

Measuring dynamical phase transitions in time series

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There is a growing interest in methods for detecting and interpreting changes in experimental time-evolution data. Based on measured time series, the quantitative characterization of dynamical phase transitions at bifurcation points of the underlying chaotic systems is a notoriously difficult task. Building on prior theoretical studies that focus on the discontinuities at $q = 1$ in the order- q dynamical Rényi entropy, we measure the derivative of its spectrum given by the variance of the logarithmic probability of trajectories. To overcome the difficulties inherent in trajectory-space descriptions of finite-length time series, we derive—within the general framework of Markov processes—a computationally efficient closed-form expression for this measure, while maintaining control over the trade-off between statistical and truncation errors. We investigate the properties of the measure and assess the efficacy of the associated method in estimating characteristic quantities of well-known dynamical systems. Furthermore, we examine its scope and limitations, including its potential utility in predicting dynamical phase transitions from time series and in characterizing the complexity of the underlying behavior. Grounded in the thermodynamic formalism of chaotic systems, the developed framework bridges dynamical systems theory, network theory, and time-series analysis, extending classical concepts such as bit-number variance or varentropy in phase-space statistics, permutation entropy in time-series analysis, and path-length statistics in network science.

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I. COMPLEX SYSTEMS AND TIME SERIES

Recently, in the era of complexity science, the significance of tools for characterizing quantitatively the temporal evolution of real-world complex systems has surged [1,2]. In the absence of defining equations of motion, the focus shifts toward analyzing the observed time series [3–7]. Objective characterization of changes in the dynamics is important from the point of view of prediction and control [8,9]. In biological time series, for example, accurately detecting epileptic seizures in electroencephalogram recordings and identifying cardiac fibrillation in electrocardiograms (ECG) data are vital [10–12]. Therefore, the study of critical transitions and the identification of change points are fundamental aspects of complex systems [13–19].

Qualitative changes in the dynamics of complex systems are typically accompanied by abrupt modifications in the phase-space distribution of the system. This can be viewed in analogy with physical systems where quantities like entropy, partition function, free energy, and diffusion coefficient, defined via phase-space distribution, contribute to a powerful

thermodynamic formalism of phase transitions. This formalism has also been adopted in the context of chaotic systems [20,21]. Its applicability has been successfully demonstrated in mostly low-dimensional systems covering both phase-space [22,23] and trajectory (history)-space statistics [24–27]. However, analytical relations can be exploited only in a limited number of dynamical systems where the equations of motion are given. In the absence of such equations, such as for experimental time series or Markov processes, it is a challenge to retain the thermodynamic formalism by estimating the relevant statistical quantities related to phase transitions. For a numerical measurement of the entropy, a symbolic representation of time series is realized in one of two ways: spatial encoding (threshold-based phase-space partitioning) or temporal encoding (ordinal patterns) [3,28–30]. As a result, the problem can be transferred to the context of symbolic dynamics, setting the stage for a computational and information-theoretical perspective [31,32].

Here, we briefly review the role of order- q Rényi entropy in characterizing dynamical properties as they manifest in the trajectory space. Based on previous studies [24–27], we propose to measure dynamical phase transitions via the derivative of the entropy at $q = 1$ exhibiting singularities at the edge of chaos. For the trajectory-space description, we employ the Markov-chain formalism, which is the most widely used and possibly the only general-purpose method covering both dynamical systems and time series [3,15,33]. Within this framework, we derive a computationally efficient closed-form expression of this measure. Here, we present examples for one- and two-dimensional maps; however, the method can be applied in higher dimensions, too. It can be generalized

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to continuous time dynamical systems and multivariate time series by adequate time discretization, for example, by constructing the corresponding Poincaré map, as performed in Refs. [3,34].

II. DYNAMICAL SYSTEMS

For discrete-time dynamical systems, we need an appropriate partitioning of the phase space by defining a set of n nonoverlapping cells that cover the attractor entirely. Quantities that are solely dependent on the natural distribution, ρ^* , on the attractor [21,22] remain invariant under the reshuffling of the data points, being unsuitable for measuring the more relevant trajectory-level information [32]. To that end, a trajectory of the system can be defined as a string of symbols, namely, coarse-grained states $\mathcal{X}(t) = \{s_1, s_2, \dots, s_t\}$ if $\mathbf{x}(\tau = 1) \in \text{cell } s_1$, $\mathbf{x}(\tau = 2) \in \text{cell } s_2$, $\dots$, $\mathbf{x}(\tau = t) \in \text{cell } s_t$, where $\mathbf{x}(\tau)$ denotes the state of the dynamical system at time step τ . Let us denote by $\mathcal{P}(\mathcal{X}(t))$ the joint probability of the trajectory $\mathcal{X}(t)$ of t consecutive steps. The corresponding order- q dynamical Rényi entropy in the probability space $\mathcal{P}(t)$ of all possible trajectories $\mathcal{X}(t)$ is defined as [32,35–37]

$$H_q(\mathcal{P}(t)) = \frac{1}{1-q} \ln \sum_{\mathcal{X}(t)} [\mathcal{P}(\mathcal{X}(t))]^q. \quad (1)$$

While the above expression usually diverges with the length of the trajectories t , the entropy rate,

$$K_q(\mathcal{P}) = \lim_{t \rightarrow \infty} \frac{1}{t} H_q(\mathcal{P}(t)), \quad (2)$$

characterizes the scaling behavior in the limit of infinite time. The above quantity typically depends on the partitioning. Using the generating partition, the supremum over partitions is reached [32]. Since such a partitioning is generally not known, one may choose instead a grid of cells of equal size. A sufficiently high resolution is also expected to provide a good estimation of the supremum [38]. Alternatively, one may also use numerical or machine-learning algorithms for estimating optimal partitions from observed data (see, e.g., [2,39,40]).

The Rényi entropy at $q = 1$, denoted here by S , is called the Kolmogorov-Sinai (KS) entropy or metric entropy and it is of special interest as it measures the entropy production rate due to the chaotic nature of the dynamics. Using Eq. (2), this measure can be expressed as the mean

$$S = K_1(\mathcal{P}) = - \lim_{t \rightarrow \infty} \frac{1}{t} \langle \ln \mathcal{P}(t) \rangle_{\mathcal{P}}, \quad (3)$$

over all trajectories $\mathcal{X}(t)$ with probability distribution $\mathcal{P}(t)$ [32]. Based on Refs. [24,41], there exists a dynamical phase transition at borderline cases of chaos; hence, the derivative of the Rényi entropy with respect to q diverges in $q = 1$. This derivative can be expressed as the varentropy [42] of trajectories, formally,

$$\Lambda = -2K'_1(\mathcal{P}) = \lim_{t \rightarrow \infty} \frac{1}{t} \Delta_{\mathcal{P}}^2 \ln(\mathcal{P}(t)), \quad (4)$$

where $\Delta_{\mathcal{P}}^2(\cdot) = \langle (\cdot)^2 \rangle_{\mathcal{P}} - \langle \cdot \rangle_{\mathcal{P}}^2$ denotes the variance [43]. The time-normalized variance of logarithmic trajectory probabilities (4) is also interpreted as a diffusion coefficient in Ref. [27].

The direct estimation of trajectory probabilities $\mathcal{P}(t)$, therefore the above mean and variance, from measured time series of finite length is not feasible. As an alternative, here we model infinite-length trajectories indirectly via a Markov-chain approximation of the dynamics.

III. MARKOV CHAINS

Discrete-time autonomous dynamical systems with a continuous state space can be approximated by time-homogeneous discrete-time Markov chains with finite-state space. This model requires two elements. First, the states are discretized, for example, by choosing a suitable partitioning as described above. Second, the transition probabilities between states i and j are defined as a conditional probability $w_{ij} = p(s_{\tau+1} = j | s_{\tau} = i)$, where $i, j = 1, \dots, N \leq n$, where n is the number of cells and N is the number of symbols present in the encoded time series. The transition matrix, $(\mathbf{W})_{ij} = w_{ij}$, corresponding to such a Markov chain is also referred to as the transfer operator within Ulam's scheme [44], while its network representation is called a state-transition network (STN) [34]. This approximation becomes exact if the coarse graining corresponds to Markov partitioning, one that is only known exactly for a handful of systems and can be approximated or optimized numerically in some other cases as well [28]. Additionally, the first-order Markov-chain description of the dynamics can be improved by considering higher-order states corresponding to symbolic sequences $\{s_{\tau-m+1}, \dots, s_{\tau}\}$ of length m , which leads to an m th order Markov process, $p(s_{\tau-m+2}, \dots, s_{\tau+1} | s_{\tau-m+1}, \dots, s_{\tau}) = p(s_{\tau+1} | s_{\tau-m+1}, \dots, s_{\tau})$, in terms of the original symbolic states. The number of symbols encoding m th-order states with nonzero probability during the dynamics is typically $N \ll n^m$. The stationary distribution of the Markov chain $\rho^{\top}$, is the left eigenvector of the transition probability matrix $\mathbf{W}$ associated with the unit eigenvalue. In the special case of first-order states, $m = 1$, this eigenvector coincides with the coarse-grained natural distribution on the attractor, $\rho = \rho^*$.

For estimating the dynamical entropy rates K_q , we define the trajectory $\mathcal{X}(t)$ as a sequence of states/nodes visited during a random walk of t steps on the network, i.e., a realization of the Markov chain. The probability of such a trajectory can be given as

$$\mathcal{P}(\mathcal{X}(t)) = \rho_{s_1} \mathcal{P}(\mathcal{X}(t) | s_1), \quad \mathcal{P}(\mathcal{X}(t) | s_1) = \prod_{\tau=1}^{t-1} (w_{s_{\tau} s_{\tau+1}}). \quad (5)$$

Using the Markov-chain description, the so-called truncated Rényi-entropy spectrum [25,41,45] is obtained as (see, e.g., Ref. [46] and Sec. B in the Supplemental Material [47])

$$\tilde{K}_q = \ln \alpha_{\max}(q) / (1 - q) \quad (6)$$

where $\alpha_{\max}(q)$ is the largest eigenvalue of the $(\mathbf{W}_q)_{ij} = w_{ij}^q$ matrix (element-wise q power). The truncated entropy, $\tilde{K}_q$, is expected to exceed the exact value, K_q , for reasons that are straightforward to show in the $q = 1$ case from the properties of conditional entropies (see also Ref. [45]). The superior efficacy of the Markov-chain-based expression (6) over the direct estimation of trajectory probabilities used in Eq. (2)

is demonstrated in Sec. C in the Supplemental Material [47] for two prototypical one-dimensional systems: the piecewise-linear asymmetric tent map [21] for which the analytically known Rényi-entropy spectrum is reproduced numerically using Eq. (6), and in the case of the critical map [24] exhibiting intermittent dynamics, the discontinuity at $q = 1$ is confirmed together with the exact value of the KS entropy.

In the case of the logistic map, $x_{\tau+1} = rx_{\tau}(1 - x_{\tau})$, the truncated entropy exhibits a phase transitionlike discontinuity at $q = 1$ only in the vicinity of critical values of the parameter r corresponding to chaos-to-periodic bifurcation points [e.g., in the case of subduction [48] at $r = 3.82842$, compare the lines denoted by the square-shaped marker in panels (a) and (c) of Fig. 1]. Around these points, the evolution of the system presents properties characteristic of phase transitions in physical systems such as critical slowing down. In the case of limit cycles, the full entropy spectrum is identically zero, for partially predictable chaos [49]; however, it is characterized by relatively low, quasiconstant values [see the star- and circle-shaped markers in panel (a) of Fig. 1, respectively]. Finally, for $r = 4$, namely, for fully developed chaos, all Rényi entropies are $K_q = \ln 2$ (see the dashed line in Fig. 1(a) and its numerical estimate denoted by the yellow line with the diamond-shaped marker) [21], which is exactly reproduced by its truncated version in Eq. (6) when using the Markov partitions $[0, 0.5)$ and $[0.5, 1)$ (not shown here).

The same can be done if the map is higher dimensional. Here, we consider the well-known two-dimensional Henon map [50], $x_{\tau+1} = 1 - ax_{\tau}^2 + y_{\tau}$, $y_{\tau+1} = bx_{\tau}$, with $b = 0.3$ and control parameter a . For chaotic dynamics at $a = 1.4$, the accepted value of the topological entropy $h_t \approx 0.465$ is reproduced by $\tilde{K}_0 \approx h_t$ [33,51]. Furthermore, the KS entropy is equal to the maximal Lyapunov exponent $\tilde{K}_1 \approx \lambda \approx 0.42$, as expected by Pesin's relation [32]. A similar phase transition can be observed in the vicinity of the critical values of the control parameter [e.g., $a \approx 1.2265$, compare panels (b) and (d) of Fig. 1]; see also Ref. [34].

IV. RANDOM-WALK STATISTICS

The critical behaviors illustrated above can be described by the trajectory-space-dependent quantity Λ in Eq. (4), a measure similar to specific heat in thermodynamics and bit-number variance in state-space description [21–23]. Estimation of the two measures from Eqs. (3) and (4) based on the truncated Rényi entropy (6) would imply eigenvalue calculation and numerical differentiation, entailing superfluous errors and increased computational complexity. Instead, we use their statistical interpretation expressed by the right-hand side of Eqs. (3) and (4), which can be estimated within the framework of first-order Markov processes as discussed below.

According to Eq. (5), the quantity $\mathcal{L}(t) \equiv -\ln \mathcal{P}(\mathcal{X}(t)|s_1)$ can be interpreted as the total length of a random-walk trajectory, $\mathcal{X}(t)$, on the STN, made up of steps of length $l_{\tau} = -\ln w_{s_{\tau}, s_{\tau+1}}$ with $\mathcal{L}(t) = \sum_{\tau=1}^t l_{\tau}$. Due to the Markov-chain central limit theorem [52], the distribution of total path lengths $\mathcal{L}(t)$, over all possible realizations of random walks, $\mathcal{X}(t)$, approaches a normal distribution in the limit of $t \rightarrow \infty$, which can be fully characterized by its mean, $\langle \mathcal{L}(t) \rangle_{\mathcal{P}}$, and variance, $\Delta_{\mathcal{P}}^2 \mathcal{L}(t)$ (see Sec. C in the Supplemental Material [47] for

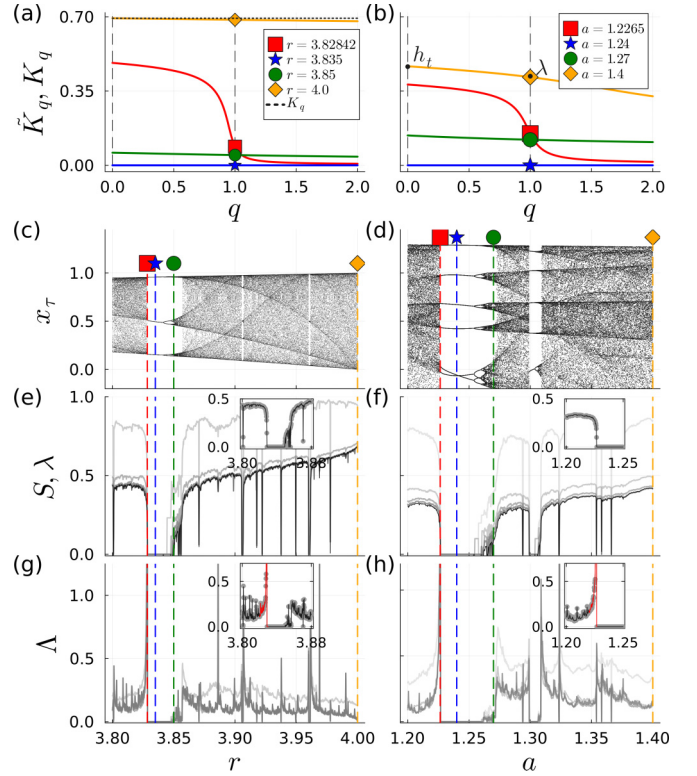


FIG. 1. Matching the classical picture of the logistic map (left column) and the Henon map (right column) to its Markov-chain-based model using $t = 10^8$ long time series. For the logistic map the $[0, 1]$ interval, while for the Henon map the phase plane $[-2, 2] \times [-2, 2]$ is partitioned into $n = 2^5$ and $n = 2^5 \times 2^5$ equally sized cells, respectively. (a) and (b) The spectrum of the truncated Rényi entropy $\tilde{K}_q$ computed by using Eq. (6) and states of order $m = 12$ for four different parameter values (given in the legends). The location of markers corresponds to the KS entropy $S = \tilde{K}_1$ given by Eq. (7). The parameter values r and a used as examples in panels (a) and (b), respectively, are indicated by the corresponding markers and the vertical dashed lines in the panels below. (a) For the logistic map, the thin dashed line denotes the theoretical Rényi entropy $K_q = \ln 2$, for $r = 4$ [21]. (b) For the Henon map, the topological entropy $h_t \approx 0.465 \approx \tilde{K}_0$ and the maximal Lyapunov exponent $\lambda \approx 0.42 \approx S$ are shown for $a = 1.4$ for comparison [51]. (c) and (d) The bifurcation diagrams of the above systems (see Sec. C in the Supplemental Material [47] for a broader range of the control parameters). (e) and (f) The KS entropy $S(m)$ and (g) and (h) the Lyapunov measure $\Lambda(m)$ from Eqs. (7) and (10), respectively. Lines in increasingly darker shades of gray correspond to Markov chains using states of order $m = 1, 2, 4, 12$, respectively. The analytical results (gray lines) given in Eq. (10) are compared to the statistics of 10^3 simulated random walks (gray circular markers) on the corresponding STNs in the insets for order $m = 12$. In panels (e) and (f), the largest Lyapunov exponent λ is also shown by the thin black line for comparison. Note that $S(12) \approx \lambda$ for $\lambda > 0$.

numerical estimates of the path-length distributions). These two quantities describing the statistics of random-walk path lengths turn out to be closely related to the phase-transition measures proposed in Eqs. (3) and (4) as discussed below.

The truncated estimation of the entropy rate from Eq. (3) can be given as the time-normalized mean path

length $\langle \mathcal{L}(t) \rangle_P / t$ (see Appendix A), which reduces to the Kolmogorov-Sinai entropy rate of the underlying Markov process [34] (see Appendix B):

$$S = \langle l \rangle = - \sum_{i,j=1}^N \rho_i w_{ij} \ln w_{ij} = \boldsymbol{\rho}^\top \mathbf{L}_1 \mathbf{1}, \quad (7)$$

where $\langle \cdot \rangle$ denotes the average over the ensemble of random walkers, $\boldsymbol{\rho}^\top$ and $\mathbf{1} = (1, 1, \dots, 1)$ are the left and right eigenvectors of the stochastic matrix $\mathbf{W}$ with the unit eigenvalue, respectively, and $(\mathbf{L}_1)_{ij} = -w_{ij} \ln w_{ij}$ is the probability-weighted edge-length matrix. In the context of STNs, this entropy is equivalent to the average of the entropies associated with individual nodes (see Sec. D in the Supplemental Material [47]).

Similarly, the diffusion coefficient (4), also referred to as Lyapunov measure [34], can be given as the time-normalized variance, $\Delta_P^2 \mathcal{L}(t) / t$, of random-walk path lengths on the same STN (see Appendix A). Employing common Markov-chain statistics [34,53],

$$\Lambda = \sigma_l^2 + 2 \sum_{\tau=1}^{\infty} (\langle l_1 l_{1+\tau} \rangle - \langle l_1 \rangle \langle l_{1+\tau} \rangle), \quad (8)$$

where the first term denotes the variance of the individual edge lengths,

$$\sigma_l^2 = \langle l^2 \rangle - \langle l \rangle^2, \quad \langle l^2 \rangle = \sum_{i,j=1}^N \rho_i w_{ij} \ln^2 w_{ij}, \quad (9)$$

sampled according to the Markov process, while the second term is the sum of autocovariances for all possible time lags τ , with l_1 being the edge length in the first step. Using the transition probability matrix $\mathbf{W}$, the Lyapunov measure Λ can be expressed in finite form (see Appendix B) as

$$\Lambda = \boldsymbol{\rho}^\top \mathbf{L}_2 \mathbf{1} - (\boldsymbol{\rho}^\top \mathbf{L}_1 \mathbf{1})^2 + 2 \boldsymbol{\rho}^\top \mathbf{L}_1 \mathbf{B} \mathbf{L}_1 \mathbf{1}, \quad (10)$$

where $(\mathbf{L}_2)_{ij} = w_{ij} \ln^2 w_{ij}$ and $\mathbf{B} \equiv (\mathbf{I} - \mathbf{W} + \mathbf{1} \boldsymbol{\rho}^\top)^{-1} - \mathbf{1} \boldsymbol{\rho}^\top$, allowing for computationally efficient common matrix algebra (see Appendix D).

The equivalence of the closed-form expressions of the two measures in Eqs. (7) and (10) and the corresponding path-length statistics obtained from the direct simulation of the underlying random walk is demonstrated for the logistic and the Henon maps in the insets of panels (e), (g), (f), and (h), respectively, of Fig. 1. As expected based on Pesin's relation, the Kolmogorov-Sinai entropy [gray lines in Figs. 1(e) and 1(f)] matches the Lyapunov exponent λ (black line), computed for all control parameter values using Benettin's method [54,55]. The two get closer as the order, m , of the states increases (darker shades of gray), $S(m) \rightarrow \lambda$. However, the Lyapunov measure tends to diverge in the neighborhood of certain bifurcation points irrespective of the details of the partitioning and the used order, m , for symbolic encoding [see the red peaks in the insets of panels Figs. 1(g) and 1(h)]. On the other hand, the width and height of the peaks can be controlled via the applied resolution n (not shown here) and the order m . Systems undergoing parameter drift produce similar divergences during their quasistationary evolution prior to a dynamical phase transition (see Sec. G of

the Supplemental Material [47]). Hence, an abrupt increase in the Lyapunov measure, for example, preceding the collapse of chaos-to-periodic behavior, can serve as a precursor of such change points. From a different perspective, the above property—vanishing and low values for periodic and fully developed chaos, respectively, and divergence at the edge of chaos—suggests the interpretation of Λ as a measure of dynamical complexity [32,56,57].

The robustness of the studied measures with respect to additive measurement noise is conditioned by the robustness of the chosen symbolization procedure [58,59] (see also Sec. E in the Supplemental Material [47]). The results obtained by ordinal partitioning (OP) [3] show that the peaks preceding critical transitions are retained even for noise levels as high as 10% relative to the total signal if the pattern length of the OP matches the periodicity of the dynamics. Simple measures such as variance and the lag-1 autocorrelation [18,60] while providing efficient early warning alternatives, are rather limited to bifurcations (tipping points) involving fixpoints [8]. For the type of transitions considered here, i.e., from chaos-to-periodic behavior, even if these measures exhibit a local increase or decrease, there is no global criterion for identifying transitions due to global trends and lack of a baseline (see Sec. F of the Supplemental Material [47]; similar observations have been reported on cardiac data [61]). On the other hand, Λ not only exhibits a more pronounced local relative increase but also attains globally large values at the critical transitions while remaining low otherwise. These properties are also retained in the context of real-world data, e.g., ECG available from the Long-Term Atrial Fibrillation database [62,63], where noise and nonstationarity are simultaneously present. The extraction of the above measures from empirical time series can be realized using sliding windows (see Sec. G in the Supplemental Material [47]). The signal provided by the time-dependent Lyapunov measure at the transition to fibrillation is both clear and robust across samples [in contrast to the variance σ^2 and lag-1 autocorrelation $ACF(1)$], sometimes preceding its onset and hence serving as an early warning indicator (see Fig. 2 and Sec. H in the Supplemental Material [47] for further details and comparison with bit-number variance [22,23] and permutation entropy [14,56]).

V. CONCLUSIONS

We have demonstrated how time-series analysis can benefit from trajectory-space statistics when combined with the Markov process model for estimating trajectory probabilities (see Appendix C for further discussion and comparison with phase-space statistics). The proposed Lyapunov measure can detect dynamical phase transitions manifesting as discontinuities in the dynamical Rényi entropy (e.g., at intermittency).

The formalism developed here allows for any symbolic representation of the time series, including ordinal partition networks [29]. The proposed method can be employed for characterizing dynamical systems and time series even at high-resolution coarse graining and high-order symbolic representation, allowing cost-effective numerical estimation of the two statistical measures. Our transition matrix-based procedure can be applied in higher dimensions, and it can be generalized to continuous time dynamical systems and mul-

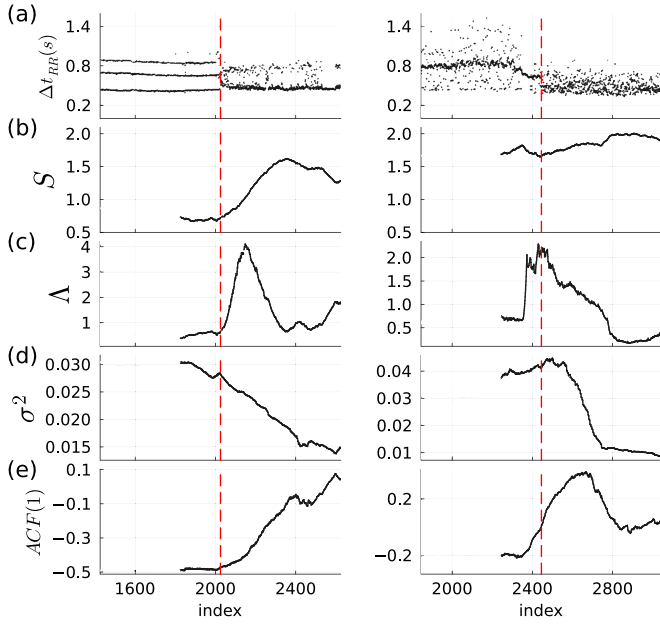


FIG. 2. Sliding-window analysis of ECG signals. Discrete time series of RR-interval lengths in seconds, $\Delta t_{RR}(s)$ [panels in row (a)], taken from two different samples (shown in the two columns, respectively). Comparison of Kolmogorov-Sinai entropy S [panel (b)], Lyapunov measure Λ [panel (c)], variance σ^2 [panel (d)] and lag-1 autocorrelation $ACF(1)$ [panel (e)], using a window of 400 data points. The obtained measures computed from each window are plotted against the index corresponding to the last data point in the respective window. Prefibrillation as well as fibrillation segments are also shown, with the vertical dashed lines denoting the fibrillation onset taken from the dataset. For each time series, S and Λ are estimated using 30 bins that divide the $(0.2, 1.2)/(0.2, 1.55)$ RR-interval ranges in the case of the samples shown in the left/right columns, respectively.

tivariate time series [3,33,34] (see Sec. I in the Supplemental Material [47] for a demonstration on the Rössler map).

The natural connection between the KS and permutation entropies [56,58] makes our method expressed by Eq. (7) combined with ordinal pattern symbolization an efficient extension for estimating permutation entropy for arbitrarily long sequences. The corresponding Lyapunov measure can be interpreted as an associated permutation complexity.

The primary role of the transition matrix $\mathbf{W}$ as the sole input to Eqs. (7) and (8) enables a straightforward application of the method to the characterization of any state-transition network, but not necessarily limited to such systems. We expect the method to yield pertinent insights for networks whose topology emerges from underlying dynamics akin to random walks (e.g., human mobility, citation, web graph). In Ref. [34], we showed that both highly cyclic structures—corresponding to periodic dynamics—and fully random networks—associated with strong chaos—suppress the variance of path lengths, while intermediate levels of structural homogeneity tend to maximize it. This behavior renders the complexity interpretation of Λ meaningful also in the context of networks.

In summary, we have outlined the mathematical foundations of a method that enables the measurement of dynamical

phase transitions in time series, facilitates the detection of early warning signals of critical transitions in intermittent chaotic dynamics, and extends and connects established measures and concepts in dynamical systems theory, time-series analysis, and network science.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [62,65].

APPENDIX A: PATH-LENGTH STATISTICS AND ENTROPIES

Let us consider a dynamical system with the set of symbolized trajectories $\mathcal{X}(t) \equiv \{\mathcal{X}(t)\}$ of joint probabilities $\mathcal{P}(t) \equiv \{\mathcal{P}(\mathcal{X}(t))\}$. Using the notations $\mathcal{P}(t) \equiv \rho_{s_1} \mathcal{P}(\mathcal{X}(t)|s_1)$ for the set of probabilities of all trajectories of t steps starting from state s_1 with probability ρ_{s_1} and $\mathcal{L}(t) \equiv -\ln \mathcal{P}(\mathcal{X}(t)|s_1)$ for the length of trajectories with given initial state s_1 , the Rényi-entropy rate (2) for $q = 1$ can be written as

$$\begin{aligned} K_1(\mathcal{P}) &= -\lim_{t \rightarrow \infty} \frac{1}{t} \langle \ln \mathcal{P}(t) \rangle_{\mathcal{P}} \\ &= -\lim_{t \rightarrow \infty} \frac{1}{t} (\langle \ln \rho \rangle_{\rho} - \langle \mathcal{L}(t) \rangle_{\mathcal{P}}) \\ &= \lim_{t \rightarrow \infty} \frac{1}{t} \langle \mathcal{L}(t) \rangle_{\mathcal{P}}, \end{aligned} \quad (\text{A1})$$

where averaging is done over all states s_i , realizations of trajectories $\mathcal{X}(t)$ of length t , and initial states s_1 , respectively.

Similarly, for the derivative with respect to q evaluated in $q = 1$, Eq. (2) yields [43]

$$K'_1(\mathcal{P}) = -\lim_{t \rightarrow \infty} \frac{1}{2t} \Delta_{\mathcal{P}}^2 \ln(\mathcal{P}(t)), \quad (\text{A2})$$

where $\Delta_{\mathcal{P}}^2 \ln(\mathcal{P}(t)) = \langle \ln^2(\mathcal{P}(t)) \rangle_{\mathcal{P}} - \langle \ln(\mathcal{P}(t)) \rangle_{\mathcal{P}}^2$ denotes the variance of the logarithm of trajectory probabilities $\mathcal{P}$ of length t . Generally, $\Delta^2(x+y) = \Delta^2 x + \Delta^2 y + 2\text{Cov}(x, y)$ for random variables x and y , with $\text{Cov}(x, y)$ denoting their covariance. Since the covariance between ρ_i and $\mathcal{P}(\mathcal{X}(t)|s_1)$

goes to zero as the number of steps, t , goes to infinity, $\text{Cov}(\rho_i, \mathcal{P}(\mathcal{X}(t)|s_1)) \rightarrow 0$, we get

$$\begin{aligned} K'_1(\mathcal{P}) &= -\lim_{t \rightarrow \infty} \frac{1}{2t} (\Delta_\rho^2 \ln \rho + \Delta_{\mathcal{P}}^2 \mathcal{L}(t)) \\ &= -\lim_{t \rightarrow \infty} \frac{1}{2t} \Delta_{\mathcal{P}}^2 \mathcal{L}(t). \end{aligned} \quad (\text{A3})$$

APPENDIX B: LYAPUNOV MEASURE AS ENSEMBLE AVERAGES

In order to compute the Lyapunov measure Λ , first we need to estimate the autocovariances in Eq. (8),

$$\text{Cov}(l_1, l_{1+\tau}) = \langle l_1 l_{1+\tau} \rangle - \langle l_1 \rangle \langle l_{1+\tau} \rangle, \quad (\text{B1})$$

for all possible time lags τ , where l_1 is the edge length in the first step. Due to the stationarity of the process, considering an ensemble of random walkers with initial distribution ρ , the ensemble-averaged step length is constant along the $\tau = 1, \dots, t$ steps of the random walks, $\langle l \rangle = \langle l_\tau \rangle$, and it can be expressed as

$$\langle l \rangle = -\sum_{i=1}^N \rho_i \sum_{j=1}^N w_{ij} \ln w_{ij} = \rho^\top \mathbf{L}_1 \mathbf{1}, \quad (\text{B2})$$

where $(\mathbf{L}_1)_{ij} = -w_{ij} \ln w_{ij}$ is the probability-weighted edge-length matrix, and $\rho^\top$ and $\mathbf{1} = (1, 1, \dots, 1)$ are the left and right eigenvectors of the stochastic transition matrix $(\mathbf{W})_{ij} = w_{ij}$ with unit eigenvalue, respectively. Note also that for $t \gg 1$, the ensemble-averaged edge lengths during the random walks do not depend on the starting positions of the walks.

Now, considering time lags $\tau \in \{1, 2, \dots\}$ we calculate the τ th-order covariance of step lengths l ,

$$\begin{aligned} \langle l_1 l_{1+\tau} \rangle &= \sum_{s_1=1}^N \rho_{s_1} \sum_{s_2=1}^N w_{s_1 s_2} (-\ln w_{s_1 s_2}) \sum_{s_3=1}^N w_{s_2 s_3} \\ &\quad \dots \sum_{s_{\tau+1}=1}^N w_{s_\tau s_{\tau+1}} (-\ln w_{s_\tau s_{\tau+1}}) \\ &= \rho^\top \mathbf{L}_1 \mathbf{W}^{\tau-1} \mathbf{L}_1 \mathbf{1}. \end{aligned}$$

Using the identity

$$(\mathbf{W} - \mathbf{1}\rho^\top)^k = \mathbf{W}^k - \mathbf{1}\rho^\top, \quad \rho^\top \mathbf{W} = \rho^\top, \quad \mathbf{W}\mathbf{1} = \mathbf{1}, \quad (\text{B3})$$

for any $k \geq 1$, for the infinite sum of covariances we need to calculate

$$\begin{aligned} \mathbf{B} &= \sum_{\tau=1}^{\infty} (\mathbf{W}^{\tau-1} - \mathbf{W}^\infty) = \sum_{k=0}^{\infty} (\mathbf{W}^k - \mathbf{1}\rho^\top) \\ &= (\mathbf{I} - \mathbf{1}\rho^\top) + \sum_{k=1}^{\infty} (\mathbf{W} - \mathbf{1}\rho^\top)^k, \end{aligned}$$

where $\mathbf{W}^\infty \equiv \lim_{k \rightarrow \infty} \mathbf{W}^k$. Denoting with $\mathbf{A} = \mathbf{W} - \mathbf{1}\rho^\top$ and knowing that $\mathbf{W}^\infty = \mathbf{1}\rho^\top$, the sum

$$\lim_{k \rightarrow \infty} \sum_{i=1}^k \mathbf{A}^i = \lim_{k \rightarrow \infty} \mathbf{A}(\mathbf{I} - \mathbf{A})^{-1}(\mathbf{I} - \mathbf{A}^{k+1}) = \mathbf{A}(\mathbf{I} - \mathbf{A})^{-1},$$

since from Eq. (B3) $\lim_{k \rightarrow \infty} \mathbf{A}^k = \mathbf{0}$.

Finally, we have

$$\mathbf{B} = (\mathbf{I} - \mathbf{1}\rho^\top) + (\mathbf{W} - \mathbf{1}\rho^\top)(\mathbf{I} - \mathbf{W} + \mathbf{1}\rho^\top)^{-1}, \quad (\text{B4})$$

and hence the infinite sum of autocovariances from Eq. (B1) is given by

$$\begin{aligned} \sum_{\tau=1}^{\infty} \text{Cov}(l_1, l_{1+\tau}) &= \sum_{\tau=1}^{\infty} \rho^\top \mathbf{L}_1 (\mathbf{W}^{\tau-1} - \mathbf{W}^\infty) \mathbf{L}_1 \mathbf{1} \\ &= \rho^\top \mathbf{L}_1 \mathbf{B} \mathbf{L}_1 \mathbf{1}. \end{aligned} \quad (\text{B5})$$

Bringing everything together, the variance of individual edge lengths is

$$\sigma_l^2 = \langle l^2 \rangle - \langle l \rangle^2 = \rho^\top \mathbf{L}_2 \mathbf{1} - (\rho^\top \mathbf{L}_1 \mathbf{1})^2, \quad (\text{B6})$$

where $(\mathbf{L}_2)_{ij} = w_{ij} \ln^2 w_{ij}$, the entropy rate can be expressed by using Eq. (B2) as

$$S = \rho^\top \mathbf{L}_1 \mathbf{1}, \quad (\text{B7})$$

while the Lyapunov measure is given by the

$$\Lambda = \rho^\top \mathbf{L}_2 \mathbf{1} - (\rho^\top \mathbf{L}_1 \mathbf{1})^2 + 2\rho^\top \mathbf{L}_1 \mathbf{B} \mathbf{L}_1 \mathbf{1} \quad (\text{B8})$$

closed-form expression, where

$$\mathbf{B} \equiv (\mathbf{I} - \mathbf{W} + \mathbf{1}\rho^\top)^{-1} - \mathbf{1}\rho^\top. \quad (\text{B9})$$

For systems defined by a random transition matrix $\mathbf{W}$ with uniformly distributed elements, the Lyapunov measure Λ approaches 1/4 as the number of states goes to infinity [34].

APPENDIX C: ROLE OF TRAJECTORY-SPACE STATISTICS

For memoryless dynamics, the KS entropy and the Lyapunov measure reduce to the Shannon entropy of states and the corresponding bit-number variance, which rely solely on the state distribution [21–23]. However, for general dynamics, the former two measures calculated from trajectories convey additional information on the underlying behavior of the system telling apart meaningful dynamics from random noise with the same statistics [4,64]. For example, the tent map, which does not exhibit criticality, and the (always) critical map produce visually similar time series, x_τ , and Rényi-entropy spectra of states, $H_q(\rho^*)$, for parameters $r = 0.8$ and $r = 2$, respectively. Therefore, natural distribution-based measures such as the Shannon entropy and bit-number variance cannot reliably indicate critical dynamics. Moreover, for these parameters, even some of the trajectory-based quantities can fail to reveal criticality having basically identical Lyapunov exponents λ , Kolmogorov-Sinai entropies, $S = \lambda = 0.5$, and topological entropies, $h_t = \ln 2$ [21,24]. However, the Rényi-entropy spectrum of trajectories exhibits qualitative differences (see Sec. C in the Supplemental Material [47]): the critical map, unlike the tent map, has a divergent derivative at $q = 1$, which can be grasped by the Lyapunov measure.

APPENDIX D: NUMERICAL ESTIMATION OF S AND Λ

For large symbol numbers N (high phase-space resolution n or high-order representations m), the transition matrix $\mathbf{W}$, is

typically sparse resulting in a storage cost of $\mathcal{O}(N)$. Therefore, the proposed matrix algebra expressions for computing the two measures in Eqs. (7) and (10) involve a computational cost of $\mathcal{O}(N)$.

The third term in Eq. (10) contains a matrix inverse but in conjunction with an inner product, allowing for the application of a linear solver instead of inversion. More precisely, we are looking for the vector

$$\mathbf{z} = (\mathbf{I} - \mathbf{W} + \mathbf{1}\rho^\top)^{-1}\mathbf{L}_1\mathbf{1}.$$

The sparseness of $\mathbf{W}$ allows for the use of high-efficiency iterative solvers. The solution in $\mathbf{z}$ is obtained as the fixpoint

of the iteration

$$\mathbf{z}' = \mathbf{W}\mathbf{z} - \mathbf{1}\langle\mathbf{z}\rangle + \mathbf{L}_1\mathbf{1},$$

where $\langle\mathbf{z}\rangle \equiv \rho^\top\mathbf{z}$. Using a random vector as an initial value of $\mathbf{z}$, the iteration converges for all systems studied here.

The necessary functionalities such as computing the symbolic representation, the transition matrix, and the corresponding measures are implemented in our Julia package, `StateTransitionNetworks.jl`. The full code base has been released on Github (see Ref. [65]). The main results included in this work can be repeated from scratch with the codes in the `stn_paper` directory (see the attached README file).

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