Generalized uncertainty relations for semi-Markov processes

Tan Van Vu and Yoshihiko Hasegawa
Department of Information and Communication Engineering, Graduate School of Information Science and Technology, The University of Tokyo, Tokyo 113-8656, Japan
E-mail: tan@biom.t.u-tokyo.ac.jp and hasegawa@biom.t.u-tokyo.ac.jp

Abstract. The thermodynamic and kinetic uncertainty relations provide finite-time bounds on the observable fluctuation in Markov processes. Herein, we generalize these bounds for semi-Markov processes. Specifically, we prove that, unlike in the Markovian case, the fluctuation of time-antisymmetric observables is bounded not only by entropy production but also by a memory term. For generic observables, we analogously show that the fluctuation is bounded by both dynamical activity and a memory term. Our results indicate that memory plays an important role in the bounds. Interestingly, with a proper form of the waiting-time distribution, the memory can decrease the observable fluctuation. When the waiting-time distribution is Poissonian (i.e., the process becomes Markov), the memory terms vanish, and the derived bounds reduce to the conventional bounds.

1. Introduction
Owing to substantial progress in stochastic thermodynamics [1] over the last two decades, many powerful relations have been discovered in nonequilibrium systems. In recent years, a trade-off between current fluctuation and entropy production, known as the thermodynamic uncertainty relation (TUR), was found for continuous-time Markov jump processes [2, 3]. The TUR states that a high precision of currents cannot be attained without increasing dissipation, quantified by the entropy production. Quantitatively, the TUR imposes the following bound on the fluctuation of currents:

$$\frac{\langle \phi \rangle}{\langle \phi \rangle^2} \geq \frac{2}{\langle \sigma \rangle},$$

where $\phi$ is an arbitrary time-integrated current, $\langle \phi \rangle$ and $\langle \langle \phi \rangle \rangle := \langle \phi^2 \rangle - \langle \phi \rangle^2$ are its mean and variance, respectively, and $\langle \sigma \rangle$ is the average entropy production. The bound has been generalized and refined intensively in other contexts [4–20]. Unlike the TUR, which applies only to time-antisymmetric observables, another inequality called the kinetic uncertainty relation (KUR) [21, 22] places a constraint on the fluctuation of generic observables, reads as

$$\frac{\langle \langle \phi \rangle \rangle}{\langle \phi \rangle^2} \geq \frac{1}{\langle n \rangle},$$

where $\phi$ is a generic observable and $\langle n \rangle$ is the average number of jumps occurred during observation time, which is also known as dynamical activity of the system. The term $\langle n \rangle$ reflects the kinetic aspect and complementarily characterizes the physics of the system along with entropy production [23, 24].
It is well-known that Markov jump processes are memoryless, i.e., the jump probability is independent of the elapsed time since the last jump occurred. However, most processes in nature, ranging from physical [25–27] to biological [28, 29] systems, typically have memory effects due to hidden and unobserved variables. Therefore, Markov processes cannot provide reliable approximations for many stochastic dynamics. To effectively model such systems, semi-Markov processes may be required. In contrast to Markov processes, semi-Markov processes have a memory and have successfully been applied to study chemical and biological systems [30–32]. It is a fundamental question to ask how the fluctuation of observables is constrained in the presence of memory.

In the present paper, we generalize the uncertainty relations, TUR and KUR, for semi-Markov processes. Using the Cramér–Rao inequality, we prove that the fluctuation of observables is constrained not only by entropy production, either dynamical activity but also by memory terms characterized by waiting-time distributions. When the waiting-time distribution is Poissonian, the memory terms vanish, and our bounds reduce to the conventional ones. Therefore, the derived bounds can be regarded as generalizations of the TUR and the KUR. Our results also reveal whether the memory can cooperatively constrain the fluctuation of observables or not.

2. Semi-Markov processes

In this section, we give a brief introduction of semi-Markov processes, including the definition, statistic properties, and total entropy production. More details on the structure and the properties of semi-Markov processes can be found in references [33, 34].

2.1. Definition and notions

Following reference [34], we describe here the definition and notions of semi-Markov processes. We consider continuous-time jump processes on a finite space $\Omega$. Unlike in the Markov cases, semi-Markov processes have non-Poissonian waiting-time distributions. The probability of a jump from state $x$ to $y$ at a certain time depends only on the states $x, y$, and the time $t$ since the last jump occurred. Specifically, transitions in the process are characterized by a density function $K(x, y, t)$. This function satisfies the normalization condition, i.e., $\sum_{y \in \Omega} \int_0^\infty K(x, y, t) dt = 1$ for all $x \in \Omega$. Using function $K(x, y, t)$, we define the waiting-time distribution at state $x$, $K(x, t)$, and the transition probability from $x$ to $y$ regardless of the waiting time, $p(x, y)$, as follows:

$$K(x, t) := \sum_{y \in \Omega} K(x, y, t), \quad p(x, y) := \int_0^\infty dt K(x, y, t).$$

(3)

It is obvious that $\int_0^\infty dt K(x, t) = 1$ and $\sum_{y \in \Omega} p(x, y) = 1$. The effective escape rate $\bar{\lambda}(x)$ is equal to the reciprocal of the average waiting time and can be calculated as

$$\bar{\lambda}(x) := \left( \int_0^\infty dt tK(x, t) \right)^{-1}.$$

(4)

When the waiting time does not depend on the future state, but depends only on the present state, i.e., $K(x, y, t) = p(x, y)K(x, t)$, we say that the semi-Markov process is time-direction independence. Throughout the paper, we exclusively focus on processes satisfying this condition. Note that, when $K(x, t) = \lambda(x)e^{-\lambda(x)t}$, the process becomes Markov.

In the stationary state, the probability distribution $\pi(x)$ satisfies the relation $\sum_{y \in \Omega} j(x, y) = 0$, where $j(x, y)$ is the probability current defined by

$$j(x, y) = \pi(x)\lambda(x)p(x, y) - \pi(y)\lambda(y)p(y, x).$$

(5)
2.2. Total entropy production

Let $\Gamma = [x_0, t_1, x_1, t_2, \ldots, x_{n-1}, t_n, x_n]$ be a trajectory observed during the time interval $[0, T]$. Here, $t_i$ $(1 \leq i \leq n)$ denotes the time that a jump from state $x_{i-1}$ to $x_i$ occurred and $0 \leq t_1 < t_2 < \cdots < t_n \leq T$. At the start time $t = 0$, the system is already at state $x_0$, and its age is stationarily distributed. The probability distribution of path $\Gamma$ has the following density:

$$P[\Gamma] = \pi(x_0)\tilde{\lambda}(x_0)\kappa(x_0, x_1, t_1)K(x_1, x_2, t_2 - t_1) \ldots K(x_{n-1}, x_n, t_n - t_{n-1})\kappa(x_n, T - t_n).$$

(6)

Here,

$$\kappa(x, y, t) := \int_t^\infty d\tau K(x, y, \tau), \quad \kappa(x, t) := \int_t^\infty d\tau K(x, \tau).$$

(7)

For each trajectory $\Gamma$, considering its time-reversed counterpart $\Gamma^\dagger = [x_n, T - t_n, x_{n-1}, T - t_{n-1}, \ldots, x_1, T - t_1, x_0]$. The total entropy production characterizes the irreversibility in the system and can be defined by the log-ratio of probabilities of observing forward and time-reversed trajectories as

$$\sigma[\Gamma] := \ln \frac{P[\Gamma]}{P[\Gamma^\dagger]}.$$  

(8)

From the equality $\langle e^{-\sigma} \rangle = 1$, one can easily prove that $\langle \sigma \rangle \geq 0$, which represents the second law in thermodynamics. Using the formula of the path probability in equation (6), we obtain

$$\sigma = \ln \pi(x_0) - \ln \pi(x_n) + \sum_{i=1}^n \ln \frac{\tilde{\lambda}(x_{i-1})p(x_{i-1}, x_i)}{\lambda(x_i)p(x_i, x_{i-1})}.\,$$

(9)

The first term in the right-hand side of equation (9), $\ln \pi(x_0) - \ln \pi(x_n)$, represents the change in the system entropy. The second term is interpreted as the entropy flux into the environment. In the stationary state, the average entropy production is equal to

$$\langle \sigma \rangle = \sum_{i=1}^n \ln \frac{\pi(x_{i-1})\tilde{\lambda}(x_{i-1})p(x_{i-1}, x_i)}{\pi(x_i)\lambda(x_i)p(x_i, x_{i-1})} = \frac{T}{2} \sum_{x,y} j(x, y) \ln \frac{\pi(x)\tilde{\lambda}(x)p(x, y)}{\pi(y)\lambda(y)p(y, x)}.$$

(10)

3. Main results

We consider a generic observable $\phi[\Gamma] = \sum_{i=0}^{n-1} \gamma(x_i, x_{i+1})$, where $\gamma : \Omega \times \Omega \mapsto \mathbb{R}$ is a real-valued function. When $\gamma(x, y)$ is asymmetric, i.e., $\gamma(x, y) = -\gamma(y, x)$, $\phi$ is a time-antisymmetric observable and called a current. We modify the original dynamics by a perturbation parameter $\theta$ and obtain a modified dynamics. Let $P_\theta[\Gamma]$ be the probability of observing the trajectory $\Gamma$ in the modified dynamics, then by applying the Cauchy–Swartchz inequality to $\langle \partial_\theta \phi \rangle^2$, we obtain [13]

$$\left\langle \left( \frac{\partial \phi}{\partial \theta} \right)^2 \right\rangle \geq \frac{\mathcal{I}(\theta)}{\left\langle \partial_\theta \phi \right\rangle^2},$$

(11)

where $\mathcal{I}(\theta) := \langle (\partial_\theta \ln P_\theta[\Gamma])^2 \rangle = -\langle \partial_\theta^2 \ln P_\theta[\Gamma] \rangle$ is the Fisher information, which places a lower bound on the precision of unbiased estimators. Here $\langle \cdot \rangle_{\theta}$ and $\langle \cdot \rangle_{\theta}$ denote the mean and variance in the modified dynamics. Equation (11) is also known as the Cramér–Rao inequality in the context of estimation theory.

3.1. Thermodynamic bound on fluctuations of currents

Consider a modified process with the following waiting-time kernel:

$$K_\theta(x, t) = (1 + \alpha_x \theta)K(x, (1 + \alpha_x \theta)t), \quad p_\theta(x, y) = \frac{(1 + \alpha_{xy}\theta)p(x, y)}{1 + \alpha_x \theta}.$$  

(12)
Here, $\alpha_{xy}$ and $\alpha_x$ are defined as follows:

$$
\alpha_{xy} = 1 - \left( \frac{\pi(y)\lambda(y)p(y,x)}{\pi(x)\lambda(x)p(x,y)} \right)^{1/2}, \quad \alpha_x = \sum_{y \in \Omega} \alpha_{xy}p(x,y).
$$

(13)

When $\theta = 0$, the modified dynamics become the original ones. Note that when $\theta \ll 1$, both $1 + \alpha_x \theta$ and $1 + \alpha_{xy} \theta$ are ensured to be positive; thus, $K_\theta(x,t)$ and $p_\theta(x,y)$ are well defined. It can be easily confirmed that they satisfy normalization conditions, i.e., $\int dt K_\theta(x,t) = 1$ and $\sum_{y \in \Omega} p_\theta(x,y) = 1$ for all $x$. This modified dynamics have the following properties: (i) the effective escape rates are scaled $\tilde{\lambda}_\theta(x) = (1 + \alpha_x \theta) \lambda(x)$, (ii) the stationary distribution remains unchanged $\pi_\theta(x) = \pi(x)$, and (iii) the probability currents are scaled $j_\theta(x,y) = (1 + \theta) j(x,y)$. Since $\phi$ is a current, its average can be expressed as $\langle \phi \rangle = T \sum_{x,y} \gamma(x,y) j(x,y)/2$. Consequently, the average of current $\phi$ in the modified dynamics is scaled $\langle \phi \rangle_\theta = (1 + \theta) \langle \phi \rangle$; thus, $\partial_\theta \langle \phi \rangle_\theta = \langle \phi \rangle$. The path probability density in the modified dynamics is expressed as

$$
P_\theta[\Gamma] = \pi_\theta(x_0)\lambda_\theta(x_0)\kappa_\theta(x_0,x_1,t_1)K_\theta(x_1,x_2,t_2-t_1) \ldots K_\theta(x_{n-1},x_n,t_n-t_{n-1})\kappa_\theta(x_n,T-t_n)
= \pi(x)(1 + \alpha_{xy} \theta) \lambda(x) \prod_{i=0}^{n-1} (1 + \alpha_{x_i,x_{i+1}} \theta)p(x_i,x_{i+1}) \prod_{i=1}^{n} K(x_i,(1 + \alpha_{x_i} \theta)(t_{i+1} - t_i))
\times \int_{t_1}^{\infty} d\tau K(x_0,(1 + \alpha_{x_0} \theta)\tau)(1 + \alpha_{x_n} \theta) \int_{T-t_n}^{\infty} d\tau K(x_n,(1 + \alpha_{x_n} \theta)\tau).
$$

(14)

Using equation (14), the Fisher information $\mathcal{I}(0)$ can be calculated as

$$
\mathcal{I}(0) = \left( \sum_{i=0}^{n-1} \alpha_{x_i,x_{i+1}}^2 \right) = \left( \alpha_{x_0}^2 f(x_0,t_1) + \alpha_{x_n}^2 f(x_n,T-t_n) + \sum_{i=1}^{n} \alpha_{x_i}^2 g(x_i,t_{i+1} - t_i) \right),
$$

(15)

where $f(x,t) := t^2 \partial_t^2 \ln \int_0^\infty d\tau K(x,\tau)$ and $g(x,t) := t^2 \partial_t^2 \ln K(x,t)$. The first term in the right-hand side of equation (15) can be reduced to a closed form as

$$
\left( \sum_{i=0}^{n-1} \alpha_{x_i,x_{i+1}}^2 \right) = T \sum_{x,y} \pi(x)\lambda(x)p(x,y) \left[ 1 - \left( \frac{\pi(y)\lambda(y)p(y,x)}{\pi(x)\lambda(x)p(x,y)} \right)^{1/2} \right]^2
= T \sum_{x,y} \sqrt{\pi(x)\lambda(x)p(x,y)} - \sqrt{\pi(y)\lambda(y)p(y,x)}^2.
$$

(16)

Applying the inequality

$$
\left( \sqrt{a} - \sqrt{b} \right)^2 \leq \frac{1}{4} (a - b) \ln \frac{a}{b}
$$

(17)

to equation (16), we obtain

$$
\left( \sum_{i=0}^{n-1} \alpha_{x_i,x_{i+1}}^2 \right) \leq T \frac{1}{4} \sum_{x,y} j(x,y) \ln \frac{\pi(x)\lambda(x)p(x,y)}{\pi(y)\lambda(y)p(y,x)} = \frac{\langle \sigma \rangle}{2}.
$$

(18)

Finally, by letting $\theta = 0$ in equation (11), we obtain the following bound on the fluctuation of currents:

$$
\frac{\langle \langle \phi \rangle \rangle}{\langle \phi \rangle^2} \geq \frac{2}{\langle \sigma \rangle + \chi_t},
$$

(19)

where $\chi_t$ is a memory term defined as

$$
\chi_t := -2 \left( \alpha_{x_0}^2 f(x_0,t_1) + \alpha_{x_n}^2 f(x_n,T-t_n) + \sum_{i=1}^{n} \alpha_{x_i}^2 g(x_i,t_{i+1} - t_i) \right).
$$

(20)

Equation (19) is our first main result. When the process becomes Markov, $f(x,t) = g(x,t) = 0$, thus, $\chi_t = 0$, and the derived inequality reduces to the conventional TUR.
3.2. Kinetic bound on fluctuations of generic observables
Consider another modified semi-Markov process with the following waiting-time kernel:

$$K_\theta(x, t) = (1 + \theta)K(x, (1 + \theta)t), \quad p_\theta(x, y) = p(x, y).$$  \hfill (21)

Unlike in the previous modification, we change only the waiting-time distribution and keep the transition probabilities unchanged. When $\theta = 0$, the modified process becomes the original one. It can be easily confirmed that $\int dt K_\theta(x, t) = 1$ and $\sum_{y \in \Omega} p_\theta(x, y) = 1$ for all $x \in \Omega$. This modified dynamics have the following properties: (i) the effective escape rates are scaled $\bar{\lambda}_\theta(x) = (1 + \theta)\bar{\lambda}(x)$, and (ii) the stationary distribution remains unchanged $\pi_\theta(x) = \pi(x)$. In the stationary state, the average of $\phi$ can be calculated as $\langle \phi \rangle = T \sum_{x,y} \gamma(x, y)\pi(x)\bar{\lambda}(x)p(x, y)$. It is easy to verify that $\langle \phi \rangle_\theta = (1 + \theta)\langle \phi \rangle$; thus, $\partial_\theta \langle \phi \rangle_\theta = \langle \phi \rangle$.

Since

$$P_\theta[\Gamma] = \pi_\theta(x_0)\bar{\lambda}_\theta(x_0)\kappa_\theta(x_0, x_1, t_1)K_\theta(x_1, x_2, t_2 - t_1) \ldots K_\theta(x_{n-1}, x_n, t_n - t_{n-1})\kappa_\theta(x_n, T - t_n)$$

$$= \pi(x_0)(1 + \theta)\bar{\lambda}(x_0) \sum_{i=0}^{n-1} p(x_i, x_{i+1}) \prod_{i=1}^{n-1}(1 + \theta)K(x_i, (1 + \theta)(t_{i+1} - t_i))$$

$$\times (1 + \theta) \int_{t_1}^\infty d\tau K(x_0, (1 + \theta)\tau)(1 + \theta) \int_{T-t_n}^\infty d\tau K(x_n, (1 + \theta)\tau).$$ \hfill (22)

Using equation (22) and performing simple calculations, we obtain an expression of $\mathcal{I}(0)$

$$\mathcal{I}(0) = \langle n \rangle - \left\{ f(x_0, t_1) + f(x_n, T - t_n) + \sum_{i=1}^{n-1} g(x_i, t_{i+1} - t_i) \right\}. \hfill (23)$$

The first term in the right-hand side of equation (23) is equal to the average number of jumps occurred during observation time and is identified as the dynamical activity of the system. It can be analytically calculated as

$$\langle n \rangle = T \sum_{x,y} \pi(x)\bar{\lambda}(x)p(x, y) = T \sum_x \pi(x)\bar{\lambda}(x). \hfill (24)$$

Substituting $\theta = 0$ in equation (11), we obtain a kinetic bound on the fluctuation of observables

$$\frac{\langle \{ \phi \} \rangle}{\langle \phi \rangle^2} \geq \frac{1}{\langle n \rangle} + \chi_k,$$ \hfill (25)

where $\chi_k$ is a memory term defined by

$$\chi_k := - \left\{ f(x_0, t_1) + f(x_n, T - t_n) + \sum_{i=1}^{n-1} g(x_i, t_{i+1} - t_i) \right\}. \hfill (26)$$

Equation (25) is our second main result. In the Markovian case, $\chi_k = 0$, and our result covers the conventional KUR derived for Markov processes.

We make several remarks about our main results, equations (19) and (25). The derived bounds hold for arbitrary observation times and are generalizations of the conventional bounds [equations (1) and (2)]. When the waiting-time distribution satisfies $f(x, t) \leq 0$, $g(x, t) \leq 0$ for all $x \in \Omega$, the memory terms are positive; thus, the bounds are lower than the conventional bounds. This implies that memory can reduce the fluctuation of observables in such cases; for example, when the waiting-time distributions are Gamma distributions,

$$K(x, t) = \frac{b_2^{a_x} t^{a_x - 1} e^{-b_x t}}{G(a_x)},$$ \hfill (27)

where $G(z)$ is the Gamma function and $a_x > 1, b_x > 0$ are constants. It is worth note that the bounds are tighter than the conventional ones when $\chi < 0$ (e.g., when $a_x < 1$).
4. Conclusion
In summary, we have derived finite-time bounds on the fluctuation of observables in steady-state semi-Markov processes. For observables that are antisymmetric under time reversal, we prove that the fluctuation is bounded not only by entropy production but also by the memory term $\chi_t$. For generic observables, the memory term $\chi_k$ and dynamical activity simultaneously constrain the fluctuation. The memory terms can be positive or negative, depending on the form of the waiting-time distribution. The sign of the memory terms indicates whether memory can reduce the fluctuation of observables or not. Our results can be applied to study fluctuations in stochastic systems modeled by semi-Markov processes, such as dynamics of kinesin molecules [35] and biochemical reaction networks [36–38] where several reactions are unobserved, or the network topology is not fully revealed. Moreover, we anticipate that the derived bound [equation (19)] can be used to infer dissipation in living systems whose underlying dynamics are semi-Markov.

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