Pattern identification using lattice spin systems: A thermodynamic formalism

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The paper addresses data-driven statistical pattern identification in complex dynamical systems, where the concept is built upon thermodynamic formalism of symbolic data sequences in the setting of lattice spin systems. The transfer matrix approach has been used for generation of pattern vectors from time series data of observed parameters. Efficacy of pattern identification is demonstrated for early detection of anomalies (i.e., deviations from the nominal pattern) on an experimental apparatus of nonlinear active electronic circuits.
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A critical issue in the study of natural and human-engineered complex systems is to adequately describe the dynamics of the underlying process by a computationally tractable mathematical model in closed form. However, high dimensionality, underlying chaotic behavior, nonlinear and nonstationary dynamics, and noisy excitation often restrict applications of the fundamental laws of physics because of inadequate modeling accuracy and precision.[1] As such, the problem is investigated using alternative means of extraction of useful information from the time series data of selected observables (e.g., sensor information).

Analysis of dynamical systems using the tools of statistical mechanics,[2] called *thermodynamic formalism*,[3,4] has been a subject of significant interest over the last few decades in the field of applied physics and computational mechanics. In statistical mechanics, the macroscopic behavior of a system, represented by a few intensive parameters (e.g., pressure and temperature), is expressed in terms of the expected values obtained from the probability distributions of the microstates. These distributions are postulated based on the microscopic activities of individual particles and their (possible) mutual interactions. Similarly, in a dynamical system, the macroscopic properties that represent the expected behavior of the system can be derived from statistical patterns (e.g., probability distributions and statistical correlations) generated from time series data of observable sensor and/or analytical measurements.[5] These statistical patterns provide a link between the microscopic and macroscopic behavior of a dynamical system.

The paper presents data-driven pattern identification in dynamical systems using the transfer matrix method of lattice spin systems.[2,4,6] The pattern identification problem is formulated such that both stationary and quasistatically evolving dynamics of the underlying system can be described in terms of the behavioral patterns of an analogous lattice spin system. The analogy is developed for a one-dimensional Potts model that describes a lattice spin system using a spin alphabet $\mathcal{S}$ with $|\mathcal{S}|\geqslant 2$. (Note that the Potts model is a generalization of the Ising model that is restricted to the binary alphabet, i.e., $|\mathcal{S}|=2$.) The key contributions of the paper are delineated below.

(1) Pattern identification in dynamical systems built upon the concepts of statistical mechanics of lattice spin systems.
(2) Construction of an appropriate Hamiltonian from the symbol sequence to establish an analogy between the methods of symbolic dynamics and the transfer matrix analysis of lattice spin systems.
(3) Representation of an r-Markov sequence ($r\geqslant 1$) by a Potts model with interactions of range r, such that the nearest-neighbor interactions (i.e., $r=1$) correspond to a standard Markov sequence [see Eqs. (4) and (7)].
(4) Concept validation with experimental data of an active nonlinear electronic system

The tools of symbolic dynamics are often used to study the behavior of complex dynamical systems,[7] where the state trajectory is represented by a sequence of symbols.[5,7] Let $\Omega\subset\mathbb{R}^n$ be a compact (i.e., closed and bounded) region within which the (stationary) motion is circumscribed under a given exogenous stimulus. The region Ω is partitioned as $\{\Phi_1,\ldots,\Phi_{|\Sigma|}\}$ consisting of $|\Sigma|$ mutually exclusive (i.e., $\Phi_j\cap\Phi_k=\varnothing$, $\forall j\neq k$), and exhaustive (i.e., $\cup_{j=1}^{|\Sigma|}\Phi_j=\Omega$) cells, where Σ is the *symbol alphabet* that labels the partition segments. Each initial state $\mathbf{x}_0\in\Omega$ generates a sequence of symbols defined by the mapping $\mathcal{M}:\Omega\rightarrow\Sigma$ such that

$$\mathbf{x}_0 \rightarrowtail \sigma_0\sigma_1\sigma_2,\cdots,\sigma_k,\cdots, \tag{1}$$

where $\sigma_i \triangleq \mathcal{M}(\mathbf{x}_i)$. The mapping in Eq. (1) is called *symbolic dynamics* as it attributes a legal (i.e., physically admissible) symbol sequence to the system dynamics starting from a given initial condition. This symbolic representation of quasistationary time series of observed parameters is constructively similar to the structure of a lattice spin system such that an observed symbol $\sigma_k\in\Sigma$ at time k is analogous to a spin $s_k\in\mathcal{S}$ at a lattice site k.[6] Since the Potts model represents a lattice system with a spin alphabet $\mathcal{S}$, an analogy is formulated with the symbol sequence generated from a dynamical system with a symbol alphabet Σ, such that $|\mathcal{S}|=|\Sigma|\geqslant 2$. The equivalence is illustrated in Fig. 1 for the simplest case of an Ising model with $\mathcal{S}=\{\uparrow,\downarrow\}$, which is analogous to the symbol sequence generated with $\Sigma=\{0,1\}$. In general, spin systems can be translated into symbolic stochastic processes and vice versa.[4]

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$\boxed{\ldots \uparrow\downarrow\downarrow\uparrow\downarrow\uparrow \ldots \uparrow\uparrow\downarrow\uparrow\downarrow \ldots \equiv \ldots 100101 \ldots 11010 \ldots}$

FIG. 1. Equivalence of the one-dimensional structure of Ising model and a symbolic sequence with alphabet set $\Sigma = \{0,1\}$.

The local space-time behavior of a thermodynamic system's constituents is described by a Hamiltonian; an analogous approach for dynamical systems is presented here. Since stationary (possibly Markov) symbol chains are frequently used to construct statistical models of dynamical systems, the Hamiltonian $\mathcal{H}_{\bar{\sigma}}$ for an observed symbol sequence $\bar{\sigma}$ can be expressed as a function of the conditional probability of occurrence of $\bar{\sigma}$ at the initial state q_0. In this paper, $\mathcal{H}_{\bar{\sigma}}$ is defined as

$$\mathcal{H}_{\bar{\sigma}} \triangleq -\ln[P(\bar{\sigma}|q_0)], \tag{2}$$

where $q_0 \equiv \sigma_{r-1}, \ldots, \sigma_0$ is the initial state of length r, $\bar{\sigma} \equiv \sigma_{n+r-1}, \ldots, \sigma_r$ is the observed sequence of length n, and $P(\star|\bullet)$ is the conditional probability of $\star$ given $\bullet$. Equation (2) implies that $\mathcal{H}_{\bar{\sigma}}$ is non-negative and finite (i.e., $0 \leqslant \mathcal{H}_{\bar{\sigma}} < \infty$). Given the initial state q_0, a deterministic sequence whose probability of occurrence is one has zero energy (i.e., $\mathcal{H}_{\bar{\sigma}}=0$); similarly, a sequence that is forbidden from state q_0 must have energy tending to infinity. In general, all sequences that have the same probability of occurrence from a given initial state q_0 form an equivalence class of systems having the same energy in the statistical mechanical sense.

Let r be the order of the Markov model of the dynamical system which is analogous to the effect of range r interactions in a spin system. In general, for $r \geqslant 1$, $\mathcal{H}_{\bar{\sigma}}$ from Eq. (2) can be factored into the structure of a generalized Ising model (i.e., the Potts model) as derived below,

$$\begin{aligned}\mathcal{H}_{\bar{\sigma}} &= -\ln[P(\bar{\sigma}|\sigma_{r-1}, \ldots, \sigma_0)] \\ &= -\ln[P(\sigma_{n+r-1}, \ldots, \sigma_r|\sigma_{r-1}, \ldots, \sigma_0)] \\ &= -\ln[P(\sigma_{n+r-1}|\sigma_{n+r-2}, \ldots, \sigma_0), \ldots, P(\sigma_r|\sigma_{r-1}, \ldots, \sigma_0)] \\ &\Rightarrow \mathcal{H}_{\bar{\sigma}} = -\ln\left[\prod_{k=0}^{n-1} P(\sigma_{k+r}|\sigma_{k+r-1}, \ldots, \sigma_0)\right].\end{aligned} \tag{3}$$

For an r-Markov process, Eq. (3) reduces to

$$\mathcal{H}_{\bar{\sigma}} = -\ln\left[\prod_{k=0}^{n-1} P(\sigma_{k+r}|\sigma_{k+r-1}, \ldots, \sigma_k)\right]. \tag{4}$$

Since $P(\bar{x}\bar{y}|\bar{y}\bar{z}) = P(\bar{x}|\bar{y}\bar{z})P(\bar{y}|\bar{y}\bar{z}) = P(\bar{x}|\bar{y}\bar{z})$, where $\bar{x}$, $\bar{y}$, and $\bar{z}$ are any finite adjacent strings on a symbol sequence, we obtain

$$P(\sigma_{k+r}, \ldots, \sigma_{k+1}|\sigma_{k+r-1}, \ldots, \sigma_k) = P(\sigma_{k+r}|\sigma_{k+r-1}, \ldots, \sigma_k) \tag{5}$$

for $\bar{x}=\sigma_{k+r}$, $\bar{y}=\sigma_{k+r-1}, \ldots, \sigma_{k+1}$, and $\bar{z}=\sigma_k$. It follows from Eqs. (4) and (5) that

$$\mathcal{H}_{\bar{\sigma}} = -\ln\left[\prod_{k=0}^{n-1} P(\sigma_{k+r}, \ldots, \sigma_{k+1}|\sigma_{k+r-1}, \ldots, \sigma_k)\right] \Rightarrow \mathcal{H}_{\bar{\sigma}} = -\sum_{k=0}^{n-1} \ln[P(\eta_{k+1}^r|\eta_k^r)], \tag{6}$$

where $\eta_k^r \equiv \sigma_{k+r-1}, \ldots, \sigma_k$ and $\eta_{k+1}^r \equiv \sigma_{k+r}, \ldots, \sigma_{k+1}$ are the states of length r. Equation (6) has the structure of a generalized Ising model, where the interaction energies are represented by the logarithms of the transition probabilities between the adjacent states on a symbol sequence.[1,4] For a Markov process ($r=1$), i.e., nearest-neighbor interactions, Eq. (6) reduces to

$$\mathcal{H}_{\bar{\sigma}} = -\sum_{k=0}^{n-1} \ln[P(\sigma_{k+1}|\sigma_k)]. \tag{7}$$

The analytical solution of one-dimensional spin systems with finite-range interactions is derived by expressing the partition function in terms of its finite-dimensional transfer matrix; all thermodynamic information is encoded in the transfer matrix.[4] The solution assumes cyclic periodic conditions ($\sigma_{n+k-1}=\sigma_{k-1}$ for $k=1, \ldots, r$), which are statistically irrelevant for sufficiently large data sequences.[2] Analogous to statistical mechanics, the partition function for a dynamical system (assuming the inverse temperature β equal to 1) is defined as

$$\mathcal{Z}_n = \sum_{\bar{\sigma}} \exp(-\mathcal{H}_{\bar{\sigma}}) = \sum_{\sigma_r} \cdots \sum_{\sigma_{n+r-1}} \exp(-\mathcal{H}_{\bar{\sigma}}), \tag{8}$$

where the summation is taken over all possible symbol sequences of length n.[2] Equations (6) and (8) yield

$$\begin{aligned}\mathcal{Z}_n &= \sum_{\sigma_r} \cdots \sum_{\sigma_{n+r-1}} \exp\left(\sum_{k=0}^{n-1} \ln[P(\eta_{k+1}^r|\eta_k^r)]\right) \\ &= \sum_{\sigma_r} \cdots \sum_{\sigma_{n+r-1}} \prod_{k=0}^{n-1} P(\eta_{k+1}^r|\eta_k^r) \Rightarrow \mathcal{Z}_n \\ &= \sum_{\sigma_r} \cdots \sum_{\sigma_{n+r-1}} \prod_{k=0}^{n-1} \mathcal{T}_{\eta_k^r, \eta_{k+1}^r},\end{aligned} \tag{9}$$

where $\mathcal{T}_{\eta_k^r,\eta_{k+1}^r} = P(\eta_{k+1}^r|\eta_k^r)$. Since with symbol alphabet Σ, η_k^r, and η_{k+1}^r can each have $|\Sigma|^r$ possible configurations, a $|\Sigma|^r \times |\Sigma|^r$ transfer matrix $\mathcal{T}$ (Ref. 4) is defined whose $(i,j)^{\text{th}}$ term is $\mathcal{T}_{\eta^r(j),\eta^r(i)}$, where $\eta^r(i)$ and $\eta^r(j)$ represent the ith and the jth configurations of states of length r, respectively. For example, if $\Sigma=\{0,1\}$ and $r=2$, then $|\Sigma|^r=4$, where the possible states are $\{00,10,01,11\}$ and the 4×4 transfer matrix includes all transition probabilities between these states. It can be shown[2,4] that Eq. (9) is the same as $\mathcal{Z}_n = \mathrm{Trace}(\mathcal{T}^n)$.

The statistical information of an r-Markov process is encoded in the transfer matrix $\mathcal{T}$. The elements of $\mathcal{T}$ are state transition probabilites that are calculated from the observed symbol sequences at nominal and different anomalous conditions. The gradual evolution of $\mathcal{T}$ with respect to the nominal condition represents the growth of small (parametric or nonparametric) changes in the dynamical system. For pattern identification, the symbol sequence derived from partitioning the time series data under the nominal condition, generates the *transfer matrix* $\mathcal{T}^0$ that, in turn, is used to obtain the *pattern vector* $\mathbf{p}^0$, where $\mathbf{p}^0$ is the left eigenvector of $\mathcal{T}^0$ corresponding to the (unique) unit eigenvalue (Note that $\mathcal{T}$ is an irreducible stochastic matrix). Similarly, the pattern vectors $\mathbf{p}^1, \mathbf{p}^2, \ldots \mathbf{p}^m, \ldots$. can be generated at subsequent anomalous conditions based on the respective time series data. (Note that the partitioning is fixed at the nominal condition). Since anomaly is defined as a deviation from the nominal behavior, a scalar macroscopic variable ψ is defined such that

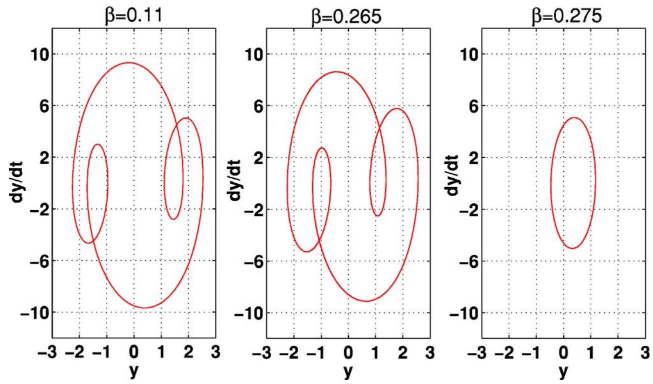

FIG. 2. (Color online) Phase plots in electronic circuit experiments.

$$\psi_m = d(\mathbf{p}^m, \mathbf{p}^0), \tag{10}$$

where $d(\bullet,\bullet)$ is a distance function (for example, the standard Euclidean norm). In general, any analytical variable derived from the statistical pattern vectors can serve as a macroscopic parameter.

This statistical mechanical concept of pattern identification has been validated on the experimental data collected from a laboratory apparatus[8] built upon an active nonlinear electronic system that emulates the second-order nonautonomous, forced Duffing equation modeled as

$$\frac{d^2y}{dt^2} + \beta\frac{dy}{dt} + y(t) + y^3(t) = A\cos(\omega t). \tag{11}$$

The dissipation parameter β is varied slowly with respect to the response of the dynamical system; $\beta=0.11$ is the nominal condition and a change in the value of β is indicative of an anomaly in the behavior of the dynamical system. Specifically, the objective is early detection of small changes in the parameter β well before it manifests into a drastic phenomenon (e.g., chaos) in the system dynamics. With amplitude $A=22.0$ and $\omega=5.0$, a sharp change in the behavior is noticed around $\beta=0.275$, possibly due to bifurcation. The phase plots, depicting this drastic change behavior, are shown in Fig. 2.

Sets of time series data of the observed sensor variable y were generated for different values of β. The data set at the nominal condition (i.e., $\beta=0.11$) was used to create a partitioning using the *maximum entropy principle*[8] with $|\Sigma|=6$ and is kept invariant for other data sets. As the dynamical behavior of the system changes due to variations in β, the statistical characteristics of the symbol sequences are also altered, leading to the evolution of transfer matrix $\mathcal{T}$. Anomaly is then captured using Eq. (10). The results are presented in Fig. 3 for $r=1$ and $r=2$. It is seen that results do not improve significantly for $r=2$ indicating that $r=1$ is adequate for pattern identification in this system. With β increasing from 0.11, there is a gradual increase in the distortion measure ψ before the abrupt change in the vicinity of

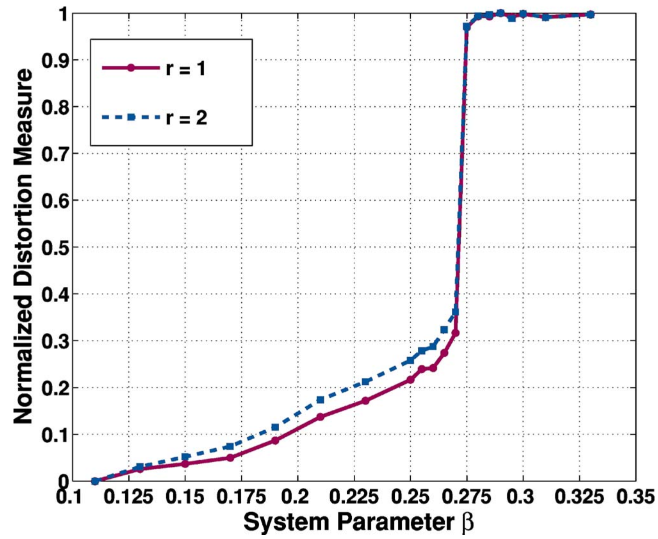

FIG. 3. (Color online) Early detection of anomalies in electronic circuit experiments.

$\beta=0.275$. This indicates growth and detection of the evolutionary changes much before a drastic change occurs in the dynamical behavior.

The major conclusion of this paper is that thermodynamic formalism is a useful tool for dynamic data-driven pattern identification in dynamical systems. The underlying concept is built upon the fundamental principles of *symbolic dynamics* and *statistical mechanics*. The method of transfer matrix analysis of spin systems is demonstrated for extraction of statistical information from symbol sequences that are generated from the time series data of observed process variables. The concepts presented in this paper may also be extended to higher dimensions using multidimensional spin system models for sensor data fusion and pattern identification, which is a topic of future research.

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