Decision Making in the Arrow of Time

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(Received 6 August 2015; published 16 December 2015)

We show that the steady-state entropy production rate of a stochastic process is inversely proportional to the minimal time needed to decide on the direction of the arrow of time. Here we apply Wald's sequential probability ratio test to optimally decide on the direction of time's arrow in stationary Markov processes. Furthermore, the steady-state entropy production rate can be estimated using mean first-passage times of suitable physical variables. We derive a first-passage time fluctuation theorem which implies that the decision time distributions for correct and wrong decisions are equal. Our results are illustrated by numerical simulations of two simple examples of nonequilibrium processes.

DOI: 10.1103/PhysRevLett.115.250602 PACS numbers: 05.70.Ln, 02.50.Le, 05.40.-a

Processes that take place far from thermodynamic equilibrium are in general irreversible and are associated with entropy production. Irreversibility implies that a sequence of events that takes place during a process occurs with different probability than the same sequence in time-reversed order. Irreversibility and the thermodynamic arrow of time can be illustrated considering a movie displaying the evolution of a complex dynamic process. Such a movie can be run either forward in time or in reverse. For an irreversible process it is possible to decide whether the movie is run forward or in reverse defining the direction of the arrow of time by the direction in which entropy increases on average [1]. For a system at thermodynamic equilibrium, however, even though all atoms or molecules move rapidly in all directions, it is impossible when watching a movie to tell whether it runs forward or in reverse. This raises the following question: Can the time τ_{dec} needed to decide between two hypotheses (movie run forward or in reverse) be related quantitatively to the degree of irreversibility and the rate of entropy production?

Decision theory provides a general theoretical framework to optimally make decisions based on observations of stochastic processes [2]. An important question of decision theory is, what is the earliest time to make a decision d between two competing hypothesis H_1 and H_0 with a given reliability, while observing a stochastic process? In 1943, Wald made a pioneering contribution to this problem by introducing the sequential probability ratio test (SPRT) [3], which provides the minimal mean decision time for a broad class of stochastic processes [4]. Wald's SPRT states that the decision $d = 1$ ($d = 0$) should be made when the cumulated logarithm of the likelihood ratio $\mathcal{L}(t)$ for the first time exceeds (falls below) a prescribed threshold L_1 (L_0) (see Fig. 1). The thresholds L_1 and L_0 are determined by the maximally allowed probabilities to make a wrong decision, $\alpha_1 = P(d = 1|H_0)$ and $\alpha_0 = P(d = 0|H_1)$. Here, α_1 (α_0) is the probability to incorrectly make the decision $d = 1$ ($d = 0$) when the hypothesis H_0 (H_1) is true.

In this Letter, we derive a general relation between the average entropy production rate in a nonequilibrium steady state and the mean time to decide whether a stationary stochastic process runs forward (H_1) or backward in time (H_0) using the SPRT. Furthermore, we introduce a fluctuation

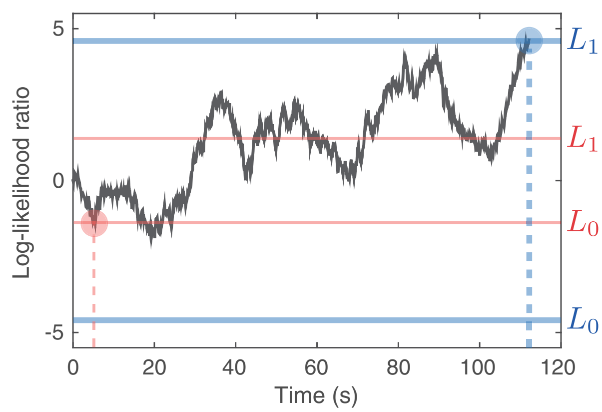

FIG. 1 (color online). Log-likelihood ratio of the sequential probability ratio test in the arrow of time as a function of time in a drift-diffusion process with diffusion coefficient $D = 0.52\ \mu\mathrm{m}^2/\mathrm{s}$ and drift velocity $v = 65\ \mu\mathrm{m/s}$. The simulation time step is $\Delta t = 0.1$ ms. The thresholds of the test are shown as horizontal lines for symmetric error probabilities equal to 20% (thin and red) and 1% (thick and blue). The thresholds L_0 and L_1 correspond to the choice of one of the two hypotheses: the sequence runs forward (L_1) or backward (L_0) in time. With 20% error probability, the decision is made faster (red circle and vertical thin red dashed line) than for 1% error probability (blue circle and vertical thick blue dashed line).

theorem for the first-passage time probability distribution of the total entropy changes and obtain a fluctuation theorem for the decision time distribution of the SPRT in the arrow of time. Our work reveals that entropy production can be estimated measuring first-passage times of stationary stochastic processes.

We consider a physical system in a nonequilibrium steady state. We denote by $X_t = \{X(s)\}_{s=0}^{t}$ a path describing the evolution of a state as a function of time t. We denote by $\tilde{X}_t$ the time-reversed path $\tilde{X}_t = \{X(t-s)\}_{s=0}^{t}$ [5]. The state of the system is characterized by the path probability $P(X_t)$. The entropy production associated with the path X_t can be defined as [6]

$$\Delta S_{\mathrm{tot}}[X_t] = k \ln \frac{P(X_t)}{P(\tilde{X}_t)}, \tag{1}$$

where k is Boltzmann's constant. We now perform a SPRT of two hypotheses. Given a path X_t, we want to decide whether it corresponds to a forward or time-reversed trajectory of the nonequilibrium steady state. We therefore consider the hypothesis $H_{\rightarrow} = H_1$ that the path runs forward in time with the conditional probability $P(X_t|H_{\rightarrow}) = P(X_t)$, and the hypothesis $H_{\leftarrow} = H_0$ that the dynamics is time reversed, for which $P(X_t|H_{\leftarrow}) = P(\tilde{X}_t)$. Using the SPRT, the decision is made when the log-likelihood ratio or Turing's weight of evidence [7]

$$\mathcal{L}(t) = \ln \frac{P(X_t|H_{\rightarrow})}{P(X_t|H_{\leftarrow})} \tag{2}$$

reaches for the first time one of the thresholds $L_1 = L$ and $L_0 = -L$, where we have chosen for simplicity a SPRT with symmetric decision error probabilities $\alpha_0 = \alpha_1 = \alpha$. When $\mathcal{L}(t)$ is continuous, we have $L = \ln[(1-\alpha)/\alpha]$ [3].

The entropy production and the log-likelihood ratio are related by

$$\mathcal{L}(t) = \frac{\Delta S_{\mathrm{tot}}[X_t]}{k}. \tag{3}$$

This provides a connection between decision theory and stochastic thermodynamics. Moreover, it allows us to obtain relations between average decision times in the SPRT and the average rate of entropy production. Applying the SPRT to continuous-time Markov processes (see Supplemental Material [8] and Ref. [11]), we show that the mean decision time for a stochastic process with continuous $\mathcal{L}(t)$ is given by

$$\langle \tau_{\mathrm{dec}} \rangle = \frac{L(1-2\alpha) + \langle \mathcal{L}_{\mathrm{ex}} \rangle_{\mathrm{dec}}}{\langle d\mathcal{L}/dt \rangle}. \tag{4}$$

Here $\langle \cdots \rangle$ denotes an ensemble average in steady state. An average over the ensemble which starts from an initial distribution of states that equals the distribution of states at the decision times is denoted by $\langle \cdots \rangle_{\mathrm{dec}}$. The excess log-likelihood ratio $\mathcal{L}_{\mathrm{ex}}$ is defined as

$$\mathcal{L}_{\mathrm{ex}} = \int_0^{\infty} \left[\frac{d\mathcal{L}}{dt'} - \left\langle \frac{d\mathcal{L}}{dt'} \right\rangle \right] dt'. \tag{5}$$

The mean decision time of the SPRT for independent identically distributed (i.i.d.) observations is a special case of Eq. (4) for which $\langle \mathcal{L}_{\mathrm{ex}} \rangle_{\mathrm{dec}} = 0$. This is because for an i.i.d. process the state distribution is identical to the stationary distribution.

We now apply the theory of decision times to the SPRT on the arrow of time of a nonequilibrium process. The relation (3) together with our Eq. (4) describing the average decision time can be used to express the average entropy production rate in steady state as

$$\frac{1}{k} \left\langle \frac{dS_{\mathrm{tot}}}{dt} \right\rangle = \frac{L(1-2\alpha) + \langle \Delta S_{\mathrm{ex}} \rangle_{\mathrm{dec}}/k}{\langle \tau_{\mathrm{dec}} \rangle}, \tag{6}$$

where

$$\Delta S_{\mathrm{ex}} = \int_0^{\infty} \left[\frac{dS_{\mathrm{tot}}}{dt'} - \left\langle \frac{dS_{\mathrm{tot}}}{dt'} \right\rangle \right] dt' \tag{7}$$

denotes the excess total entropy change.

In the limit of small α, the mean decision time becomes large, $\langle \Delta S_{\mathrm{ex}} \rangle_{\mathrm{dec}} / \langle \tau_{\mathrm{dec}} \rangle$ becomes small, and, thus, Eq. (6) simplifies to

$$\frac{1}{k} \left\langle \frac{dS_{\mathrm{tot}}}{dt} \right\rangle \simeq \frac{L(1-2\alpha)}{\langle \tau_{\mathrm{dec}} \rangle}. \tag{8}$$

Equations (6) and (8) show that the minimal average time needed to decide whether a process runs forward or backward in time is inversely proportional to the average entropy production rate. Approaching thermodynamic equilibrium, the mean decision time diverges because $\mathcal{L}(t) = 0$ in this limit. If the reliability of the decision is increased, decision times increase correspondingly. Because the average entropy production rate is a property of the process only and not of the SPRT, the ratio given in the right-hand side of Eq. (8) is thus independent of the error probability α.

Making decisions in the arrow of time provides a novel way to estimate the entropy production rate of nonequilibrium Markovian processes. Estimators for the steady-state entropy production rate can be obtained from the first-passage times τ of a suitable physical observable $\Gamma(X_t)$. If we use the first passage of a physical observable through a threshold value to decide on the arrow of time and if this decision has an error probability α, then it follows from the optimality of the SPRT that $\langle \tau \rangle \geq \langle \tau_{\mathrm{dec}} \rangle$; i.e., the mean first-passage time $\langle \tau \rangle$ is larger or equal to the mean decision time of the SPRT given in Eq. (8). The resulting estimator of the entropy production provides a lower bound to the exact value:

$$\frac{1}{k}\left\langle\frac{dS_{\mathrm{tot}}}{dt}\right\rangle \geq \frac{D[\rightarrow\|\leftarrow]}{\langle\tau\rangle}, \tag{9}$$

where $D[\rightarrow\|\leftarrow] = D[P(d|H_{\rightarrow})\|P(d|H_{\leftarrow})] = \ln[(1-\alpha)/\alpha](1-2\alpha)$ is the Kullback-Leibler divergence between the conditional probabilities of the decision variable. When decisions in the direction of time are made based on the log-likelihood ratio, i.e., when $\Gamma = \Delta S_{\mathrm{tot}}/k$, Eq. (9) becomes an equality.

The stochastic nature of decision making in the arrow of time can be characterized by the probability density $P(\tau_{\mathrm{dec}})$ of making a decision at time τ_{dec}. The connection between decision theory and thermodynamics implies a relation between the decision time distribution and the distribution of entropy production ΔS_{tot}. For Markovian processes, the probability density $P(\Delta S_{\mathrm{tot}};t)$ of entropy production ΔS_{tot} during the time interval t is related by a fluctuation theorem to the probability density to reduce entropy by the same amount: $P(\Delta S_{\mathrm{tot}};t)/P(-\Delta S_{\mathrm{tot}};t) = \exp(\Delta S_{\mathrm{tot}}/k)$ [12–16]. In addition, we find that the probability distribution of the first-passage time τ of entropy production also obeys the following detailed fluctuation theorem if the transition probabilities are translationally invariant [17] (see Supplemental Material [8]):

$$\frac{P(\tau;\Delta S_{\mathrm{tot}})}{P(\tau;-\Delta S_{\mathrm{tot}})} = \exp(\Delta S_{\mathrm{tot}}/k). \tag{10}$$

Here, $P(\tau;\Delta S_{\mathrm{tot}})d\tau$ denotes the probability to reach the value ΔS_{tot} for the first time in the time interval $[\tau,\tau+d\tau]$ given that the entropy production has not reached $-\Delta S_{\mathrm{tot}}$ before.

The relation between entropy production and the log-likelihood ratio [Eq. (3)] together with the first-passage time fluctuation theorem [Eq. (10)] implies for the SPRT in the arrow of time

$$\frac{P(\tau_{\mathrm{dec}};L)}{P(\tau_{\mathrm{dec}};-L)} = \exp(L). \tag{11}$$

Here, $P(\tau_{\mathrm{dec}};L)$ is the probability distribution of the decision time of the SPRT for a given error rate α. $P(\tau_{\mathrm{dec}};L)$ is also the distribution of first-passage times to reach the threshold L for the first time without reaching the threshold $-L$ before, given $H_{\rightarrow}$ is true. The probability distributions in Eq. (11) are equal to the joint probability densities to make a decision $d\in\{\rightarrow,\leftarrow\}$ at time τ_{dec}, $P(\tau_{\mathrm{dec}},\rightarrow) = P(\tau_{\mathrm{dec}};L)$, and $P(\tau_{\mathrm{dec}},\leftarrow) = P(\tau_{\mathrm{dec}};-L)$. Equation (11) thus implies

$$\frac{P(\tau_{\mathrm{dec}},\rightarrow)}{P(\tau_{\mathrm{dec}},\leftarrow)} = \exp(L). \tag{12}$$

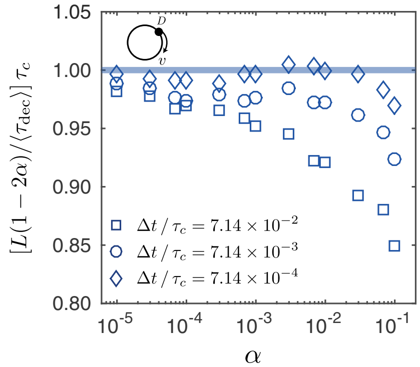

FIG. 2 (color online). Estimation of the steady-state entropy production rate of a drift-diffusion process with periodic boundary conditions (e.g., particle in a ring, see inset) by a sequential probability ratio test in the arrow of time. The estimator $L(1-2\alpha)/\langle\tau_{\mathrm{dec}}\rangle$ is shown as a function of the error probability α for different simulation time steps $\Delta t/\tau_c$ and normalized by $\tau_c = 1/[\langle dS_{\mathrm{tot}}/dt\rangle/k] = D/v^2$. For the vertical axis we use the empirical mean of τ_{dec}, and L is the threshold for the decision. The data are obtained from 1000 numerical simulations with drift velocity $v = 65\ \mu\mathrm{m/s}$ and diffusion coefficient $D = 0.52\ \mu\mathrm{m}^2/\mathrm{s}$. The horizontal line corresponds to the steady-state entropy production rate.

From Eq. (12) it follows that $P(d=\rightarrow)/P(d=\leftarrow) = \exp(L)$, consistent with previous results obtained for two-boundary first-passage time processes [18,19]. Using $P(\tau_{\mathrm{dec}},d) = P(\tau_{\mathrm{dec}}|d)P(d)$, we then find that the conditional probability densities for the decision time obey

$$P(\tau_{\mathrm{dec}}|\rightarrow) = P(\tau_{\mathrm{dec}}|\leftarrow). \tag{13}$$

This implies that even though decisions are made with different probabilities, the conditional decision time distributions have the same shape for both outcomes. We therefore call Eq. (13) the fluctuation theorem in the arrow of time (FTAT). Equations (8) and (13) are the main results of this Letter.

To illustrate how Eq. (8) provides an estimator for the steady-state entropy production rate, we discuss two paradigmatic examples of nonequilibrium stochastic processes. We first consider a drift-diffusion process with periodic boundary conditions of a particle with position $x(t)$, average drift velocity v, and diffusion coefficient D. If Einstein's relation holds, $D = kT/\gamma$, where γ is a friction coefficient, the steady-state entropy production rate is $\langle dS_{\mathrm{tot}}/dt\rangle/k = v^2/D = F^2/(\gamma kT)$, where $F = \gamma v$ is the friction force and T is the temperature of the thermal bath [20]. Figure 2 shows $L(1-2\alpha)/\langle\tau_{\mathrm{dec}}\rangle$ obtained from 1000 numerical simulations of the SPRT in the arrow of time (markers) as a function of the error probability α for different values of the simulation time step Δt together with $\langle dS_{\mathrm{tot}}/dt\rangle/k$ (blue solid line). For the drift-diffusion process, the log-likelihood ratio for the SPRT in the arrow of time is simply given by $\mathcal{L}(t) = (v/D)[x(t)-x(0)]$. As long as the simulation time step obeys $\Delta t \ll \tau_c$, where

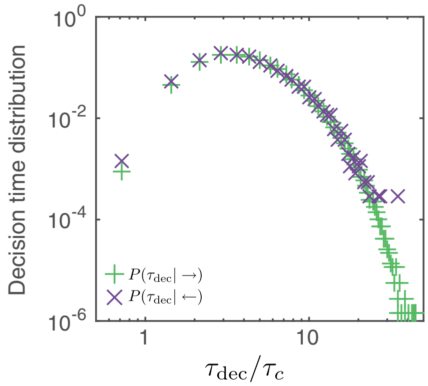

FIG. 3 (color online). Conditional distributions of the decision time $P(\tau_{\rm dec}|\rightarrow)$ and $P(\tau_{\rm dec}|\leftarrow)$ obtained from 10^6 numerical simulations of a drift-diffusion process with diffusion $D = 0.52\ \mu{\rm m}^2/{\rm s}$ and drift $v = 65\ \mu{\rm m/s}$. The simulation time step is $\Delta t = 0.1$ ms and the error probability $\alpha = 0.01$.

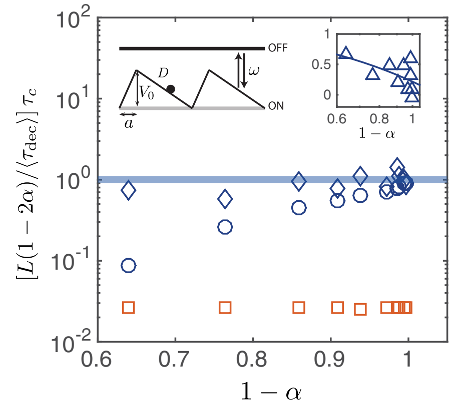

FIG. 4 (color online). Estimation of the entropy production rate using the SPRT in the arrow of time in a flashing ratchet model using the right-hand side in Eq. (8) (blue open circles) and the right-hand side in Eq. (6) (blue open diamonds) as a function of the reliability of the test. Red open squares are given by the ratio between $D[\rightarrow \| \leftarrow]$ and the mean first-passage time $\langle\tau\rangle$ of the position of the particle in Eq. (9). The results were obtained from 1000 numerical simulations with time step $\Delta t = 1\ \mu$s, diffusion coefficient $D = 1\ \mu{\rm m}^2/{\rm ms}$, $V_0 = 10$ kT, $a = 1/3\ \mu$m, and $\omega = 10$ kHz. The characteristic time $\tau_c = 0.07$ ms is the numerical estimate of $k/\langle dS_{\rm tot}/dt\rangle$ obtained from a single stationary trajectory of 10^7 data points. Inset: Correction term in Eq. (6) given by $[\langle\Delta S_{\rm ex}\rangle_{\rm dec}/k\langle\tau_{\rm dec}\rangle]\tau_c$ as a function of $1-\alpha$ (blue triangles). The solid line is a linear fit of the data.

$\tau_c = k/\langle dS_{\rm tot}/dt\rangle = D/v^2$, the SPRT in the arrow of time provides an accurate estimator of entropy production independent of the error probability α. For larger Δt, the estimator is only accurate for small α but provides a lower bound to the steady-state entropy production rate for larger α. In our simulations, we also calculated empirical conditional decision time probabilities $P(\tau_{\rm dec}|\rightarrow)$ (green) and $P(\tau_{\rm dec}|\leftarrow)$ (purple), which are shown in Fig. 3 for $\alpha = 0.01$. Figure 3 demonstrates the validity of the FTAT given in Eq. (13) for the drift-diffusion process.

The drift-diffusion process is a simple example and serves as an illustration of our results. We now test whether our results also hold in more complex nonequilibrium stochastic processes that involve discontinuous jumps of the state variables. We therefore discuss the SPRT in the arrow of time for the case of a flashing ratchet with periodic boundary conditions. We consider a Brownian particle with diffusion coefficient D, subject to a piecewise linear periodic potential that is switched on and off stochastically at a constant rate ω [21]. The log-likelihood ratio of the SPRT in the arrow of time in steady state can be approximated by the cumulated work W exerted on the particle during switches, $\mathcal{L}(t) = W(t)/kT$. Here $W(t) = \sum_i \Delta V_i$, where ΔV_i is the potential energy change during the switching event i and the sum is done over all switches that occur before time t [22]. Figure 4 shows the estimate of $L(1-2\alpha)/\langle\tau_{\rm dec}\rangle$ as a function of the reliability $1-\alpha$. The plot shows that the SPRT in the arrow of time provides a lower bound for the steady-state entropy production rate (blue open circles) and converges for high reliability to the correct value. In addition, Fig. 5 shows the conditional distributions of the decision times revealing that the FTAT holds to good approximation for high error probabilities despite the fact that the propagator is not translationally invariant.

When using the estimator given by Eq. (6), which includes the excess entropy production, the entropy production rate is estimated more accurately at low reliabilities (Fig. 4, blue diamonds). The inset in Fig. 4 confirms that the correction term in Eq. (6) tends to zero for α small. Note that the estimator $L(1-2\alpha)/\langle\tau_{\rm dec}\rangle$ in Eq. (8) provides a lower bound at small α because of the discontinuous jumps in the state variables. Using an heuristic estimator given by the ratio $D[\rightarrow \| \leftarrow]/\langle\tau\rangle$, where τ is the first-passage time of the position of the particle, also bounds from below the steady-state entropy production, as follows from Eq. (9) (Fig. 4, red squares).

The dynamics of a stochastic nonequilibrium process provides evidence on the arrow of time to an observer. Reliable decisions on the direction of the arrow of time can be made measuring first-passage times of physical observables.

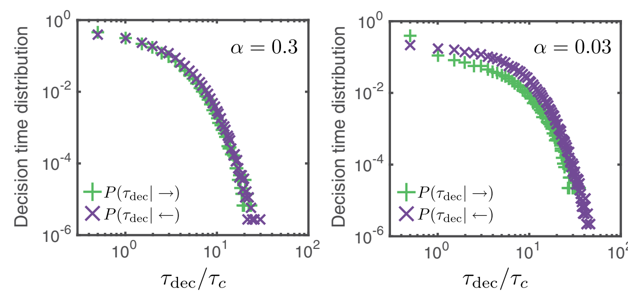

FIG. 5 (color online). Conditional distributions of the decision time $P(\tau_{\rm dec}|\rightarrow)$ and $P(\tau_{\rm dec}|\leftarrow)$ obtained from 10^6 numerical simulations of the flashing ratchet with the same simulation parameters as in Fig. 4. The two figures show the distributions for two different error probabilities α.

When the physical observable used is the entropy production, the decision time is minimized. In addition, measuring first-passage times of physical observables provides estimators for the steady-state entropy production rate that are lower bounds to the true value. This follows from the optimality of the SPRT. Using this method to estimate entropy production, it is not necessary to sample the whole space of stochastic trajectories as required in previous approaches [23–25]. Interestingly, our fluctuation theorem for the two-boundary first-passage time distribution of entropy production [Eq. (10)] implies that the shape of the distributions of decision times for correct and wrong decisions are equal even though the probabilities in both cases are different. The connection between decision theory and thermodynamics provided here could be of particular interest in the context of nonequilibrium processes that involve feedback control, often found in biology and engineering.

We acknowledge fruitful discussions with Mostafa Khalili-Marandi. This work is partially supported by the German Research Foundation (DFG) within the Cluster of Excellence "Center for Advancing Electronics Dresden" and within the CRC 912 "Highly Adaptive Energy-Efficient Computing." E. R. acknowledges funding from Grupo Interdisciplinar de Sistemas Complejos (GISC, Madrid, Spain) and from Spanish Government, Grants ENFASIS (FIS2011-22644) and TerMic (FIS2014-52486-R).

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