A generic scheme for choosing models and characterizations of complex systems

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It is argued that the two problems of choosing characterizations and models of complex systems should not be considered independently. A particular criterion for these choices, oriented on the potential usefulness of the results, is considered, and a generic formalization applicable to realistic experiments is developed. It is applied to Kuramoto-Sivashinsky chaos.

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The systematic characterization of self-organized structures is a long-standing challenge to the science of structure formation. ‘Labyrinths’, ‘breathers’, ‘dendrites’, ‘worms’, ‘spiral-defect chaos’, or ‘scale-free networks’ are only few of the words that were introduced to describe real and numerical experimental observations. Images and natural language can usually communicate what is meant, but as the number of observed structures increases and distinctions become finer, a more systematic approach seems desirable. The problem is felt particularly strong for the large variety of spatially irregular structures and spatio-temporally chaotic states that have been found.

In search for appropriate characterizations researchers do often concentrate on those properties of the experimental data that are easily modeled – those properties of the data or the underlying structures that are governed by their own rules (one might call them “coherent structures”). In this case, the choice of the characterization depends on the available models. On the other hand, only when a particular set of properties of experimental data has been found to be characteristic for an observed structure, one can meaningfully ask for a model that reproduces this structure, i.e., a model that reproduces data with these properties. Modeling requires prior characterization.

Intuition is the fallback most researchers rely on when facing this circular relationship of modeling and characterizing. In fact, intuition is an excellent guide. But for some problem areas, e.g., those involving spatio-temporal chaos, progress appears to have slowed down also due to a lack of intuition about what the characteristic properties and what appropriate models are. Even when intuition is successful in choosing models and characterizations, it is legitimate to ask if these choices are subjective in the sense that they depend essentially on the way humans observe the world (other beings might decide very differently), or if they are the solution of some objective problem, that our intuition is just highly efficient in solving. Most of the approaches to the related problem of emergence (e.g., [2, 3]) are based on the a priori assumption of some limitation to observation (coarse graining), thus involving an “inherently subjective” component. For an argument in favor of the objectivity of the choices it is therefore important to formulate a criterion that does not depend on such artificial limitations.

Here, a proposal for such a criterion is introduced. It is first stated on a heuristic level and then modeled in a mathematical language; thus modeling the problem of modeling. This involves the combination of concepts from computer science that proved powerful in the context of structure formation – algorithmic complexity (program length) [1, 2] and computational complexity (execution time) [4, 5] – with ideas from statistical test theory [6]. It is shown that the circular relation between models and characterizations is, in this case, not vicious: the criterion leads to nontrivial choices. As an example, the formalism is applied to the spatio-temporally chaotic solutions of the Kuramoto-Sivashinsky Equation.

Consider the following requirements for models and characterizations:

Characterizations should be easily communicated and verified, be specific, and should, over a wide control-parameter range, apply to experimental data and be reproducible in models.

Models should be easily communicated and easily evaluated, show little artifacts, and reproduce given characterizations.

The practical relevance of most of these requirements is obvious. To see why it is desirable that characterizations are reproducible in models, notice that, from such models, larger, composed models could be constructed, that can then be used to explore and characterize situations not accessible experimentally (e.g., climate models). Even though the existence of models of sub-systems that reproduce the properties relevant for the composed model is not guaranteed, in case that they exist, it is good to know them. Now, as the general criterion, choose those pairs of models and characterizations that jointly satisfy conditions [1] and [2] as well as possible.

In order to formalize this criterion and make it accessible to a rigorous analysis, both characterizations and models are represented by computer programs: programs that test data for particular properties, and programs that generate data. The practical use of these programs is illustrated in Fig. [1].
to produce random results, the program has access to a source of independent, evenly distributed random bits. Subsequent runs of a generator are fully independent.

As in conventional statistical test theory \( \mathbb{A} \), the \emph{power function} is introduced. Denote by \( t_x(\{y_i\}) \) the output of the test \( t \) at control parameter \( x \in C[t] \) when applied to the sequence of experimental results \( \{y_i\} \in D^\infty \) (for formal simplicity, the sequences \( \{y_i\} \) are assumed infinite, even though the tests use only finite subsequences). Let \( \{Y_i\} \) be a sequence of i.i.d. random results with values in \( D^\infty \). Define the power of the test function \( t_x \) when applied to \( \{Y_i\} \) as the probability to reject \( \{Y_i\} \), i.e.,

\[
pow(t_x, \{Y_i\}) := \Pr[t_x(\{Y_i\}) = 0] \quad (x \in C[t]).
\] (3)

Unlike in conventional test theory, there is no independent null hypothesis \( H_0 \) here that states the distribution or the class of distributions of \( \{Y_i\} \) that is tested for. Instead, given a test function \( t_x \), the null hypothesis, i.e., the class of distributions, is defined by the condition

\[
pow(t_x, \{Y_i\}) \leq \alpha,
\] (4)

where \( 0 < \alpha < 1 \) is a fixed significance level \( \mathbb{A} \).

The ease or difficulty of communicating a test \( t \) or model \( g \), mentioned in requirements \( \mathbb{B} \), is measured by the lengths \( L(t) \), \( L(g) \) of the programs \( t \) and \( g \). The value of \( L(\cdot) \) depends on the machine model. In the example below, MMIX, an idealized modern microprocessor is used \( \mathbb{C} \).

The ease or difficulty of verifying characterizations and evaluating models is measured by the execution times \( T(g), T(t) \) of the programs. To be specific, define \( T(\cdot) \) as the maximum of the expectation value of the runtime over all \( x \in C \) and all distributions of data. Below, time is measured by the number of “oops” (symbol: \( 1 \times \)) counted by the MMIX emulation \texttt{mix-sim} \( \mathbb{D} \).

The often-encountered tradeoff between \( L \) and \( T \) is taken into account by assuming that there is a cost function depending on both resources, which increases strictly monotonically with \( L \) at fixed \( T \) and with \( T \) at fixed \( L \) but is otherwise unspecified. With this in mind, define the relations \( \preceq \) (\emph{always cheaper or equal}) and \( \prec \) (\emph{always cheaper}) for programs \( p_1, p_2 \) by

\[
p_1 \preceq p_2 \iff L(p_1) \leq L(p_2) \text{ and } T(p_1) \leq T(p_2)
\] (5)

and

\[
p_1 \prec p_2 \iff p_1 \preceq p_2 \text{ and not } p_2 \preceq p_1.
\] (6)

It turns out that the machine dependence of relations \( \preceq \) and \( \prec \) for implementations of algorithms on different processor models is weak. In principle, other resources could also be taken into account in definition \( \mathbb{E} \) such as, for tests, the number of experimental runs required.

Since for every program \( p \) there is only a finite number of programs with smaller or equal length, there is also
only a finite number of programs $p'$ such that $p' \prec p$ or $p' \preceq p$. Below we need Lemma 1: Every nonempty set $P$ of tests or generators contains an element $p$ which is minimal with respect to the relation $\prec$, i.e., such that no $p' \in P$ satisfies $p' \prec p$. This is a direct consequence of the previous note and the transitivity and antireflexivity of $\prec$. In general, there are several minimal elements, each using its own mix of resources. This reflects the intuition that there are several “good” models and characterizations for one experiment.

These concepts from statistics and computer science are now combined to formalize requirement (2), except for the condition regarding artifacts. Denote by $g_x$ the sequence $\{Y_i\}$ of random outputs of generator $g$ at control parameter $x$. Define for given $C$, $D$ the notion of an optimal generator $g$ relative to a test $t$ and a power threshold $1 > \gamma > \alpha$ by

$$\text{opt}_t^\gamma g \overset{\text{def}}{=} \bigwedge_{x \in C[t]} \text{pow}(t_x, g_x) \leq \alpha \text{ and } \bigvee_{g' \prec g \atop x \in C[t]} \text{pow}(t_x, g'_x) > \gamma \text{ and } \bigvee_{g' \preceq g \atop x \in C[t]} \text{pow}(t_x, g'_x) \geq \text{pow}(t_x, g_x),$$

(7a)

(7b)

(7c)

where the quantifiers $\bigwedge$ (for all) and $\bigvee$ (there is) have been introduced for brevity. Line (7a) states that $g$ satisfies $t$, line (7b) says that all cheaper generators are rejected by $t$ with power $> \gamma$, and line (7c) handles the generators that use the same resources as $g$. The test $t$ is specific to $g$ in the sense that it does not apply to any $g' \prec g$.

In order to disentangle the circularity between models and characterizations, consider now the problem of specifying a generator by characterizing its output. For a i.i.d. random sequence $\{Y_i\}$ denote by $p[\{Y_i\}]$ the distribution function of its elements, i.e., $p[\{Y_i\}](y) := \Pr[Y_1 = y]$ for $y \in D$. Call a generator $g$ an optimal implementation with respect to a set $C \subset C$ if there is no generator $g' \prec g$ such that $p[g'_x] \equiv p[g_x]$ for all $x \in C$. Theorem 1: Given $C$ and $D$, there is for every $C \subset C$, every optimal implementation $g$ with respect to $C$, and every $1 > \gamma > \alpha$, a test $t$ such that $\text{opt}_t^\gamma g$ and $C[t] = C$. Outline of the proof: Explicitly construct $t$. $x \in C$ can be tested for by keeping a list of $C$ in $t$. Since there is only a finite number of $g' \preceq g$, the test must distinguish $p[g_x]$ from a finite number of different distributions $p[g'_x]$ for all $x \in C$, with certainty $\gamma$ if $g' \prec g$. This can be achieved by comparing a sufficiently accurate representation of $p[g_x]$, stored in $t$ for all $x \in C$, with a histogram sampled from $g'_x$. With a high number of samples, any degree of certainty can be reached. The cost of testing is not taken into account, yet.

The following definition formalizes the criterion stated above for choosing models and characterizations; to find pairs $(t, g)$ jointly satisfying conditions (12) as well as possible. Only the validity of characterizations for experiments is not contained in the definition: Given $C$ and $D$, call a pair $(t, g)$ a basic model specifying characterization (b.m.s.c.) iff there is a $1 > \gamma > \alpha$ such that $\text{opt}_t^\gamma g$ and there is no $t' \prec t$ with $C[t] \subset C[t']$ and $\text{opt}_{t'}^\gamma g$.

This optimization with respect to $t$ implies the avoidance of artifacts, when artifacts are considered as properties that are specific and are cheaper to communicate and verify than the property $t$ that $g$ is supposed to model. The definition of a b.m.s.c. involves the simultaneous minimization of cost with respect to $t$ and $g$. An answer to the question if there are any nontrivial solutions to this double optimization problem – i.e., if the circular relation between models and characterizations as considered here is vicious – is given by Theorem 2: Given $C$ and $D$, there is for every $C \subset C$ and every optimal implementation $g$ with respect to $C$, a test $t$ such that $(t, g)$ is a b.m.s.c. and $C \subset C[t]$. Proof: Fix some $1 > \gamma > \alpha$. By Theorem 1, the set $S := \{t|t \text{opt}_t^\gamma g \text{ and } C \subset C[t]\}$ is nonempty. Theorem 2 is satisfied by any $t \in S$ which is minimal with respect to the half ordering $\prec$. By Lemma 1 such an element exists. D

Only for a few b.m.s.c. $(t, g)$ the test $t$ also applies to a given experiment. Generally, there will be some fundamental level of description (the Schrödinger equation, say) at which a 1-to-1 model $g$ of the experiment can be constructed, and then a corresponding test $t$ exists by Theorem 2. But these b.m.s.c. are often too expensive. Finding cheaper b.m.s.c. that apply to the data requires intuition, insight, and experience, and goes beyond the scope of this work. The goal here was only to investigate if an objective, well-posed problem of modeling and characterizing exists, and to model it so that among several solutions conceived some are selected.

As an example for an application, assume some idealized experiment, the fundamental description of which is given by the Kuramoto-Sivashinsky (KS) equation

$$\partial_t u = -\partial^2_x u - \partial^4_x u + u \partial^2_x u,$$

(8)

with periodic boundary conditions $u(\tau, \xi) = u(\tau, \xi + \Xi)$, as they apply for experiments in a ring-channel geometry. In each experimental run, 128 equally spaced points of $u$ at distance $\Delta \xi = 0.8 \,(\Xi = 128 \times 128)$ are sampled 200 times in $\Delta \tau = 0.2$ sampling intervals, while $u$ is evolving along the chaotic KS attractor. The data format $D$ is given by all sequences of $128 \times 200 = 25600$ 8-byte floating point numbers. There is no control parameter: $x$ is always the empty string and the only element of $C$.

The systematic construction of a pair $(t, g)$ likely to be a b.m.s.c. of the experiment goes from the generator $g$ over a corresponding test $t$ to a verification that the experiment passes the test $t$. Practically finding a suitable $g$ requires a preliminary approximation of $t$ characterizing the experiment. This first, exploratory step is not described here.
The code for the generator $g$ is a minimal-length implementation of Eq. (8) on an MMIX processor. A discretization $u_{p,q}$ locally approximately proportional to a solution $u(10^p \Delta \tau, q \Delta x)$ of Eq. (8) is obtained by an Euler integration with in-place update of the form

$$u_{p+1,q} = c_1 (u_{p,q+2} + u_{p+1,q-2}) + c_2 (u_{p,q+1} + u_{p+1,q-1}) + (c_3 + u_{p,q+1} - u_{p+1,q-1}) u_{p,q},$$

where $(c_1, c_2, c_3) \approx (-0.05, 0.18, 0.75)$. Including code to handle the periodic boundaries, to initialize $u_{0,q}$ with random numbers $O(10^{-2})$, to drop a transient of 16 time units, and to output $y$ (Fig. 2b), this requires $L(g) = 260$ bytes and $T(g) = 34$ Mv for a single run.

For the test $t$, a code is used that implicitly computes the stripes $\partial u(t, \xi) > 0$ (Fig. 2b) using data of every $k$-th sampling interval ($k \approx 5$). Then it determines for each of $N = 20$ runs the total numbers of beginnings $n_b$, ends $n_e$, mergers $n_m$, and splits $n_s$ of the stripes along the time axis, as well as the average number $l$ of stripes. The value of $N$ implicitly determines $\delta$.

If a combination $(n_b, n_e, n_m, n_s, l)$ is repeated for two runs, the test rejects the data stream in order to enforce randomness. The averages $\overline{n_b}, \overline{n_e}, \overline{n_m}, \overline{n_s}, \overline{l}$ of these statistics over all $N$ runs are determined. The data is rejected if $\overline{n_e} > m_e \approx 15.2$ or $\overline{n_s} > m_s \approx 0.4$, which enforces the tree-like geometry of the stripes and consequently a minimal accuracy of $g$. Data is rejected if $(\overline{n_l} - m_l)^2 > v_l$ or $(\overline{n_b} - m_b)^2 > v_b$, which sets the length and time scales of the tree structure $\{(m_l, v_l, m_b, v_b) \approx (14., 0.03, 22., 1.5)\}$. Finally, data is rejected if the difference between the initial and final number of stripes is large, i.e., $(\overline{n_l} + \overline{n_m} - \overline{n_b} - \overline{n_s})^2 > v_a \approx 1.7$, which enforces the suppression of a transient in the generator. Within the statistical error, $t$ accepts $g$ at the $\alpha = 0.1$ significance level: $\text{pow}(t_x, g_x) = 0.105(3) \lesssim \alpha$. Using precise numerical simulations of Eq. (8), it was verified that solutions of the fundamental description (Fig. 2b) are rejected by $t$ with a probability of only 0.031($\alpha < \alpha$. That is, $t$ characterizes the “experimental” data and is even robust to small deviations from the fundamental description $\mathcal{B}$. A compiler-optimized implementation of $t$ requires $L(t) = 1192$ bytes and $T(t) = 3.8$ Mv = $N \times 0.19$ Mv.

In principle, the precise values of the tuning parameters in $t$ could be determined by locally solving the optimization problem for the condition for the pair $(t, g)$ to be a $b.m.s.c.$ to the precision of the coding of the parameters. Regarding the question if this pair is also a global solution of the optimization problem for a $b.m.s.c.$, it can only be said that this is a plausible conjecture. It has been checked that the direct verification of Eq. (9) would yield a test that is shorter than the tree-test $t$, but requires much more time. Likewise, generators more explicitly coded to generate tree structures accepted by $t$ could be faster than $g$, but the examples investigated indicate that, due to several conditional branches, they would always be longer. Thus, no counterexamples could be found. Notice that the information reduction performed by $t$ in concentrating on the stripes $\partial u > 0$ is not externally imposed. Rather, it is the a consequence of the rather small number of competing generators to be excluded.

To the degree that the pair $(t, g)$ described here it is a $b.m.s.c.$, it is also of practical relevance. The tree-test $t$ provides a fast, rather simple, and robust way to identify KS chaos. There seems to be no other simple “explanation” for the structure identified by $t$. On the other hand, $g$ provides a simple and, as it turns out, cooperatively fast method to obtain approximations of KS chaos on digital computers, which is important whenever resources are scarce.

A formal scheme combining computation and statistics for choosing models and characterizations has been laid out. It models the main aspects of the practical problem. The question if the choices are “intuitive” is presumably hard to answer systematically. At least, it has been argued, they are useful: not because nature is a computer, but because people use computers.

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[10] This suppresses simple characterizations that are valid only in complex subsets of $C$.
[11] From $t_x$, computable tests for the same $H_0$ at other significance levels can be constructed.