
590 # variable (H), when variable Cod2y is chosen as the class
591 # variable in the naive Bayes structure.
```

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