

Supplementary Materials to *Early Warning Signals of Complex Critical Transitions in Deterministic Dynamics*

S1.1 Methods

S1.1.1 Regime boundary detection algorithm

In order to determine where regimes such as a chaotic regime end and start, the periodicity of the time series needs to be determined for each value of the bifurcation parameter. Ideally, the exact moment of transition is found analytically, yet for complex bifurcations whose timing depends sensitively on the initial condition and rate of parameter change, this is not possible [1]. We thus resort to numerical methods.

Given that most EWS studies into complex bifurcations rely on only one or a few simulations [2–4], no systematic way of finding regime boundaries seems to be used in the literature. For some bifurcations, it is possible to find the critical transition point analytically, but this will not correspond to the simulated transition under intrinsic noise. Empirical studies into transitions may rely on change point analysis [5, 6], which detects a shift in statistical properties such as the mean or variance. Though this may work well for simple bifurcations, these methods are not well suited for complex bifurcations, where the difference between regimes may be subtle (e.g. period-doubling bifurcations) and differences within the regime are substantial. Given the lack of guidance in the literature, we thus developed our own algorithm for detecting regime boundaries.

Algorithm 1: Regime boundary detection

Data: Time series with step-wise changes in bifurcation parameter range s

Result: Regime boundaries

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1 Find peaks and troughs in time series
2 for each step  $s_i$  in the bifurcation parameter range  $s$  do
3   Get peaks and troughs  $p = p_j, \dots, p_N$  corresponding to step  $s_i$ 
4   for period  $k = 1, \dots, K$  do
5     Group  $p$  according to group indices  $g = j \bmod k$  with  $j = 1, \dots, N$ 
6     Compute Euclidean distance  $D_j = \|p_j\|$  for each group  $g_j$ 
7     Set fit  $f_k$  as maximum distance  $\max(D)$  across groups
8   end
9   if Distance between fits is less than  $\delta_{node}$  then
10    Set behaviour as node
11  else
12    Choose best  $k$  based on best fit  $f^*$  weighted by  $\delta_k$ 
13    if Best fit  $f^* > \delta_{ampl}$  &  $f^* > \delta_{idx}$  then
14      Set behaviour as chaotic
15    else
16      Set behaviour as period  $k$ 
17    end
18  end
19 end
20 Smooth over exceptions in behaviour ( $\delta_{smooth}$ )
21 Flag steps which touch basin boundary  $[x_{min}, x_{max}]$ 
22 Flag chaotic behaviour where the spread of peaks and troughs covers an area larger than  $\delta_{band}$ 
23 Find regimes by grouping consecutive sequences in behaviour which are of length  $l \geq \delta_l$ 

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Rather than analysing the complete time series, a more efficient method finds the periodicity by using the amplitude and timing of the time series' peaks and troughs [7]. A first intuitive approach to finding the time series' periodicity may be to count the number of distinct peak coordinates using a histogram. However, this only works for simple oscillations with clearly separable peak coordinates which do not repeat. For instance, an oscillation with a pattern $[a, b, a, c]$ is not the same as $[a, b, c]$, yet a histogram will depict both as a period-3 oscillation. The order of the peaks thus needs to be included to accurately identify the period, which a histogram discards.

Incorporating a temporal aspect, a second approach to determining periodicity may be to find peaks in the autocorrelation function. However, repeated peak coordinates in the oscillation again make such an approach difficult. The first local maximum in the autocorrelation does not correspond to the period in patterns such as $[a, b, a, c]$, where the autocorrelation will peak at lag 2 and more strongly at lag 4. Oscillations with a long period and subtle differences between peak amplitudes are again difficult to pick up.

The present paper used a third, more computationally expensive approach because of its greater accuracy over the former two approaches. The period k was determined by assessing which k had the best fit when the peaks and troughs are partitioned according to their position in the period. For instance, to test whether the time series is of period $k = 3$, its peaks and troughs y_i are grouped using $i \bmod k$, resulting in a grouping sequence $g = 1, 2, 3, 1, 2, 3, \dots$ which correspond to indices in an oscillation of period $k = 3$ (algorithm 1, line 5). For each group g , the (Euclidean) distance between peaks is computed (algorithm 1, line 6). If the time series is indeed period-3, the distance for all groups $y_{g=1}, y_{g=2}, y_{g=3}$ should be minimal. The maximum distance across groups is taken as an indicator of fit (algorithm 1, line 7), such that the best fit (i.e. the smallest maximum distance) across all $k = 1, \dots, K$ yields the period of the signal. This procedure can be completed for both the amplitudes of the peaks and troughs (i.e. coordinates) as well as their timing (i.e. indices).

Completing this procedure for all time series per step in the bifurcation parameter gives the evolving order of periodicity across the bifurcation range. Some parameters were added to account for several weaknesses. Firstly, a time series was identified as a node if all fits were the same within some margin of error δ_{node} (algorithm 1, line 10). Secondly, as multiples of the true period will lead to a better fit simply because each group g will have fewer peaks resulting in smaller distances, a penalty δ_k is added for higher k (algorithm 1, line 12). This ensures that a higher k needs to result in a better fit than lower k . Thirdly, as the algorithm will always find a best-fitting k even when the time series is chaotic, behaviour was defined as chaotic if the best fit exceeded the maximum thresholds $\delta_{\text{ampl}}, \delta_{\text{idx}}$ for the allowed maximum distance in the amplitude and timing of the peak (algorithm 1, line 13). Finally, the maximum period K to look for is defined as the maximum period which still repeats at least once given the length of the time series N : $K = \text{floor}(N/2)$.

To add more granularity to the regimes, we distinguish between regimes which touch the basin boundary and those that do not, as well as between different types of chaos. More fine-grained behaviours help to identify more critical transitions. To help detect boundary crises, the algorithm flags time series of which a chosen variable reaches a specified minimum x_{min} and maximum x_{max} (algorithm 1, line 21). These correspond to the edges of the basin that are touched right before a boundary crisis happens, which are $x_{\text{min}} = 0$ and $x_{\text{max}} = 1$ for variable x_1 and x_2 , in our case. Secondly, to help detect interior crises, the algorithm separates chaotic time series that have well separated chaotic bands and those that cover the entire area between the lowest and highest value (δ_{band} , algorithm 1, line 22).

The result of this procedure yields the type of behaviour corresponding to each step in the bifurcation parameter. To finally identify regime boundaries across the parameter range, we defined regimes as a consecutive sequence of the same behaviour of a minimal length δ_l which may be interrupted by behaviours of length less than δ_l (algorithm 1, line 23). This ensured that brief outliers given some flaws in the algorithm or the parameter settings were not seen as transition points, which may also be smoothed using δ_{smooth} (algorithm 1, line 20). Though the algorithm of course has its weaknesses (e.g. too high periodicity is classified as chaos if only short time series are available), it detected regime boundaries quite well as

assessed visually (Supplementary Figures S2-S4). Even for limit cycles with growing amplitude across the bifurcation range, in which case peak coordinates do not match, the algorithm identified the whole stretch as belonging to the same cycle.

S1.1.2 Simulation details

Default parameter settings for the regime boundary detection algorithm which yielded good performance as found via experimentation may be found in Table S1. Some deviations from the defaults needed to be made in order to either obtain the desired type of critical transition, or simply to save computational power and storage space (Table S2). For instance, as the default method was not able to generate a

Table S1 Default parameter settings of regime boundary detection algorithm

Parameter	Default value	Meaning
δ_k	.1	Penalty term to fit for higher k
δ_{smooth}	0	Number of steps in bifurcation parameter to smooth regimes over
δ_{node}	.001	Maximum difference between fit for each k below which time series is classified as a node
δ_{ampl}	.025	Distance between peak amplitudes above which time series is classified as chaotic
δ_{idx}	2	Distance between peak indices above which time series is classified as chaotic
δ_{band}	.7	Maximum percentage of area covered between minimum and maximum value to be flagged as separated (cf. merged) chaotic bands
δ_l	5	Minimum length for a consecutive sequence of the same behaviour to be classified as a regime
x_{min}	0	Minimum edge of basin boundary
x_{max}	1	Maximum edge of basin boundary

Table S2 Details of simulation parameters per bifurcation

s	Δ_s	Bifurcation	Changes to default settings
[1.15, .9]	-.0001	Saddle-node	$\delta_k = 1; T = 100; N_{\text{noise}} = 250; N_{\text{sim}} = 1$
[.6, .85]	.001	Hopf (Period 1 to 2)	$\delta_k = 1; T = 200; N_{\text{noise}} = 250; N_{\text{sim}} = 1$
[.85, .985]	.0001	Period 2 to 4	$\delta_l = 8$
		Period 4 to 8	
		Period 8 to 16	
		Mixed-Periodic to Chaotic	
[.985, .8]	-.0001	Chaotic to Mixed-Periodic	$\delta_k = .01; \delta_{\text{ampl}} = .01$
		Period 16 to 8	
		Period 8 to 4	
		Period 4 to 2	
		Reverse Hopf (Period 2 to 1)	
[1.01, 1.02]	.00005	Interior crisis: chaos expansion	$\delta_{\text{smooth}} = 5; \delta_l = 1$
[1.03, 1.01]	-.0001	Interior crisis: chaos reduction	$\delta_k = 1; \delta_{\text{smooth}} = 10; \delta_{\text{ampl}} = .01$
[1.1, 1.3]	.001	Boundary crisis	$\Delta_t = .1; \delta_l = 20; \delta_k = 1; \delta_{\text{ampl}} = .1; \text{Euler simulation}$

Algorithm 2: Data simulation and EWS analysis

Result: Performance as measured by AUC per EWS per bifurcation type

```
1 for each range  $s$  do
  // Simulate transition and null models and compute EWS
2 for each simulation in  $1 : N_{sim}$  do
3   Generate time series of a GLV forced through range  $s$ 
4   Apply regime boundary detection algorithm to find regime boundaries  $[s_1, s_2]$  and initial
     condition  $x_0$  of desired critical transitions
5   for each desired critical transition do
6     for transition and null model do
7       Generate time series using  $[s_1, s_2]$  and  $x_0$ 
8       for each downsampling frequency  $f_s$  do
9         for each observational noise intensity  $\sigma_{obs}$  do
10          for each noise iteration in  $1 : N_{noise}$  do
11            Distort time series by downsampling to  $f_s$  and adding observational
              noise  $\sigma_{obs}$ 
12            for each step in  $[s_1, s_2]$  do
13              Compute all EWS on distorted time series
14            end
15          end
16        end
17      end
18    end
19  end
20 end
  // Compute performance
21 for each desired critical transition do
22   for each metric in EWS do
23     for each downsampling frequency  $f_s$  do
24       for each observational noise intensity  $\sigma_{obs}$  do
25         Compute ROC curve by finding the number of false positives in null models
           and true positives in transition models for each critical cut-off value  $\sigma_{crit}$  until
           FPR = 0 and TPR = 0
26         Integrate ROC curve to obtain AUC
27         Find the optimal critical cut-off value  $\sigma_{crit}^*$  corresponding to the maximum
           Youden's  $J$  statistic,  $J = \text{TPR} - \text{FPR}$ 
28         Save warnings in transition models when setting  $\sigma_{crit}^*$ 
29       end
30     end
    // Summarise across conditions
31    Compute median timing of saved warning signals
32    Assess whether saved warnings either all fell above, all below, or both above and
      below the confidence band
33  end
34 end
35 end
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boundary crisis, the time step and solver were changed to $\Delta_t = .1$ and Euler integration only for this bifurcation type.

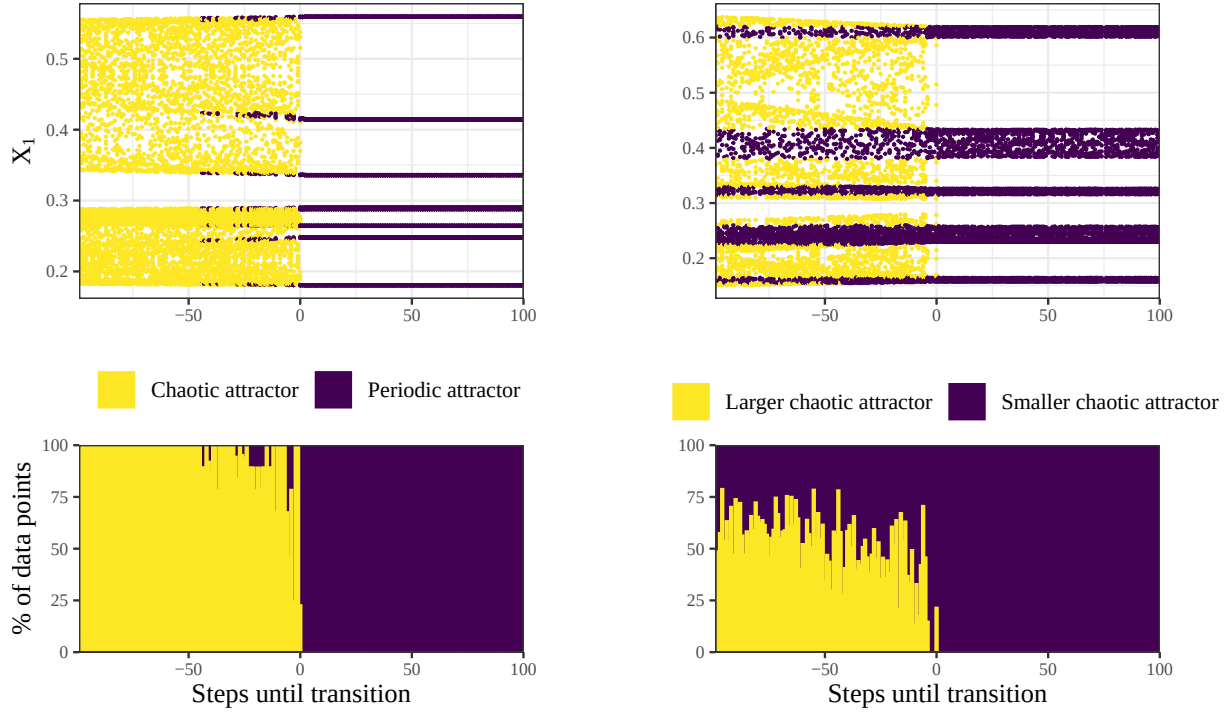


Fig. S1 Illustration of intermittency between a periodic and chaotic attractor (top, left panel), or between two chaotic attractors (top, right panel). The new attractor (purple, after the transition) is already embedded within the current attractor (yellow and purple, before the transition) before the bifurcation occurs. The time spent in the new attractor increases when approaching the bifurcation point (bottom panel), which could potentially be used as a warning signal

Note that in order to fairly evaluate which bifurcation types can be anticipated, we chose to have the same amount of data for each bifurcation. However, as some bifurcations are inherently faster than others (e.g. a period-4 to period-8 bifurcation is intrinsically shorter than a period-2 to period-4 bifurcation because of Feigenbaum’s constant), the step size Δ_s in the bifurcation parameter could not be held constant. That is, the transition and null models of each bifurcation type had the same number of steps in the bifurcation parameter, the same number of time points for each step, the same time step, and the same sampling frequency, but had different Δ_s .

S1.1.3 Chaotic features: Intermittency and transients

A typical feature within chaotic dynamics is *intermittency*: recurrent switches between two or more attractors. Intermittent switches may occur between a periodic and chaotic attractor (Supplementary Figure S1, left panel), or between two chaotic attractors (Supplementary Figure S1, right panel). Intermittency in a subduction is related to the traditional Pomeau–Manneville dynamics intermittency [8], whereas interior crises show crisis-induced intermittency [9].

Importantly, these intermittent switches change in character as a bifurcation point is approached (Supplementary Figure S1, bottom panel). For instance, the intermittency route to chaos contains short bursts of chaotic behaviour amidst regularity, which increase in length and frequency until the system fully occupies the chaotic attractor after the bifurcation point. Approached from the other direction, a dominant chaotic attractor may show brief bursts of regularity of increasing length and frequency as the bifurcation point is approached. Though the study of how these changes in intermittency express themselves in warning signs is beyond the scope of this paper, they offer a potential warning sign for chaotic bifurcations.

Similarly, another feature tied to transitional chaotic dynamics are *chaotic transients*. A chaotic transient is non-asymptotic behaviour where the system gets trapped in a remnant of the basin of attraction of the chaotic attractor that existed before the crisis occurred. It will trace an orbit much the like now extinguished chaotic attractor, before switching to another attractor [9–12]. Crucially, though, chaotic transients are typically found just *beyond* the bifurcation [13], as they commonly arise either from a ghost attractor or an unstable saddle (crawl-by transients) [13, 14]. As such, they would not help to anticipate the transition, yet are still highly relevant to understand critical transitions. Though dynamics are conventionally understood through attracting invariant sets, *non-attracting* invariant sets play an especially important part on non-asymptotic timescales. Chaotic transients may hinder the detection of the bifurcation, by mimicking the behaviour of the destroyed attractor, or may help to assess how far past the bifurcation point the system is, by the difference in duration of the transient [15, 16]. Factors such as skewed noise, multiple intrinsic time scales in slow-fast systems, and space and time delays in high-dimensional systems may create or lengthen long transients [13]. As only deterministic dynamics were considered here, transients could become much more relevant with the addition of state perturbations.

S1.2 Results

S1.2.1 Bifurcation diagrams

The bifurcation diagrams of the all variables for $s \in [.6, 1.3]$, $s \in [1.3, .6]$ (reverse order of s), and of the saddle-node bifurcation are shown in Figures S2-S4.

In complex systems such as the GLV, regions of the control parameter space may be *multistable*: differences in initial conditions can lead the system to converge to different attractors. As an illustration, Supplementary Figure S5 shows the GLV for $s \in [.96, .985]$ starting from three different initial conditions. Though these initial conditions converge to roughly the same bifurcation sequence, there are slight differences in the exact values of the control parameter at which these bifurcations occur. Some bifurcations may not happen at all. For example, the periodic windows interspersed in the chaotic regime do not occur for all conditions. Because of this dependence on initial conditions, we generated multiple realisations for each bifurcation type.

S1.2.2 Predictability of bifurcations

Performance per condition (downsampling frequency $f_s \in [10, 1, .1]$ and observational noise intensity $\sigma_{\text{obs}} \in [0.0001, .02, .04]$) for each critical transition is shown in Figures S6-S11. The direction of EWS when setting an optimal cut-off value σ_{crit}^* using Youden’s J statistic is shown in Figure S12. Finally, some examples of complex warning patterns are illustrated in Figure S13.

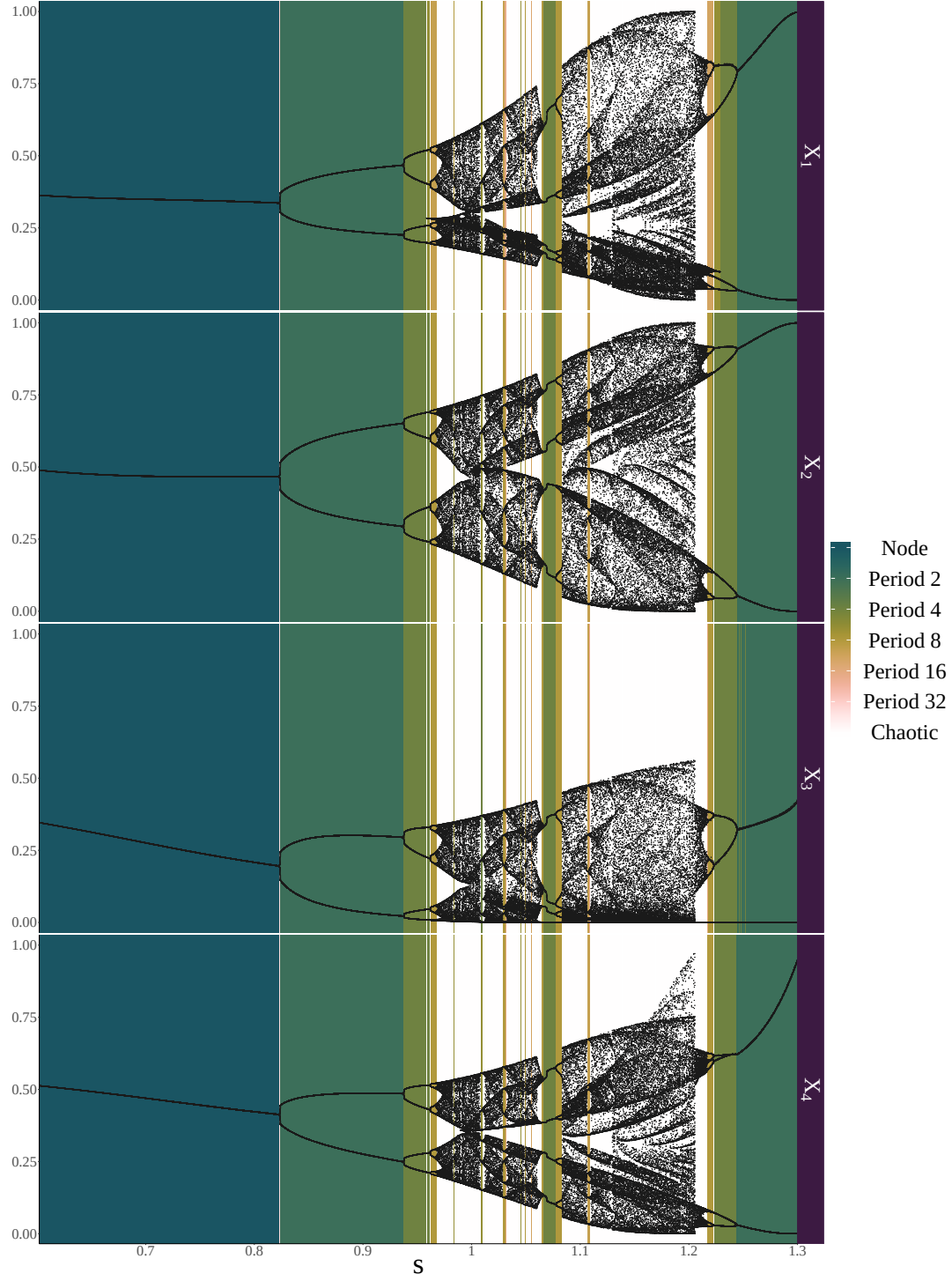


Fig. S2 Bifurcation diagram of all variables X_i in the Generalised Lotka-Volterra model, showing the sequence of transitions as the control parameter s is increased from $[.6, 1.3]$. For each step in s , the peaks and troughs (i.e. local minima and maxima) of the corresponding time series are shown as black points, corresponding to each value of the bifurcation parameter s (x-axis). Coloured bars indicate the periodicity of the time series as found using our regime boundary detection algorithm, where white indicates chaotic or transitioning regimes

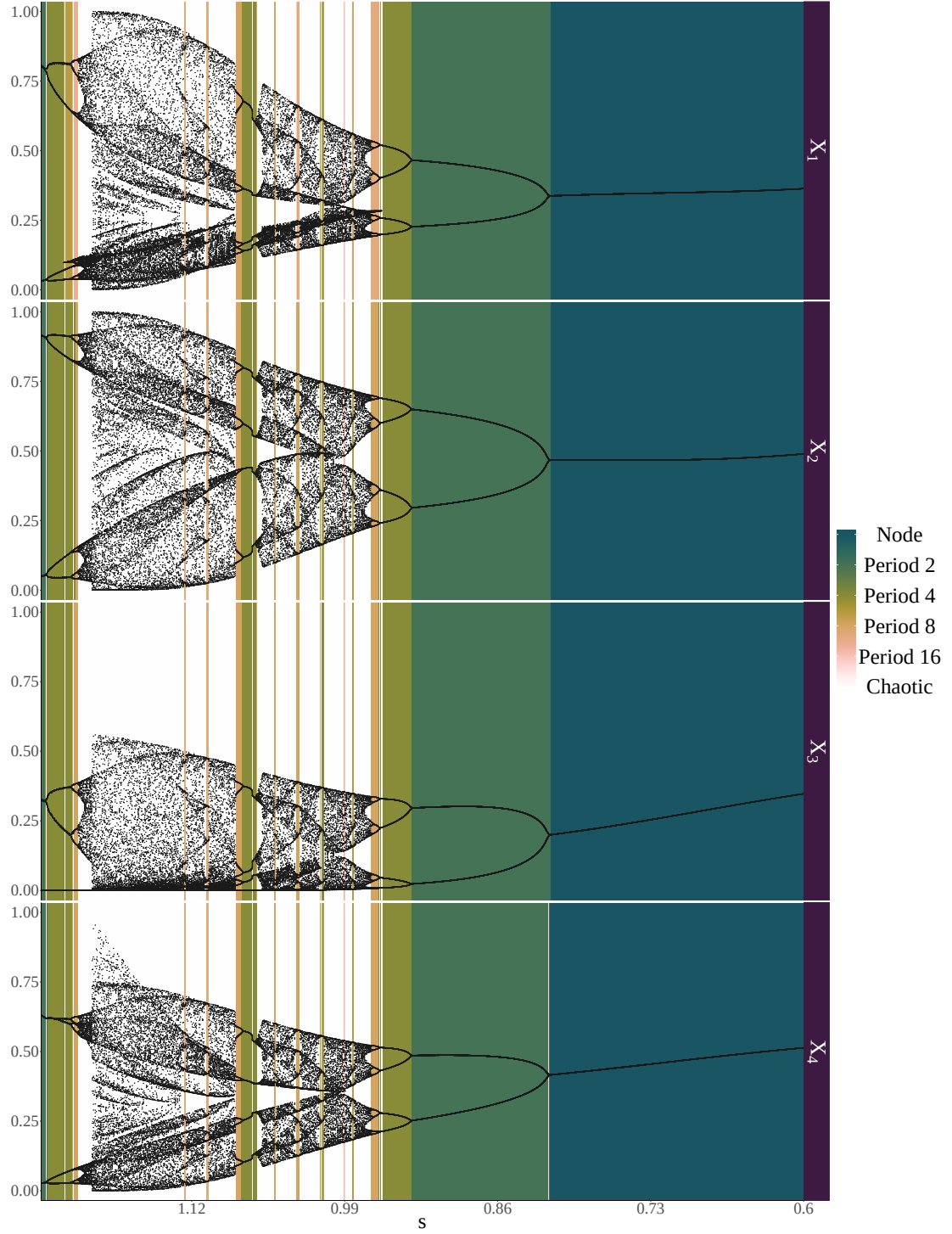


Fig. S3 Bifurcation diagram of all variables X_i in the Generalised Lotka-Volterra model, showing the sequence of transitions as the control parameter s is decreased from $[1.25, .6]$. For each step in s , the peaks and troughs (i.e. local minima and maxima) of the corresponding time series are shown as black points, corresponding to each value of the bifurcation parameter s (x-axis). Coloured bars indicate the periodicity of the time series as found using our regime boundary detection algorithm, where white indicates chaotic or transitioning regimes

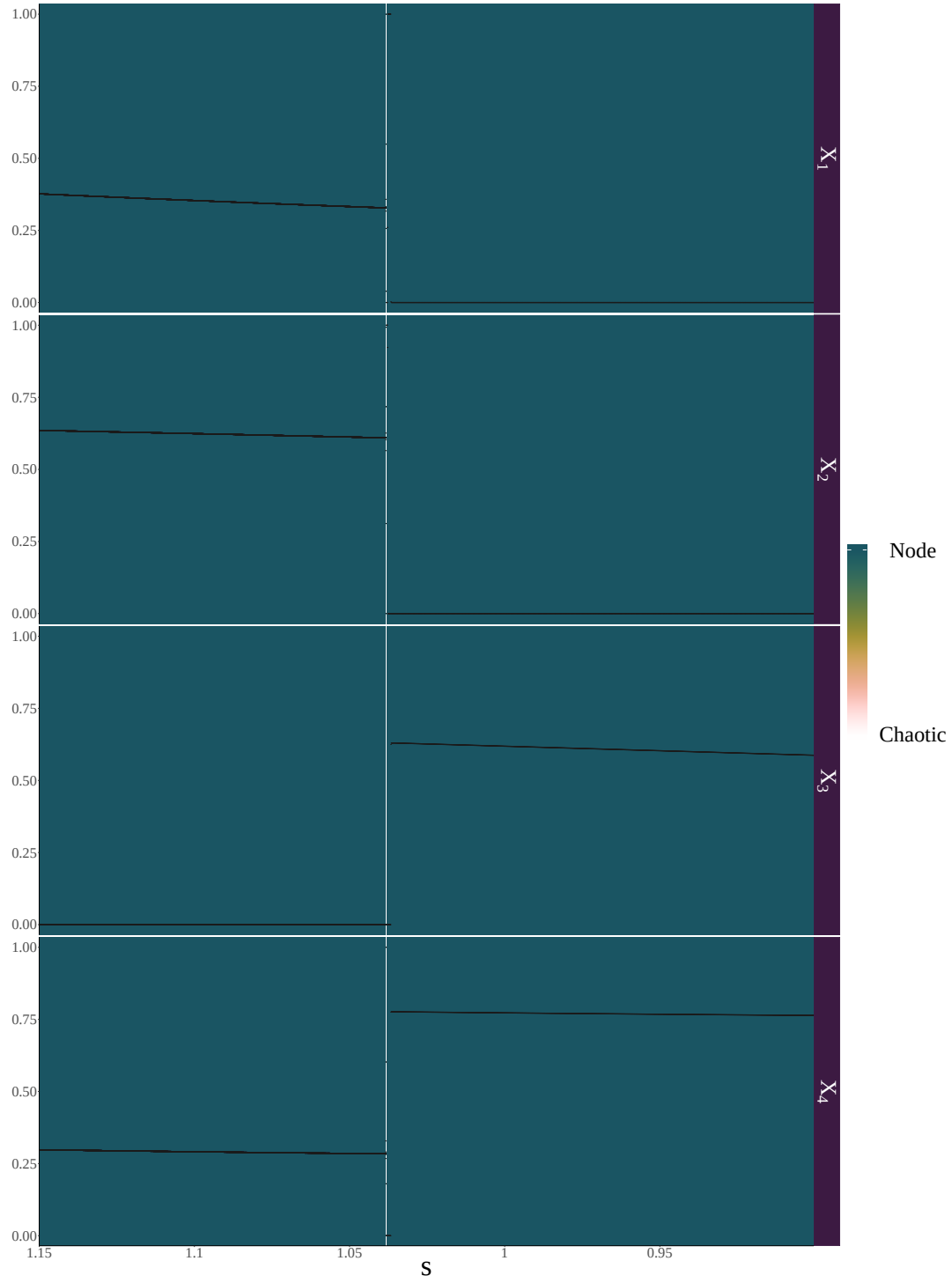


Fig. S4 Bifurcation diagram of all variables X_i in the Generalised Lotka-Volterra model, showing the saddle-node bifurcation as the control parameter s is decreased from [1.15, .9]. For each step in s , the peaks and troughs (i.e. local minima and maxima) of the corresponding time series are shown as black points, corresponding to each value of the bifurcation parameter s (x-axis). Coloured bars indicate the periodicity of the time series as found using our regime boundary detection algorithm, where white indicates chaotic or transitioning regimes

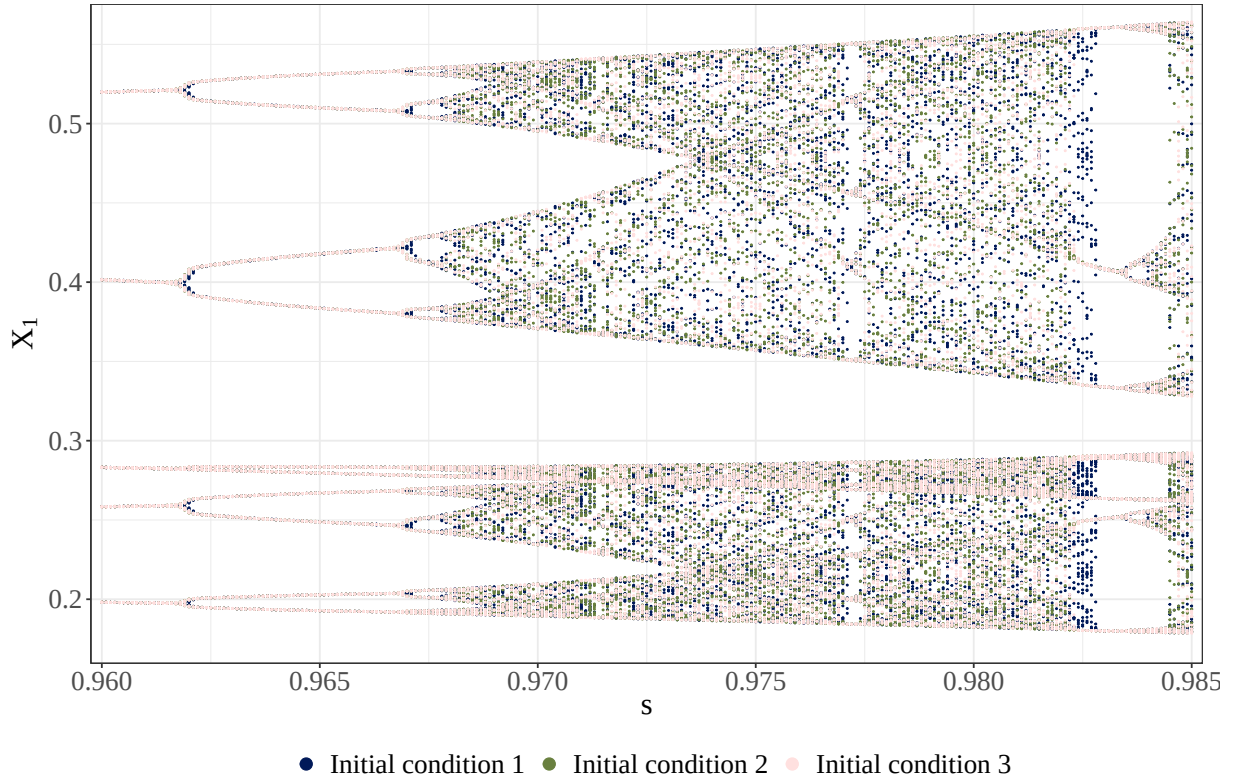


Fig. S5 Bifurcation diagram of the Generalised Lotka-Volterra model starting from three different initial conditions (only the first variable X_1 , $s \in [.96, .985]$), showing that differences in initial conditions can lead the system to converge to different attractors and bifurcation sequences

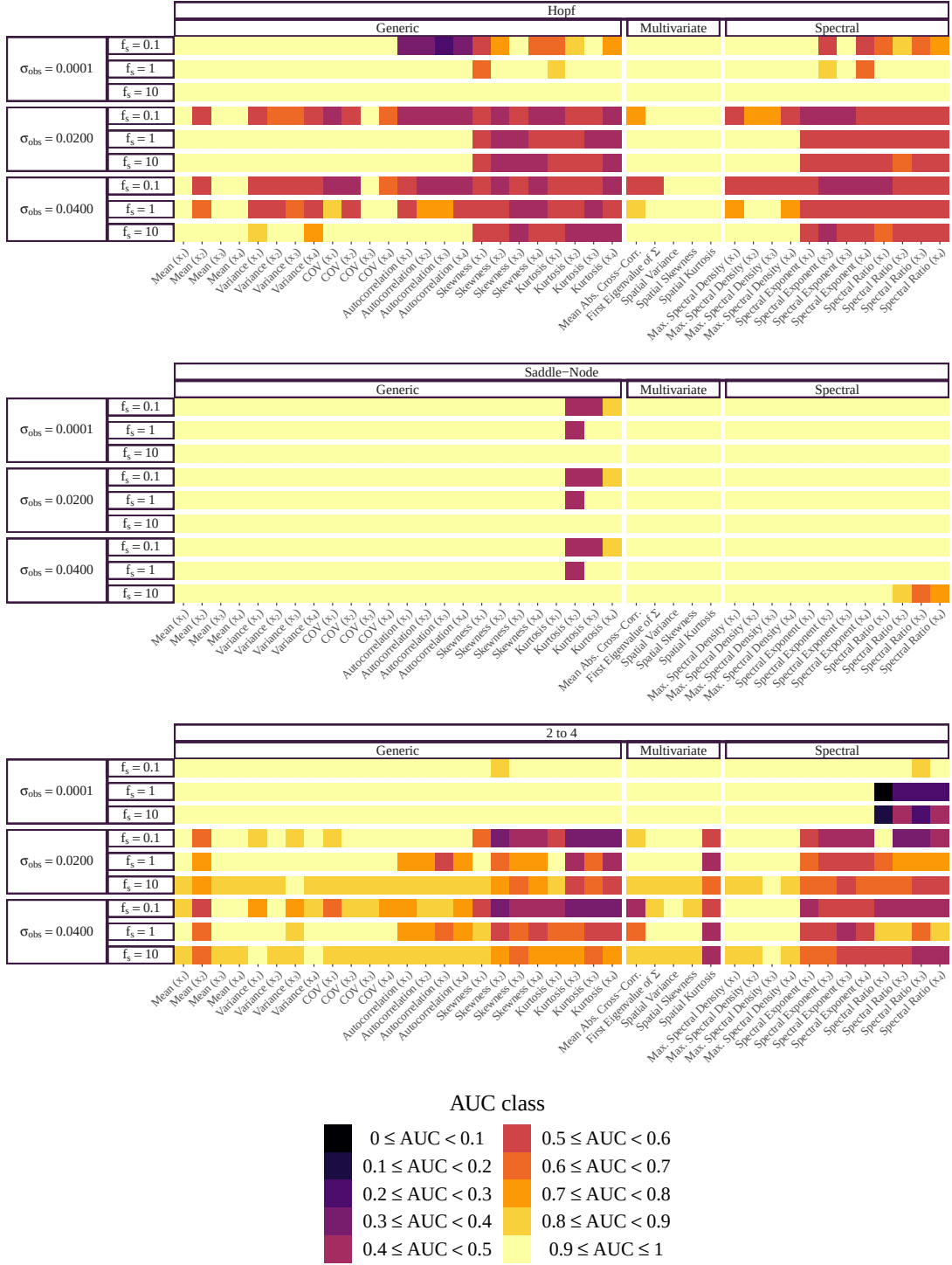


Fig. S6 The performance metric AUC per condition (downsampling frequency $f_s \in [10, 1, .1]$ and observational noise intensity $\sigma_{\text{obs}} \in [0.0001, .02, .04]$) for the Hopf and saddle-node bifurcation and the period-doubling bifurcation from period 2 to 4. Brighter, yellow colours indicate EWS are better able to predict an upcoming transition, whereas darker, purple colours indicate EWS do poorly in anticipating a transition

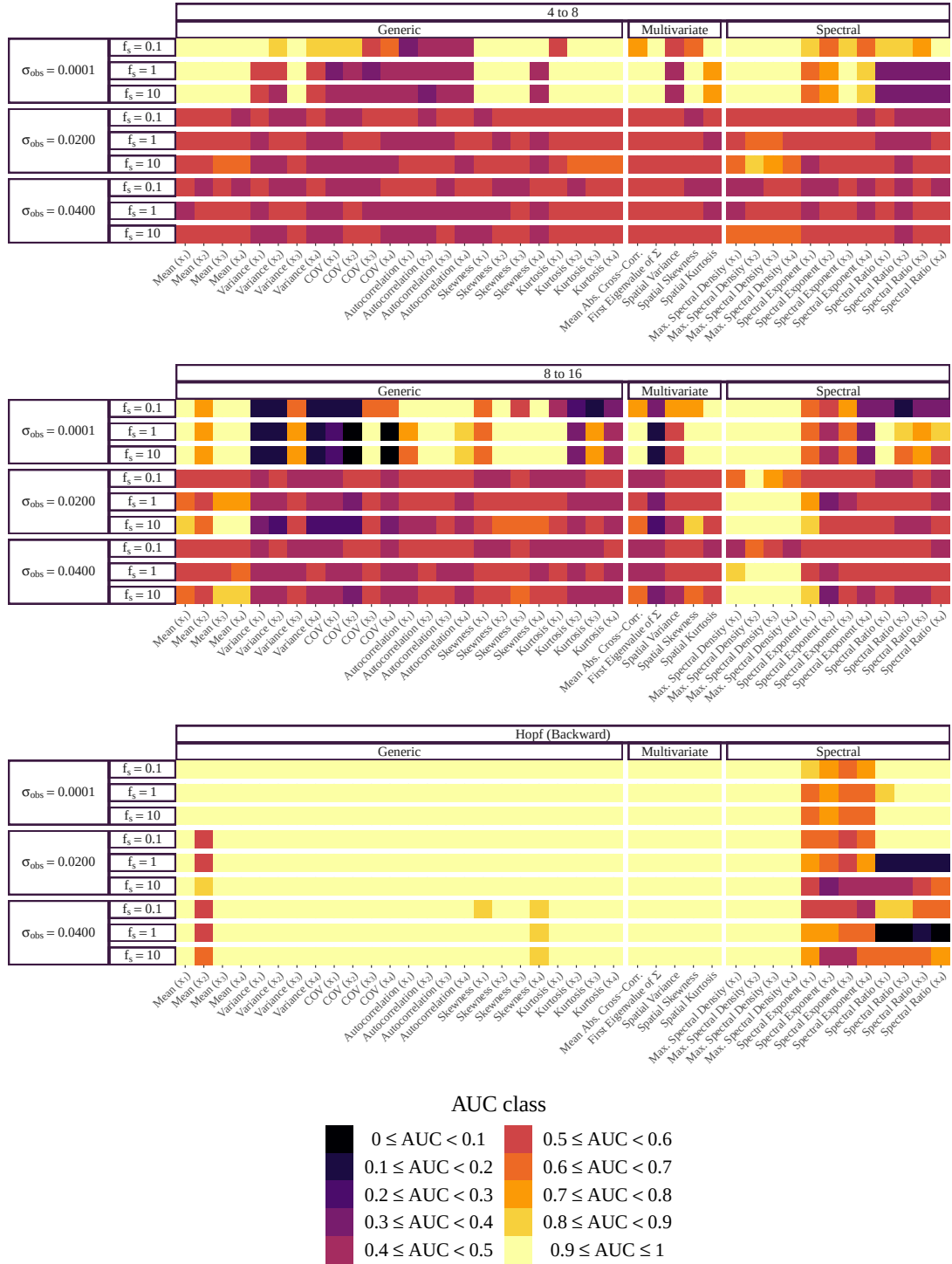


Fig. S7 The performance metric AUC per condition (downsampling frequency $f_s \in [10, 1, .1]$ and observational noise intensity $\sigma_{\text{obs}} \in [0.0001, .02, .04]$) for the period-doubling bifurcations from period 4 to 8 and 8 to 16, and period-halving from period 2 to 1 (i.e. the backwards Hopf bifurcation). Brighter, yellow colours indicate EWS are better able to predict an upcoming transition, whereas darker, purple colours indicate EWS do poorly in anticipating a transition

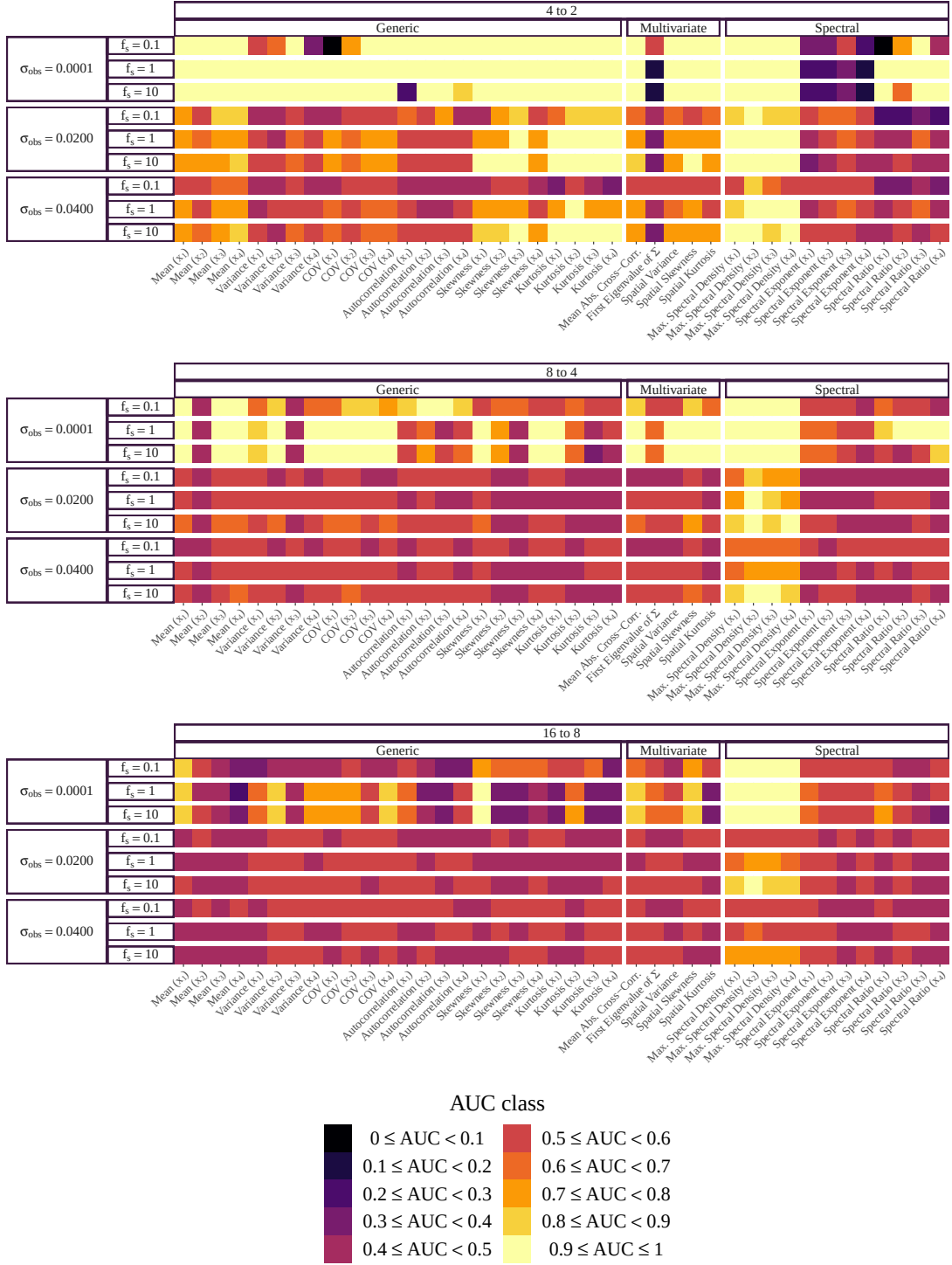


Fig. S8 The performance metric AUC per condition (downsampling frequency $f_s \in [10, 1, .1]$ and observational noise intensity $\sigma_{\text{obs}} \in [0.0001, .02, .04]$) for the period-halving bifurcations from period 4 to 2, period 8 to 4, and 16 to 8. Brighter, yellow colours indicate EWS are better able to predict an upcoming transition, whereas darker, purple colours indicate EWS do poorly in anticipating a transition

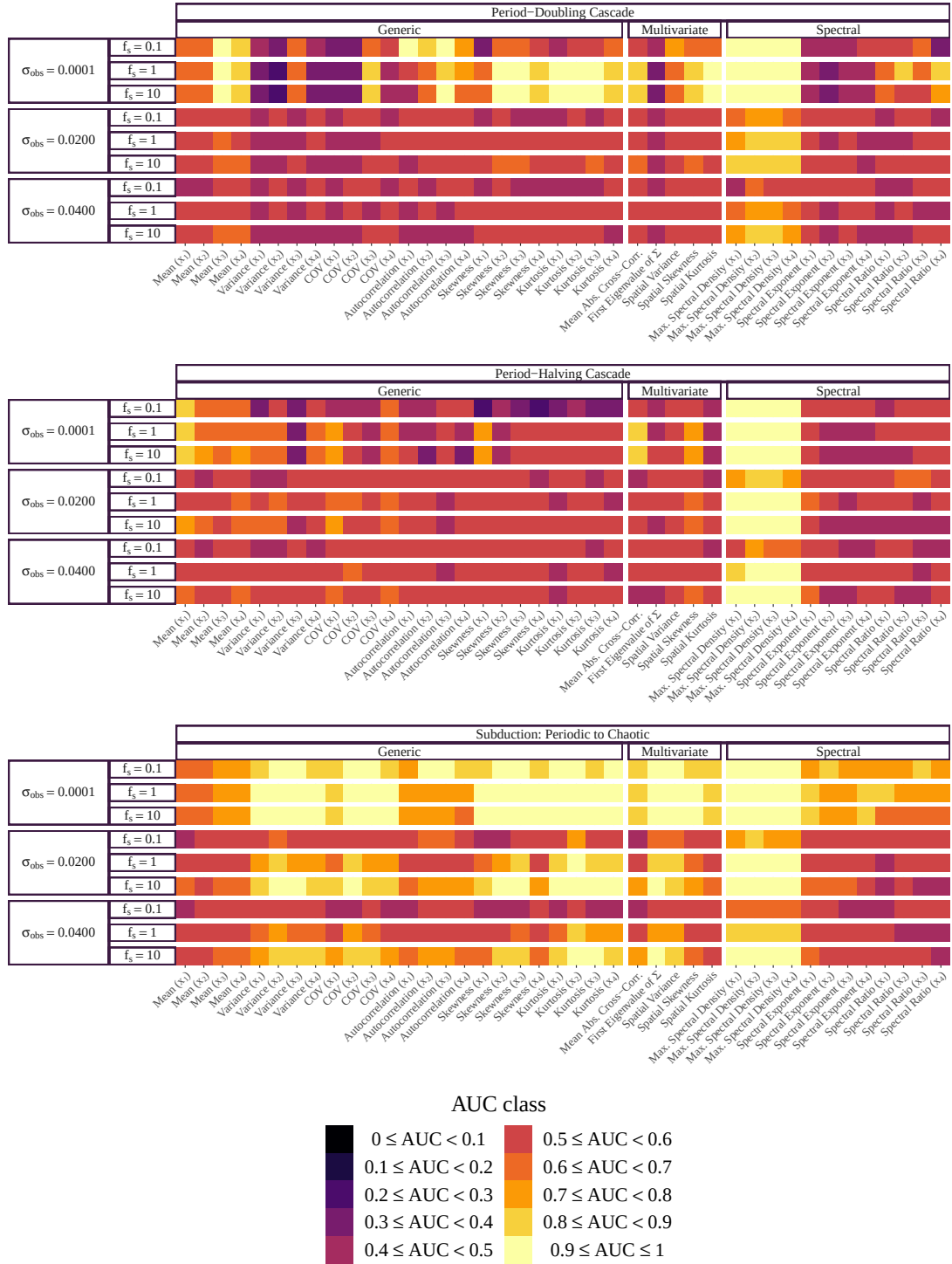


Fig. S9 The performance metric AUC per condition (downsampling frequency $f_s \in [10, 1, .1]$ and observational noise intensity $\sigma_{\text{obs}} \in [0.0001, .02, .04]$) for the period-doubling cascade, the period-halving cascade, and the subduction (periodic to chaotic). Brighter, yellow colours indicate EWS are better able to predict an upcoming transition, whereas darker, purple colours indicate EWS do poorly in anticipating a transition

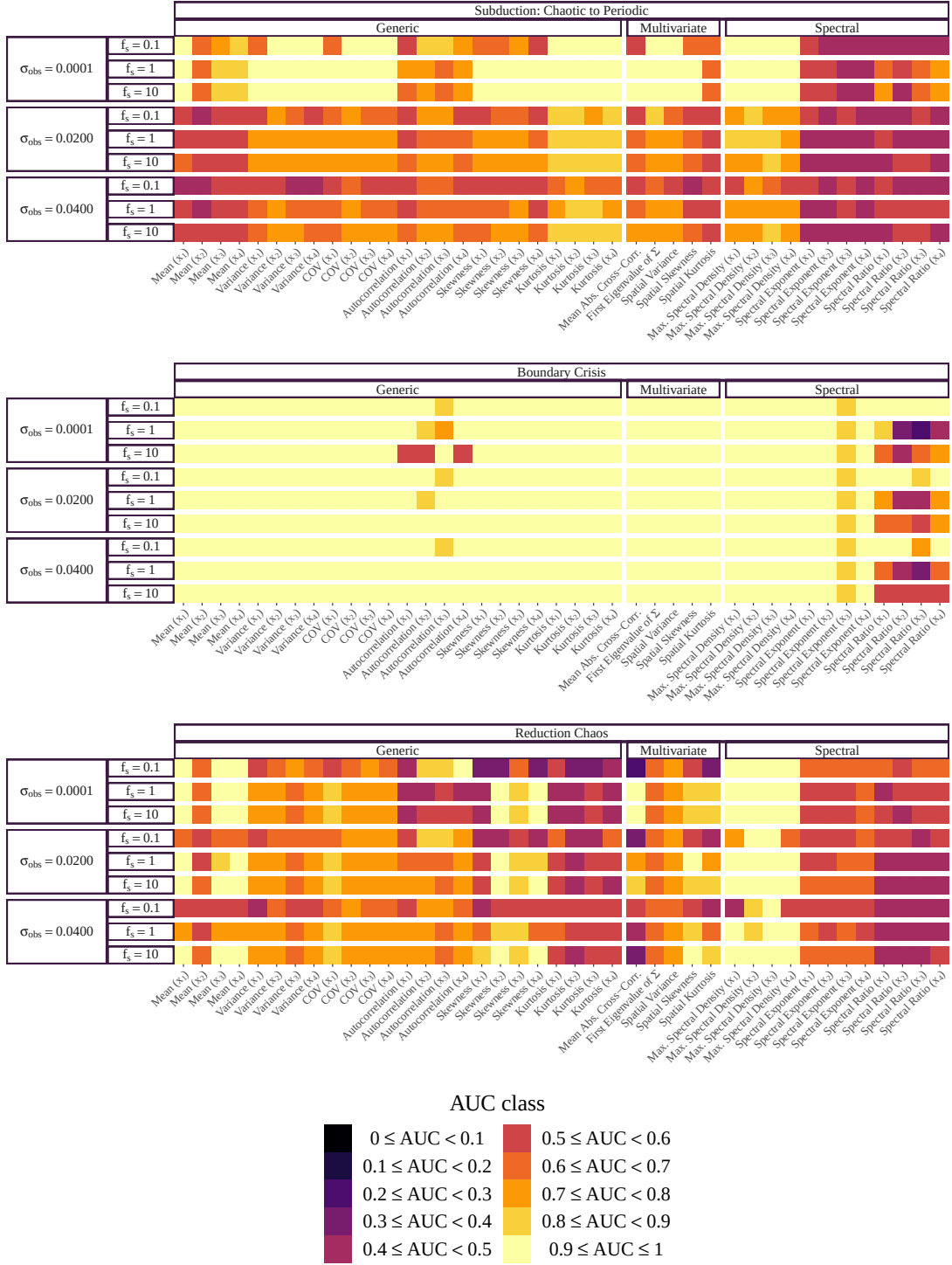


Fig. S10 The performance metric AUC per condition (downsampling frequency $f_s \in [10, 1, .1]$ and observational noise intensity $\sigma_{\text{obs}} \in [0.0001, .02, .04]$) for the subduction (chaotic to periodic), boundary crisis, and interior crisis (chaos reduction). Brighter, yellow colours indicate EWS are better able to predict an upcoming transition, whereas darker, purple colours indicate EWS do poorly in anticipating a transition

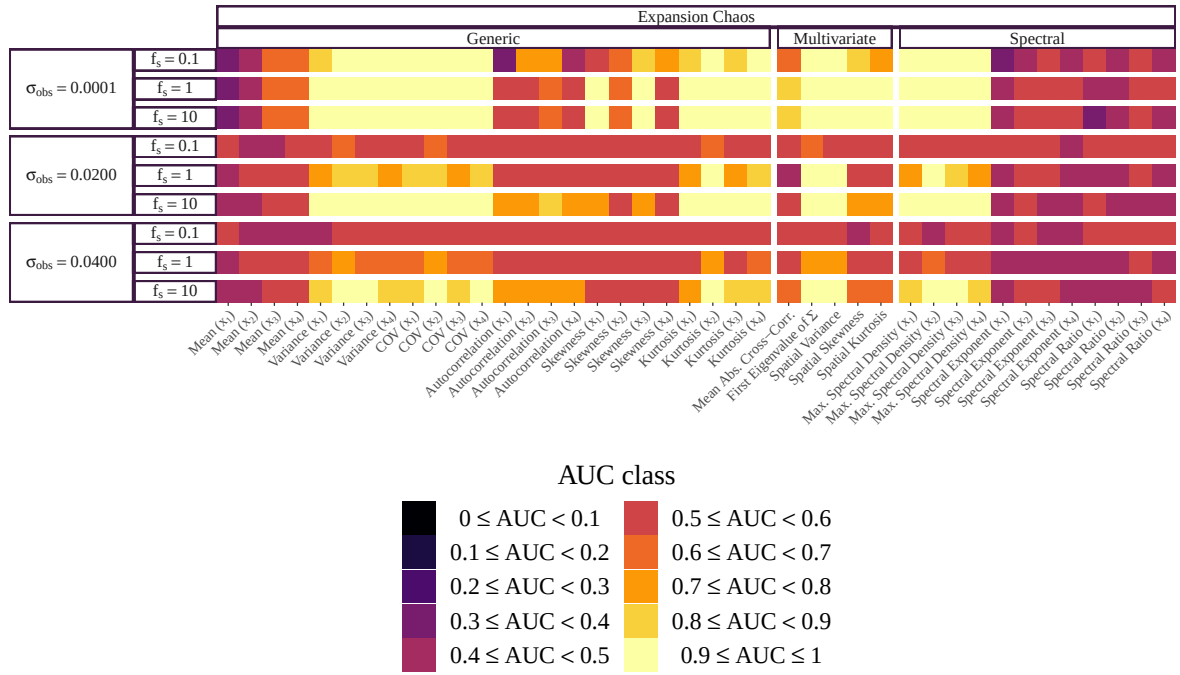


Fig. S11 The performance metric AUC per condition (downsampling frequency $f_s \in [10, 1, .1]$ and observational noise intensity $\sigma_{\text{obs}} \in [0.0001, .02, .04]$) for the interior crisis (chaos expansion). Brighter, yellow colours indicate EWS are better able to predict an upcoming transition, whereas darker, purple colours indicate EWS do poorly in anticipating a transition

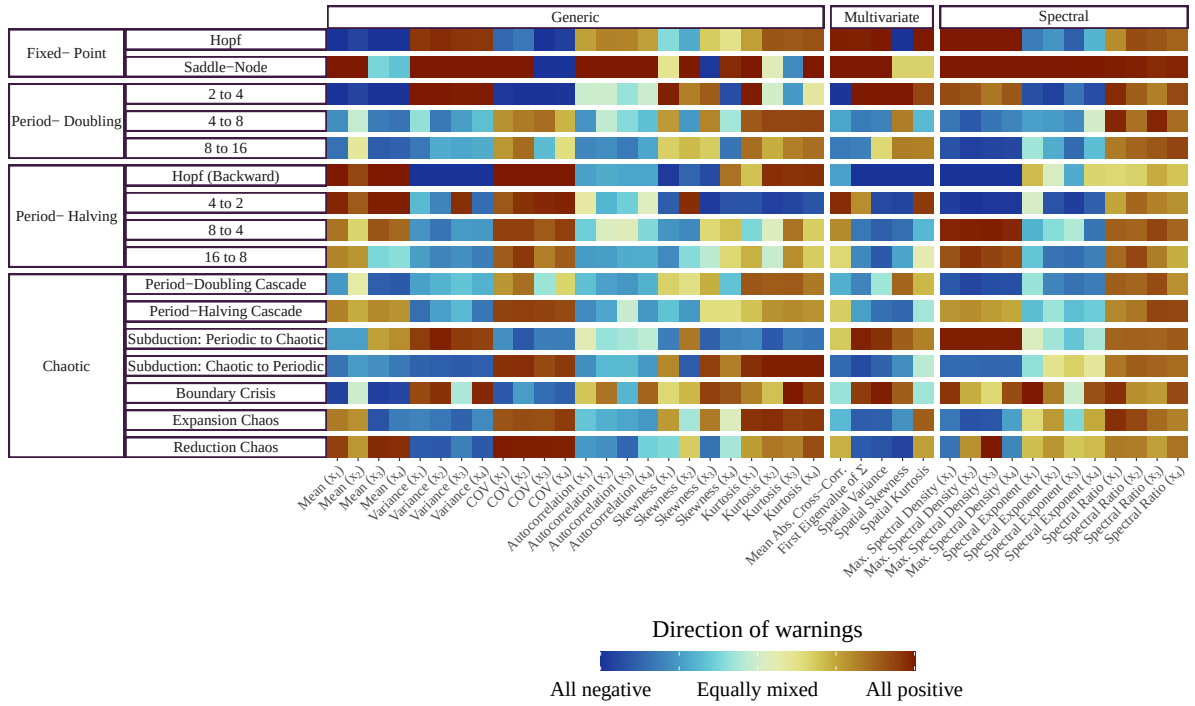


Fig. S12 Direction of EWS when setting an optimal cut-off value σ_{crit}^* , showing the lack of a universal signature of an upcoming transition. A warning may be given by a signal that increases or decreases as compared to baseline. Across simulations, warnings may show a consistent pattern of either increasing (brown-red) or decreasing (blue), or both may occur (mixed, white)

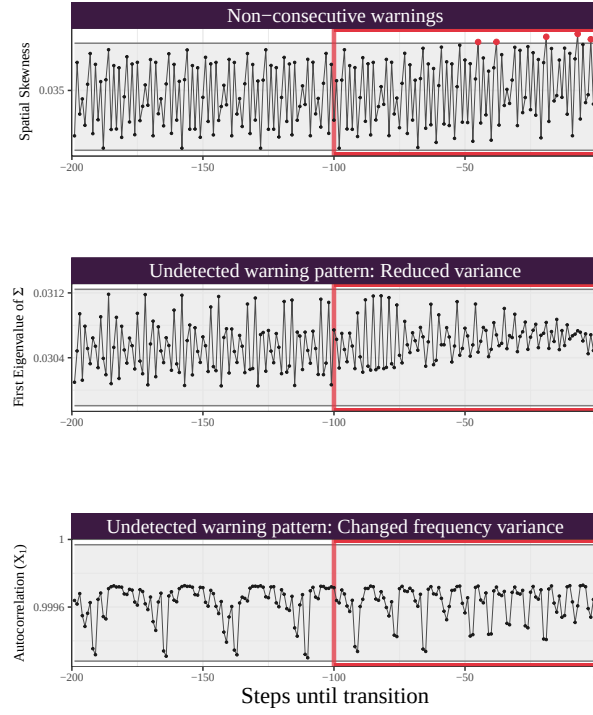


Fig. S13 Complex warning patterns that are not detected well by standard methods. Warning signs are shown for a period-doubling bifurcation (period-4 to period-8, top panel), a period-halving bifurcation (period-4 to period-2, middle panel), and a period-halving cascade from chaos to periodic behaviour (bottom panel). The transition period in which s is changing is indicated in red, which is preceded by a baseline period. Confidence bands are constructed with $\sigma_{\text{crit}} = 2$

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