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# Monte Carlo Simulation of Random Walks with Residence Time Dependent Transition Probability Rates

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An exact, computer-oriented, Monte Carlo procedure is derived for numerically simulating continuous-time/discrete-state random walks in which the transition probability per unit time from state $S_m$ to state $S_n$ may depend upon the residence time $\tau$ in the state $S_m$. Conditions for applicational feasibility of the simulation procedure are briefly indicated, and explicit stepping algorithms for some simple $\tau$-dependencies are obtained.

## 1. INTRODUCTION

Consider a system that executes a "random walk" over a discrete (possibly infinite) set of states $S_1$, $S_2$,..., according to the following transition rule:

> If the system is in the state $S_m$ at time $t$, having arrived there at time $t - \tau$ ($\tau \geqslant 0$), then the probability that it will step to some other state $S_n$ in the next infinitestimal time interval $(t, t + \mathrm{dt})$ is
>
> $$A_{nm}(\tau)\, dt. \tag{1}$$

The function $A_{nm}(\tau)$ is assumed here to be a given, nonnegative function of the integer state labels $n$ and $m$ and the nonnegative real variable $\tau$.[1] If $A_{nm}(\tau)$ is constant with respect to $\tau$, then the infinitesmal transition probability depends on the past only through the current state $S_m$, and the random walk is termed a "Markov process." The more general case in which the infinitesimal transition probability also depends upon how long a time $\tau$ the system has been in the current state $S_m$ is sometimes referred to as a "semi-Markov process" [1].

The purpose of this article is to present a computer-oriented Monte Carlo procedure for *numerically simulating* the random walk process (1). This simulation procedure is essentially a generalization of an algorithm presented in an earlier issue of this journal for simulating the stochastic time evolution of a spatially homogeneous, chemically

[1] The form of the dependence on $n$ and $m$ will of course depend upon how one chooses to label the states. It is immaterial for our purposes whether one uses an explicit, fixed labeling scheme, or a highly implicit labeling scheme that changes after each step. This point will receive further attention in Section 3.



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reacting system [2]; in that case, the system executes a Markov random walk over the space of the molecular population numbers of the participating chemical species, with the form of the stepping probability rate function being determined by the various chemical reaction channels. That computational algorithm will here be generalized to cover semi-Markov random walks. It will be shown that this generalized simulation procedure is *exact* in the sense that it is a mathematically rigorous consequence of (1). However, whether or not the simulation procedure is *feasible* will depend on the specifics of the random walk at hand. Roughly speaking, the method should be feasible whenever the walk is such that, for a given $m$, $A_{nm}(\tau)$ vanishes for all but a relatively few values of $n$, and the $\tau$-dependence of the nonvanishing $A_{nm}(\tau)$ is not too complicated. No specific applications of the algorithm will be attempted here; however, it should be noted that possible candidates for this do exist in certain generalized random walks currently being considered elsewhere as models for transient photocurrents in amorphous semiconductors [3–6] and for exciton transport in photosynthetic units [7].

Rigorous analytical treatments of random walk processes are usually based on the so-called "master equation", which is the time-evolution equation for the function $\tilde{P}(m, t) \equiv$ probability of being in the state $S_m$ at time $t$. Unfortunately, the master equation is usually quite formidable, and can seldom be solved even with the help of a powerful computer. For a *Markov* random walk, the master equation does have the virtue of being linear in $\tilde{P}(m, t)$, and this circumstance permits one to readily deduce time-evolution equations for the physically significant averages or *moments* of $\tilde{P}(m, t)$. Although these moment equations are seldom solvable exactly, they can usually be reduced through suitable approximations to a tractable system of ordinary differential equations (e.g., the set of coupled "reaction-rate" equations for a spatially homogeneous chemically reacting system). A more common, but less rigorous, way of obtaining these simplified rate equations for a Markov process is to regard $A_{nm}\,dt$ as measuring the *number* of $S_m \to S_n$ transitions in time $dt$ instead of the *probability* of an $S_m \to S_n$ transition in time $dt$; this has the effect of approximating the given discrete, stochastic random walk process by a continuous, deterministic rate process. However, it is not at all obvious how to create such an approximate rate formalism when $A_{nm}$ is a function of the residence time in the state $S_m$. Indeed, the master equation for a semi-Markov random walk turns out to involve a time-convolution integral [7–11], and this indicates that the corresponding time-evolution equations for the various moments of $\tilde{P}(m, t)$ will have a much more complicated structure than they would have in the pure Markov case.

These considerations suggest that a reliable numerical simulation method might be a very useful tool for studying specific examples of the random walk (1). Moreover, the existence of a viable simulation technique for the process (1) might encourage investigators in the physical, biological, and social sciences to experiment more freely with models of this type in their respective fields of research.

It should be noted that (1) is not the only way to specify a semi-Markov process. A specification format that turns out to be especially convenient from the standpoint of the master equation is [7–11]:

If the system arrives in the state $S_m$ at time $t$, then the probability that it will *next* step to state $S_n$ in the infinitesimal time interval $(t + \tau, t + \tau + d\tau)$ is

$$\pi(n, m)\, \psi(\tau \mid m)\, d\tau. \tag{2}$$

Here, $\psi(\tau \mid m)$ is the probability density function for the pausing time $\tau$ in the state $S_m$, and $\pi(n, m)$ is the stepping probability from state $S_m$ to state $S_n$. The precise mathematical relationship between formats (1) and (2) will be elaborated on in the next section. However, the focus of this paper will be primarily on the specification format (1). This choice reflects the writer's own opinion, based on past experiences with physical systems that behave in a Markovian fashion, that the function $A_{nm}(\tau)$ will probably have a more direct relationship to the physical parameters of a real physical system than will the pair of functions $\pi(n, m)$ and $\psi(\tau \mid m)$. In any event, this paper will be concerned chiefly with the simulation of those stochastically evolving systems which are such that (1) provides a more "natural" specification of the transition dynamics than (2).

## 2. The Transition Probability Density Function

Since (1) does not specify $A_{nm}(\tau)$ for $n = m$, we shall for convenience put

$$A_{nm}(\tau) \equiv 0. \tag{3}$$

Then if we define

$$A_m(\tau) \equiv \sum_n A_{nm}(\tau), \tag{4}$$

it follows from (1) and the addition law of probability theory that

$$A_m(\tau)\, dt = \text{probability that the system in state } S_m \text{ at time } t, \text{ having arrived there at time } t - \tau, \text{ will step away from } S_m \text{ during } (t, t + dt). \tag{5}$$

The key theoretical construct upon which our Monte Carlo simulation procedure is based is the *transition probability density function* $P(\tau, n \mid m, t)$, which is defined by the statement

$$P(\tau, n \mid m, t)\, d\tau \equiv \text{probability that, given the system arrives in the state } S_m \text{ at time } t, \text{ the } \textit{next} \text{ transition will occur in the infinitesimal time interval } (t + \tau, t + \tau + d\tau) \textit{ and} \text{ will be to the state } S_n. \tag{6}$$

$P(\tau, n \mid m, t)$ is a joint probability density function of the real variable $\tau$ and the

integer variable $n$, conditioned on $m$ and $t$. For a random walk specified by (2), $P(\tau, n \mid m, t)\, d\tau$ is evidently equal to $\pi(n, m)\, \psi(\tau \mid m)\, d\tau$. However, in order to set the stage for an explicit Monte Carlo simulation procedure for a random walk specified by (1), we shall require an expression for $P(\tau, n \mid m, t)$ in terms of the given function $A_{nm}(\tau)$. This will also allow us to elucidate the precise connection between (1) and (2).

Using (1), the probability in (6) may be expressed as

$$P(\tau, n \mid m, t)\, d\tau = \mathscr{P}(\tau \mid m, t) \cdot A_{nm}(\tau)\, d\tau, \tag{7}$$

where the auxiliary quantity $\mathscr{P}(\tau \mid m, t)$ is defined by

$$\mathscr{P}(\tau \mid m, t) \equiv \text{probability that, given the system arrives in the state } S_m \text{ at time } t, \textit{no} \text{ transition will occur in the time interval } (t, t + \tau). \tag{8a}$$

To obtain an expression for $\mathscr{P}(\tau \mid m, t)$, we need only observe that it must satisfy [cf. (5)]

$$\mathscr{P}(\tau + d\tau \mid m, t) = \mathscr{P}(\tau \mid m, t)[1 - A_m(\tau)\, d\tau],$$

or equivalently

$$d\mathscr{P}(\tau \mid m, t)/\mathscr{P}(\tau \mid m, t) = -A_m(\tau)\, d\tau.$$

Integrating this last relation subject to the required initial condition $\mathscr{P}(0 \mid m, t) = 1$ gives

$$\mathscr{P}(\tau \mid m, t) = \exp\left[-\int_0^\tau A_m(\tau')\, d\tau'\right]. \tag{8b}$$

Substituting this into (7) yields the result

$$P(\tau, n \mid m, t) = A_{nm}(\tau) \exp\left[-\int_0^\tau A_m(\tau')\, d\tau'\right]. \tag{9}$$

Before we proceed to cast (9) into a form more suitable for Monte Carlo purposes, let us digress here to establish the connection between (1) and (2). As noted earlier, for systems described by (2), $P(\tau, n \mid m, t)$ is equal to $\pi(n, m)\, \psi(\tau \mid m)$. Combining this with (9) gives

$$\pi(n, m)\, \psi(\tau \mid m) = A_{nm}(\tau) \exp\left[-\int_0^\tau A_m(\tau')\, d\tau'\right]. \tag{10}$$

Now $\pi(n, m)$ in (2) is presumed to satisfy $\sum_n \pi(n, m) = 1$, so by summing (10) over $n$ and recalling the definition (4) we obtain for $\psi(\tau \mid m)$ the formula

$$\psi(\tau \mid m) = A_m(\tau) \exp\left[-\int_0^\tau A_m(\tau')\, d\tau'\right]. \tag{11a}$$

Substituting this back into (10) then gives for $\pi(n, m)$ the formula

$$\pi(n, m) = A_{nm}(\tau)/A_m(\tau). \tag{11b}$$

Equations (11) define the translation from the random walk specification (1) into the random walk specification (2). We notice from (11b) that the function $\pi$ must be written $\pi(n, m, \tau)$ unless the ratio $A_{nm}(\tau)/A_m(\tau)$ is independent of $\tau$ for all $n$ and $m$. One case in which that ratio is obviously independent of $\tau$ is for the Markov process, $A_{nm}(\tau) = a_{nm}$ ; substituting into (11a) and (11b) shows that, for this case, $\psi(\tau \mid m) = a_m \exp(-a_m\tau)$ and $\pi(n, m) = a_{nm}/a_m$ , where $a_m \equiv \sum_n a_{nm}$ .

We can "invert" Eqs. (11) by first integrating (11a) over $\tau$, solving for the integral of $A_m$ , and differentiating the result, to obtain

$$A_m(\tau) = \psi(\tau \mid m)\Big/\left[1 - \int_0^\tau \psi(\tau' \mid m)\, d\tau'\right].$$

Then putting this into (11b) and solving for $A_{nm}(\tau)$ gives

$$A_{nm}(\tau) = \pi(n, m)\, \psi(\tau \mid m)\Big/\left[1 - \int_0^\tau \psi(\tau' \mid m)\, d\tau'\right] \tag{12}$$

as the formula for translating the random walk specification (2) into the random walk specification (1). We see from (12) that if $\pi$ is independent of $\tau$ then $A_{nm}(\tau)$ will have the functional form $f(n, m)\, g(\tau, m)$. We also see from (12) that if $\int_0^{\tau_m} \psi(\tau' \mid m)\, d\tau' = 1$ for some *finite* $\tau_m$ , and hence also $\psi(\tau \mid m) \equiv 0$ for $\tau > \tau_m$ , then $A_{nm}(\tau)$ diverges at $\tau = \tau_m$ and is indeterminate for $\tau > \tau_m$ . The reason for this apparently bizarre behavior can be readily understood from (1), though, if one merely considers that definition for the situation in which the system is *certain* to leave the state $S_m$ by the time $t + \tau_m$ . Obviously, random walks having this property are more naturally described in terms of (2) rather than (1).

For the purpose of deriving a Monte Carlo method for numerically simulating the random walk defined in (1), it will prove convenient to express the probability (6) in the "conditioned" form

$$P(\tau, n \mid m, t)\, d\tau = P_1(m, t) \cdot P_2(\tau \mid m, t)\, d\tau \cdot P_3(n \mid m, t; \tau), \tag{13}$$

where the quantities on the right are defined as follows:

$P_1(m, t) \equiv$ probability that the system, arriving in $S_m$ at time $t$, will eventually leave $S_m$ (i.e., will not stay in $S_m$ forever); (14a)

$P_2(\tau \mid m, t)\, d\tau \equiv$ probability that the system, arriving in $S_m$ at time $t$, will next leave $S_m$ in $(t + \tau, t + \tau + d\tau)$, *given* that the system does eventually leave $S_m$ ; (14b)

$P_3(n \mid m, t; \tau) \equiv$ probability that the system, arriving in $S_m$ at time $t$, will jump next to $S_n$ , *given* that the next jump is made at time $t + \tau$. (14c)

We shall now use (9) to obtain explicit expressions for these three probabilities in terms of the given function $A_{nm}(\tau)$. For convenience, we first define the quantity

$$B_m(\tau) \equiv \int_0^\tau A_m(\tau')\, d\tau', \tag{15}$$

so that (9) takes the form

$$P(\tau, n \mid m, t) = A_{nm}(\tau) \exp[-B_m(\tau)]. \tag{16}$$

The definition in (14a) implies that $P_1(m, t)$ may be calculated as

$$\begin{aligned} P_1(m, t) &= \int_0^\infty \sum_n P(\tau, n \mid m, t)\, d\tau \\ &= \int_0^\infty A_m(\tau) \exp[-B_m(\tau)]\, d\tau, \end{aligned}$$

where we have used (16) and (4). Changing integration variables here from $\tau$ to $B_m(\tau)$ [see (15)], this integral is easily evaluated to give

$$P_1(m, t) = 1 - \exp[-B_m(\infty)]. \tag{17a}$$

We note in passing that, if $B_m(\infty) < \infty$, there is a nonzero probability, namely, $\exp[-B_m(\infty)]$, that the system will never leave the state $S_m$ . We do *not* disallow this possibility.

Now denoting by $\bar{P}(\tau, n \mid m, t)$ the *normalized* transition probability density function—i.e., $\bar{P}(\tau, n \mid m, t)\, d\tau$ is the probability that the system, upon arriving in $S_m$ at $t$, will next jump to $S_n$ in $(t + \tau, t + \tau + d\tau)$, *given* that it does indeed make another jump—we evidently have

$$\bar{P}(n, \tau \mid m, t) = P(n, \tau \mid m, t)/P_1(m, t).$$

The definitions in (14b) and (14c) imply that $P_2(\tau \mid m, t)$ and $P_3(n \mid m, t; \tau)$ may be calculated from $\bar{P}(n, \tau \mid m, t)$ according to

$$P_2(\tau \mid m, t) = \sum_n \bar{P}(n, \tau \mid m, t)$$

and

$$P_3(n \mid m, t; \tau) = \bar{P}(n, \tau \mid m, t)/P_2(\tau \mid m, t).$$

These calculations are easy, and they yield

$$P_2(\tau \mid m, t) = \{1 - \exp[-B_m(\infty)]\}^{-1} A_m(\tau) \exp[-B_m(\tau)], \tag{17b}$$

$$P_3(n \mid m, t; \tau) = A_{nm}(\tau)/A_m(\tau). \tag{17c}$$

As a check on the above results, it will be observed that when the expressions in (17a), (17b) and (17c) are substituted into the right side of (13), the result agrees exactly with (16).

## 3. The Simulation Procedure

In order to simulate the random walk defined by (1), we must be able to do the following: For the system arriving in any state $S_m$ at any time $t$, we must be able to determine at what time $t + \tau$ the next step should occur, and to which state $S_n$ that next step should be. The reason for introducing the transition probability density function $P(\tau, n \mid m, t)$ in the previous section is that it allows us to state this requirement in more precise mathematical terms: For the system arriving in any state $S_m$ at any time $t$, we must be able to draw or "generate" a pair of numbers $(\tau, n)$ from the set of random pairs whose joint probability density function is $P(\tau, n \mid m, t)$.

For the purpose of accomplishing this task on a digital computer we shall assume that we have access to a "unit-interval uniform random number generator." This is simply a computer subprogram which, when called, calculates and returns a random number $r$ from the uniform distribution in the unit interval. More precisely, the a priori probability that any generated value $r$ lies inside any given subinterval of the unit interval is equal to the length of that subinterval and is independent of its location:

$$\text{For any } 0 \leqslant a \leqslant b \leqslant 1, \qquad \text{Prob}\{a \leqslant r \leqslant b\} = b - a. \tag{18}$$

For brevity we shall refer to any unit-interval uniform random number generator subprogram as URN. Nowadays, virtually every large computer facility has an URN subprogram in its library file that is fast, easy to use, and sufficiently "random" for our purposes. Assuming ready access to such a subprogram, our procedure for generating a random pair $(\tau, n)$ according to $P(\tau, n \mid m, t)$ is as follows:

> Draw two random numbers $r_1$ and $r_2$ from the unit-interval uniform distribution (i.e., from URN). If the inequality

$$\ln(1/r_1) < \int_0^\infty A_m(\tau')\, d\tau' \tag{19a}$$

is satisfied, then choose $\tau$ so that

$$\int_0^\tau A_m(\tau')\, d\tau' = \ln(1/r_1), \tag{19b}$$

and next choose $n$ so that

$$\sum_{n'=1}^{n-1} A_{n'm}(\tau) < r_2 A_m(\tau) \leqslant \sum_{n'=1}^{n} A_{n'm}(\tau), \tag{19c}$$

where $\tau$ is the value determined in (19b). If the inequality (19a) is *not* satisfied, then take $\tau = \infty$ (i.e., terminate the random walk in the state $S_m$).

That this algorithm indeed generates a random pair $(\tau, n)$ distributed according to the joint probability density function $P(\tau, n \mid m, t)$ of Section 2 is proved in Section 4.[2] The solution of (19b) for $\tau$ is to be accomplished analytically if possible, but numerically if necessary; the solution of (19c) for $n$ may be effected by means of a simple do-loop in the computer program. Using this algorithm, our procedure for numerically simulating the random walk (1) is now fairly straightforward:

*Step* 0 *(initialization).* Set the variable $m$ (the current state index) to the prescribed initial value $m_0$, and set the variable $t$ (the current time) to 0.

*Step* 1. Establish, relative to the current state $S_m$, an indexing scheme $n = 1, 2, \ldots, N_m$ for all states $S_n$ for which $A_{nm}(\tau)$ is not identically zero; then calculate the function

$$A_m(\tau) \equiv \sum_{n=1}^{N_m} A_{nm}(\tau).$$

*Step* 2. Using the functions $A_{nm}(\tau)$ and $A_m(\tau)$ established in Step 1, generate a random pair $(\tau, n)$ with the generating algorithm (19).

*Step* 3. Replace $t$ and $m$ by $t + \tau$ and $n$, respectively; then return to Step 1.

The 1–2–3 sequence above is to be iterated until $t$ has reached some predetermined value, or until the system "sticks" in some state $S_m$ because of the failure of the inequality (19a). Notice that, if the integral on the right of (19a) is infinite for all states $S_m$, as is the case with many random walks, then (19a) will always be satisfied and that test may be omitted.

If the random walk is such that $N_m$ in Step 1 is normally very large, or the functions $A_{nm}(\tau)$ and $A_m(\tau)$ are very complicated, then this simulation procedure will obviously be too cumbersome to implement. When these parameters are "reasonable," the key to a successful implementation may well lie in how efficiently one can accomplish the "reindexing of states" in Step 1. In that connection, we might take note of what

[2] For a random walk specified according to (2) with $\int_0^{\tau_m} \psi(\tau \mid m)\, d\tau = 1$ for finite $\tau_m$, it is simpler to use the following generating procedure: Draw two random numbers $r_1$ and $r_2$ from URN; choose $\tau$ so that $\int_0^\tau \psi(\tau' \mid m)\, d\tau' = r_1$, and choose $n$ so that $\sum_{n'=1}^{n-1} \pi(n', m) < r_2 \leqslant \sum_{n'=1}^{n} \pi(n', m)$.

amounts to an *implicit* reindexing scheme used in simulating the time evolution of a spatially homogeneous chemically reacting system (which constitutes a Markovian random walk over the space of the molecular population numbers) [2]: Instead of dealing directly with the possible states $S_n$ to which the system may jump from the current state $S_m$, attention is focused on the possible reactions $R_\mu$ that may occur in that state. Unlike the possible "next states," the possible "next reactions" do not change from state to state, so a considerable simplification is achieved by replacing in the transition probability density function the "next state" index $n$ by the "next reaction" index $\mu$; once the next reaction $R_\mu$ has been selected, the system can then be "moved" to the next state by simply altering the molecular population numbers in accordance with $R_\mu$. Generalizing from this, it may be that the reindexing of states in Step 1 can be most easily accomplished implicitly, by focusing on the single-step *transition channels* instead of on the possible next states themselves.

If we carry out the simulation procedure described above, we will obviously produce only *one* realization of the random walk defined by (1). If we want to calculate *ensemble averages* of the kind that are (in principle) calculable from the grand probability function $\tilde{P}(m, t)$, then we will have to carry out *many* simulation runs, all identical except for the URN values used. The ensemble average of any state function at time $t$ may then be calculated as the direct (equally weighted) average of the values found for the state function at time $t$ in these simulation runs. The number of runs required for this type of calculation will depend strongly on the system under consideration, the state function whose average is sought, and the level of statistical accuracy that is desired. Obviously there will be instances in which such a calculation will not be feasible because an unaffordably large number of runs is required. But in situations where the master equation is simply too complicated to handle, the simulation approach may be the best that one can do. Even for cases in which the master equation *is* tractable the simulation procedure can still be useful, because its ability to follow *individual realizations* of a random walk provides a nice complement to the ensemble average characterization provided by the grand probability function $\tilde{P}(m, t)$.

## 4. Proof of the Generating Algorithm

In this section we shall prove that the random pair $(\tau, n)$ generated by the algorithm (19) is indeed distributed according to the joint probability density function $P(\tau, n \mid m, t)$ in Section 2. For this purpose, we define the following three probabilities with respect to the algorithm (19):

$$P_1^*(m, t) \equiv \text{probability that (19a) will be satisfied, so that the random walk does not terminate in } S_m\text{;} \tag{20a}$$

$$P_2^*(\tau \mid m, t) \equiv \text{probability density function for the } \tau\text{-value selected by (19b);} \tag{20b}$$

$$P_3^*(n \mid m, t; \tau) \equiv \text{probability that (19c) will select the value } n. \tag{20c}$$

Our proof will consist of showing that $P_1^*$, $P_2^*$, and $P_3^*$ defined above are identical respectively, to the functions $P_1$, $P_2$, and $P_3$ in Section 2 [see Eqs. (14) and (17)].

First, using (20a), (19a), and the definition (15),

$$\begin{aligned} P_1^*(m, t) &= \text{Prob}\{\ln(1/r_1) < B_m(\infty)\} \\ &= \text{Prob}\{\exp[-B_m(\infty)] < r_1 < 1\}. \end{aligned}$$

But since $r_1$ is a random number from the uniform distribution in the unit interval, then we have from (18)

$$P_1^*(m, t) = 1 - \exp[-B_m(\infty)]. \tag{21a}$$

Comparing (21a) with (17a), we see that $P_1{}^*(m, t) = P_1(m, t)$.

If (19a) is satisfied, $r_1$ can *then* be regarded as a random number from the uniform distribution in the interval $(\exp[-B_m(\infty)], 1)$; i.e., when we come to (19b), $r_1$ is a random number whose probability density function is

$$\begin{aligned} p(r_1) &= \{1 - \exp[-B_m(\infty)]\}^{-1}, && \text{for } \exp[-B_m(\infty)] < r_1 < 1; \\ &= 0, && \text{otherwise.} \end{aligned}$$

The transformation (19b) produces from $r_1$ a new random variable $\tau$, whose probability density function is determined by the rule

$$P_2^*(\tau \mid m, t) = p(r_1) \mid dr_1/d\tau \mid = \{1 - \exp[-B_m(\infty)]\}^{-1} \mid dr_1/d\tau \mid$$

Now (19b) implies that

$$r_1 = \exp\left[-\int_0^\tau A_m(\tau')\, d\tau'\right]$$

so

$$dr_1/d\tau = -A_m(\tau) \exp\left[-\int_0^\tau A_m(\tau')\, d\tau'\right] = -A_m(\tau) \exp[-B_m(\tau)],$$

where we have used (15). Substituting this into the above equation for $P_2{}^*(\tau \mid m, t)$ gives

$$P_2^*(\tau \mid m, t) = \{1 - \exp[-B_m(\infty)]\}^{-1} A_m(\tau) \exp[-B_m(\tau)]. \tag{21b}$$

Comparing (21b) with (17b), we see that $P_2^*(\tau \mid m, t) = P_2(\tau \mid m, t)$.

Finally, the probability that (19c) will be satisfied for the index $n$ is evidently

$$P_3^*(n \mid m, t; \tau) = \text{Prob}\left\{\sum_{n'=1}^{n-1} A_{n'm}(\tau)/A_m(\tau) < r_2 \leqslant \sum_{n'=1}^{n} A_{n'm}(\tau)/A_m(\tau)\right\}.$$

But since $r_2$ is a random number from the unit-interval uniform distribution, then by (18) we have

$$P_3^*(n \mid m, t; \tau) = \left[\sum_{n'=1}^{n} A_{n'm}(\tau)/A_m(\tau)\right] - \left[\sum_{n'=1}^{n-1} A_{n'm}(\tau)/A_m(\tau)\right]$$

or

$$P_3^*(n \mid m, t; \tau) = A_{nm}(\tau)/A_m(\tau). \tag{21c}$$

Comparing (21c) with (17c), we see that $P_3^*(n \mid m, t; \tau) = P_3(n \mid m, t; \tau)$.

Since $P_1$, $P_2$, and $P_3$ condition $P(\tau, n \mid m, t)$ according to (13), we may therefore conclude that $P(\tau, n \mid m, t)$ is indeed the joint probability density function of the $(\tau, n)$ pair generated by the algorithm (19).

## 5. Some Examples

We conclude by working out the stepping algorithm (19) for three simple functional forms of $A_{nm}(\tau)$.

Example 1. $A_{nm}(\tau) = a_{nm}$ (constant). (22a)

This, as mentioned earlier, is the transition probability rate for the Markov process. Defining

$$a_m \equiv \sum_n a_{nm}, \tag{22b}$$

it follows that $A_m(\tau) = a_m$, so

$$\int_0^\tau A_m(\tau')\, d\tau = a_m \tau.$$

For $\tau = \infty$ this integral diverges (assuming $a_m \neq 0$), so the check (19a) may be omitted. (19b) becomes

$$a_m \tau = \ln(1/r_1)$$

and can be solved explicitly for $\tau$. Hence, the stepping algorithm is:

Draw $r_1$ and $r_2$ from URN; take

$$\tau = (1/a_m) \ln(1/r_1), \tag{23a}$$

and take $n$ so that

$$\sum_{n'=1}^{n-1} a_{n'm} < r_2 a_m \leqslant \sum_{n'=1}^{n} a_{n'm}. \tag{23b}$$

This is the generating procedure used in [2] to simulate the stochastic behavior of a chemically reacting system, except that there, as noted earlier, the state index was replaced by a transition channel index in order to facilitate Step 1 of the simulation procedure.

EXAMPLE 2. $A_{nm}(\tau) = a_{nm}\tau^{\alpha_m} \qquad (\alpha_m > -1).$ (24a)

Defining

$$a_m \equiv \sum_n a_{nm}\,, \tag{24b}$$

it follows that $A_m(\tau) = a_m\tau^{\alpha_m}$, so

$$\int_0^\tau A_m(\tau')\,d\tau' = a_m\tau^{(\alpha_m+1)}/(\alpha_m + 1).$$

Since $\alpha_m > -1$, this integral diverges for $\tau = \infty$ (assuming $a_m \neq 0$), so the check (19a) may be omitted. (19b) becomes

$$a_m\tau^{(\alpha_m+1)}/(\alpha_m + 1) = \ln(1/r_1)$$

which can be solved explicitly for $\tau$. Equation (19c) may be simplified by noting that $A_{nm}(\tau)/A_m(\tau) = a_{nm}/a_m$. Hence, the stepping algorithm is:

Draw $r_1$ and $r_2$ from URN; take

$$\tau = [(\alpha_m + 1)(1/a_m)\ln(1/r_1)]^{1/(\alpha_m+1)}, \tag{25a}$$

and take $n$ so that

$$\sum_{n'=1}^{n-1} a_{n'm} < r_2 a_m \leqslant \sum_{n'=1}^{n} a_{n'm}\,. \tag{25b}$$

Notice that, for $\alpha_m = 0$, (25) reduces to (23), as expected.

EXAMPLE 3. $A_{nm}(\tau) = a_{nm}e^{-\alpha_m\tau} \qquad (\alpha_m > 0).$ (26a)

This case should not be confused with the (Markovian) case in which $\psi(\tau \mid m)$ in (2) is an exponentially decaying function of $\tau$. Defining

$$a_m \equiv \sum_n a_{nm}\,, \tag{26b}$$

it follows that $A_m(\tau) = a_m e^{-\alpha_m\tau}$, so

$$\int_0^\tau A_m(\tau')\,d\tau' = (a_m/\alpha_m)[1 - e^{-\alpha_m\tau}].$$

Since

$$\int_0^\infty A_m(\tau')\,d\tau' = a_m/\alpha_m < \infty$$

then the test (19a) *cannot* be omitted. Equation (19b) reads

$$(a_m/\alpha_m)[1 - e^{-\alpha_m \tau}] = \ln(1/r_1)$$

which can be solved explicitly for $\tau$. Equation (19c) may be simplified by noting that $A_{nm}(\tau)/A_m(\tau) = a_{nm}/a_m$. Hence, the stepping algorithm is:

Draw $r_1$ and $r_2$ from URN. If $\ln(1/r_1) \geqslant a_m/\alpha_m$ then terminate the random walk in the present state $S_m$; if $\ln(1/r_1) < a_m/\alpha_m$, take

$$\tau = (1/\alpha_m) \ln\{1/[1 - (\alpha_m/a_m) \ln(1/r_1)]\}, \tag{27a}$$

and take $n$ so that

$$\sum_{n'=1}^{n-1} a_{n'm} < r_2 a_m \leqslant \sum_{n'=1}^{n} a_{n'm}. \tag{27b}$$

In the foregoing three examples it will be noted that the $n$-selection algorithms are identical; it is only in the $\tau$-selection algorithms for Examples 2 and 3 that the residence time parameter $\alpha_m$ enters. This implies that these three random walks will differ only in their "time schedules" and not in their "routes" (except that in the third example the journey may be abruptly terminated). It is obvious from (19c) and (4) that this will be the case for *all* random walks whose transition probability rate functions $A_{nm}(\tau)$ have the form $a_{nm} f(\tau, m)$, $f$ being an arbitrary function.

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