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Construction of Equivalent Stochastic Differential Equation Models

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Abstract: It is shown how different but equivalent Itô stochastic differential equation models of random dynamical systems can be constructed. Advantages and disadvantages of the different models are described. Stochastic differential equation models are derived for problems in chemistry, textile engineering, and epidemiology. Computational comparisons are made between the different stochastic models.

Keywords: Chemical reactions; Cotton fiber breakage; Epidemiology; Mathematical model; Stochastic differential equation.

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1. INTRODUCTION

Often, in modeling a random dynamical problem, a system of Itô stochastic differential equations is developed and studied. There appear to be three procedures for developing stochastic differential equation (SDE) models for applications in population biology, physics, chemistry, engineering, and mathematical finance. In the first modeling procedure, a discrete stochastic model is developed by studying changes in the system components over a small time interval (e.g., [1–12]). This approach is a natural extension of the procedure used for many years in modeling deterministic dynamical processes in physics and engineering, where changes in the system are studied over a small time interval and a differential equation is obtained as the time interval approaches zero. Similarities between the forward Kolmogorov equations satisfied by the probability distributions of discrete- and continuous-time stochastic models let us infer that an Itô SDE model is close to the discrete stochastic model. In this procedure, the number of Wiener processes in the resulting SDE model never exceeds the number of components in the system. In the second procedure, the dynamical system is carefully studied to determine all of the different independent random changes that occur in the system. Appropriate terms are determined for these changes in developing a discrete-time stochastic model which is then approximated by a system of stochastic differential equations (e.g., [13–17]). As the total number of different random changes may exceed the number of components in the system, a stochastic differential equation model is obtained where the number of Wiener processes may exceed the number of equations. This procedure yields systems of stochastic differential equations that are generally easy to solve numerically. A third procedure is direct formulation of a system of stochastic differential equations and is the most commonly used procedure in constructing SDE models. For a given random dynamical system, specific functional forms are assumed for the elements of the drift vector and diffusion matrix. Frequently, for mathematical simplicity, these elements are assumed to be linear functions of the component processes (e.g., [18, 19]). These three procedures have been used in modeling many dynamical processes that experience random influences. In this investigation, only the first two procedures are discussed.

In the next section, two stochastic differential equation systems are studied which are produced by the first and second modeling procedures. The two systems of stochastic differential equations are structurally different yet have identical probability distributions. In addition, by identifying relations between Wiener trajectories, it is shown that a sample path solution of one system is also a sample path solution of the other system. As the stochastic models can be interchanged, conceptual or computational advantages possessed by either model can

be employed in any particular problem. In Section 3, it is shown how the two stochastic models are derived from first principles, that is, from the possible changes that may occur in the system. In Section 4, three examples from chemistry, textile engineering, and epidemiology are discussed, illustrating the derivations of the stochastic models and some computational comparisons between them.

2. EQUIVALENT SDE SYSTEMS

Let

$$\vec{f} : [0, T] \times \mathbb{R}^d \to \mathbb{R}^d,$$
$$G : [0, T] \times \mathbb{R}^d \to \mathbb{R}^{d \times m},$$

and

$$B : [0, T] \times \mathbb{R}^d \to \mathbb{R}^{d \times d}.$$

In addition, let $\vec{X}(t) = [X_1(t), X_2(t), \ldots, X_d(t)]^T$, $\vec{X}^*(t) = [X_1^*(t), X_2^*(t), \ldots, X_d^*(t)]^T$, $\vec{W}(t) = [W_1(t), W_2(t), \ldots, W_m(t)]^T$, and $\vec{W}^*(t) = [W_1^*(t), W_2^*(t), \ldots, W_d^*(t)]^T$, where $W_i(t)$, $i = 1, \ldots, m$ and $W_j^*(t)$, $j = 1, \ldots, d$ are independent Wiener processes and $m \geq d$. Considered in this article are the two Itô SDE systems:

$$d\vec{X}(t) = \vec{f}(t, \vec{X}(t))dt + G(t, \vec{X}(t))d\vec{W}(t), \tag{2.1}$$

and

$$d\vec{X}^*(t) = \vec{f}(t, \vec{X}^*(t))dt + B(t, \vec{X}^*(t))d\vec{W}^*(t). \tag{2.2}$$

Matrices G and B are related through the $d \times d$ matrix V, where $V(t, \vec{z}) = G(t, \vec{z})G^T(t, \vec{z})$ and $B(t, \vec{z}) = V^{1/2}(t, \vec{z})$ for $\vec{z} \in \mathbb{R}^d$. It is assumed that $\vec{f}$, G, and B satisfy certain continuity and boundedness conditions [20, 21] so that (2.1) and (2.2) have pathwise unique solutions. Since $\vec{W}$ and $\vec{W}^*$ are not defined on the same probability space, neither are X and X^*. However, it is shown that solutions to (2.1) and (2.2) have the same probability distribution. In addition, one can define a measure-preserving map between the probability spaces in such a way that the corresponding sample paths X and X^* are identical.

Notice that the $d \times d$ symmetric positive semidefinite matrix V has entries

$$v_{i,j}(t, \vec{X}) = \sum_{l=1}^{m} g_{i,l}(t, \vec{X}) g_{j,l}(t, \vec{X}) \tag{2.3}$$

for $i, j = 1, \ldots, d$ and $d \times d$ symmetric positive semidefinite matrix B has entries that satisfy

$$v_{i,j}(t, \vec{X}) = \sum_{l=1}^{d} b_{i,l}(t, \vec{X}) b_{j,l}(t, \vec{X}) \tag{2.4}$$

for $i, j = 1, \ldots, d$. In component form, systems (2.1) and (2.2) can be expressed as

$$X_i(t) = X_i(0) + \int_0^t f_i(s, \vec{X}(s))ds + \int_0^t \sum_{j=1}^{m} g_{i,j}(s, \vec{X}(s))dW_j(s) \tag{2.5}$$

for $i = 1, 2, \ldots, d$, where f_i is the ith entry of $\vec{f}$ and $g_{i,j}$ is the i, j entry of the $d \times m$ matrix G and

$$X_i^*(t) = X_i^*(0) + \int_0^t f_i(s, \vec{X}^*(s))ds + \int_0^t \sum_{j=1}^{d} b_{i,j}(s, \vec{X}^*(s))dW_j^*(s) \tag{2.6}$$

for $i = 1, \ldots, d$ and $b_{i,j}$ is the i, j entry of the $d \times d$ matrix B.

It is now shown that solutions to (2.1) and (2.2) possess the same probability distributions; they are equivalent in distribution. To see this, consider the forward Kolmogorov equation or Fokker-Planck equation for the probability density function $p(t, \vec{x})$ associated with the stochastic differential system (2.1),

$$\frac{\partial p(t, \vec{x})}{\partial t} = \frac{1}{2} \sum_{i=1}^{d} \sum_{j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j} \left[p(t, \vec{x}) \sum_{l=1}^{m} g_{i,l}(t, \vec{x}) g_{j,l}(t, \vec{x}) \right] - \sum_{i=1}^{d} \frac{\partial [p(t, \vec{x}) f_i(t, \vec{x})]}{\partial x_i}. \tag{2.7}$$

In particular, if $\vec{z}_1, \vec{z}_2 \in \mathbb{R}^d$ and $\vec{z}_1 \leq \vec{z}_2$, then

$$P(\vec{z}_1 \leq \vec{X}(t) \leq \vec{z}_2) = \int_{z_{1,d}}^{z_{2,d}} \int_{z_{1,d-1}}^{z_{2,d-1}} \cdots \int_{z_{1,1}}^{z_{2,1}} p(t, \vec{x}) dx_1 \, dx_2, \ldots, dx_d.$$

As the elements of V satisfy

$$v_{i,j}(t, \vec{x}) = \sum_{l=1}^{m} g_{i,l}(t, \vec{x}) g_{j,l}(t, \vec{x}) = \sum_{l=1}^{d} b_{i,l}(t, \vec{x}) b_{j,l}(t, \vec{x}),$$

systems (2.1) and (2.2) have the same forward Kolmogorov equation. Hence, the probability density functions for $\vec{X}(t)$ and $\vec{X}^*(t)$ are identical.

In addition to solutions of (2.1) and (2.2) having the same probability distribution, it is useful conceptually and for sample path approximation to be aware that a sample path solution of one equation

is also a sample path solution of the second equation defined on an augmented probability space. It will be shown that stochastic differential equations (2.1) and (2.2) possess the property that a sample path solution of one equation is also a sample path solution of the second equation, and the correspondence is measure preserving. More specifically, given a Wiener trajectory $\vec{W}(t)$ with sample path solution $\vec{X}(t)$ to (2.1), there exists a Wiener trajectory $\vec{W}^*(t)$ with the sample path solution $\vec{X}^*(t) = \vec{X}(t)$ to (2.2). Conversely, given a Wiener trajectory $\vec{W}^*(t)$ with sample path solution $\vec{X}^*(t)$ to (2.2), there exists a Wiener trajectory $\vec{W}(t)$ with the sample path solution $\vec{X}(t) = \vec{X}^*(t)$ to (2.1).

Assume now that a Wiener trajectory $\vec{W}(t)$ for $0 \le t \le T$ is given and the sample path solution to (2.1) is $\vec{X}(t)$. It is now shown that there exists a Wiener trajectory $\vec{W}^*(t)$ such that (2.2) has the same sample path solution as (2.1), i.e., $\vec{X}^*(t) = \vec{X}(t)$ for $0 \le t \le T$. To see this, an argument involving the singular value decomposition of $G(t) = G(t, \vec{X}(t))$ is employed. Consider, therefore, the singular value decomposition of $G(t) = P(t)D(t)Q(t)$ for $0 \le t \le T$, where $P(t)$ and $Q(t)$ are orthogonal matrices of sizes $d \times d$ and $m \times m$, respectively, and $D(t)$ is a $d \times m$ matrix with $r \le d$ positive diagonal entries. (It is assumed that the rank of $G(t)$ is r for $0 \le t \le T$. This assumption can be generalized so that the rank of $G(t)$ is a piecewise constant function of t on a partition of $[0, T]$.) It follows that $V(t) = G(t)G(t)^T = P(t)D(t)D^T(t)P^T(t) = [B(t)]^2$, where $B(t) = P(t)(D(t)D^T(t))^{1/2}P^T(t)$. The vector $\vec{W}^*(t)$ of d independent Wiener processes is now defined as

$$\vec{W}^*(t) = \int_0^t P(s)((D(s)(D(s))^T)^{1/2})^+ D(s)Q(s)d\vec{W}(s) + \int_0^t P(s)d\vec{W}^{**}(s)$$

for $0 \le t \le T$, where $\vec{W}^{**}(s)$ is a vector of length d with the first r entries equal to 0 and the next $d - r$ entries independent Wiener processes, and where $((D(t)D^T(t))^{1/2})^+$ is the $d \times d$ pseudoinverse of $(D(t)D^T(t))^{1/2}$. (If Σ is a $d \times m$ matrix with nonzero entries $\sigma_{i,i}$ for $i = 1, 2, \ldots, r$ with $r \le d \le m$, then Σ^+ is a $m \times d$ matrix with nonzero entries $1/\sigma_{i,i}$ for $i = 1, 2, \ldots, r$. See, e.g., [22] or [23] for more information about the singular value decomposition and pseudoinverses.) Notice that $E(\vec{W}^*(t)(\vec{W}^*(t))^T) = tI_d$, where I_d is the $d \times d$ identity matrix verifying that $\vec{W}^*(t)$ is a vector of d independent Wiener processes. The diffusion term on the right side of (2.2) with $\vec{X}^*(t)$ replaced by $\vec{X}(t)$ satisfies

$$\begin{aligned}
&B(t, \vec{X}(t))d\vec{W}^*(t) \\
&\quad = B(t)\big(P(t)\big((D(t)(D(t))^T\big)^{1/2}\big)^+ D(t)Q(t)d\vec{W}(t) + P(t)d\vec{W}^{**}(t)\big) \\
&\quad = P(t)(D(t)D^T(t))^{1/2}P^T(t)\big(P(t)\big((D(t)(D(t))^T\big)^{1/2}\big)^+ D(t)Q(t)d\vec{W}(t) \\
&\qquad + P(t)d\vec{W}^{**}(t)) \\
&\quad = G(t, \vec{X}(t))d\vec{W}(t).
\end{aligned}$$

Hence, $d\vec{X}(t) = \vec{f}(t, \vec{X}(t))dt + B(t, \vec{X}(t))d\vec{W}^*(t)$; $\vec{X}(t)$ is the sample path solution of (2.2).

Conversely, assume a Wiener trajectory $\vec{W}^*(t)$ for $0 \le t \le T$ is given and the sample path solution to (2.2) is $\vec{X}^*(t)$. It is now shown that there exists a Wiener trajectory $\vec{W}(t)$ such that (2.1) has the same sample path solution as (2.2), that is, $\vec{X}(t) = \vec{X}^*(t)$ for $0 \le t \le T$. In this case, the singular value decomposition of G has the form $G(t, \vec{X}^*(t)) = G(t) = P(t)D(t)Q(t)$ for $0 \le t \le T$, where $P(t)$ and $Q(t)$ are orthogonal matrices of sizes $d \times d$ and $m \times m$, respectively, and $D(t)$ is a $d \times m$ matrix with $r \le d$ positive diagonal entries. The vector $\vec{W}(t)$ of m independent Wiener processes is now defined as

$$\vec{W}(t) = \int_0^t Q^T(s)D^+(s)(D(s)(D(s))^T)^{1/2}P^T(s)d\vec{W}^*(s) + \int_0^t Q^T(s)d\vec{W}^{***}(s)$$

for $0 \le t \le T$ where $\vec{W}^{***}(s)$ is a vector of length m with the first r entries equal to 0 and the next $m - r$ entries independent Wiener processes, and where $D^+(t)$ is the $m \times d$ pseudoinverse of $D(t)$. Notice that $E(\vec{W}(t)(\vec{W}(t))^T) = tI_m$, where I_m is the $m \times m$ identity matrix. The diffusion term in (2.1) with $\vec{X}(t)$ replaced by $\vec{X}^*(t)$ satisfies

$$\begin{aligned}
&G(t, \vec{X}^*(t))d\vec{W}(t)\\
&\quad = G(t)\big(Q^T(t)D^+(t)\big(\big(D(t)\big(D(t)\big)^T\big)^{1/2}\big)P^T(t)d\vec{W}^*(t) + Q^T(t)d\vec{W}^{***}(t)\big)\\
&\quad = P(t)D(t)Q(t)\big(Q^T(t)D^+(t)\big(\big(D(t)(D(t))^T\big)^{1/2}\big)P^T(t)d\vec{W}^*(t)\\
&\qquad + Q^T(t)d\vec{W}^{***}(t))\\
&\quad = B(t, \vec{X}^*(t))d\vec{W}^*(t).
\end{aligned}$$

Thus, $d\vec{X}^*(t) = \vec{f}(t, \vec{X}^*(t))dt + G(t, \vec{X}^*(t))d\vec{W}(t)$; $\vec{X}^*(t)$ is the sample path solution of (2.1).

In effect, a sample path solution of system (2.1) with $m \ge d$ Wiener processes is also a sample path solution of stochastic system (2.2) with d Wiener processes, where the $d \times d$ matrix B satisfies $B^2 = GG^T$. That the correspondence is measure-preserving follows from the two ways of writing (2.7). In summary, the following result has been proved.

Theorem 2.1. *Solutions to SDE systems* (2.1) *and* (2.2) *possess the same probability distribution. In addition, a sample path solution of one equation is a sample path solution of the second equation.*

3. EQUIVALENT SDE MODELING PROCEDURES

In this section, it is shown how to formulate a stochastic differential equation (SDE) model from a random dynamical system consisting

of d components, where $m \geq d$ distinct independent random changes may occur to the components of the system during a small interval of time. Two modeling procedures are described for formulating an SDE model as discussed in the previous sections. In the first procedure, the m changes are collectively considered and means and covariances are determined. The first approach produces an SDE system with d Wiener processes. In the second procedure, each change is considered separately. The second approach produces an SDE system with m Wiener processes. In both procedures, the number of equations in the SDE model equals the number of components, d. In addition, the two SDE models are equivalent in that solutions to both models have the same probability distribution and a sample path solution of one SDE model is also a sample path solution of the other SDE model.

Consider a stochastic modeling problem that involves d component processes $S_1, S_2, \ldots, S_d$, $\vec{S} = [S_1, S_2, \ldots, S_d]^T$. Suppose that there are a total of $m \geq d$ possible changes that can occur to at least one of the variables S_i in a small time interval Δt. Suppose, in addition, that the probabilities of these changes can be defined as $p_j \Delta t \equiv p_j(t, \vec{S})\Delta t$ for $j = 1, 2, \ldots, m$, where the jth change alters the ith component by the amount $\lambda_{j,i}$ for $i = 1, 2, \ldots, d$. Let

$$f_i\big(t, \vec{S}(t)\big) = \sum_{j=1}^{m} p_j\big(t, \vec{S}(t)\big)\lambda_{j,i} \tag{3.1}$$

for $i = 1, 2, \ldots, d$. Notice that (3.1) can be used to define a deterministic model consisting of a system of ordinary differential equations (ODEs):

$$d\vec{S}(t) = \vec{f}\big(t, \vec{S}(t)\big)dt, \tag{3.2}$$

where $\vec{f} = (f_1, f_2, \ldots, f_d)^T$. For Δt small, the ODE system (3.2) can be approximated using Euler's method by the formula

$$S_{n+1,i} = S_{n,i} + f_i\big(t_n, \vec{S}_n\big)\Delta t, \tag{3.3}$$

where $t_n = n\Delta t$ and $S_{n,i} \approx S_i(t_n)$ for $i = 1, \ldots, d$ and $n = 0, 1, \ldots$.

Assuming that Δt is a small but fixed time interval, an accurate discrete-time stochastic model can be formulated by considering the random changes at each time step. Let $\vec{r}_j$ represent a random change of the jth kind, where to order $O\big((\Delta t)^2\big)$, $\vec{r}_j$ is defined as follows:

$$\vec{r}_j = \begin{cases} [\lambda_{j,1}, \lambda_{j,2}, \ldots, \lambda_{j,d}]^T & \text{with probability } p_j\Delta t \\ [0, 0, \ldots, 0]^T & \text{with probability } 1 - p_j\Delta t. \end{cases}$$

For Δt small, $(\vec{r}_j)_i$ has approximate mean $\lambda_{j,i}p_j\Delta t$ and variance $\lambda_{j,i}^2 p_j \Delta t$. An accurate yet simple stochastic model for $\vec{S}_{n+1}$, given the vector

$\vec{S}_n$, is

$$\vec{S}_{n+1} = \vec{S}_n + \sum_{j=1}^{m} \vec{r}_j \tag{3.4}$$

for $n = 0, 1, \ldots$. In component form, (3.4) becomes

$$S_{n+1,i} = S_{n,i} + \sum_{j=1}^{m} (\vec{r}_j)_i \tag{3.5}$$

for $i = 1, \ldots, d$ and $n = 0, 1, \ldots$.

In the first modeling procedure, it can be shown [1, 5] that if the changes are small and Δt is small, then the probability distribution associated with the discrete-time stochastic system (3.4) can be approximated by the solution to the forward Kolmogorov equation

$$\frac{\partial p(t, \vec{x})}{\partial t} = -\sum_{i=1}^{d} \frac{\partial \left[p(t, \vec{x}) f_i(t, \vec{x}) \right]}{\partial x_i} + \frac{1}{2} \sum_{i=1}^{d} \sum_{j=1}^{d} \frac{\partial^2}{\partial x_i \partial x_j} \left[p(t, \vec{x}) v_{i,j}(t, \vec{x}) \right], \tag{3.6}$$

where $v_{i,j}$ is the (i, j)th entry of $d \times d$ matrix $V = \sum_{j=1}^{m} p_j \vec{\lambda}_j (\vec{\lambda}_j)^T$ and $\vec{f} = \sum_{j=1}^{m} p_j \vec{\lambda}_j$. (See, e.g., [1, 4–6] for more information about this procedure.) The probability distribution $p(t, x_1, x_2, \ldots, x_d)$ that solves (3.6) is identical to the distribution of solutions corresponding to the SDE system

$$\begin{cases} d\vec{S}(t) = \vec{f}\left(t, \vec{S}(t)\right) dt + B\left(t, \vec{S}(t)\right) d\vec{W}^*(t) \\ \vec{S}(0) = \vec{S}_0, \end{cases} \tag{3.7}$$

where the $d \times d$ matrix $B = V^{1/2}$ and $\vec{W}^*(t)$ is a vector of d independent Wiener processes. This first procedure gives the minimal number d of Gaussian processes that can be used to describe this process.

The discrete stochastic model (3.4) is closely related to the SDE model (3.7). Specifically, the probability distribution of solutions to (3.4) is approximately the same as the probability distribution of solutions to (3.7). In addition, it is useful to notice that the drift vector and diffusion matrix, $\vec{f}$ and B of the SDE model are equal to the expected change divided by Δt and the square root of the covariance matrix of the change divided by Δt, respectively. Specifically, letting $\vec{\lambda}_j = [\lambda_{j,1}, \lambda_{j,2}, \ldots, \lambda_{j,n}]^T$, then the expected change in $\vec{S}$ and the covariance in the change are

$$E\left(\Delta \vec{S}\right) = \sum_{j=1}^{m} p_j \vec{\lambda}_j \Delta t = \vec{f} \Delta t \quad \text{and} \quad E\left(\Delta \vec{S} \left(\Delta \vec{S}\right)^T\right) = \sum_{j=1}^{m} p_j \vec{\lambda}_j (\vec{\lambda}_j)^T \Delta t = V \Delta t \tag{3.8}$$

where $B = V^{1/2}$.

In the second modeling procedure, the m random changes in (3.4) are approximated using m independent normal random variables, $\eta_j \sim N(0, 1)$, $j = 1, 2, \ldots, m$. The normal approximation may be justified by arguments involving the Central Limit Theorem or by normal approximations to Poisson random variables. Equation (3.4) for small but fixed Δt is therefore approximated by

$$S_{n+1,i} = S_{n,i} + f_i\big(t_n, \vec{S}_n\big)\Delta t + \sum_{j=1}^{m} \lambda_{j,i} p_j^{1/2} (\Delta t)^{1/2} \eta_j \tag{3.9}$$

for $n = 0, 1, \ldots,$ where f_i is defined in (3.1). (See, e.g., [14–17] for more information about this procedure.) Notice the similarity between the deterministic equation (3.3) and the stochastic equation (3.9). The discrete stochastic model (3.9) is an Euler-Maruyama approximation and converges strongly (in the mean-square sense [20]) as $\Delta t \to 0$ to the SDE system

$$\begin{cases} d\vec{S}(t) = \vec{f}\big(t, \vec{S}(t)\big)dt + G\big(t, \vec{S}(t)\big)d\vec{W}(t), \\ \vec{S}(0) = \vec{S}_0, \end{cases} \tag{3.10}$$

where the i, j entry in the matrix G is $g_{i,j} = \lambda_{j,i} p_j^{1/2}$ for $i = 1, 2, \ldots, d$, $j = 1, 2, \ldots, m$, and $\vec{W}(t)$ is a vector of m independent Wiener processes. Thus, the SDE system (3.10) is closely related to the discrete model (3.4). Notice that the SDE system (3.10) has m Wiener processes and the $d \times d$ matrix $V = GG^T$ has entries

$$(V)_{i,l} = \big(GG^T\big)_{i,l} = \sum_{j=1}^{M} g_{i,j} g_{l,j} = \sum_{j=1}^{M} p_j \lambda_{ji} \lambda_{jl} = v_{i,l} \tag{3.11}$$

for $i, l = 1, \ldots, d$. Furthermore, the entries of G are easy to write down given the probabilities of the different changes based on the discrete-time Markov chain (3.4).

Notice that the $d \times m$ matrix G satisfies $V = GG^T$ and the SDE system (3.10) can be replaced by the system (3.7) by the argument in the previous section. Indeed, the forward Kolmogorov equations are identical for both systems (3.7) and (3.10) and a sample path solution of one system is a sample path solution of the other system. Finally, notice that system (3.7) is generally more complicated than (3.10), as the $d \times d$ matrix B is the square root of V even though G is $d \times m$. Consequently, system (3.10) is generally easier to solve computationally. However, if the number of changes, m, is much greater than the number of system components, d, then equation (3.10) loses much of its computational advantages.

It is interesting to note that there are other SDE systems equivalent to (3.10) that can be generated from the probabilities of the changes.

For example, if the diffusion matrix G is replaced by $-G$ in (3.10), this alternate system's solutions will have the same probability distribution. In general, there are other diffusion matrices H with the property $HH^T = V = GG^T$ that can replace G in (3.11). This is due to the fact that for a multivariate Gaussian process there are many ways in which the process can be written.

It is important to understand that stochastic differential equation models (3.7) and (3.10) approximate the actual randomly varying system as time and system variables are continuous in the SDE models whereas discrete changes may be occurring at discrete times in the actual randomly varying system. It is generally recommended when formulating a mathematical model for a given process that the model be thoroughly tested with Monte Carlo calculations or with experimental data to verify the model's accuracy.

It is useful to briefly discuss square roots of symmetric positive semidefinite matrices because of their relevance to the stochastic system (3.7). It is well-known that a symmetric positive semidefinite matrix has a unique symmetric positive semidefinite square root [25, 26]. Clearly, when V is put in the canonical form $V = P^T DP$, where $P^T P = I$ and $d_{ii} \geq 0$ for $i = 1, 2, \ldots, n$, then $V^{1/2} = P^T D^{1/2} P$. However, for a large matrix, it is computationally intensive to accurately compute all of the eigenvalues and eigenvectors of V which are needed to determine P and D. For a 2×2 matrix, the positive semidefinite square root can be readily calculated. Indeed,

$$V^{1/2} = \begin{bmatrix} a & b \\ b & c \end{bmatrix}^{1/2} = \frac{1}{d} \begin{bmatrix} a+w & b \\ b & c+w \end{bmatrix},$$

where $w = \sqrt{ac - b^2}$ and $d = \sqrt{a + c + 2w}$. For a general $n \times n$ symmetric positive semidefinite matrix V with $n \geq 3$, there is no explicit formula for $V^{1/2}$ and, therefore, it must be calculated numerically. However, many numerical procedures are available for computing $V^{1/2}$ (e.g., [24–26]).

In summary, two equivalent procedures were described for constructing an Itô SDE model for a dynamical system consisting of d components with $m \geq d$ different and independent random changes. In the first procedure, means and covariances of the random changes are calculated which then determines the SDE model. In the second procedure, each independent random change is explicitly included. Several examples arising in chemistry, textile engineering, and epidemiology are described in the next section, where the two modeling procedures are compared.

4. EXAMPLES AND COMPUTATIONAL COMPARISONS

4.1. Chemical Reactions

In this section, chemical reactions between molecules are modeled in a stochastic manner (similar to the investigations described in [13–15]). It is shown how an SDE model can be developed using the two modeling procedures. It is assumed that a fixed volume contains a uniform mixture of d different chemical species that interact through m different chemical reactions. The reaction rates are either proportional to the rates that the molecules collide or, if the reaction is spontaneous, the reaction rate is just proportional to the number of molecules of the particular chemical species. Given the initial numbers of molecules of the d different chemical species, the objective is to find the molecular population levels at a later time.

To illustrate the modeling procedure for chemical reactions, it is useful to consider a specific problem. Therefore, suppose that there are three chemical species S_1, S_2, and S_3 interacting through molecular collisions or spontaneously in the four ways described in Table 1. In Table 1, μ_1, μ_2, μ_3, and μ_4 are reaction rate constants and X_1, X_2, and X_3 are the number of molecules of species S_1, S_2, and S_3, respectively. The second reaction is assumed to be spontaneous and so the probability of a reaction only depends on the number of molecules, X_3. For the first reaction, the rate depends on a collision occurring between species S_1 and S_2 and is therefore proportional to the product of X_1 and X_2. The third reaction depends on a collision involving two molecules of S_2 and one molecule of S_3. As there are $X_2(X_2-1)/2$ ways to select two molecules from a total of X_2 molecules, the rate of this reaction depends approximately on the product of $X_2^2/2$ with X_3. The fourth reaction depends on two molecules of S_1 interacting and is approximately proportional to $X_1^2/2$. For a thorough discussion of reaction rate dynamics, see [13–15].

To form the SDE model using the first procedure discussed in the previous section, $E(\Delta\vec{X})$ and $E\left((\Delta\vec{X})(\Delta\vec{X})^T\right)$ need to be computed. To find these expectations, the possible changes for the reactions given in

Table 1. Probabilities for reactions among three chemical species

Reaction	Probability
$S_1 + S_2 \to S_3$	$p_1 = \mu_1 X_1 X_2 \Delta t$
$S_3 \to S_1 + S_2$	$p_2 = \mu_2 X_3 \Delta t$
$2S_2 + S_3 \to 2S_1$	$p_3 = \mu_3 X_2^2 X_3 \Delta t/2$
$2S_1 \to 2S_2 + S_3$	$p_4 = \mu_4 X_1^2 \Delta t/2$

Table 1 are listed in Table 2 along with their associated probabilities. Then

$$\begin{aligned} E(\Delta\vec{X}) &= \sum_{i=1}^{4} p_i (\Delta\vec{X})_i \\ &= \begin{bmatrix} -\mu_1 X_1 X_2 + \mu_2 X_3 + \mu_3 X_2^2 X_3 - \mu_4 X_1^2 \\ -\mu_1 X_1 X_2 + \mu_2 X_3 - \mu_3 X_2^2 X_3 + \mu_4 X_1^2 \\ \mu_1 X_1 X_2 - \mu_2 X_3 - \mu_3 X_2^2 X_3/2 + \mu_4 X_1^2/2 \end{bmatrix} \Delta t \\ &= \vec{f}(X_1, X_2, X_3)\Delta t \end{aligned}$$

and

$$\begin{aligned} E\big((\Delta\vec{X})(\Delta\vec{X})^T\big) &= \sum_{i=1}^{4} p_i (\Delta\vec{X})_i (\Delta\vec{X})_i^T \\ &= \begin{bmatrix} a+4b & a-4b & -a-2b \\ a-4b & a+4b & -a+2b \\ -a-2b & -a+2b & a+b \end{bmatrix} \Delta t \\ &= V(X_1, X_2, X_3)\Delta t, \end{aligned}$$

where $a = \mu_1 X_1 X_2 + \mu_2 X_3$ and $b = \mu_3 X_2^2 X_3/2 + \mu_4 X_1^2/2$. It follows that the SDE model for this example problem has the form

$$\begin{cases} d\vec{X}(t) = \vec{f}(X_1, X_2, X_3)dt + (V(X_1, X_2, X_3))^{1/2}\, d\vec{W}^*(t) \\ \vec{X}(0) = [X_1(0), X_2(0), X_3(0)]^T, \end{cases} \tag{4.1}$$

where $\vec{W}^*(t) = [W_1^*(t), W_2^*(t), W_3^*(t)]^T$.

Using the second modeling procedure for this example gives the SDE model:

$$\begin{cases} d\vec{X}(t) = \vec{f}(X_1, X_2, X_3)dt + G(X_1, X_2, X_3)d\vec{W}(t) \\ \vec{X}(0) = [X_1(0), X_2(0), X_3(0)]^T, \end{cases} \tag{4.2}$$

Table 2. Possible molecular population changes in a small time period Δt

Possible change	Probability
$(\Delta\vec{X})_1 = [-1, -1, +1]^T$	$p_1 = \mu_1 X_1 X_2 \Delta t$
$(\Delta\vec{X})_2 = [+1, +1, -1]^T$	$p_2 = \mu_2 X_3 \Delta t$
$(\Delta\vec{X})_3 = [+2, -2, -1]^T$	$p_3 = \mu_3 X_2^2 X_3 \Delta t/2$
$(\Delta\vec{X})_4 = [-2, +2, +1]^T$	$p_4 = \mu_4 X_1^2 \Delta t/2$

Table 3. Calculated mean molecular levels and standard deviations at time $t = 1.0$ using a Monte Carlo procedure

Chemical species	$E(X_i)$	$\sigma(X_i)$
S_1	79.21	7.28
S_2	37.61	5.84
S_3	131.19	5.54

where $\vec{W}(t) = [W_1(t), W_2(t), W_3(t), W_4(t)]^T$ is a vector of four independent Wiener processes and the 3×4 matrix G has the form

$$G = \begin{bmatrix} -(\mu_1 X_1 X_2)^{1/2} & (\mu_2 X_3)^{1/2} & 2(\mu_3 X_2^2 X_3/2)^{1/2} & -2(\mu_4 X_1^2/2)^{1/2} \\ -(\mu_1 X_1 X_2)^{1/2} & (\mu_2 X_3)^{1/2} & -2(\mu_3 X_2^2 X_3/2)^{1/2} & 2(\mu_4 X_1^2/2)^{1/2} \\ (\mu_1 X_1 X_2)^{1/2} & -(\mu_2 X_3)^{1/2} & -(\mu_3 X_2^2 X_3/2)^{1/2} & (\mu_4 X_1^2/2)^{1/2} \end{bmatrix}.$$

Stochastic differential equation models of the form (4.2) are referred to as chemical Langevin systems [15].

To verify the accuracy and illustrate the close agreement between the SDE models (4.1) and (4.2), calculational results using the models were compared with those obtained using a Monte Carlo procedure. In the Monte Carlo procedure, the molecular process was checked at each small interval of time to see if any reaction occurred. The calculational results for the Monte Carlo procedure are summarized in Table 3 for 5,000 sample paths. In these calculations, the values of the reaction rate constants were taken as $\mu_1 = 0.02$, $\mu_2 = 0.4$, $\mu_3 = 0.001$, and $\mu_4 = 0.03$. The initial numbers of molecules were assumed to be $X_1(0) = X_2(0) = X_3(0) = 100$ and the final time was taken as $t = 1.0$. Next, the SDE models (4.1) and (4.2) were numerically solved using the Euler-Maruyama method with 5,000 sample paths. The results using these two SDE models are compared in Table 4, where a sample path using (4.1) is plotted in Figure 1 and a sample path using model (4.2)

Table 4. Calculated mean molecular levels and standard deviations at time $t = 1.0$ using SDE models (4.1) and (4.2)

Model	Chemical species	$E(X_i)$	$\sigma(X_i)$
(4.1)	S_1	79.31	7.62
	S_2	37.44	6.14
	S_3	131.17	6.43
(4.2)	S_1	79.39	7.69
	S_2	37.47	6.13
	S_3	131.09	5.85

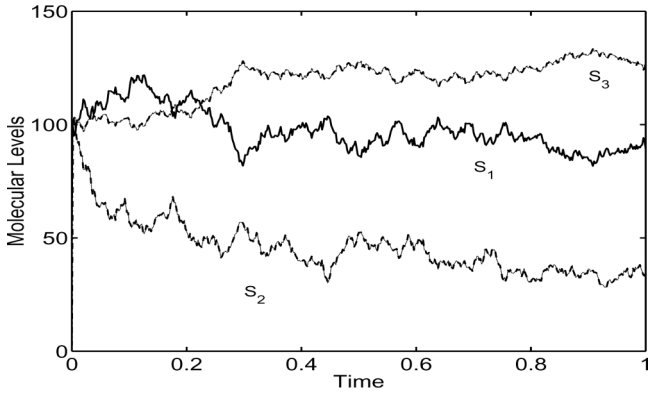

Figure 1. Molecular population levels for one sample path of SDE (4.1).

is plotted in Figure 2. Notice the good agreement between the two SDE models as well as the good agreement between the SDE models and the Monte Carlo approach.

4.2. Cotton Fiber Breakage

In cotton thread manufacture, the cotton fiber length distribution determines many of the characteristics of the thread [12, 27, 28]. Fiber length is a good indicator of spinning efficiency, yarn strength, and yarn uniformity. Fiber length distribution is affected by breakage during processing. In cotton processing, fiber breakage occurs in ginning and carding. Breakage of the fibers in cotton processing generally results in lower quality yarn.

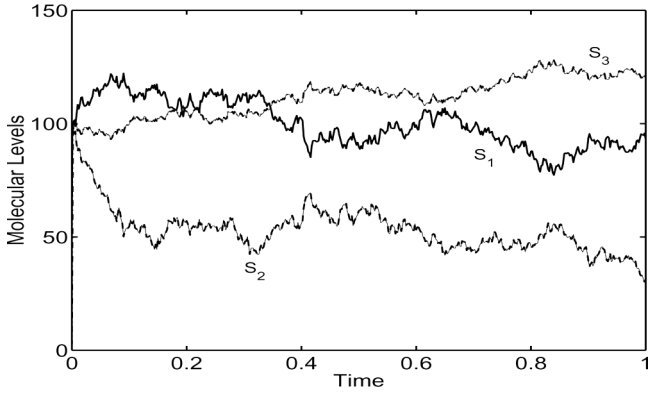

Figure 2. Molecular population levels for one sample path of SDE (4.2).

The development of an SDE model for fiber-length distributions provides insight into the fiber breakage phenomenon and the origin of different fiber-length distributions. By comparing calculations of the stochastic model with fiber-length data, fiber breakage parameters can be estimated and the distribution characteristics can be investigated.

In the stochastic model, the fibers are grouped by length. In this manner, the cotton fiber distribution can be considered as a population distribution. The SDE model is derived by carefully considering the population process and breakage possibilities over a short time interval using the stochastic modeling techniques described previously. First, a discrete stochastic model is derived where the breakage phenomenon is carefully studied for a short time interval. A system of stochastic differential equations is then identified whose probability distribution approximates that of the discrete-time stochastic model.

In developing an SDE model, d populations, $\{N_k(t)\}_{k=1}^{d}$, of fibers having different lengths are considered as functions of time t. Some terminology and notation associated with the stochastic model are required and introduced next.

L = fiber length, where $0 \le L \le L_{max}$.

$L_k = kh$ for $k = 0, 1, \ldots, d$, where $h = L_{max}/m$.

$N_k(t)$ = number of fibers of length L_k for $k = 1, 2, \ldots, d$.

$q_k\,dt$ = fraction of fibers of length L_k broken in time dt.

$S_{k,l}$ = fraction of fragments of length L_l formed from breakage of fibers of length L_k.

$p_{k,l}(t)dt = N_k(t)S_{k,l}q_k dt$ = probability of a fragment of length L_l being formed from breakage of a fiber of length L_k in time t to $t + dt$.

From the preceding definitions, it follows that $\sum_{l=1}^{k-1} S_{k,l} = 1$, $S_{k,k-l} = S_{k,l}$, and the number of independent random changes in any interval of time is $d(d-1)/2$.

To develop the SDE system using the first modeling procedure, the changes in the fiber populations are carefully studied and tabulated for a small time interval dt. Then the mean change $E\big(\Delta\vec{N}(t)\big)$ and the covariance in the change $E\Big(\big(\Delta\vec{N}(t)\big)\big(\Delta\vec{N}(t)\big)^T\Big)$ for the small time interval are calculated. For example, consider the special case where $d = 8$, that is, there are 8 groups of fibers. Consider a fiber in the seventh group breaking into two fibers, one in group 5 and one in group 2. The change produced is

$$\big(\Delta\vec{N}\big)^{7,5} = [0, 1, 0, 0, 1, 0, -1, 0]^T \tag{4.3}$$

with probability $p_{7,5}(t)dt = N_7(t)S_{7,5}q_7 dt$. The value of the expected change $E(\Delta\vec{N}(t))$ for the small time interval is calculated by summing the products of the changes with the respective probabilities. In general, for any value of d, it can be shown that the lth component of $E(\Delta\vec{N}(t))$ has the form

$$E\big(\Delta\vec{N}(t)\big)_l = 2\sum_{k=l+1}^{d} p_{k,l}(t)dt - \sum_{k=1}^{l-1} p_{l,k}(t)dt.$$

In addition, the covariance matrix has the form

$$E\big(\big(\Delta\vec{N}(t)\big)\big(\Delta\vec{N}(t)\big)^T\big) = \sum_{k=1}^{d}\sum_{l=1}^{k-1} C^{k,l}p_{k,l}(t)dt,$$

where $C^{k,l} = (\Delta\vec{N})^{k,l}((\Delta\vec{N})^{k,l})^T$ and $(\Delta\vec{N})^{k,l}$ is the change produced for a fiber of group k breaking into a fiber of group l and group $k-l$. For example, for the special case where $d = 8$ and a fiber in the seventh group breaks into two fibers, one in group 5 and one in group 2, then the corresponding term in the covariance matrix is:

$$C^{7,5} = \big(\Delta\vec{N}\big)^{7,5}\big(\big(\Delta\vec{N}\big)^{7,5}\big)^T = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Now, the expected change and the covariance matrix are defined by

$$\mathrm{E}\big(\Delta\vec{N}\big) = \vec{f}\big(t, \vec{N}(t)\big)dt \quad \text{and} \quad \mathrm{E}\big(\Delta\vec{N}\Delta\vec{N}^T\big) = V\big(t, \vec{N}(t)\big)dt.$$

Then, as explained earlier, the probability distribution $p(t, \vec{N})$ of the fiber-length populations with time t can be approximated by the solution to the forward Kolmogorov equation,

$$\frac{\partial p(t,\vec{N})}{\partial t} = -\sum_{i=1}^{d}\frac{\partial}{\partial N_i}[f_i(t,\vec{N})p(t,\vec{N})] + \frac{1}{2}\sum_{i=1}^{d}\sum_{j=1}^{d}\frac{\partial^2}{\partial N_i \partial N_j}\left[\sum_{k=1}^{d} v_{i,k}(t,\vec{N})v_{j,k}(t,\vec{N})p(t,\vec{N})\right].$$

The SDE system corresponding to this forward Kolmogorov equation has the following form:

$$d\vec{N}(t) = \vec{f}\big(t, \vec{N}(t)\big)dt + \big(V\big(t, \vec{N}(t)\big)\big)^{1/2} d\vec{W}^*(t), \tag{4.4}$$

where $\vec{N}(t) = [N_1(t), N_2(t), \ldots, N_d(t)]^T$ are the fiber populations in each length group and $\vec{W}^*(t) = [W_1^*(t), \ldots, W_d^*(t)]^T$ is an d-dimensional Wiener process. Equation (4.4) is an SDE model for the fiber-length populations as a function of time t.

In the second modeling procedure, the independent random changes are explicitly modeled. Let $(\Delta\vec{N})^{k,l}$ be the change to the vector $\vec{N}(t)$ (see Equation (4.3)), with probability $p_{k,l}(t)dt$ due to a breakage of a fiber in group k to produce one fiber each in groups l and $k-l$. Then the SDE model using the second approach can be written in the form

$$d\vec{N}(t) = \vec{f}\big(t, \vec{N}(t)\big)dt + \sum_{k=1}^{d}\sum_{l=1}^{k-1}\big(\Delta\vec{N}\big)^{k,l}(p_{k,l}(t))^{1/2}\,dW_{k,l}(t), \tag{4.5}$$

where $p_{k,l}(t) = N_k(t)S_{k,l}q_k$, $W_{k,l}(t)$ for $l = 1, 2, \ldots, k-1$ and $k = 1, 2, \ldots, d$ are m independent Wiener processes, and the ith element of vector $(\Delta\vec{N})^{k,l}$ is

$$\big((\Delta\vec{N})^{k,l}\big)_i = \begin{cases} -1, & \text{if } i = k \\ 1, & \text{if } i = l \quad \text{or } i = k-l \\ 0, & \text{otherwise.} \end{cases}$$

Notice, for SDE model (4.5), that $m = d(d-1)/2$ Wiener processes are required whereas SDE model (4.4) only requires d Wiener processes.

To compare the stochastic models (4.4) and (4.5), Monte Carlo simulations are performed. In the Monte Carlo calculations, at each small time step, each fiber is checked for breakage. If breakage occurs, the fiber is randomly divided. Considered in these calculations is the situation where breakage occurs randomly and the probability for breakage is proportional to the length of the fiber. Under this breakage assumption,

$$q_k S_{k,j}\,dt = \mu\left(\frac{h}{L_{max}}\right)dt,$$

where μ is a constant which determines the rate of fiber breakage fraction of fibers of length k broken in time dt and

$$S_{k,j} = \frac{h}{L_{k-1}} = \frac{1}{k-1},$$

where $S_{k,j}$ fraction of fragments of length L_j formed from breakage of fiber of length L_k. The parameter μ is set equal to unity in the calculations and it is assumed that there are initially 100 fibers each one inch in length. Two hundred sample paths were computed for each SDE model (4.4) and (4.5). The calculational results are compared in

Table 5. Monte Carlo and SDE calculational results on fiber lengths at time $t = 1.0$

Avg. number of fibers	Standard dev. in no. of fibers	Average fiber length	Standard dev. in fiber length
200.5 (MC)	10.57 (MC)	0.5001 (MC)	0.0263 (MC)
197.8 (SDE (4.4))	11.47 (SDE (4.4))	0.5068 (SDE (4.4))	0.0265 (SDE (4.4))
196.3 (SDE (4.5))	10.25 (SDE (4.5))	0.5109 (SDE (4.5))	0.0271 (SDE (4.5))

Table 5. The results indicate very good agreement between the two different modeling procedures.

Additional computations produce fiber-length distributions having a bimodal structure. Bimodal distributions are commonly seen in fiber-length data. Results of an example calculation are illustrated in Figure 3. For this calculation, it is assumed that the fibers are distributed initially as $N_k(0) = 2(k - 20)$ for $k = 20, 21, \ldots, 35$ and $N_k(0) = 2(50 - k)$ for $k = 36, 37, \ldots, 50$, where $N_k(0)$ is the initial number of fibers of length $L_k = 0.02k$.

4.3. Epidemic Model with Vaccination

In the last example, the impact of vaccination on a population is studied. Individuals within the population are classified according to the following four disease stages: susceptible, infective, recovered (and immune), and vaccinated, S, I, R, and V, respectively. The vaccine is assumed to be imperfect; vaccinated individuals may still transmit the

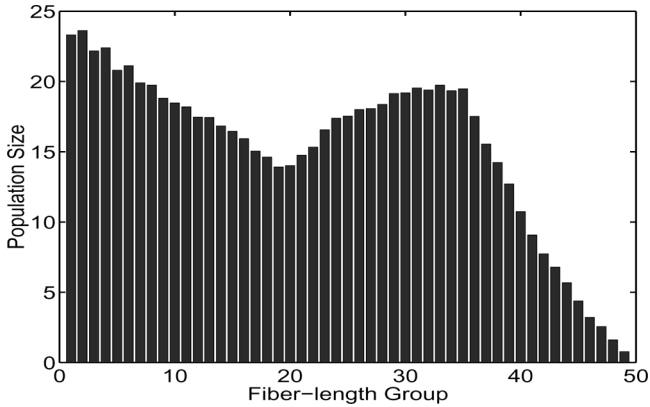

Figure 3. Average fiber length distribution after random breakage for time $t = 1.0$ (SDE model (4.4)).

disease. The deterministic model was originally formulated by Arino et al. [29]. A stochastic formulation of this model using the procedure that leads to (3.7) was formulated by Allen and van den Driessche [30]. The alternate but equivalent stochastic formulation that leads to (3.10) is derived here in addition to a slightly simpler but equivalent SDE model.

For large populations, the SDE models can be derived directly from the deterministic epidemic model because the changes that occur can be clearly identified in the deterministic model. The ODE model with vaccination is given by the following system:

$$\begin{aligned}
\frac{dS}{dt} &= d(N-S) - \beta\tfrac{SI}{N} - \phi S + \theta V + \nu R \\
\frac{dI}{dt} &= \beta\tfrac{SI}{N} + \sigma\beta\tfrac{VI}{N} - (d+\gamma)I \\
\frac{dR}{dt} &= \gamma I - (d+\nu)R \\
\frac{dV}{dt} &= \phi S - (d+\theta)V - \sigma\beta\tfrac{VI}{N}.
\end{aligned} \tag{4.6}$$

The total population size is constant, $N = S(t) + I(t) + R(t) + V(t)$. The per capita birth rate equals the death rate, d. Parameters β, γ, and ϕ are the transmission rate, recovery rate, and vaccination rate, respectively. The vaccine does not provide lifelong protection and wanes at a rate θ. In addition, natural immunity is not lifelong; loss of natural immunity occurs at a rate ν. The parameter σ is the vaccine efficacy, $0 \le \sigma \le 1$. If $\sigma = 0$, then the vaccine is perfect but if $\sigma > 0$, the vaccine is imperfect; vaccinated individuals transmit the disease. This model has some interesting properties. In [29], it was shown for certain parameter regions that both the disease-free equilibrium and an endemic equilibrium are stable; the system exhibits what is known as bistability. In practical terms, the disease is difficult to control with vaccination when parameter values lie in the region of bistability.

Because the population size is constant, system (4.6) can be reduced to three differential equations. The three variables $I(t)$, $R(t)$, and $V(t)$ are sufficient to model the disease dynamics; $S(t) = N - I(t) - R(t) - V(t)$. Let X_i, $i = 1, 2, 3$ denote the random variables for I, R, and V, respectively, and let X_0 denote $N - X_1 - X_2 - X_3$. There are seven possible changes in the vector $\vec{X} = [X_1, X_2, X_3]^T$ for a small time interval Δt, assuming at most one change can occur. These changes are given in Table 6.

Applying the first modeling procedure yields the following system for the epidemic model:

$$\begin{cases} d\vec{X}(t) = \vec{f}\big(t, \vec{X}(t)\big)dt + B\big(t, \vec{X}(t)\big)d\vec{W}^*(t) \\ \vec{X}(0) = [X_1(0), X_2(0), X_3(0)]^T, \end{cases} \tag{4.7}$$

Table 6. Possible changes in the process for the epidemic model when Δt is small

Possible change	Probability
$(\Delta\vec{X})_1 = [1, 0, 0]^T$	$p_1 = (\beta X_0 X_1/N)\Delta t$
$(\Delta\vec{X})_2 = [-1, 0, 0]^T$	$p_2 = dX_1\Delta t$
$(\Delta\vec{X})_3 = [-1, 1, 0]^T$	$p_3 = \gamma X_1\Delta t$
$(\Delta\vec{X})_4 = [0, -1, 0]^T$	$p_4 = (d+v)X_2\Delta t$
$(\Delta\vec{X})_5 = [1, 0, -1]^T$	$p_5 = (\sigma\beta X_1 X_3/N)\Delta t$
$(\Delta\vec{X})_6 = [0, 0, -1]^T$	$p_6 = (d+\theta)X_3\Delta t$
$(\Delta\vec{X})_7 = [0, 0, 1]^T$	$p_7 = \phi X_0\Delta t$

where $\vec{W}^*(t) = [W_1^*(t), W_2^*(t), W_3^*(t)]^T$ is a vector of three independent Wiener processes. The drift vector $\vec{f}$ has the form

$$\vec{f}(t, \vec{X}(t)) = \begin{bmatrix} \beta\frac{X_0X_1}{N} + \sigma\beta\frac{X_1X_3}{N} - (d+\gamma)X_1 \\ \gamma X_1 - (d+v)X_2 \\ \phi X_0 - (d+\theta)X_3 - \sigma\beta\frac{X_1X_3}{N} \end{bmatrix} \tag{4.8}$$

and the 3×3 matrix $B = V^{1/2}$. Matrix V is

$$\begin{bmatrix} \beta\frac{X_0X_1}{N} + \sigma\beta\frac{X_1X_3}{N} + (d+\gamma)X_1 & -\gamma X_1 & -\sigma\beta\frac{X_1X_3}{N} \\ -\gamma X_1 & \gamma X_1 + (d+v)X_2 & 0 \\ -\sigma\beta\frac{X_1X_3}{N} & 0 & \phi X_0 + (d+\theta)X_3 + \sigma\beta\frac{X_1X_3}{N} \end{bmatrix}$$

This procedure was applied in [30].

Applying the second modeling procedure yields the following stochastic system for the epidemic model:

$$\begin{cases} d\vec{X}(t) = \vec{f}(t, \vec{X}(t))dt + G(t, \vec{X}(t))d\vec{W}(t) \\ \vec{X}(0) = [X_1(0), X_2(0), X_3(0)]^T, \end{cases} \tag{4.9}$$

where $\vec{W}(t) = [W_1(t), W_2(t), \ldots, W_7(t)]^T$ is a vector of 7 independent Wiener process, the drift vector $\vec{f}$ is given in (4.8), and the diffusion matrix G is a 3×7 matrix of the form

$$\begin{bmatrix} \left(\beta\frac{X_0X_1}{N}\right)^{1/2} & (dX_1)^{1/2} & -(\gamma X_1)^{1/2} & \left(\sigma\beta\frac{X_1X_3}{N}\right)^{1/2} & 0 & 0 & 0 \\ 0 & 0 & (\gamma X_1)^{1/2} & 0 & [(d+v)X_2]^{1/2} & 0 & 0 \\ 0 & 0 & 0 & -\left(\sigma\beta\frac{X_1X_3}{N}\right)^{1/2} & 0 & [(d+\theta)X_3]^{1/2} & (\phi X_0)^{1/2} \end{bmatrix}$$

so that $GG^T = V$.

A simpler SDE model, equivalent to the two preceding models (4.7) and (4.9), is given by the system

$$\begin{cases} d\vec{X}(t) = \vec{f}(t, \vec{X}(t))dt + H(t, \vec{X}(t))d\vec{W}'(t) \\ \vec{X}(0) = [X_1(0), X_2(0), X_3(0)]^T, \end{cases} \tag{4.10}$$

where $\vec{W}'(t) = [W_1'(t), W_2'(t), W_3'(t), W_4'(t), W_5'(t)]^T$ is a vector of 5 independent Wiener processes, $\vec{f}$ is given in (4.8), and H is the 3×5 matrix

$$\begin{bmatrix} \left(\beta \frac{X_0 X_1}{N} + dX_1\right)^{1/2} & -(\gamma X_1)^{1/2} & \left(\sigma\beta \frac{X_1 X_3}{N}\right)^{1/2} & 0 & 0 \\ 0 & (\gamma X_1)^{1/2} & 0 & [(d+v)X_2]^{1/2} & 0 \\ 0 & 0 & -\left(\sigma\beta \frac{X_1 X_3}{N}\right)^{1/2} & 0 & [(d+\theta)X_3 + \phi X_0]^{1/2} \end{bmatrix}.$$

Note that $HH^T = V$. A similar set of Itô SDEs was formulated by Greenwood et al. [16] for an SIR epidemic model.

Numerical simulations of the three SDE models, (4.7), (4.9), and (4.10), for the epidemic model with vaccination are compared. The mean and standard deviation for each random variable and for each model are computed at $t = 5$ years using the Euler-Maruyama method with 10,000 sample paths. See Table 7. The parameter values are chosen in the region of bistability but the initial conditions are such that almost all sample paths are close to the stable endemic equilibrium [29, 30]. In the deterministic model, the stable endemic equilibrium is $(\bar{I}, \bar{R}, \bar{V}) = (193.25, 284.95, 447.41)$. The means and standard deviations illustrate the close agreement among the three SDE models.

The probability distributions associated with each of the random variables are close to normal at $t = 5$. Graphed in Figure 4 are the

Table 7. Mean and standard deviation for the three SDE epidemic models at $t = 5$ years. The units of the parameter values are per year: $\gamma = 365/21$, $d = 1/75$, $v = 365/32$, $\phi = 365/20$, and $\theta = 1/5$ [29, 30]. Vaccine efficacy is $\sigma = 0.10$. Initial conditions are $X_1(0) = 5$, $X_2(0) = 0 = X_3(0)$

Model	Variables	$E(X_i)$	$\sigma(X_i)$
	X_1	188.67	24.03
(4.7)	X_2	278.38	28.77
	X_3	458.96	46.14
	X_1	188.53	24.38
(4.9)	X_2	278.32	29.38
	X_3	459.66	47.29
	X_1	189.24	23.51
(4.10)	X_2	279.14	27.56
	X_3	457.72	43.95

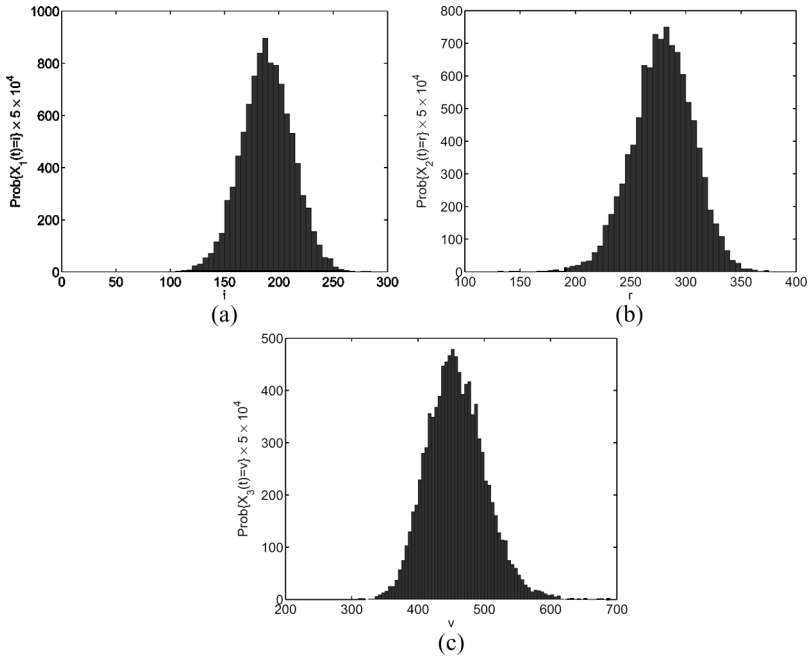

Figure 4. Probability histograms at time $t = 5$ for (a) X_1 (infectives), (b) X_2 (recovered and immune), and (c) X_3 (vaccinated).

probability histograms for the three random variables based on 10,000 sample paths using SDE model (4.10).

5. SUMMARY AND CONCLUSIONS

Two procedures are described for formulating a stochastic differential equation model for a random dynamical system consisting of d components, where $m \geq d$ distinct independent random changes may occur to the components during a small interval of time. The first procedure produces a diffusion matrix B of dimension $d \times d$ and the second procedure produces a diffusion matrix G of dimension $d \times m$. The two distinct systems of Itô stochastic differential equations are shown to be equivalent in the sense that solutions of the systems possess the same probability distribution and a sample path solution of one system is a sample path solution of the other system.

Each modeling procedure possesses certain conceptual and computational advantages that can be interchanged in any particular problem. The first procedure has certain conceptual advantages as the procedure is a natural extension of the modeling procedure applied for

many years in modeling deterministic dynamical processes in physics and engineering, where changes in the deterministic system are studied over a small interval of time and a differential equation is obtained as the time increment approaches zero. Also, for the first procedure, similarities are straightforward to obtain between the forward Kolmogorov differential equations satisfied by the probability distributions of the discrete- and continuous-time stochastic models and these similarities alow one to infer an Itô SDE model from the discrete stochastic model [1, 5]. However, because the system produced in the first procedure requires computation of a square root of a matrix, whereas the system produced in the second procedure does not, the second system with the larger diffusion matrix may be a computationally simpler system provided that m is not excessively large compared with d.

Finally, it is shown how both systems are easy to formulate and provide alternate ways to develop stochastic differential equation models based on underlying discrete-time stochastic processes. Stochastic differential equation models are formulated and computationally compared for example problems arising in chemistry, textile engineering, and epidemiology. The computational results illustrate the equivalence of the probability distributions for the two SDE models.

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