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On spurious detection of linear response and misuse of the fluctuation–dissipation theorem in finite time series

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ABSTRACT

Using a sensitive statistical test we determine whether or not one can detect the breakdown of linear response given observations of deterministic dynamical systems. A goodness-of-fit statistics is developed for a linear statistical model of the observations, based on results for central limit theorems for deterministic dynamical systems, and used to detect linear response breakdown. We apply the method to discrete maps which do not obey linear response and show that the successful detection of breakdown depends on the length of the time series, the magnitude of the perturbation and on the choice of the observable.

We find that in order to reliably reject the assumption of linear response for typical observables sufficiently large data sets are needed. Even for simple systems such as the logistic map, one needs of the order of 10^6 observations to reliably detect the breakdown with a confidence level of 95%; if less observations are available one may be falsely led to conclude that linear response theory is valid. The amount of data required is larger the smaller the applied perturbation. For judiciously chosen observables the necessary amount of data can be drastically reduced, but requires detailed *a priori* knowledge about the invariant measure which is typically not available for complex dynamical systems.

Furthermore we explore the use of the fluctuation–dissipation theorem (FDT) in cases with limited data length or coarse-graining of observations. The FDT, if applied naively to a system without linear response, is shown to be very sensitive to the details of the sampling method, resulting in erroneous predictions of the response.

1. Introduction

An important question in the study of probabilistic properties of dynamical systems is how to determine the response of a system if subjected to a small perturbation. For example, in climate science we would like to know how the global mean temperature changes upon increasing CO_2 levels. This problem was solved in statistical physics in the context of thermostatted Hamiltonian systems, establishing the framework of linear response theory [1–4]. In essence, linear response theory employs a Taylor expansion of the perturbed invariant measure around the unperturbed equilibrium measure; with a manipulation of terms in this expansion one may then approximate averages of observables in the perturbed system entirely from knowledge of the statistics of the unperturbed system.

The study of linear response involves two issues: proving differentiability of the response and finding an expression for the derivative of the response. To establish linear response, the invariant measure needs to be differentiable with respect to the parameter describing the magnitude of the perturbation. For the existence of an analytical formula for the response in terms of the equilibrium fluctuations of the unperturbed system, which is the statement of the celebrated fluctuation–dissipation theorem (FDT), the invariant measure needs additionally to be differentiable with respect to the phase space variables.

Applying this framework to deterministic dynamical systems, in particular to forced dissipative systems whose dynamics evolves on an attractor of zero Lebesgue measure in the full space, has been a challenge. In a series of papers, Ruelle showed that the response is linear for the class of uniformly hyperbolic Axiom A systems, i.e. the invariant measure is differentiable with respect to the magnitude of the perturbation [5–8].

Due to the singular nature of the invariant measure of forced dissipative systems the fluctuation–dissipation theorem, however, cannot hold. Heuristically this failure can be understood by realizing that typical perturbations will have a non-zero projection

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along the stable manifold, generally transverse to the attractor, whereas the invariant measure is supported entirely on the attractor. Therefore one cannot estimate the response by solely considering correlations of the unperturbed system. A linear response formula can still be expressed, but involves the full linear tangent dynamics and must take into account the evolution of exponentially attenuated perturbations along stable directions rather than just the unperturbed fluctuations along the unstable manifolds as in the FDT.

The hope that linear response theory can be extended to more general chaotic dynamical systems has been dampened by numerical results on the tent map [9] and rigorous analysis by Baladi and co-workers [10–14]. In particular, it was shown that the logistic map does not obey linear response. This is due to the non-smooth changes of the invariant measure when perturbing from a chaotic parameter value to a periodic one or vice versa. Even worse, even when restricting to the Cantor set of chaotic parameter values the measure is not differentiable in the sense of Whitney. On the other hand, there are numerical simulations suggesting that linear response might exist for some examples of non-uniformly hyperbolic systems [15–17] including the Lorenz '63 system which involves homoclinic tangencies. Furthermore, the lack of structural stability, which was believed to be an obstruction to linear response theory in the climate system [18], does not preclude the existence of linear response as was rigorously shown in [19]. The current belief in the mathematical community is that a sufficient condition for the existence of linear response is the summability of the correlation function; the summability of the correlation function is, however, shown not to be necessary for general observables [20,21].

Notwithstanding the lack of rigorous mathematical proofs for its validity for general forced dissipative non-equilibrium systems, linear response theory has been taken up in the climate sciences to predict the response of the climate, as was first proposed by Leith [22]. Linear response theory and the fluctuation–dissipation theorem have since been used with some success by several groups. They have been applied to various toy models related to atmospheric chaos [23,17,24–27], barotropic models [28–30], quasi-geostrophic models [31], atmospheric models [32–38] and coupled climate models [39–42]. These successes have led scientists to believe that high-dimensional complex systems may very well obey linear response. The standard argument is that complex systems involve a multitude of interacting processes on several temporal and spatial scales and behave effectively stochastically with a smooth invariant measure [23]. This point of view seems at least reasonable for observables of the slow dynamics of complex multi-scale systems which in the limit of infinite time-scale separation are asymptotically stochastic [43–45]. In the case of stochastic dynamical systems linear response theory can indeed be justified [46,47]. However, several instances are now known where atmospheric and oceanic dynamics exhibits a rough dependence on parameters [48], and where, even if linear response theory is observed, the fluctuation–dissipation theorem is not valid [49].

On a more fundamental level, however, it is by no means clear that high-dimensional complex systems do obey linear response theory. In this paper we do not attempt to answer this question. Rather, we consider the following practical issue: systems which do not obey linear response theory are observed with *finite* time series. In such cases we seek to show that the breakdown might not be detectable, and the system's observed behavior may appear consistent with linear response theory. Moreover, the choice of the observable is crucial for the detectability of the breakdown of linear response in finite time series. In particular, we will show that global observables are less able to detect the non-smoothness of the invariant measure whereas local observables which hone in on the roughness of the invariant measure will make the non-smoothness apparent for smaller amounts of data. Finally, the perturbation size also impacts on the detectability of breakdown, with smaller perturbations requiring more data for successful breakdown detection.

This work is motivated by the contradiction between the reported success of linear response theory in the climate sciences and rigorous mathematical results proving the non-existence of linear response theory for a large class of dynamical systems.

The paper is organized as follows. In Section 2 we briefly review linear response theory and the fluctuation–dissipation theorem. In Section 3 we propose a goodness-of-fit test to probe for the validity of linear response in time series. In Section 4 we discuss the logistic map, demonstrate the mechanism leading to the breakdown of linear response for this one-dimensional map and show how this breakdown might not be apparent with time series of insufficient length. We show the effect of finite data size as well as how the choice of the observable can either mask or emphasize the non-smoothness of the invariant measure. In Section 6 we show further that in situations where linear response does not exist, an application of the FDT cannot provide any reliable statistical information, not even in an averaged sense. We conclude with a summary in Section 7.

2. Linear response theory

We consider here a family of dynamical systems $f_\varepsilon : M \to M$ on some space M. We assume that the map f_ε depends smoothly on the parameter ε and that for each ε the dynamical systems admit a unique invariant physical measure μ_ε, e.g. absolutely continuous measures or Sinai–Ruelle–Bowen measures (SRB). An ergodic measure is called physical if for a set of initial conditions of nonzero Lebesgue measure the temporal average of a typical observable converges to the spatial average over this measure. Considering an observable $A : M \to \mathbb{R}$, we are interested in the change of the average of the observable

$$\langle A\rangle_\varepsilon = \int_M A\, d\mu_\varepsilon$$

upon varying ε. A system is said to have *linear response* if the derivative

$$\langle A\rangle'_{\varepsilon_0} := \frac{\partial}{\partial\varepsilon}\langle A\rangle_\varepsilon|_{\varepsilon_0}$$

exists. It is obvious that a sufficient condition for linear response is that the invariant measure μ_ε is differentiable with respect to ε. If the limit does not exist, we say there is a breakdown of linear response. We assume that the observable captures sufficient dynamic information about the dynamical system; for example, an odd observable on a system symmetric about 0 would be identically zero regardless of whether the system had a linear response or not.

One may further ask whether, if linear response exists, a computable analytical expression for the linear response

$$\langle A\rangle_\varepsilon \approx \langle A\rangle_{\varepsilon_0} + \langle A\rangle'_{\varepsilon_0}\,\delta\varepsilon \tag{1}$$

can be found for small values of $\delta\varepsilon = \varepsilon - \varepsilon_0$. To write down an expression of the linear response, we introduce a vector field X as $X \circ f_{\varepsilon_0} := \partial_\varepsilon f_\varepsilon|_{\varepsilon=\varepsilon_0}$. Note that the introduction of the vector field X is the standard way of formulating perturbations in statistical physics as $f_\varepsilon = f_{\varepsilon_0} + \delta\varepsilon X(f_{\varepsilon_0})$. The linear response $\langle A\rangle'_{\varepsilon_0}$ can then be formally expressed as

$$\frac{\partial}{\partial\varepsilon}\langle A\rangle_\varepsilon|_{\varepsilon_0} = \sum_{n=0}^{\infty}\langle X(x)\nabla(A\circ f^n_{\varepsilon_0})(x)\rangle_{\varepsilon_0}, \tag{2}$$