Irreversibility and Fluctuation Theorem in Stationary Time Series

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The relative entropy between the joint probability distribution of backward and forward sequences is used to quantify time asymmetry (or irreversibility) for stationary time series. The parallel with the thermodynamic theory of nonequilibrium steady states allows us to link the degree of asymmetry in the time signal with the distance from equilibrium and the lack of detailed balance among its states. We study the statistics of time asymmetry in terms of the fluctuation theorem, showing that this type of relationship derives from simple general symmetries valid for any stationary time series.

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Detecting time asymmetry or irreversibility in stationary time series is important not only because time series may be easier to predict and model in one direction, but especially because irreversibility is a symptom of non-Gaussian forcing and dynamic nonlinearities [1,2]. Moreover, when time series represent the evolution of either stochastic or deterministic dynamical systems, irreversibility takes on a special meaning linked to the lack of equilibrium and detailed balance of the probability fluxes among the system states. Despite its importance, however, the issue of time irreversibility has received relatively less attention compared to other aspects of nonlinear time series analysis, with a few notable exceptions [1–11]. In thermodynamics and statistical mechanics, reversibility is synonymous with equilibrium. Steady-state systems that are in equilibrium obey detailed balance, while nonequilibrium steady-state (NESS) systems are time irreversible and have a positive internal entropy production rate [12]. Recently, a renewed interest has been sparked by the discovery of general relationships valid also far from equilibrium [13,14]. The fluctuation theorem (FT), in particular, links the probability of realizations that consume entropy to those that produce it as a function of the system size. The theorem was originally proposed for many particle systems [15,16], and was then verified experimentally [17] and derived theoretically for Markovian processes [18–22].

In this Letter we borrow from the thermodynamics of NESS and information theory to propose a consistent framework to quantify the degree of asymmetry in stationary time series. We also show that FT-type relationships derive from simple symmetries between forward and backward sequences which are valid with great generality for any discrete and continuous stationary time series independently of their dynamics.

Measure of asymmetry.—Let us begin by considering a stationary time series x assumed for now to be discrete in time. The series may be naturally discrete or have been discretized from a continuous series after suitable coarse graining. Let the joint probability distribution of a sequence of n consecutive values of the time series be $p(x_1, x_2, \ldots, x_n)$, and the corresponding distribution of the reverse sequence $\hat{p}(x_1, x_2, \ldots, x_n)$. The fundamental symmetry

$$\hat{p}(x_1, x_2, \ldots, x_n) = p(x_n, x_{n-1}, \ldots, x_1) \tag{1}$$

links the forward and the backward distributions. This property is very general and independent of any stationarity assumption. With these definitions, a stationary time series is said to be reversible (or time symmetric) if and only if $p(x_1, x_2, \ldots, x_n) = \hat{p}(x_1, x_2, \ldots, x_n)$ for any n. Thus, any time series generated as a Bernoulli sequence is reversible. In the case of Markov chains with transition matrix P_{ij} and steady-state distribution π_i, time symmetry (or reversal) holds if [23] $\pi_i P_{ij} = \pi_j P_{ji}$, and the chain is said to be in detailed balance. Although the backward sequence is still generated by a Markov chain [23], this has a different transition matrix, $\hat{P}_{ij} = \frac{\pi_j}{\pi_i} P_{ji}$. For stationary Markov processes this property is generalized as $\hat{p}(x_1|x_2)p(x_2) = p(x_2|x_1)p(x_1)$ (see [24], p. 83).

For general stationary time series the degree of time irreversibility and nonequilibrium can be determined by how different the backward and forward joint probability distributions are. A natural statistic to quantify the difference between p and $\hat{p}$ is the relative entropy or Kullback-Leibler distance [25]

$$\langle Z_n \rangle = \sum p(x_1, x_2, \ldots, x_n) \log \frac{p(x_1, x_2, \ldots, x_n)}{\hat{p}(x_1, x_2, \ldots, x_n)}, \tag{2}$$

where the sum is intended over all the possible states x_1, $x_2, \ldots, x_n$ [26]. Equation (2) can be interpreted as the mean of the difference between the "surprise" of finding a given sequence in forward time, i.e., $\log p$, and in reverse time, i.e., $\log \hat{p}$, or equivalently

$$Z_n = \log \frac{p(x_1, x_2, \ldots, x_n)}{\hat{p}(x_1, x_2, \ldots, x_n)}. \tag{3}$$

$\langle Z_n \rangle$ is always positive and it is zero only if the two distributions are equal [25]. It can be shown to be symmetric, $\langle Z_n \rangle = \langle \hat{Z}_n \rangle$, because of Eq. (1), and that $\langle Z_n \rangle \geq \langle Z_{n-1} \rangle$. The same measure is used to quantify the lack of equilibrium and detailed balance in NESS systems [18,19]. $\langle Z_n \rangle$ can also be expressed as a difference between the so-called block entropy [28], H_n, and another form of entropy, H_n^R, introduced in the context of NESS thermodynamics [19]. Division by n transforms these quantities into entropy rates, the limits of which, under suitable conditions, converge to

$$\lim_{n\to\infty} \frac{\langle Z_n \rangle}{n} = \lim_{n\to\infty}\left(\frac{H_n^R}{n} - \frac{H_n}{n}\right) = h^R - h = \sigma, \quad (4)$$

where h is the Kolmogorov-Sinai entropy, and σ is related to the internal entropy generation rate (it is always positive and zero only for time-reversible stationary time series). It is important to note that $\langle Z_n \rangle$ is infinite if at least one sequence is not found in reverse, i.e., if $\hat{p}$ is zero for at least one sequence. This is the case, for example, of irreversible periodic signals and of Markov chains that have asymmetric zeros in their transition matrices.

The behavior of $\langle Z_n \rangle / n$ as a function of n is of particular interest in time series as it describes the degree of temporal asymmetry at different scales. In the trivial case of Bernoulli sequences, as well as in the case of two state Markov processes [4], $\langle Z_n \rangle$ is always zero, while for Markov chains with three or more states one gets [19,20] $\langle Z_n \rangle = n \sum \pi_i P_{ij} \log[\pi_j P_{ij}/(\pi_i P_{ji})]$, for $n \geq 2$, which shows, as expected from the behavior of H_n/n [28], that the corresponding rates are constant and equal to σ for $n \geq 2$.

Fluctuation theorem.—An important property for Z_n can be derived solely from (1) and the moment generating function (MGF) of Z_n, $G_n(k) = \langle e^{-kZ_n} \rangle$. In fact, writing

$$G_n(k) = \sum p(x_1, x_2, \ldots, x_n)\left[\frac{p(x_1, x_2, \ldots, x_n)}{\hat{p}(x_1, x_2, \ldots, x_n)}\right]^{-k}$$
$$= \sum p(x_1, x_2, \ldots, x_n)\left[\frac{p(x_1, x_2, \ldots, x_n)}{\hat{p}(x_1, x_2, \ldots, x_n)}\right]^{-(1-k)}, \quad (5)$$

which follows from (1) and the commutative property of summation, one obtains

$$G_n(k) = G_n(1 - k). \quad (6)$$

Equation (6) is the FT in the k domain, and implies that the MGF is symmetric around $k = \frac{1}{2}$. The fact that $G_n(0) = 1$ and the convexity of the MGF ([29], pp. 48–49) confirm that $\langle Z_n \rangle$ is always greater than or equal to zero. Equation (6) also provides a symmetry among the moments of $p/\hat{p}$. In particular, $k = 1$ corresponds to the harmonic mean of $p/\hat{p}$ which is therefore always equal to 1. A more meaningful form of the FT is obtained in terms of the probability distribution of Z_n, $p_{Z_n}(Z_n)$. Using the property of the MGF (e.g., discrete Laplace transform) that $L^{-1}\{G_n(k - a)\} = e^{aZ_n} L^{-1}\{G_n(k)\}$ and $L^{-1}\{G_n(-k)\} = p_{Z_n}(-Z_n)$, where $L^{-1}\{\cdot\}$ denotes inverse Laplace transform, it is immediate to show that

$$p_{Z_n}(-Z_n) = p_{Z_n}(Z_n) e^{-Z_n}, \quad (7)$$

which implies that the negative tail of the probability distribution decays faster than the positive one. It is important to highlight that the two equivalent properties (6) and (7) require only stationarity, which is implicit in the definition of the averaging operation of the MGF, and are a direct consequence of the symmetry property (1) used in Eq. (5).

Continuous time series.—All of the above properties remain valid for time series in continuous time and with continuous state space, with only the proviso of extending the Kullback-Leibler distance using differential entropies ([25], p. 231). A different and useful formulation valid at a point in time can also be obtained by assuming that the n points in the sequence are separated by Δt, and then considering the limit $\Delta t \to 0$. In this limit, in fact, there is a one-to-one correspondence between the joint probability density functions (PDF's) of a sequence of n points of a time series and that (distinguished by an asterisk) of its subsequent time derivatives, at a point in time,

$$p(x_1, x_2, \ldots, x_n) \Leftrightarrow p^*\left(x, \frac{dx}{dt}, \frac{d^2x}{dt^2}, \ldots, \frac{d^{n-1}x}{dt^{n-1}}\right)\Bigg|_{x=x_1}. \quad (8)$$

Taking into account that, when the continuous time series is looked at backwards in time, the odd derivatives change sign, the fundamental relationship (1) is replaced by

$$\hat{p}^*\left(x, \frac{dx}{dt}, \ldots, \frac{d^{n-1}x}{dt^{n-1}}\right) = p^*\left(x, -\frac{dx}{dt}, \ldots, (-1)^{n-1}\frac{d^{n-1}x}{dt^{n-1}}\right). \quad (9)$$

Thus, in analogy to the discrete case, one can define the continuous version of Eq. (3) as

$$Z_n^* = \log\frac{p^*}{\hat{p}^*}, \quad (10)$$

where the arguments of the joint PDF's have been dropped for conciseness. Using conditional probabilities in Eq. (10), the measure of asymmetry given by the mean of Z_n^* can be written as the mean of the asymmetries at any given level x,

$$\langle Z_n^* \rangle = \int p_X(x) \langle Z_n^* | x \rangle \, dx, \quad (11)$$

where $p_X(x)$ is the PDF of the stationary process and

$$\langle Z_n^* | x \rangle = \int \ldots \int p^*(\dot{x}, \ddot{x}, \ldots | x) \times \log \frac{p^*(\dot{x}, \ddot{x}, \ldots | x)}{p^*(-\dot{x}, \ddot{x}, \ldots | x)} d\dot{x}\, d\ddot{x} \ldots, \quad (12)$$

where we used the dot notation for time derivatives [30]. While Eqs. (11) and (12) are problematic to compute for real time series, a simple measure of asymmetry involving the first time derivative of a signal can be obtained as

$$\langle Z_2^* \rangle = \int p_X(x) \int p_{\dot{X}}(\dot{x}|x) \log \frac{p_{\dot{X}}(\dot{x}|x)}{p_{\dot{X}}(-\dot{x}|x)} dx\, d\dot{x}, \quad (13)$$

where the integrals extend over the whole domains of X and $\dot{X}$. In applications to time series, $p_{\dot{X}}(\dot{x}|x)$ can be easily computed for different values of x and then averaged out to obtain (13). Since $\langle Z_n^* \rangle$ is strictly increasing with n, $\langle Z_2^* \rangle$ provides a sufficient condition for asymmetry.

Using again the MGF and the properties of the continuous (bilateral) Laplace transforms ([29], pp. 48–49), Eqs. (6) and (7) can be shown to hold also for Z_n^*. Moreover, the FT is now also valid at a point in time (independently of stationarity) and for any x,

$$p_{Z_n^*|x,t}(-Z_n; x, t) = p_{Z_n^*|x,t}(Z_n; x, t) e^{-Z_n}. \quad (14)$$

For $n = 2$, Eq. (14) provides a relationship for the PDF of $Z_2^* = \log[p_{\dot{X}}(\dot{x}|x)/p_{\dot{X}}(-\dot{x}|x)]$ that can be readily verified in real time series. It is also interesting to derive the previous property for a general one-dimensional Langevin equation with drift $f(x)$ and diffusion $g(x)$. In this case, $\dot{X}|x$ has a Gaussian distribution with mean equal to $f(x)$ and variance $\lim_{\Delta t \to 0}[g^2(x)/\Delta t]$ [24,29,31]. It follows that $Z_2^*|x$ is a linear function of $\dot{X}|x$, i.e., $Z_2^*|x = \lim_{\Delta t \to 0}[2(\Delta x/\Delta t) f(x)/(g^2(x)/\Delta t)]$. As a result, $Z_2^*|x$ is still Gaussian with mean $\lim_{\Delta t \to 0}[2f^2(x)/(g^2(x)/\Delta t)]$ and variance always equal to twice the mean, which is exactly the condition for a Gaussian distribution to satisfy Eq. (14). Moreover, since the mean of $Z_2^*|x$ is proportional to Δt, $\langle Z_2^* | x \rangle \to 0$ for $\Delta t \to 0$. Because of the Markovian nature this is also true for $n \geq 2$ and therefore, as expected, detailed balance and reversibility are always satisfied [24,31].

Applications.—The estimation of the relative entropies as our measures of asymmetry, $\langle Z_n \rangle$ and $\langle Z_n^* \rangle$, raises several technical issues and it is prone to underestimation especially for high values of n [32,33]. Here we use only a simple binning procedure, based on equiprobabilistic partitioning, to discretize the support of the forward and backward probability distribution, limiting the estimation to relatively coarse partitioning and small values of n. A further difficulty for estimation is the occurrence of infinities. Because of statistical errors in the estimation of small probabilities for finite data sequences, we stipulate that only finite ratios of the probabilities may contribute to the estimate, thus excluding infinities generated by possible forbidden sequences in the reverse direction.

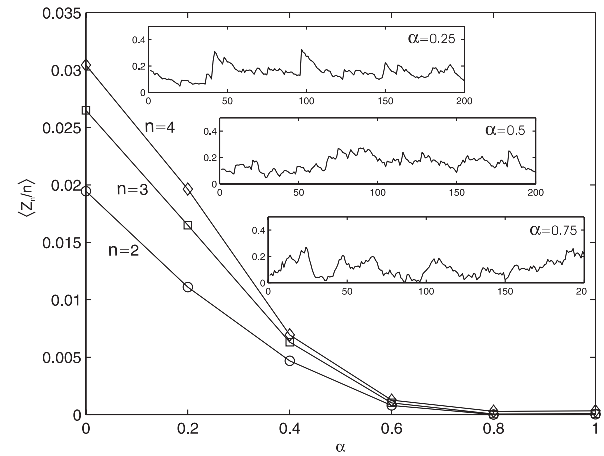

FIG. 1. Asymmetry statistic, $\langle Z_n \rangle / n$, for the stochastic process $x_t = (1 - \alpha)\eta_t + \alpha \xi_t$ ($k = 0.07$, $\gamma = 0.04$, $\lambda = 0.28$) as a function of α for different block lengths n.

We first apply our method to stochastic time series generated by $x_t = (1 - \alpha)\eta_t + \alpha \xi_t$, where η_t is the (asymmetric) jump process with exponential decays of rate k and exponentially distributed jumps of mean γ occurring as a Poisson process with rate λ, while ξ_t is an Ornstein-Uhlenbeck process with mean and variance equal to those of η_t. Figure 1 shows $\langle Z_n \rangle / n$ estimated for different α for three values of n and equiprobable partition with eight states. Notice the relatively smooth decay to zero as the Gaussian noise becomes more dominant, reflecting the decreasing asymmetries in the signal. Also, $\langle Z_n \rangle / n$ appears to increase with n before decaying to a finite limit for large n (not shown). Computations not reported here also confirm the validity of the fluctuation theorem for various n and partition number. A preliminary comparison has shown good agreement with the method by [8].

As a second application we consider 50 years of discharge measurements from the Po River, Italy. We first quantify the asymmetry of the time series by using embedding sequences [7], $x_1, x_{1+\tau}, \ldots, x_{1+(n-1)\tau}$, where τ is the delay time and n is the embedding dimension. This allows us to explore longer temporal windows focusing on optimal values of τ and without the estimation problems of high dimensional sequences. The results [Fig. 2(b)] indicate a strong asymmetry in the time series, which becomes most evident at a time scale of 10–15 days and is likely linked to the typical duration of the falling limbs of the hydrographs after flood peaks. Beyond that temporal range, the data points tend to become more and more independent and thus time reversible. We also illustrate the validity of the FT for the distributions of time derivatives for different values of x, $Z_2^*|x$. Figure 2(c) shows the resulting distribution of slopes for x equal to the mode of the series. From the distribution of slopes, $Z_2^*|x$ is found by taking $\log[p(\dot{x}|x)/p(-\dot{x}|x)]$, from which the probability distribution of $Z_2^*|x$ is derived by change of variable,

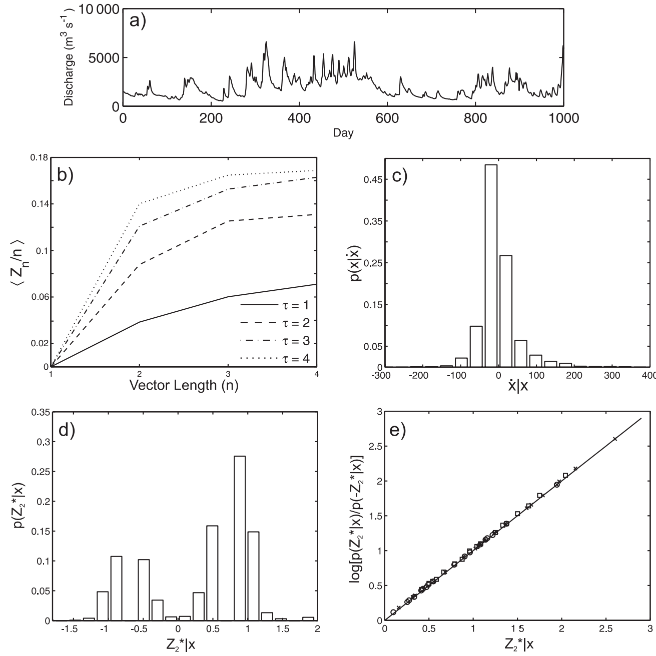

FIG. 2. (a) Portion of Po River (Italy) discharge series, (b) asymmetry measure computed for different delay times, (c) PDF of time derivative given x chosen as the mode of the distribution, (d) PDF of $Z_2^*(\dot{x}|x)$, and (e) the resulting FT for the PDF of $Z_2^*|x$ where x is chosen, respectively, as the mode (circles), mean (squares), and the median (crosses) of the discharge series.

Fig. 2(d). The general validity of the FT is illustrated in Fig. 2(e) by taking $\log[p(Z_2^*|x)/p(-Z_2^*|x)]$ for the mode, median, and mean of the time series.

We have presented a statistic measuring temporal asymmetry in time series which draws on the theory of NESS in thermodynamics and retains general applicability for both discrete and continuous cases. We have shown also that the symmetry in the PDF of $\log(p/\hat{p})$, referred to as the FT, applies generally to any stationary time series and arises from basic properties of its MGF.

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