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Review

Digital twins of nonlinear dynamical systems: a perspective

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Abstract Digital twins have attracted a great deal of recent attention from a wide range of fields. A basic requirement for digital twins of nonlinear dynamical systems is the ability to generate the system evolution and predict potentially catastrophic emergent behaviors so as to provide early warnings. The digital twin can then be used for system "health" monitoring in real time and for predictive problem solving. For example, if the digital twin forecasts a possible system collapse in the future due to parameter drifting as caused by environmental changes or perturbations, an optimal control strategy can be devised and executed as early intervention to prevent the collapse. Two approaches exist for constructing digital twins of nonlinear dynamical systems: sparse optimization and machine learning. The basics of these two approaches are described and their advantages and caveats are discussed.

1 Introduction

In applications, it is often the case that an accurate mathematical model of the underlying dynamical system is not available but time series measurements or observations of some key variables can be made. If the existing empirical data indicate that the underlying system has been functioning as designed or "healthy," how to anticipate any future potential collapse of the system, e.g., caused by slow drifting of a system parameter? Digital twins provide a viable solution. In particular, if a digital "copy" of the system can be faithfully constructed, then a computational bifurcation analysis with respect to variations in the parameter of interest can be performed to assess the possible future collapse of the system.

Recent years have witnessed a fast growing interest in building digital twins not only in many fields of science and engineering but also in industry, health care, and defense [1]. Historically, digital twins were first used for predicting the structural life of aircrafts [2]. In dynamical systems, digital twins can be exploited for predicting the future states and anticipating emergent, potentially catastrophic behaviors [3]. In medicine and health care, for a certain type of disease, mechanistic knowledge, observational or diagnostic data, medical histories, and detailed physiological modeling can be combined to construct patient-specific digital twins [4–6]. Development of digital twins of the Earth for green transition is currently underway in Europe [7, 8].

The aim of this perspective is to present an overview of the current approaches to digital twins for nonlinear dynamical systems. The need for digital twins can be appreciated through an illustrative example. As shown in Fig. 1, a dynamical system of interest generates two time series at two slightly different parameter values: one before a critical transition and another after. Before the transition, the system functions "normally" in the sense that the dynamical variable plotted has a finite mean value, in spite of the statistical fluctuations, as shown in the top panel. The variable can be, e.g., the population of a protected species in an ecosystem. After the transition, for an initial period of time, the variable exhibits a statistically indistinguishable behavior from that before the transition. However, in the long run the variable becomes zero, signifying, e.g., population extinction. If observations were made at any time before the variable begins to decrease systematically, any observation would suggest that the system is completely healthy and functional. Assume that a model of the system is not available and all information that can be obtained from the system is time series measurements. The question is, if at a time when all measurements or observations of the system give no indication of any "abnormal" behavior of the system, how can one tell that in one case the system will continue to be functional (the top panel in Fig. 1), but in another case, a catastrophic collapse will occur (the bottom panel in Fig. 1), based on measured time series only?

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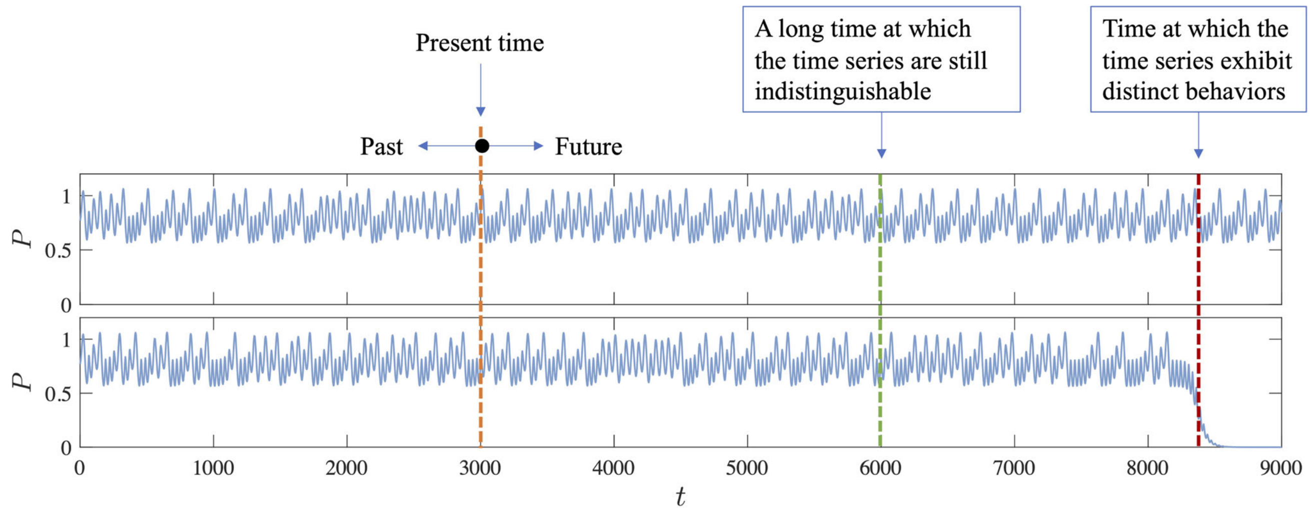

Fig. 1 A challenging prediction problem that was previously deemed unsolvable in nonlinear dynamics. Shown are two time series from a chaotic system at two different parameter values, respectively. The system exhibits a crisis, a global bifurcation that destroys the chaotic attractor, at a critical parameter value p_c. The parameter values corresponding to the time series in the top and bottom panels are before and after p_c, respectively. In the observation time interval [0, 3000] (corresponding approximately to about 80 oscillation cycles of the dynamical variable), the two time series are statistically indistinguishable with approximately identical nonzero mean values (no extinction). Even when the observation time interval is twice as long ([0, 6000]), the two time series still cannot be distinguished. Only when the observation time extends to over 8000 (corresponding to about 250 cycles of oscillation—the red dashed vertical line) will the time series exhibit completely different behavior: one sustaining (top) and another collapsing toward zero (bottom). Suppose the observation time is $t = 3000$—the present time, so the only information available about the system is the two time series. How can the future behaviors of the two time series, i.e., one corresponding to sustained or healthy behavior while another to extinction, be predicted based on the time series that cannot be distinguished?

This model-free prediction of system's future behavior is an extremely challenging problem in applied nonlinear dynamics. Digital twins provide a solution.

At the present, there are two main approaches to digital twins in nonlinear dynamical systems. One is based on reconstructing the system model by finding the accurate equations governing the dynamical evolution from measurements. Crutchfield and McNamara [9] pioneered the problem of determining the system equations from measurements based on estimating the information contained in a sequence of observations to deduce an approximate set of equations of motion representing the deterministic portion of the system dynamics. Bollt proposed the idea of constructing a dynamical system "near" the original system with a desired invariant density by exploiting the Frobenius–Perron theorem [10]. Later, Yao and Bollt developed a least-squares approximation strategy to estimate the system model and parameters [11]. In the past decade or so, a leading approach to finding system equations [12–20] is based on sparse optimization such as compressive sensing [21–26] in situations where these equations have a "sparse" structure ,[1]. The basic idea is as follows. If the vector fields are smooth, they can be approximated by some series expansions such as power or Fourier series. The task then becomes that of estimating the various coefficients in the series expansion. If most of these coefficients are non-zero, the problem is not simplified as the total number of coefficients to be determined will be large. However, if the series expansion is sparse in the sense that the vast majority of the coefficients are zero, then well-developed sparse-optimization methods such as compressive sensing can be used to uniquely solve the few non-trivial coefficients even with a small amount of data [12, 13]. With those coefficients, the system equations described by the series expansions represent a "digital copy" of the original system.

The second approach to digital twin is machine learning [27]. The basic idea is that a dynamical system functions to evolve the state vector forward in time according to a set of mathematical rules, so a digital twin must also be able to evolve the state vector forward in time even without any input. Reservoir computing [28–30] is a suitable choice because its intrinsic recurrent neural network can be trained to execute

[1] The idea of exploiting sparse optimization for discovering system equations was first published by the ASU group in 2011 [12, 13]. Five years later (in 2016), the same idea was republished and named as "SINDy" [S. L. Brunton, J. L. Proctor, and J. Nathan Kutz, "Discovering governing equations from data by sparse identification of nonlinear dynamical systems," Proc. Nat. Acad. Sci. **113** 3932–3937 (2016)]. Approximately five months before this 2016 paper was published, at a Program Review meeting, Prof. Kutz was made aware of the ASU work earlier and was provided the references.

closed-loop, self dynamical evolution with memory. In recent years, there is a great deal of interest in reservoir computing for predicting chaotic systems [31–52]. The advantage of the machine-learning approach to digital twins is its applicability to any systems, regardless of the underlying mathematical structure of the governing equations (e.g., sparse or dense in terms of some series expansion). The disadvantage is that the amount of data required for training can be quite demanding.

The sparse-optimization approach to digital twin through discovering system equations has been previously reviewed [53, 54]. The focus of this Perspective article is on the general principle of the more recent machine-learning approach.

2 Digital twins of nonlinear dynamical systems: adaptable machine learning

Dynamical systems in the real world are not only nonlinear but also complex. Even if an approximate model of the system can be found, the underlying nonlinearity is likely to cause sensitive dependence on initial conditions, parameter variations, stochastic fluctuations, and perturbations, rendering ineffective any model-based prediction method. Predicting characteristic changes in the system in advance of their occurrence thus must rely on data collected during its normal functioning phase, for which machine learning is viable and potentially powerful.

Most previous studies on reservoir computing focused on the behavior of the target dynamical system at a fixed parameter setting, i.e., once the machine has been trained through learning for certain parameter values, it is utilized to predict the state evolution of the system but at the same set of parameter values. A digital twin of the system, by its nature, must be able to faithfully generate the changes in the system behavior as some parameter varies. A basic requirement of digital twin is that it must be able to generate the correct bifurcation behaviors of the original system. That is, the digital twin must not only capture the "dynamical climate" of the original system, but also accurately reflect how the climate changes with the bifurcation or control parameter. Adaptable machine learning [45, 49] was developed to meet this challenge, where the term "adaptable" was introduced to mean that a machine trained with time series data in one parameter regime is capable of generating the dynamical behaviors of the target system in another, distinct parameter regime. The former is referred to as the parameter regime of normal system functioning from which the training data are collected, while the latter is the prediction regime in which system collapse can occur.

The adaptable machine learning framework is schematically shown in Fig. 2. Its working principle can be explained, as follows. Let p be the bifurcation parameter of the target nonlinear system. As p varies, a critical point arises: p_c, where the system functions normally for $p < p_c$ and it exhibits a transient towards collapse for $p > p_c$. Training of the digital twin is done based on the time series taken from a small number of parameter values in the normal regime, e.g., $p_1 < p_2 < p_3 < p_c$. For each parameter value, adequate training is required in the sense that the twin is able to predict correctly and accurately the oscillatory behavior at the same parameter value for a reasonable amount of time. Suppose that, currently, the system functioning is normal and it operates at the parameter value $p_0 < p_c$. In the prediction phase, suppose a parameter change $\Delta p > 0$ has occurred. The new parameter value $p_0 + \Delta p$ is then fed into the digital twin through the parameter channel. The prediction is deemed successful if the twin generates normal oscillations for $p_0 + \Delta p < p_c$ but exhibits a transient towards collapse for $p_0 + \Delta p > p_c$.

A recent work demonstrated that the machine-learning architecture of reservoir computing is effective as digital twins for a variety of nonlinear dynamical systems [27]. A reservoir computing machine consists of three main components: an input layer, a hidden layer with a high-dimensional and complex neural network (the reservoir network), and an output layer. The input layer maps the typically low-dimensional time series data into the high-dimensional state space of the reservoir network, and the output layer projects the high-dimensional dynamical evolution of the neural network state back into low-dimensional time series (readout). Training is administered to adjust the parameters associated with the projection matrix of the output layer to minimize the difference between the output and the true input time series. Because of the nature of the recurrent neural network, the input matrix and the reservoir network structure and link weights are chosen *a priori* according to the values of a few hyperparameters (e.g., the network spectral radius) and are fixed during the training and prediction phases. As a result, highly efficient learning can be achieved. In terms of hardware realization, reservoir computing can be implemented using electronic, time-delay autonomous Boolean systems [31] or high-speed photonic devices [32].

There are two major types of reservoir computing systems: echo state networks (ESNs) [28] and liquid state machines [29]. The architecture of an ESN is one that is associated with supervised learning underlying recurrent neural networks. The basic principle of ESNs is to drive a large neural network of a random or complex topology—the reservoir network—with the input signal. Each neuron in the network generates a nonlinear response signal. Linearly combining all the response signals with a set of trainable parameters yields the output signal. A schematic illustration of the proposed adaptable reservoir computing scheme is shown in Fig. 3, where the training and testing configurations are illustrated in Fig. 3a, b, respectively. The machine consists of three components: (i) an input layer that maps the low-dimensional (M) input signal into a (high) N-dimensional signal through the weighted

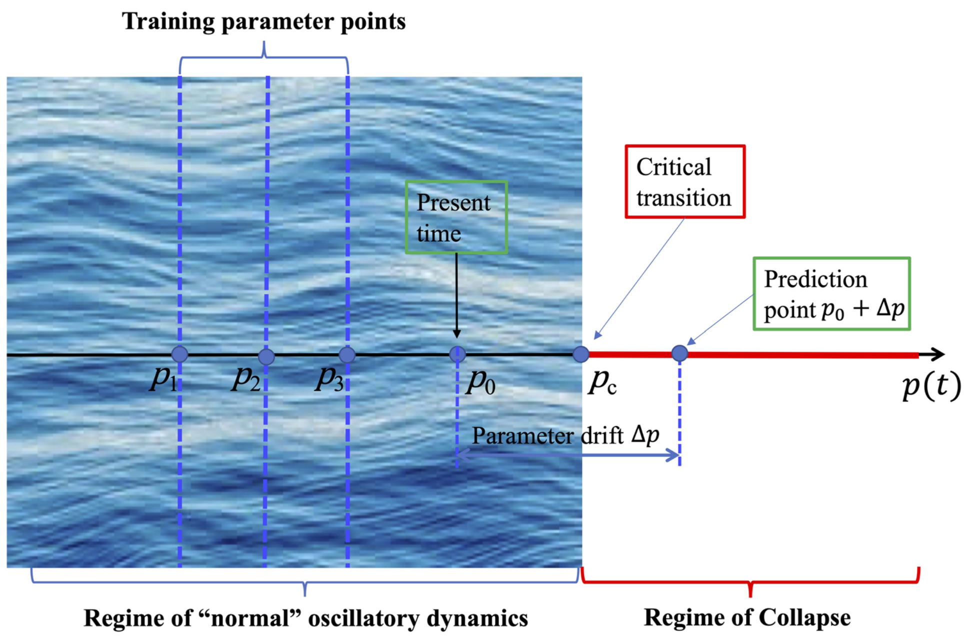

Fig. 2 Training scheme of adaptable machine learning. The target system of interest has two characteristically distinct operational regimes: normal/oscillatory and collapse regimes separated by a critical transition point p_c, where p is a bifurcation parameter. As p increases through p_c, the system transitions from the normal to the collapse regime. Suppose the parameter drifts slowly with time, and let p_0 be its value at the present time. The parameter values p_1, p_2, and p_3, as indicated by the three vertical blue dashed lines, thus occurred in the past, from which observational data or time series can be obtained. Training of the neural machine is done using these time series in the normal or pre-transition regime. The future behavior of the system can be predicted by adding a parameter variation Δp (corresponding to a specific time in the future) to p_0 and observing the dynamical state of the machine under the parameter value $p_0 + \Delta p$. For $p_0 + \Delta p < p_c$, a well trained machine shall predict that the system will still be in the normal functional regime. For $p_0 + \Delta p > p_c$, the machine would generate dynamical evolution that is indicative of system collapse

$N \times M$ matrix $\mathcal{W}_{in}$, (ii) the reservoir network of N neurons characterized by $\mathcal{W}_r$, a weighted network matrix of dimension $N \times N$, and (iii) an output layer that converts the N-dimensional signal from the reservoir network into an L-dimensional signal through the output weighted matrix $\mathcal{W}_{out}$, where $L \sim M \ll N$. The matrix $\mathcal{W}_r$ defines the structure of the reservoir neural network in the hidden layer, where the dynamics of each node are described by its internal state and a nonlinear (e.g., hyperbolic tangent) activation function. For constructing a digital twin, it is necessary to set $M = L$. As mentioned, the matrices $\mathcal{W}_{in}$ and $\mathcal{W}_r$ are generated randomly prior to training, whereas all elements of $\mathcal{W}_{out}$ are to be determined through training.

Consider the setting where the system and environmental variations are characterized by the changes in a single parameter—the "bifurcation parameter." The idea is to designate an additional input channel to feed the parameter value into each and every artificial neuron in the hidden-layer network, as shown in Fig. 3, which makes the reservoir computing machine "cognizant" of the parameter variations. The basic considerations are as follows. To predict critical transitions and system collapse, a requirement is that the time series data must be obtained while the system is still in normal operation, and it is necessary to collect data from multiple values of the bifurcation parameter in the normal phase. Because the training data come from several distinct bifurcation parameter values, it is necessary that the machine "know" the parameter values at which the data are taken, which can be accomplished by "injecting" the parameter values to all nodes of the recurrent dynamical neural network in the hidden layer.

3 Examples of digital twins of nonlinear dynamical systems

3.1 Systems for which sparse optimization methods fail

Recall that the basic requirement of any sparse optimization technique for finding the system equations is *sparsity*: when the system equations are expanded into a power series or a Fourier series, it must be that only a few terms are present so that the coefficient vectors to be determined from data are sparse [12, 53]. However, there are physical and biological systems that violate this sparsity requirement. An example is the two-dimensional Ikeda map describing the dynamics of a

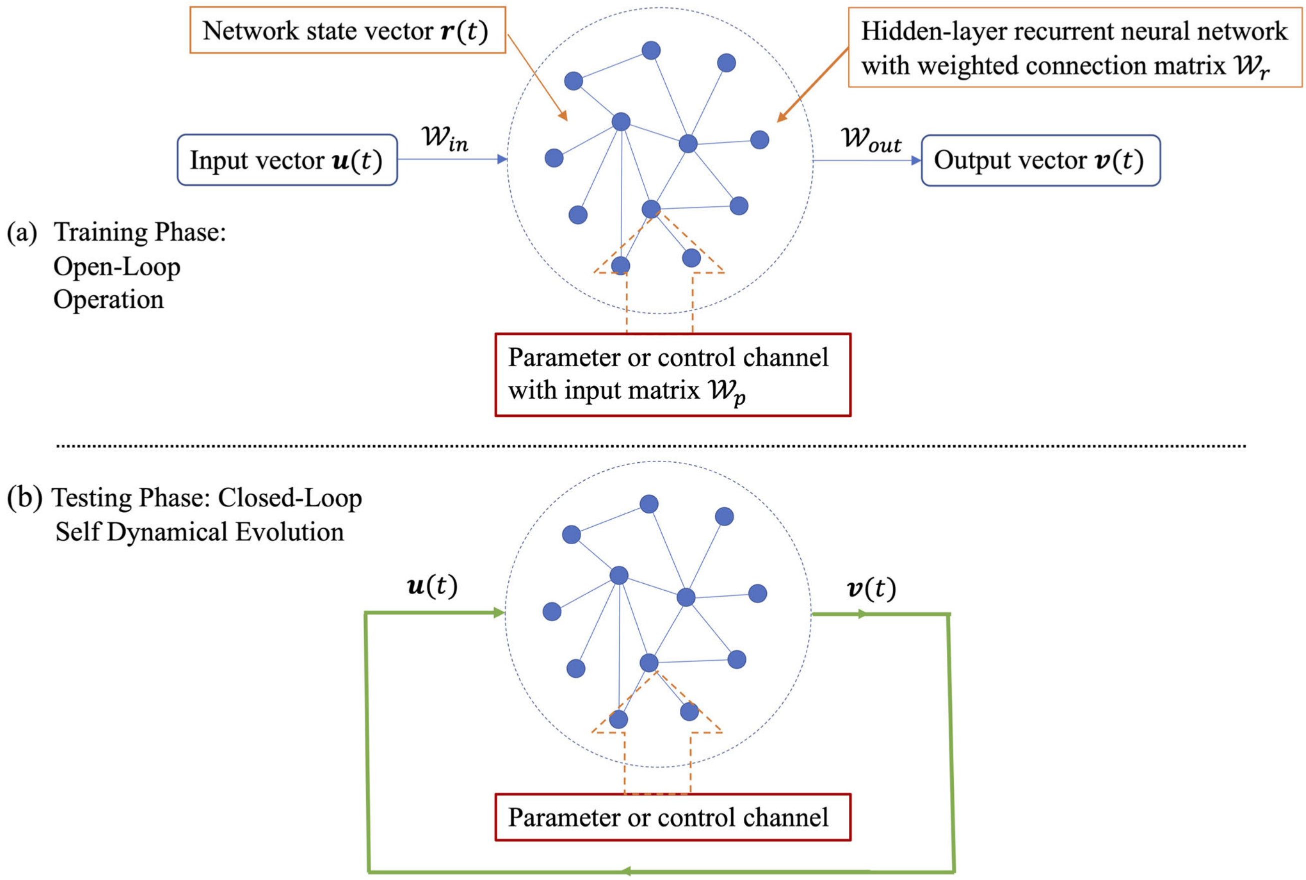

Fig. 3 Basic structure of adaptable reservoir computing. **a** Training phase. Time series data provide the input to the machine. The input matrix $\mathcal{W}_{in}$ maps the M-dimensional input data to a vector of much higher dimension N, where $N \gg M$, and the matrix $\mathcal{W}_p$ feeds the bifurcation parameter value into each and every neuron in the hidden layer as denoted by the dashed circle. The complex neural network of N interconnected neurons in the hidden layer is characterized by an $N \times N$ weighted matrix $\mathcal{W}_r$. The dynamical state of the ith neuron in the reservoir is r_i, for $i = 1, \ldots, N$, constituting the state vector $\mathbf{r}(t)$. The output matrix $\mathcal{W}_{our}$ converts the N-dimensional state vector of the reservoir network into an L-dimensional output vector, where $N \gg L$. For constructing a digital twin, it is necessary to set $M = L$. During the training phase, the vector $\mathbf{u}(t)$ is the input data, so the system is in open-loop operation. **b** In the prediction phase, the external input is cut off and the output vector $\mathbf{v}(t)$ is directly fed back as the input to the reservoir, generating a closed-loop, self-evolving dynamical system

laser pulse propagating in a nonlinear cavity: [55–57]:

$$z_{n+1} = \mu + \gamma z_n \exp\left(i\kappa - \frac{i\nu}{1+|z_n|^2}\right), \qquad (1)$$

where the dynamical variables x and y are the real and imaginary parts of the complex variable z, μ is the dimensionless laser input amplitude (a convenient bifurcation parameter), γ is the reflection coefficient of the partially reflecting mirrors of the cavity, κ is the cavity detuning parameter, and ν characterizes the detuning contributed by the nonlinear medium in the cavity. If the map functions are expanded into a power series or a Fourier series, an infinite number of terms will be present. In fact, for the Ikeda map it remains infeasible to find a suitable mathematical base to expand the map functions into a sparse series, rendering inapplicable the sparse optimization method for constructing a digital twin. It was demonstrated [49] that adaptable reservoir computing provides an effective approach to creating a digital twin of the Ikeda map, which can be used to predict bifurcations and critical transitions of the optical-cavity system.

Another example is a three-species ecosystem described by [58]

$$\begin{aligned}
\frac{\mathrm{d}R}{\mathrm{d}t} &= R\left(1 - \frac{R}{K}\right) - \frac{x_c y_c C R}{R + R_0},\\
\frac{\mathrm{d}C}{\mathrm{d}t} &= x_c C\left[\frac{y_c R}{R + R_0} - 1\right] - \frac{x_p y_p P C}{C + C_0},\\
\frac{\mathrm{d}P}{\mathrm{d}t} &= x_p P\left(\frac{y_p C}{C + C_0} - 1\right),
\end{aligned} \qquad (2)$$

where the dynamical variables R, C, P are the population densities of the three species: resource, consumer, and predator, respectively, and the system parameters are K (the carrying capacity), x_c, y_c, x_p, y_p, R_0, and C_0. For a wide range of the parameter values, the system exhibits a critical transition to species extinction. A power-series expansion of the vector field on the right side of Eq. (2) contains an infinite number terms, rendering inapplicable any sparse optimization method. It was demonstrated [45] that adaptable reservoir computing can be used to construct a digital twin of the ecosystem to predict the critical transition and the dynamical behaviors about the transition.

3.2 Predicting amplitude death

In nonlinear dynamical systems, it can happen that, when a bifurcation parameter of the system changes through a critical point, the oscillatory behaviors of the state variables halt suddenly and completely—a phenomenon called amplitude death [59, 60]. From the point of view of bifurcation, amplitude death is caused by a sudden transition of the system from an oscillatory state to a steady state. If the normal function of the system relies on oscillations, then this phenomenon will be undesired and it is important to be able to predict amplitude death before its actual occurrence. For example, in biological systems, normal conditions are often associated with oscillations, and amplitude death marks the onset of pathological conditions. To anticipate amplitude death in advance of its occurrence based on oscillatory time series collected during normal functioning is important. It was demonstrated that adaptable reservoir computing as a digital twin of the system of interest can be effective for this prediction task [61].

3.3 Predicting onset of synchronization

In complex dynamical systems consisting of a number of coupling elements, synchronization is coherent motion among the elements. Depending on the specific form of the coherent motion, different types of synchronization can emerge, including complete chaotic synchronization [62], phase synchronization [63], and generalized synchronization [64]. The occurrence of synchronization has significant consequences for the system behavior and functions. An example is the occurrence of epileptic seizures in the brain neural system, where a widely adopted assumption is that hypersynchrony is closely associated with the occurrence of epileptic seizures [65], during which the number of independent degrees of freedom of the underlying brain dynamical system is reduced. In the extensive literature in this field, there was demonstration that partial and transient phase synchrony can be exploited to detect and characterize (but not to predict) seizure from multichannel brain data [66–68]. Reliable seizure prediction remains a challenge. In general, it is of interest to predict or anticipate synchronization before its actual occurrence based on time series data obtained before the system evolves into some kind of synchronous dynamical state. In particular, given that the system operates in a parameter regime where there is no synchronization, would it be possible to predict, without relying on any model, the onset of synchronization based solely on the dynamically incoherent time series measurements taken from the parameter regime of desynchronization? A digital twin of the original system represents a viable solution.

It was demonstrated [48] that adaptable reservoir computing can be used to construct a digital twin for predicting synchronization. In particular, the digital twin can predict, with a given amount of parameter change, whether the system would remain asynchronous or exhibit synchronous dynamics. Systems tested include representative chaotic and network systems that exhibit continuous (second-order) or abrupt (first-order) transitions. Of special interest are network dynamical systems exhibiting an explosive (first-order) transition and a hysteresis loop, and it was shown [48] that the digital twin possesses the power to accurately predict these features including the precise locations of the transition points associated with the forward and backward transition paths.

4 Discussion and outlook

There exist two approaches to digital twins in nonlinear dynamical systems: sparse optimization and machine learning, where the former relies on finding the exact governing equations of the system and its applicability is thus limited. This Perspective explains the difficulty with the sparse-optimization approach and focuses on the machine-learning approach. An issue concerns the type of machine-learning scheme that can be exploited for constructing digital twins for nonlinear dynamical systems. Since a dynamical system evolves its state forward in time according to a set of mathematical rules, its digital twin must be able to evolve forward in time by itself. In this regard, reservoir computing is capable of closed-loop, self dynamical evolution with memory, so it provides a base for developing digital twins of nonlinear dynamical systems.

An important contribution to explainable machine learning as applied to nonlinear dynamical system is the mathematical understanding of the inner workings of reservoir computing by Bollt [50], leading to the development of "next-generation reservoir computing" [51]. A foundational problem underlying the development of a physical understanding of the workings of reservoir-computing based digital twins is searching for scaling laws between the complexities of a chaotic system and its digital twin. In particular, in order for the digital twin to predict the state evolution of the target system, the complexity of the former must "overpower" that of the latter. What is the meaning of "overpowering" and how can it be characterized? Are there scaling laws quantifying the relationship? Answers to these questions will provide a deeper understanding of the inner workings of reservoir-computing based digital twins.

For a chaotic system, its state evolution is determined by the trajectory movement on a dynamically invariant set, e.g., a chaotic attractor. The complexity of the chaotic system can be faithfully characterized by the information dimension of the chaotic invariant set [69, 70]. Likewise, the complexity of the digital twin is determined by its "inner" dynamical system, which is typically a complex dynamical network in the hidden layer of the reservoir computer. For a complex network, in general its complexity increases with its size. As the information dimension of the target chaotic system increases, the size of the reservoir network must increase accordingly to warrant its predictive power over the former. A universal scaling law between the network size required for accurate prediction and the information dimension of the chaotic system, if it indeed exists, would represent a meaningful way to characterize the digital twins' ability to overpower the target chaotic system.

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