Memory Index of First-Passage Time: A Simple Measure of Non-Markovian Character

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The theory is developed for the second moment of the first-passage-time variable of statistical flows with memory (non-Markovian dynamics) and applied to a model of free non-Markovian Brownian motion. More importantly, a novel quantity, called memory index σ, is introduced, giving a quantitative characterization of the influence on non-Markovian behavior. Thus, a theoretical or experimental evaluation of σ allows one to assess the quality of widely used approximative (Markovian) Fokker-Planck-type descriptions of the dynamics.

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The concept of the mean of the first-passage-time variable[1,2] enjoys great popularity among many physicists, chemists, and engineers. Its great practical use for estimating relevant time scales in nonlinear dynamical problems such as they occur in chemical kinetics, decay of metastable states, or decay of unstable states in nonequilibrium systems has been demonstrated many times.[1-10]

The main purpose of this paper is the promotion of yet another quantity: the memory index σ [defined below in (20)] of the first-passage-time random variable. A measurement of σ does not prevent major difficulties for experimentalists, yet provides a novel characterization of the quality of an *a priori* Markovian approximation of the coarse-grained dynamics of nonlinear statistical systems. A researcher interested in the theoretical modeling of the dynamics of statistical systems will almost always choose an approximative Markovian theory such as a nonlinear Fokker-Planck modeling.[1-10] It should be borne in mind, however, that such an approach has no divine right. A Markovian modeling merely serves as an *a priori* approximation over a more accurate but generally rather complex non-Markovian modeling.[8,11,12] It is of course generally understood that "strong" deviations from a Markovian description can be traced back to the coarse graining over a slow variable. In complex systems (e.g., biological systems) it can become rather difficult to collect the complete set of *all* relevant slow variables forming the approximative Markovian dynamics. A quantitative criterion testing the validity of a chosen Markovian approximation appears thus very desirable.

Limiting for the sake of simplicity the following discussion to a one-dimensional stochastic variable $x(t)$, we unavoidably must first develop a small amount of stochastic calculus. Consider an interval $I=[x_1,x_2]$ out of the state space of the dynamical variable $x(t)$. If initially the random variable $x(t)$ assumes the value $x(t_0=0)=x_0$ in I, the first passage time $\tau(x_0)$ (a random variable) is the time which elapses before $x(t)$ leaves the interval I for the first time. If $F_t(x_0)$ denotes the probability for a random walker, $x(t)$, which started our at time $t_0=0$ at x_0 to be still in interval I without ever having left this interval, one obtains for the probability density $\rho_t(x_0)$ that the first passage time $\tau(x_0)$ lies in the interval $(t, t+dt)$

$$\rho_t(x_0)=-(\partial/\partial t)F_t(x_0), \quad F_{t_0=0}(x_0)=1. \tag{1}$$

The moments $T_n(x_0)$ of the first-passage-time random variable are defined by

$$T_n(x_0)=\int_0^\infty t^n \rho_t(x_0)\,dt, \quad n=1,2,\ldots; \qquad T_0(x_0)=1. \tag{2}$$

Now let us first consider a Markovian dynamics; i.e., in terms of a master operator $\underline{\Gamma}$ the time evolution of the single-event probability density $p_t(x)$ of the stochastic variable $x(t)$ is in operator notation given by

$$\dot{p}_t=\underline{\Gamma}\,p_t. \tag{3}$$

Then, the moments T_n in (2) obey a rather simple equation[1,2]

$$\underline{\bar{\Gamma}}^\dagger T_n=-n\,T_{n-1}, \quad n=1,2,\ldots; \quad T_0=\underline{1}. \tag{4}$$

Hereby, $\underline{\Gamma}^\dagger$ denotes the adjoint operator with the kernel $\Gamma^\dagger(x,y)=\Gamma(y,x)$ and the bar over $\underline{\Gamma}^\dagger$ denotes the properly adjusted operator so as to prevent backflow of probability into the interval I. In particular, transition rates $\Gamma(y\to x)=\Gamma(x,y)$, with x in I and y not in I, are set equal to zero.[11] With such boundary conditions included in the definition of $\underline{\bar{\Gamma}}^\dagger$, T_n is formally given by iterates of the Green's function $[\underline{\bar{\Gamma}}^\dagger]^{-1}$ (inverse of adjusted rate matrix[1,11]):

$$T_n = (-1)^n n! [\underline{\bar{\Gamma}}^{\dagger}]^{-n} \underline{1}. \tag{5}$$

A non-Markovian dynamics is characterized by a retarded master operator[12,13]

$$\dot{p}_t = \int_0^t \underline{K}_{t-s} p_s \, ds, \tag{6a}$$

where

$$\underline{K}_{t-s} p_s |_x = \int K_{t-s}(x, y) p_s(y) dy. \tag{6b}$$

It has been shown previously,[11] that the probability $F_t(x_0)$ satisfies the relation

$$\dot{F}_t = \int_0^t \underline{\bar{K}}_{t-s}^{\dagger} F_s \, ds, \tag{7}$$

with the operator $\underline{\bar{K}}_t^{\dagger}$ being adjusted as above. It then follows from (1) and (2) that the mean first passage time T_1 of a non-Markovian process obeys[11,14]

$$\Omega_0^{\dagger} T_1 = -\underline{1}, \tag{8a}$$

where $\Omega_0^{\dagger}$ is given by (zeroth moment)

$$\Omega_0^{\dagger} = \int_0^{\infty} \underline{\bar{K}}_s^{\dagger} ds. \tag{8b}$$

Often, the time integral of the kernel $K_t(x, y)$ is identified with a transition kernel $\Gamma(x,y)$ of a Markovian process; i.e., $\langle x | \int_0^{\infty} K_t \, dt | y \rangle \equiv \Gamma(x, y) > 0$, $x \neq y$.[12] Hence, the mean first passage time T_1 of the non-Markovian dynamics, K_t, *coincides precisely* with T_1 of the commonly used Markovian approximation given by[12]

$$\underline{\Gamma}_{\mathrm{Markov}} \equiv \int_0^{\infty} \underline{K}_s ds. \tag{9}$$

Clearly this remarkable fact cannot hold true for all moments T_n because processes generated from a common initial probability p_0 (p_0 not the stationary probability $\bar{p}$) via (6), or via (3) with $\underline{\Gamma}$ given by (9), are markedly different. In particular, let us focus now on the second moment

$$T_2(x_0) = \int_0^{\infty} t^2 [-\partial F_t(x_0)/\partial t] dt, \tag{10}$$

which after a partial integration[15] equals

$$T_2(x_0) = 2\int_0^{\infty} t F_t(x_0) dt. \tag{11}$$

Next we use the trivial identity [see (7)]

$$-\int_0^{\infty} t \{ \partial F_t/\partial t - \int_0^t \underline{\bar{K}}_{t-s}^{\dagger} F_s ds \} dt = \underline{0}, \tag{12}$$

which readily yields

$$T_1 + \mathcal{L}\{ \underline{\bar{K}}_t^{\dagger} t * F_t;\ z=0 \} + \mathcal{L}\{ \underline{\bar{K}}_t^{\dagger} * F_t t;\ z=0 \} = \underline{0}. \tag{13}$$

The notation $\mathcal{L}\{f_t;\ z=0\}$ denotes the Laplace transform of the function f_t evaluated at $z=0$ and $f*g$ stands for a convolution between f and g. Introducing the operator $\Omega_1^{\dagger}$ (first moment)

$$\Omega_1^{\dagger} = \int_0^{\infty} s \, \underline{\bar{K}}_s^{\dagger} ds, \tag{14}$$

one can recast (13) as

$$\Omega_0^{\dagger} T_2 = -2[T_1 + \Omega_1^{\dagger} T_1]. \tag{15}$$

This relation is a central result of the paper. It determines the second moment of the first-passage-time variable and notably differs from the corresponding Markovian relation in (4) for $n=2$ if $\Omega_0^{\dagger}$ is identified with $\underline{\bar{\Gamma}}^{\dagger}$ [see (9)].

Before turning to the interpretation of the result in (15) we apply (15) to the following model of non-Markovian dynamics:

$$\dot{p}_\tau(x) = \gamma^2 \int_0^{\tau} \left\{ \frac{J_1(\tau-\mu)}{\tau-\mu} \right\} \frac{\partial}{\partial x}\left(\frac{\partial}{\partial x} + x \right) p_\mu(x) d\mu \tag{16}$$

with J_1 being a first-order Bessel function. Equation (16) can be regarded as a model for free Brownian motion presented here in absence of any rigorous derivation. Actually, (16) results as the approximative (Born approximation) generalized Fokker-Planck equation for Rubin's model[16-18] of the Brownian motion of a heavy particle (mass M) in a linear harmonic chain (angular frequency coupling ω_0) of light particles (mass m) with γ^2 being the mass ratio m/M, x the dimensionless velocity, $x = (m/kT)^{1/2} v$, of the heavy particle, and $\tau = \omega_0 t$ the dimensionless time variable.[17] Although (16) is not the exact generalized Fokker-Planck equation for Rubin's model,[17] (16) yields the *exact non-Markovian moments*, $\langle x(\tau) \times | x(0) = x_0 \rangle$ and the *exact* stationary velocity correlation function $\varphi(\tau) = \langle x(\tau) x(0) \rangle$.[17,19] Observing the integrals $\int_0^{\infty} [J_1(\tau)/\tau] d\tau = 1$, $\int_0^{\infty} J_1(\tau) d\tau = 1$, one obtains

$$\Omega_0^{\dagger} = \Omega_1^{\dagger} = \gamma^2 (x \, \partial/\partial x + \partial^2/\partial x^2) = \underline{\Gamma}_{\text{Fokker-Planck}}^{\dagger}, \tag{17}$$

or for (15), utilizing (8a),

$$\Omega_0^{\dagger} T_2 = -2[T_1 - \underline{1}], \tag{18}$$

which can easily be integrated. If $x = x_1$ is a reflecting boundary, $\partial T_2(x)/\partial x|_{x=x_1} = 0$, and $x_2 > x_1$ absorbing, $T_2(x=x_2) = 0$, one obtains in terms of the stationary probability $\bar{p}(x) = (2\pi)^{-1/2} \exp(-x^2/2)$

$$T_1(x_0) = \int_{x_0}^{x_2} [dy/\bar{p}(y)] \int_{x_1}^{y} \bar{p}(z) dz/\gamma^2, \tag{19a}$$

$$T_2(x_0) = 2\int_{x_0}^{x_2} [dy/\bar{p}(y)] \int_{x_1}^{y} \bar{p}(z) \times \{T_1(z) - 1\} dz/\gamma^2, \tag{19b}$$

or

$$[T_2^{NM}(x_0)-T_2^{M}(x_0)]/T_1^2(x_0)=-2/T_1(x_0). \quad (19c)$$

The superscript NM denotes non-Markovian dynamics given by (6) and (16), and M Markovian dynamics, (9) and (17). Note that $(T_2^{NM}-T_2^{M})/T_1^2$ is proportional to $\gamma^2=m/M$ [compare with (22) below].

The quantity

$$\sigma(x_0)\equiv\frac{T_2^{NM}(x_0)-T_2^{M}(x_0)}{T_1^2(x_0)}$$
$$=\frac{-2}{T_1^2(x_0)}[(\Omega_0^\dagger)^{-1}\Omega_1^\dagger T_1]|_{x_0}, \quad (20a)$$

or its average over a probability p_0 of starting values x_0

$$\sigma=\int_I p_0(x)\sigma(x)dx/\int_I p_0(x)dx, \quad (20b)$$

will be called *memory index of the first-passage-time random variable*. By use of the Markovian approximation (9), or equivalently $\underline{K}_t=2\underline{\Gamma}\delta(t)$, the operator $\Omega_1^\dagger$ vanishes, $\Omega_1^\dagger=\underline{0}$; i.e., the measure σ vanishes for all x_0. Hence, the quantity σ can be used as a practical quantitative measure of non-Markovian character and can be evaluated either theoretically or experimentally[5] measuring the moments $T_2^{NM}(x_0)$, $T_1(x_0)$, and calculating $T_2^{M}(x_0)$ from the Markov approximation. As mentioned earlier, the quantity σ should be "small" if there exists a clear-cut separation between macroscopic and microscopic time scales; i.e., if bath correlations are rapidly decaying.[12] However, the actual magnitude of such "small deviations from Markovian behavior" not only depends on the relaxation-time scale of bath correlations but is also a function of the strength of the heat-bath noise. This noise strength can be measured by the value of the macroscopic diffusion coefficient

$$D(x)=\tfrac{1}{2}\int(y-x)^2\Gamma_{\text{Markov}}(y,x)dy. \quad (21)$$

In most cases of practical interest, the diffusion of the intensive macrovariable [i.e., $x(t)=\langle x(t)\rangle+O(\Phi^{-1/2})$] scales as the inverse of the system size Φ,[8,9,20] e.g., $\Phi=1/\gamma^2=M/m$ in our Brownian motion example (16). If we can assume that the random walker starting at x_0 on its motion towards the exit point at x_2 (absorbing boundary) passes a region in state space where the walker must eventually overcome a barrier, or at least passes a region where it moves freely, the first moment $T_1(x_0)$ is growing at least inversely to D. Thus, for vanishing diffusion $D(x)$ $(\Phi\to\infty)$, σ in (20) approaches zero:

$$\sigma(x)\approx O(1/T_1(x))\to 0 \text{ as } D(x)\to 0. \quad (22)$$

In conclusion, appreciable deviations from the approximative Markovian dynamics are expected to occur predominantly in systems of small size. Most interesting candidates for observing an appreciable non-Markovian character as characterized by a finite memory index are quantum-optical systems[5-8,10] such as photon statistics in a single-mode laser at threshold or in absorptive optical bistability, magnetic hysteresis, noisy electronic oscillators, transport in Josephson junctions of small size, or ligand migration in biomolecules. The theoretical modeling of the dynamics of those nonlinear systems is usually based on a heuristic nonlinear Fokker-Planck equation[1-10,21] and most researchers tacitly assume that such an approximative Markovian description will model satisfactorily not only the statics and quantities like T_1 but also the dynamics as, e.g., higher-order correlation functions or higher moments T_n.

The concept put forward in this paper can also be utilized to characterize the degree to which a high-dimensional nonlinear discrete dynamics exhibiting strange attractors can be approximated by a one-dimensional map model.

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[13]Generally Eq. (6) does contain an inhomogeneous term. If, however, the physical preparation procedure is taken into account explicitly in the definition of the projection operator, this inhomogeneity disappears; see H. Grabert, P. Hänggi, and P. Talkner, Z. Phys. B26, 398 (1977), and 29, 273 (1978), and J. Stat. Phys. 22, 537 (1980).

[14]For unit-step non-Markovian birth and death processes (including those with two-step transitions) one obtains from Eq. (8a) closed-form expressions for $T_1(x_0=i)$, i in I; see Eqs. (3.7) and (3.20) in Ref. 11.

[15]With $F_{t=\infty}(x_0)=0$, one utilizes

$$\lim_{t\to\infty} t^2 F_t(x_0) = \lim_{t\to\infty} t^2 \int_t^\infty \rho_s(x_0)\,ds \le \lim_{t\to\infty} \int_t^\infty s^2 \rho_s(x_0)\,ds = 0$$

for bounded $T_2(x_0)$.

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