DISCRETE-TIME STOCHASTIC MODELS, SDEs, AND NUMERICAL METHODS

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NIMBioS Tutorial: Stochastic Models With Biological Applications

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STOCHASTIC DIFFERENTIAL EQUATIONS ARE BECOMING INCREASINGLY MORE POPULAR

(1) Random effects in biological, physical, and financial problems can be modeled using stochastic differential equations.

(2) Stochastic models are considered to be more realistic for many problems.

(3) A procedure for deriving accurate stochastic differential equation models is useful to understand.

(4) For simulating stochastic differential equations, computational procedures are generally necessary.

This Lecture Is Divided Into Several Parts

(1) A procedure is described for deriving a stochastic differential equation from an associated discrete stochastic model.

(2) Stochastic differential equation systems are derived for several population problems. (Modeling with SDEs continues in the second lecture.)

(3) Commonly used numerical procedures are described for computationally solving systems of stochastic differential equations.

To Introduce SDE Modeling, Consider The Birth-Death Process

Let $u(t)$ be the population size and let b and d be birth and death rates. The dynamics of the birth-death process is represented exactly by:

$$u(t + (\Delta t)_t) = u(t) + (\Delta u)_t, \quad u(0) = a$$

where $(\Delta t)_t$ is the time interval to the next birth or death after time t, $(\Delta u)_t = 1$ with probability $b/(b + d)$, and $(\Delta u)_t = -1$ with probability $d/(b + d)$.

In addition, $(\Delta t)_t$ is exponentially distributed and if β_t is a random number uniform on $[0, 1]$, then

$$(\Delta t)_t = -\log(\beta_t)/((b + d)u(t)).$$

The above is suitable for Monte Carlo computations, but these equations give little insight into the birth-death process.

A Deterministic ODE Model Is Often Used For The Birth-Death Process

Since $E(u(t+\Delta t)) = E(u(t)) + (b-d)E(u(t))\Delta t$ for small Δt, it follows that

$$\frac{dv(t)}{dt} = (b-d)v(t), \quad v(0) = a.$$

where $v(t) = E(u(t))$.

This ODE is so common and so well-accepted that it is often forgotten that there are two important assumptions:

(1) $v(t)$ is not the population size; it is the mean size, and

(2) $v(t)$ varies continuously, i.e., the population size can have fractional values.

In this model, we have lost information about the randomness in the birth-death process and about the population's integer size values.

An SDE Model Retains The Random Nature Of The Birth-Death Process And Gives Insight

As derived later, an SDE for the birth-death process is:

$$dy(t) = (b-d)y(t)dt + \sqrt{(b+d)y(t)}\, dW(t), \quad y(0) = a$$

where $W(t)$ is the Wiener process and $W(t_2) - W(t_1)$ is normally distributed with mean 0 and variance $t_2 - t_1$ for any $t_2 \geq t_1$.

This SDE model generalizes the deterministic ODE model. but there are an infinite number of solutions just as in nature. Each solution is called a sample path, a trajectory, or a trial.

Indeed, the sample paths have exact first and second moments. That is,

$$E(y(t)) = a \exp{(b-d)t}$$

$$\mathbf{Var}(y(t)) = a(b+d)(\exp{(2(b-d)t)} - \exp{((b-d)t)})/(b-d).$$

Calculations Indicate That An SDE For The Birth-Death Process Is Very Reasonable

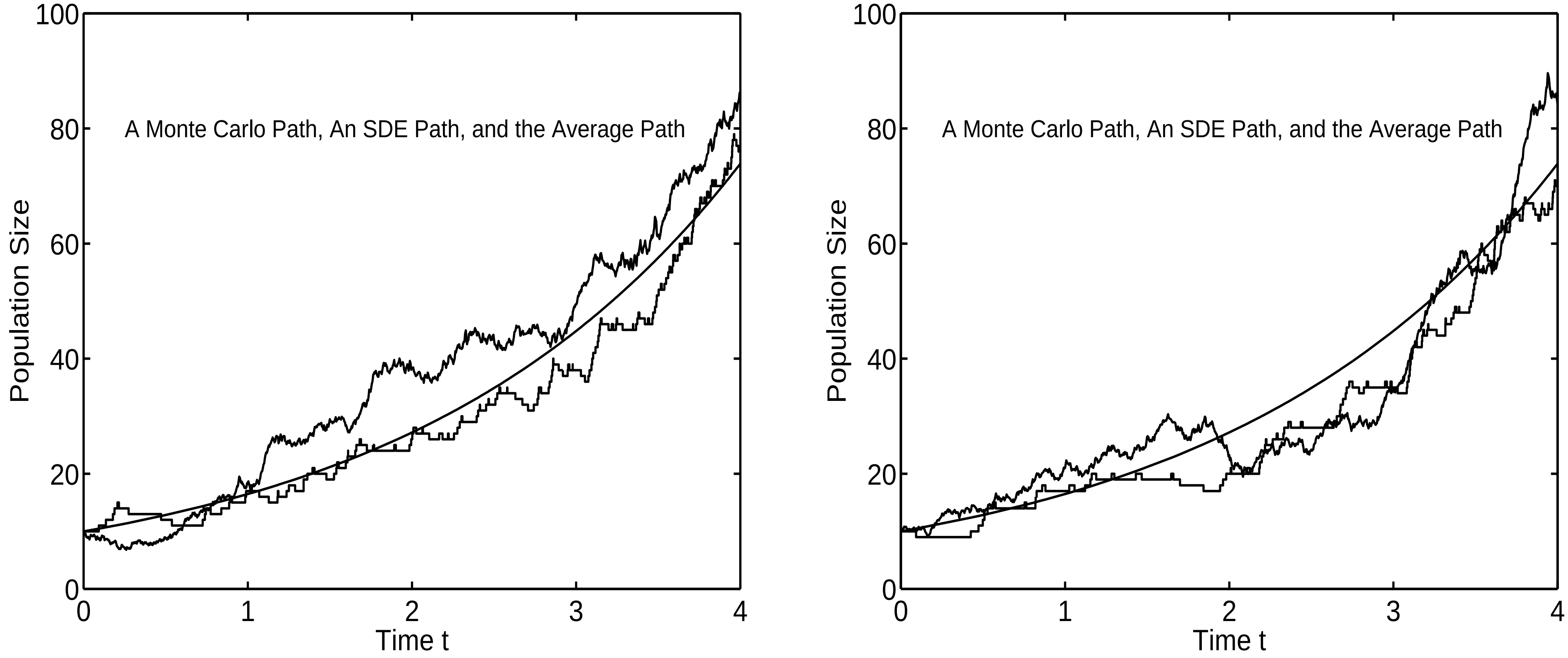


Figure 1: Calculated Sample Paths for a Birth-Death Process where b=1.0 and d=0.5

The SDE captures the random behavior of the birth-death process even though the population values are not integers.

For SDEs, It Is Very Useful To Understand Wiener Processes

The Wiener process satisfies certain properties:

(a) $W(0) = 0$**,**

(b) $W(t) \sim N(0, t)$**, that is,** $W(t)$ **is distributed normally with mean** 0 **and variance** t **for each** t**,**

(c) $W(t + \Delta t) - W(t) \sim N(0, \Delta t)$ **for each** t **and each** Δt**,**

(d) the Wiener process can be generated by the recurrence:

$$W((k+1)\Delta t) = W(k\Delta t) + \sqrt{\Delta t}\,\eta_k \quad \textbf{for} \quad k = 0, 1, 2, \ldots \quad \textbf{and} \quad \eta_k \sim N(0, 1),$$

(e) $W(t_3) - W(t_2)$ **is independent of** $W(t_2) - W(t_1)$ **for** $t_1 < t_2 < t_3$**. Indeed,**

$$E(W(t_3) - W(t_2))(W(t_2) - W(t_1)) = 0 \quad \textbf{but} \quad E(W(t_2) - W(t_1))^2 = t_2 - t_1.$$

(f) the Wiener process is continuous but nowhere differentiable.

Generation of a Wiener process gives some understanding

A sample path of a Wiener process $W(t)$ can be easily generated at a finite number of points.

Suppose that a Wiener process trajectory is desired on the interval $[t_0, t_N]$ at the points $\{t_i\}_{i=0}^N$ where $t_0 = 0$. Then, $W(t_0) = 0$ and

$$W(t_i) = W(t_{i-1}) + \eta_{i-1}\sqrt{t_i - t_{i-1}}, \quad \textbf{for} \quad i = 1, 2, \ldots, N,$$

where η_{i-1} are independent normally distributed numbers.

The values $W(t_i)$, $i = 0, 1, \ldots, N$, determine a Wiener sample path at the points $\{t_i\}_{i=0}^N$.

(Note that the normally distributed random numbers, η_{i-1} for $i = 1, 2, \ldots, N$, are generally found using pseudo-random number generators.)

Two Sample Paths (Or Trajectories) Of The Wiener Process Illustrate Its Random Behavior

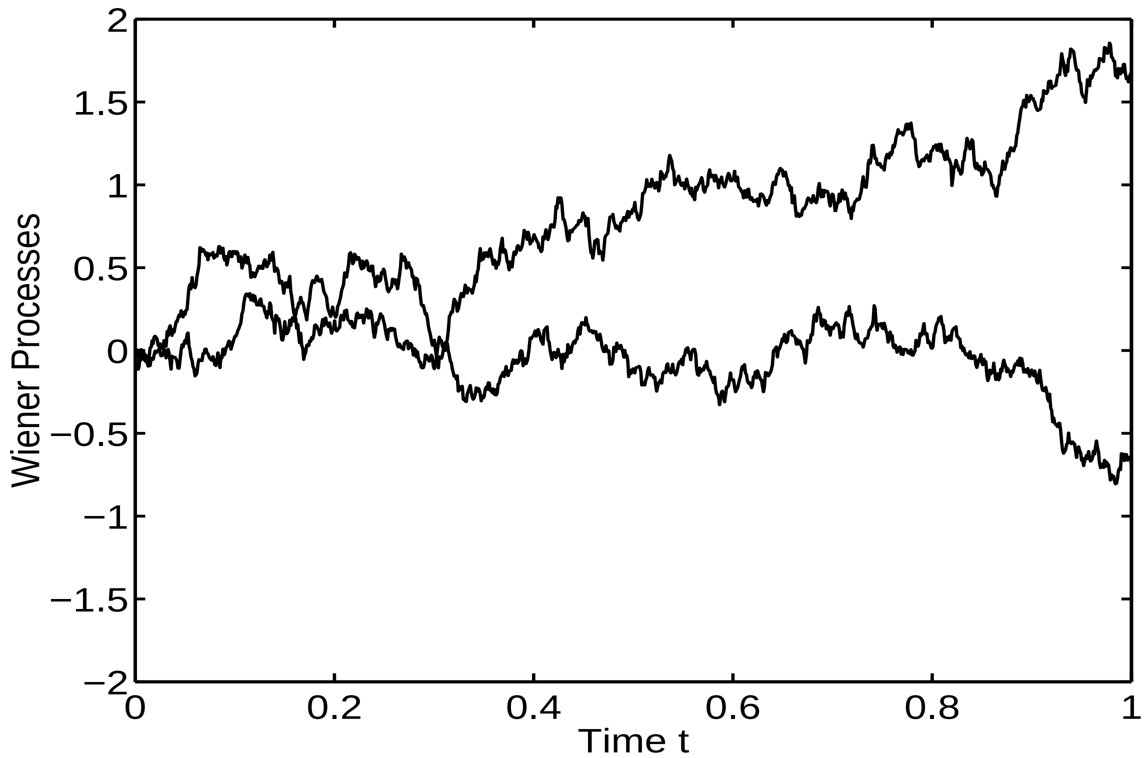


Figure 2: **Two Wiener Processes On [0,1]**

SDEs Are Defined From Stochastic Integrals

The Itô integral $\int_a^b f(t)\, dW(t)$ is defined to be

$$\int_a^b f(t)\, dW(t) = \lim_{m\to\infty} \sum_{i=0}^{m-1} f(t_i)\big(W(t_{i+1}) - W(t_i)\big)$$

where $t_i = a + i\Delta t$ and $\Delta t = (b-a)/m$.

Two useful properties are:

(1) $E(\int_a^b f(t)\, dW(t)) = 0$

(2) $E(\int_a^b f(t)\, dW(t))^2 = \int_a^b E(f(t))^2\, dt$

In addition, if $X(t) = \int_0^t f(t)\, dt + \int_0^t g(t)\, dW(t)$, we say that $X(t)$ satisfies the Itô SDE:

$$\frac{dX(t)}{dt} = f(t) + g(t)\frac{dW(t)}{dt} \quad \textbf{or} \quad dX(t) = f(t)\, dt + g(t)\, dW(t).$$

Itô Stochastic Differential Equations Are Popular

An Itô SDE has the form

$$X(t) = X(0) + \int_0^t f(s, X(s))\, ds + \int_0^t g(s, X(s))\, dW(s)$$

for $0 \leq t \leq T$ **where** $X(0)$ **is given.**

In differential form,

$$dX(t) = f(t, X(t))\, dt + g(t, X(t))\, dW(t)$$

where f **is called the drift coefficient and** g **is called the diffusion coefficient.**

To prove existence and uniqueness, it is often assumed that f **and** g **satisfy:**

Condition (a): $|f(t,x) - f(s,y)|^2 \leq k(|t-s| + |x-y|^2)$ **for** $0 \leq s, t \leq T$ **and** $x, y \in \mathbb{R}$.

Condition (b): $|f(t,x)|^2 \leq k(1 + |x|^2)$ **for** $0 \leq t \leq T$ **and** $x \in \mathbb{R}$.

Solutions of the SDE are Bounded and Continuous

Assuming that f and g satisfy (a) and (b) then there are constants c_1 and c_2 such that:

Boundedness:

$$E|X(t)|^2 \leq c_1 \textbf{ for } 0 \leq t \leq T.$$

Continuity:

$$E|X(t) - X(r)|^2 \leq c_2|t-r| \textbf{ for } 0 \leq r, t \leq T.$$

(So, given $\epsilon > 0$ there is a $\delta > 0$ such that $(E|X(t) - X(r)|^2)^{1/2} < \epsilon$ when $|t - r| < \delta$.)

Itô's Formula Is Very Useful To Understand

Itô's formula says that a smooth function, $F(t, X(t))$, of the stochastic process $X(t)$ also satisfies an SDE.

Consider the Itô SDE in differential form:

$$dX(t) = f(t, X(t))\, dt + g(t, X(t))\, dW(t) \ \textbf{ for } \ 0 \le t \le T.$$

Let F be a smooth function. Itô's formula says:

$$\begin{aligned} dF(t, X(t)) \ &= \ \left(\frac{\partial F(t, X)}{\partial t} + f(t, X) \frac{\partial F(t, X)}{\partial x} + \frac{1}{2} g^2(t, X) \frac{\partial^2 F(t, X)}{\partial x^2} \right) dt \\ &\quad + \ g(t, X) \frac{\partial F(t, X)}{\partial x} dW(t). \end{aligned}$$

Itô's formula helps us, for example, determine exact solutions or moments for certain SDEs. In doing this, useful is:

$$E\left(\int_0^t G(t, X(t))\, dW(t) \right) = 0.$$

SKETCH OF A PROOF OF ITÔ'S FORMULA

The proof of Itô's formula relies on using the Taylor series expansion to $o(\Delta t)$:

$$F(t+\Delta t, X(t+\Delta t)) - F(t, X(t)) \approx \frac{\partial F(t,X)}{\partial t}\Delta t +$$
$$+\frac{\partial F(t,X)}{\partial X}(X(t+\Delta t) - X(t)) + \frac{1}{2}\frac{\partial^2 F(t,X)}{\partial X^2}(X(t+\Delta t) - X(t))^2.$$

Dividing by Δt and using, also to order $o(\Delta t)$, the approximation:

$$X(t+\Delta t) - X(t) = \int_t^{t+\Delta t} f(s)ds + \int_t^{t+\Delta t} g(s)dW(s) \approx f(t)\Delta t + g(t)\Delta W,$$

we obtain that:

$$\frac{dF(t,X(t))}{dt} = \frac{\partial F(t,X)}{\partial t} + \frac{\partial F(t,X)}{\partial X}\left(f(t) + g(t)\frac{dW(t)}{dt}\right) + \frac{1}{2}\frac{\partial^2 F(t,X)}{\partial X^2}g^2(t)$$

where we used

$$E(\Delta W)^2 = E(W(t+\Delta t) - W(t))^2 = \Delta t.$$

Example: Finding Exact Moments For An SDE

Consider the SDE:

$$dX(t) = -\frac{1}{4}X^3(t)\,dt + \frac{1}{2}X^2(t)\,dW(t) \;\; \textbf{with} \;\; X(0) = \frac{1}{2}.$$

In this example, $E(X(t))$ **and** $E(X^3(t))$ **are to be determined exactly.**

First,

$$dE(X(t)) = -\frac{1}{4}E(X^3(t))\,dt \;\; \textbf{with} \;\; E(X(0)) = \frac{1}{2}$$

so $E(X^3(t))$ **is needed in order to find** $E(X(t))$**. Applying Itô's formula to the SDE gives**

$$dX^3(t) = \left[-\frac{3}{4}X^5(t) + \frac{3}{4}X^5(t)\right]\,dt + \frac{3}{2}X^4(t)\,dW(t) \;\; = \frac{3}{2}X^4(t)\,dW(t)$$

with $E(X^3(0)) = \frac{1}{8}$**.**

Thus, $E(X^3(t)) = \frac{1}{8}$ **and it follows that** $E(X(t)) = \frac{1}{2} - \frac{1}{32}t$.

Example: Finding Exact Moments For An SDE

Consider the stochastic differential equation

$$dX(t) = \left[\frac{1}{3}X^{1/3}(t) + 6X^{2/3}(t)\right] dt + X^{2/3}(t)\, dW(t) \ \ \textbf{with} \ \ X(0) = 1.$$

In this example, we wish to determine $E(X(t))$ **and** $E(X^2(t))$ **exactly. First notice that**

$$dE(X(t)) \neq \left[\frac{1}{3}\big(E(X(t))\big)^{1/3} + 6\big(E(X(t))\big)^{2/3}\right] dt$$

so an appropriate change of variables is required to find the moments. Let

$$Y_n(t) = (X(t))^{n/3} \ \ \textbf{for} \ \ n = 0, 1, 2, \ldots, 6.$$

Next, applying Itô's formula, the stochastic differentials are obtained

$$dY_n(t) = \left[\frac{1}{18}(n^2 - n)X^{\frac{n-2}{3}}(t) + 2nX^{\frac{n-1}{3}}(t)\right] dt + \left[\frac{n}{3}X^{\frac{n-1}{3}}(t)\right] dW(t)$$

with $Y_n(0) = 1$ **for** $n = 0, 1, 2, \ldots, 6$. **Then,**

$$dY_n(t) = \left[\frac{1}{18}(n^2 - n)Y_{n-2}(t) + 2nY_{n-1}(t)\right] dt + \left[\frac{n}{3}Y_{n-1}(t)\right] dW(t)$$

for $n = 0, 1, 2, \ldots, 6$.

Letting $Z_n(t) = E(Y_n(t)) = E((X(t))^{n/3})$**, then the initial-value system is:**

$$\frac{dZ_n(t)}{dt} = \frac{1}{18}(n^2 - n)Z_{n-2}(t) + 2nZ_{n-1}(t) \ \ \textbf{for} \ \ n = 1, 2, \ldots, 6$$

with $Z_n(0) = 1$ **for** $n = 1, 2, \ldots, 6$ **and** $Z_0(t) = 1$**. Solving this gives**

$$\begin{aligned}
Z_1(t) &= E((X(t))^{1/3}) = 2t + 1 \\
Z_2(t) &= E((X(t))^{2/3}) = 4t^2 + \frac{37}{9}t + 1 \\
Z_3(t) &= E((X(t)) = 8t^3 + \frac{38}{3}t^2 + \frac{19}{3}t + 1 \\
Z_6(t) &= E((X(t))^2) = 64t^6 + \frac{656}{3}t^5 + \frac{2660}{9}t^4 + \frac{49145}{243}t^3 + \frac{665}{9}t^2 + \frac{41}{3}t + 1.
\end{aligned}$$

In particular, $E(X(1)) = 28.0$ **and** $E(X^2(1)) = 869.0206$.

Example: Finding The Exact Solution Of An SDE

Consider the SDE (Ornstein-Uhlenbeck):

$$dX(t) = \beta(X_e - X(t))\,dt + \alpha\,dW(t), \quad X(0) = X_0$$

where β, α, X_e, and X_0 are constants. Let $F(t,X) = e^{\beta t}X(t)$. By Itô's formula,

$$d\big(e^{\beta t}X(t))\big) = \big[\beta e^{\beta t}X(t) + \beta e^{\beta t}(X_e - X(t)\big]\,dt + \alpha e^{\beta t}\,dW(t)$$

Thus,

$$e^{\beta t}X(t) - X_0 = e^{\beta t}X_e - X_e + \int_0^t e^{\beta s}\alpha\,dW(s).$$

So the exact solution is

$$X(t) = X_e + (X_0 - X_e)e^{-\beta t} + e^{-\beta t}\int_0^t e^{\beta s}\alpha\,dW(s)$$

and, at large time t, $X(t)$ is approximately normally distributed with mean X_e and variance $\alpha^2/(2\beta)$.

Example: Finding The Exact Solution Of An SDE

Consider the stochastic differential equation

$$dX(t) = f(t)X(t)\,dt + g(t)X(t)\,dW(t), \quad X(0) = X_0$$

where X_0 is a constant. For this problem, the exact solution has the form

$$X(t) = X_0 \exp\left(\int_0^t \left(f(s) - \frac{1}{2}g^2(s)\right) ds + \int_0^t g(s)\,dW(s)\right).$$

To see this, let $F(t, X) = \ln(X(t))$. Applying Itô's formula,

$$d(\ln(X(t))) = \left[f(t) - \frac{1}{2}g^2(t)\right] dt + g(t)\,dW(t).$$

Thus,

$$\ln(X(t)) - \ln(X_0) = \int_0^t \left(f(s) - \frac{1}{2}g^2(s)\right) ds + \int_0^t g(s)\,dW(s)$$

which yields the solution.

The Forward Kolmogorov Equation Is Useful To Understand

The probability distribution of solutions to a discrete-valued continuous stochastic process satisfies a system of differential equations called the forward Kolmogorov equations. An analogous result holds for the probability distribution of solutions to an SDE. The probability distribution of solutions to an SDE satisfies a PDE called the forward Kolmogorov equation.

Consider the stochastic differential equation

$$dX(t) = f(t, X(t))\, dt + g(t, X(t))\, dW(t).$$

By applying Itô's formula, it can be shown that the probability density for solutions to the SDE satisfies:

$$\frac{\partial p(t,x)}{\partial t} = -\frac{\partial (p(t,x) f(t,x))}{\partial x} + \frac{1}{2}\frac{\partial^2 (p(t,x) g^2(x,t))}{\partial^2 x}.$$

In particular, $P(a < X(t) < b) = \int_a^b p(x,t)\, dx$**.**

SKETCH OF A PROOF OF THE FORWARD KOLMOGOROV EQUATION

Consider the stochastic differential equation

$$dX(t) = f(t, X(t))\, dt + g(t, X(t))\, dW(t)$$

and let $F \in \mathbb{C}_0^\infty(\mathbb{R})$**. Applying Itô's formula to** $F(X)$ **gives**

$$\begin{aligned} dF(X) \;=\; & \left(f(t, X)\frac{\partial F(t, X)}{\partial x} + \frac{1}{2}g^2(t, X)\frac{\partial^2 F(t, X)}{\partial x^2} \right) dt \\ & + g(t, X)\frac{\partial F(t, X)}{\partial x}\, dW(t). \end{aligned}$$

Because

$$E\int_0^t g(s, X(s))\frac{\partial F(X(s))}{\partial x}\, dW(s) = 0,$$

then

$$\frac{dE(F)}{dt} = E\left[\frac{\partial F}{\partial x} f + \frac{1}{2}g^2\frac{\partial^2 F}{\partial x^2}\right].$$

Let $p(t, x)$ **be probability density for solutions to the SDE. Then,**

$$\frac{d}{dt}\int_{-\infty}^{\infty} p(t, x)F(x)\, dx = \int_{-\infty}^{\infty} p(t, x)\left[\frac{\partial F}{\partial x} f + \frac{1}{2}g^2\frac{\partial^2 F}{\partial^2 x}\right]\, dx.$$

Integrating by parts the right-hand side yields

$$\int_{-\infty}^{\infty} F(x) \left[\frac{\partial p(t,x)}{\partial t} + \frac{\partial (p(t,x) f(t,x))}{\partial x} - \frac{1}{2} \frac{\partial^2 (p(t,x) g^2(t,x))}{\partial^2 x} \right] dx = 0.$$

As the above integral holds for every function $F \in \mathbb{C}_0^\infty(\mathbb{R})$**, this implies that**

$$\frac{\partial p(t,x)}{\partial t} = - \frac{\partial (p(t,x) f(t,x))}{\partial x} + \frac{1}{2} \frac{\partial^2 (p(t,x) g^2(x,t))}{\partial^2 x}.$$

This equation is the forward Kolmogorov equation or Fokker-Planck equation for the probability distribution of solutions to the SDE.

Also, the forward Kolmogorov equation for a system of SDEs is:

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

Consider the stochastic differential equation

$$\begin{cases} dX(t) = a\,dt + b\,dW(t) \\ X(0) = x_0. \end{cases}$$

The probability density of the solutions satisfies the forward Kolmogorov equation

$$\begin{cases} \dfrac{\partial p(t,x)}{\partial t} = -\dfrac{\partial(ap(t,x))}{\partial x} + \dfrac{b^2}{2}\dfrac{\partial^2(p(t,x))}{\partial^2 x} \\ p(0,x) = \delta(x - x_0). \end{cases}$$

The solution to this partial differential equation is

$$p(t,x) = \frac{1}{\sqrt{2\pi b^2 t}} \exp\left(\frac{-(x - at - x_0)^2}{2b^2 t}\right).$$

Numerical Methods To Approximate SDEs Are Valuable

The exact solution to an SDE is generally difficult to obtain so methods to approximate the solution are important. The Euler-Maruyama method is the most commonly used numerical method.

The Euler-Maruyama method has the form

$$X_{i+1} = X_i + f(t_i, X_i)\Delta t + g(t_i, X_i)\Delta W_i, \quad X_0 = X(0)$$

for $i = 0, 1, 2, \ldots, N-1$ **where** $X_i \approx X(t_i)$**,** $t_i = i\Delta t$**,** $\Delta t = T/N$**,** $\Delta W_i = (W(t_{i+1}) - W(t_i)) \sim N(0, \Delta t)$**.**

To study the error in this method, we approximate the solution for all $t \in [0, T]$ **and not just at the nodal points** t_i**. To accomplish this, let** $\hat{X}(t) \approx X(t)$ **be defined as**

$$\hat{X}(t) = X_i + \int_{t_i}^{t} f(t_i, X_i)\, ds + \int_{t_i}^{t} g(t_i, X_i)\, dW(s)$$

for $t_i \le t \le t_{i+1}$ **and** $i = 0, 1, \ldots, N-1$**. Notice that** $\hat{X}$ **is identical to Euler's method approximation at the nodal points, that is,** $\hat{X}(t_i) = X_i$ **for** $i = 0, 1, \ldots, N$**.**

On the ith subinterval, $\hat{X}(t)$ is the solution of the SDE

$$\begin{cases} d\hat{X}(t) = f(t_i, X_i)\,dt + g(t_i, X_i)\,dW(t), \quad t_i \le t \le t_{i+1} \\ \hat{X}(t_i) = X_i. \end{cases}$$

Recall that the solution $X(t)$ satisfies the SDE

$$dX(t) = f(t, X(t))\,dt + g(t, X(t))\,dW(t), \quad t_i \le t \le t_{i+1}.$$

Define the error as $\epsilon(t) = X(t) - \hat{X}(t)$. Then the error ϵ satisfies the SDE

$$\begin{cases} d\epsilon(t) = (f(t, X(t)) - f(t_i, X_i))\,dt + (g(t, X(t)) - g(t_i, X_i))\,dW(t), \\ \epsilon(t_i) = X(t_i) - \hat{X}(t_i) \end{cases}$$

for $t_i \le t \le t_{i+1}$. Using Itô's formula, the stochastic differential for $\epsilon^2(t)$ is:

$$\begin{aligned} d(\epsilon^2(t)) &= 2\big(X(t) - \hat{X}(t)\big)\big(f(t, X(t)) - f(t_i, X_i)\big)\,dt \\ &+\big(g(t, X(t)) - g(t_i, X_i)\big)^2\,dt + 2\big(X(t) - \hat{X}(t)\big)\big(g(t, X(t)) - g(t_i, X_i)\big)\,dW(t) \end{aligned}$$

Hence, $E(\epsilon^2(t_{i+1}))$ satisfies

$$
\begin{aligned}
E(\epsilon^2(t_{i+1})) \;&=\; E(\epsilon^2(t_i)) + E\int_{t_i}^{t_{i+1}} \big(g(t,X(t)) - g(t_i,X_i)\big)^2\,dt \\
&\quad + E\int_{t_i}^{t_{i+1}} 2\big(X(t)-\hat{X}(t)\big)\big(f(t,X(t)) - f(t_i,X_i)\big)\,dt \\
&\quad + E\int_{t_i}^{t_{i+1}} 2\big(X(t)-\hat{X}(t)\big)\big(g(t,X(t)) - g(t_i,X_i)\big)\,dW(t)
\end{aligned}
$$

Using the inequality $|2ab| \le a^2 + b^2$ and properties of stochastic integrals,

$$
\begin{aligned}
E(\epsilon^2(t_{i+1})) \;&\le\; E(\epsilon^2(t_i)) + \int_{t_i}^{t_{i+1}} E(X(t)-\hat{X}(t))^2\,dt \\
&+ \int_{t_i}^{t_{i+1}} E(f(t,X(t)) - f(t_i,X_i))^2\,dt + \int_{t_i}^{t_{i+1}} E(g(t,X(t)) - g(t_i,X_i))^2\,dt.
\end{aligned}
$$

But

$$
\begin{aligned}
|f(t,X(t)) - f(t_i,X_i)|^2 \;&\le\; 2|f(t,X(t)) - f(t_i,X(t_i))|^2 \\
&\quad +2|f(t_i,X(t_i)) - f(t_i,X_i)|^2 \\
&\le\; 2k|t-t_i| + 2k|X(t)-X(t_i)|^2 + 2k|X(t_i)-X_i|^2
\end{aligned}
$$

and similarly for g**. Hence,**

$$\begin{aligned} E(\epsilon^2(t_{i+1})) &\le E(\epsilon^2(t_i)) + \int_{t_i}^{t_{i+1}} E(X(t) - \hat{X}(t))^2\,dt \\ &\quad + 4k(1+c)\int_{t_i}^{t_{i+1}} (t-t_i)\,dt + 4k\int_{t_i}^{t_{i+1}} E(\epsilon^2(t_i))\,dt \end{aligned}$$

using $E|X(t) - X(t_i)|^2 \le c|t-t_i|$**. Therefore,**

$$E(\epsilon^2(t_{i+1})) \le E(\epsilon^2(t_i))(1+4k\Delta t) + 2k(1+c)(\Delta t)^2 + \int_{t_i}^{t_{i+1}} E(\epsilon^2(s))\,ds.$$

By Bellman-Gronwall inequality with $b(t) = E(\epsilon^2(t_i))(1+4k\Delta t)$ $+2k(1+c)(\Delta t)^2$**,**

$$\begin{aligned} E(\epsilon^2(t_{i+1})) &\le E(\epsilon^2(t_i))(1+4k\Delta t) + 2k(1+c)(\Delta t)^2 \\ &\quad + \int_{t_i}^{t_{i+1}} e^{(t_{i+1}-t)}\left[E(\epsilon^2(t_i))(1+4k\Delta t) + 2k(1+c)(\Delta t)^2\right] dt \\ &= e^{\Delta t}\left[E(\epsilon^2(t_i))(1+4k\Delta t) + 2k(1+c)(\Delta t)^2\right]. \end{aligned}$$

Letting $a_i = E(\epsilon^2(t_i)), R = e^{\Delta t}(1+4k\Delta t)$**, and** $S = e^{\Delta t}2k(1+c)(\Delta t)^2$**, then**

$$a_{i+1} \le Ra_i + S \;\; \textbf{for} \;\; i = 0,1,2,\ldots,N-1.$$

These inequalities yield

$$a_N \leq S\frac{R^N - 1}{R - 1} \ \ \textbf{with} \ \ a_0 = E(\epsilon^2(0)) = 0.$$

Hence,

$$E(\epsilon^2(t_N)) \leq \frac{e^{\Delta t} 2k(1+c)(\Delta t)^2 e^{N\Delta t} e^{4kN\Delta t}}{e^{\Delta t} - 1 + e^{\Delta t} 4k\Delta t} \leq \Delta t \frac{(1+c)e^{(1+4k)T}}{2}.$$

This holds for any nodal point and, thus, the mean square error satisfies

$$E|X(t_i) - X_i|^2 \leq \hat{c}\Delta t$$

for $i = 0, 1, 2, \ldots, N$ **where** $\hat{c} = \frac{1}{2}(1+c)e^{(1+4k)T}$.

(By Chebyshev's inequality, given $\epsilon > 0$**, the probability that** $|X(t_i) - X_i| > \epsilon$ **goes to zero as** $\Delta t \to 0$**.)**

Milstein's Method Is A Well-Known Higher-Order Method

Higher order numerical methods for SDEs are similar to higher order methods for ODEs. For example, there are explicit or implicit multistep methods and Runge-Kutta methods.

A popular second-order method is Milstein's method and has mean square error proportional to $(\Delta t)^2$ rather than Δt. Milstein's method has the form

$$\begin{aligned} X_{i+1} &= X_i + f(t_i, X_i)\Delta t + g(t_i, X_i)\Delta W_i \\ &\quad + \frac{1}{2} g(t_i, X_i) \frac{\partial g(t_i, X_i)}{\partial x} [(\Delta W_i)^2 - \Delta t] \end{aligned}$$

for $i = 0, 1, 2, \ldots, N-1$ with $X_0 = X(0,)$, where $X_i \approx X(t_i)$, $\Delta W_i = (W(t_{i+1}) - W(t_i)) \sim N(0, \Delta t)$, $t_i = i\Delta t$, $\Delta t = T/N$.

Milstein's method has an additional term at each step in comparison with Euler's method.

Example: Approximation Of An SDE By Euler-Maruyama And By Milstein

Consider the stochastic differential equation

$$dX(t) = \left[\frac{1}{3}X^{1/3}(t) + 6X^{2/3}(t)\right] dt + X^{2/3}(t)\, dW(t), \quad X(0) = 1.$$

It was shown earlier that $E(X(1)) = 28.0$ **and** $E(X^2(1)) = 869.0206$. **For this problem, Euler's method has the form:**

$$X_{i+1} = X_i + \left[\frac{1}{3}X_i^{1/3} + 6X_i^{2/3}\right] \Delta t + X_i^{2/3}\sqrt{\Delta t}\, \eta_i \ \textbf{ where } \ \eta_i \sim N(0,1)$$

for $i = 0, 1, 2, \ldots, N-1$ **with** $X_0 = 1$**,** $t_i = i\Delta t$, **and** $\Delta t = 1/N$**. Milstein's method has the form**

$$X_{i+1} = X_i + \left[\frac{1}{3}X_i^{1/3} + 6X_i^{2/3}\right] \Delta t + X_i^{2/3}\sqrt{\Delta t}\, \eta_i + \frac{1}{3}X_i^{1/3}(\eta_i^2 - 1)\Delta t$$

where $\eta_i \sim N(0,1)$**.**

The calculational results for the mean square error $E|X(1)-X_N|^2$ are given in the table for 10,000 sample paths for each value of N.

Value of N	**Euler Error**	**Milstein Error**
2^9	2.80×10^{-2}	1.61×10^{-2}
2^{10}	1.04×10^{-2}	4.03×10^{-3}
2^{11}	4.20×10^{-3}	1.01×10^{-3}
2^{12}	1.89×10^{-3}	2.53×10^{-4}
2^{13}	8.76×10^{-4}	6.24×10^{-5}
2^{14}	4.12×10^{-4}	1.60×10^{-5}

Notice that the mean square errors are approximately proportional to $\Delta t = 1/N$ for Euler's method and to $(\Delta t)^2 = 1/N^2$ for Milstein's method.

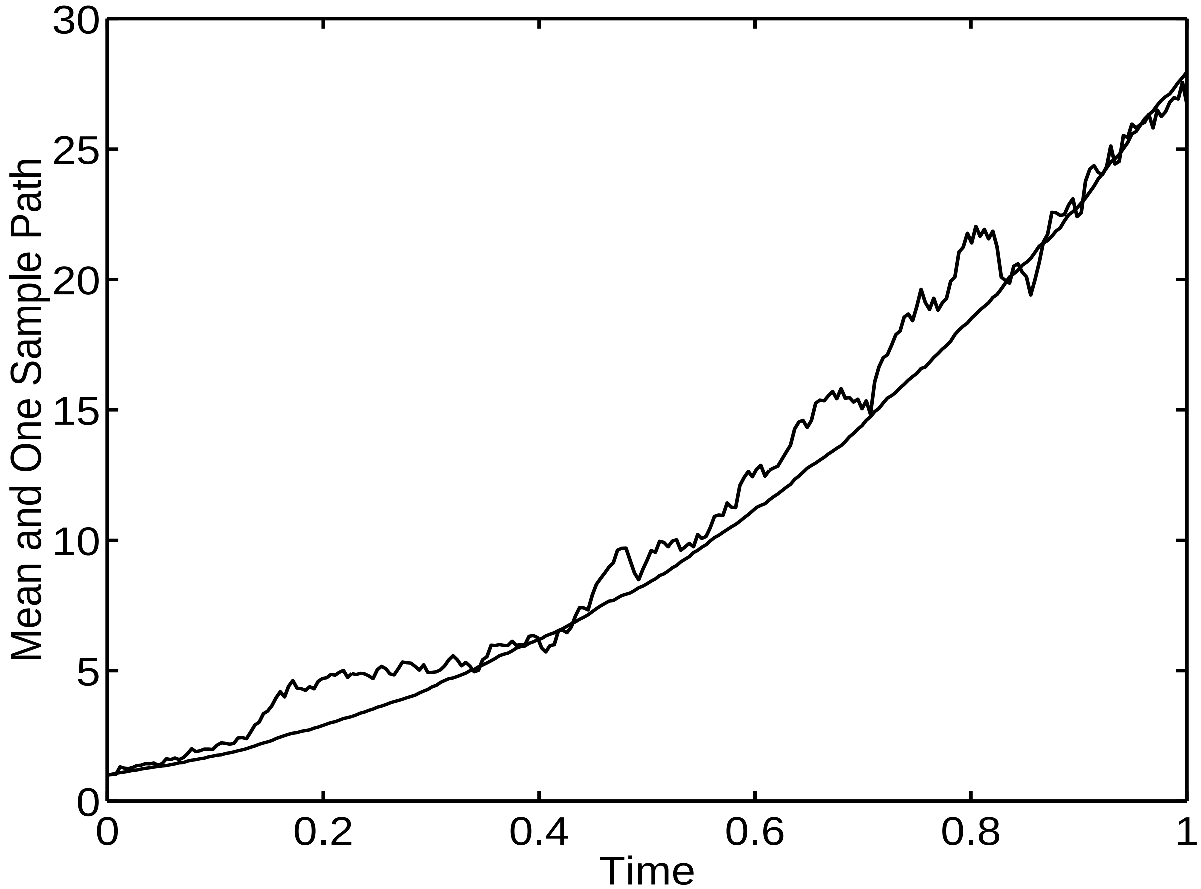


Figure 3: **Mean solution and one sample path**

The mean and one sample path are plotted in the figure for this problem.

Next, for this example, $E(X(1))$ and $E(X(1))^2$ were estimated using $E(X(1)) \approx \sum_{j=1}^{100,000} X_N^{(j)}/100,000$ and $E(X(1))^2 \approx \sum_{j=1}^{100,000}(X_N^{(j)})^2/100,000$ where $X_N^{(j)}$ is the estimate of $X(1)$ for the jth sample path using N intervals.

In the table, the errors are given in parentheses. Recall that $E(X(1)) = 28.0$ and $E(X^2(1)) = 869.0206$ are the exact values. Notice that the errors in the mean values are proportional to Δt for either numerical method. In particular, the errors in Euler's method when estimating mean values are proportional to Δt rather than $(\Delta t)^{1/2}$.

Value of N	**Euler Estimate**	**Milstein Estimate**
2^6	**27.07 (0.93)**	**27.08 (0.92)**
2^7	**27.56 (0.44)**	**27.56 (0.44)**
2^8	**27.79 (0.21)**	**27.79 (0.21)**
Value of N	**Euler Estimate**	**Milstein Estimate**
2^6	**810.15 (58.87)**	**810.18 (58.84)**
2^7	**840.89 (28.13)**	**840.93 (28.09)**
2^8	**855.33 (13.69)**	**855.31 (13.71)**

There Are Two Forms of Approximation: Strong And Weak

This example illustrates that are two kinds of approximation in computational solution of SDEs.

A method is a strong approximation of order γ if

$$(E(X(T) - X_N)^2)^{1/2} \leq c(\Delta t)^\gamma$$

where $X(T)$ is the exact solution at time T and X_N is the approximate solution.
Euler's and Milstein's methods have strong orders $\frac{1}{2}$ and 1.

However, if expectations of functions for an SDE are desired and not necessarily the pathwise approximation of a strong approximation, then a weak numerical method may be sufficient.

An approximation X_N is said to converge weakly with order β if

$$|E(F(X(T))) - E(F(X_N))| \leq c(\Delta t)^\beta$$

for all smooth functions F.
Euler's and Milstein's method both have weak order 1.

Richardson Extrapolation Can Increase The Accuracy Of Weak Approximations

Both Euler's or Milstein's method have weak-error expansions of the correct form for applying Richardson extrapolation.

The weak error for Euler's or Milstein's method has the form

$$E(F(X(T))) - E(F(X_N)) = c_1\Delta t + c_2(\Delta t)^2 + c_3(\Delta t)^3 + \dots,$$

where $\Delta t = T/N$ **and** $c_1, c_2, c_3, \dots$ **are independent of** Δt**.**

Several approximations with different values of N **can be applied to obtain a higher order approximation. Suppose that** $E(F(X_N))$**,** $E(F(X_{2N}))$**, and** $E(F(X_{4N}))$ **are three approximations to** $E(F(X(T)))$ **using step lengths of** T/N**,** $T/2N$**, and** $T/4N$ **in Euler's or in Milstein's method.**

To obtain an approximation to $E(F(X(T)))$ **of order** $(\Delta t)^2$**, let**

$$E(F(X(T))) - \left[2E(F(X_{2N})) - E(F(X_N))\right] = \hat{c}_2(\Delta t)^2 + \hat{c}_3(\Delta t)^3 + \dots.$$

To obtain an approximation to $E(F(X(T)))$ **of order** $(\Delta t)^3$**, let**

$$E(F(X(T))) - \left[8E(F(X_{4N})) - 6E(F(X_{2N})) + E(F(X_N))\right]/3 = \tilde{c}_3(\Delta t)^3 + \dots.$$

An Example Illustrates Richardson Extrapolation

For the previous example, the following approximations to $E((X(1))^2)$ **are obtained using the Euler-Maruyama method:**

$$E((X_{64})^2) = 810.15, \quad E((X_{128})^2) = 840.89, \quad \textbf{and} \quad E((X_{256})^2) = 855.33.$$

To obtain $O((\Delta t)^2)$ **and** $O((\Delta t)^3)$ **approximations, respectively, to** $E((X(1))^2)$ **we calculate**

$$2E((X_{128})^2) - E((X_{64})^2) = 871.63$$

and

$$[8E((X_{256})^2) - 6E((X_{128})^2) + E((X_{64})^2)]/3 = 869.15.$$

As $E((X(1))^2) = 869.02$ **exactly, the original Euler approximations are much improved through extrapolation.**

Systems Of SDEs Can Be Treated In A Similar Manner

Itô's formula and numerical methods can be extended to systems. Let

$$\vec{X}(t) = [X_1(t), X_2(t), \ldots, X_d(t)]^T$$
$$\vec{W}(t) = [W_1(t), W_2(t), \ldots, W_m(t)]^T$$
$$\vec{f} : [0,T] \times \mathbb{R}^d \to \mathbb{R}^d \text{ and } g : [0,T] \times \mathbb{R}^d \to \mathbb{R}^{d\times m},$$

where $W_i(t), 1 \leq i \leq m$ **are independent Wiener processes.**

Then a system of stochastic differential equations has the form

$$d\vec{X}(t) = \vec{f}(t, \vec{X}(t))\, dt + g(t, \vec{X}(t))\, d\vec{W}(t).$$

In component form, the system is

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

for $i = 1, 2, \ldots, d$.

Itô's Formula Generalizes For Systems Of SDEs

Let

$$\vec{F} : [0,T] \times \mathbb{R}^d \to \mathbb{R}^k \ \textbf{ and let } \ \vec{Y}(t,\omega) = \vec{F}(t, \vec{X}(t,\omega)).$$

Then the pth component of $\vec{Y}(t,\omega)$ satisfies:

$$dY_p(t) \ = \ \left[\frac{\partial F_p}{\partial t} + \sum_{i=1}^{d} f_i \frac{\partial F_p}{\partial x_i} + \sum_{i=1}^{d}\sum_{j=1}^{d}\sum_{l=1}^{m} \frac{1}{2} g_{i,l} g_{j,l} \frac{\partial^2 F_p}{\partial x_i \partial x_j}\right] dt$$

$$+ \sum_{l=1}^{m}\sum_{i=1}^{d} g_{i,l} \frac{\partial F_p}{\partial x_i} dW_l(t)$$

for $p = 1, 2, \ldots, k$**.**

Example of Itô's Formula For An SDE With $d = 1$ and $m = 2$

Consider the SDE:

$$\begin{cases} dX(t) = t^2 X(t)\, dt + t\, dW_1(t) + X(t)\, dW_2(t), \quad 0 \le t \le T \\ X(0) = 1, \end{cases}$$

where $d = 1$ **and** $m = 2$**.**

For this problem, $f_1 = t^2 X, \;\; g_{1,1} = t$**,** **and** $g_{1,2} = X$**.**

Consider using Itô's formula to find the SDE for $F = X^2$**. Applying Itô's formula,**

$$\begin{cases} d(X^2(t)) = \left[2t^2 X^2(t) + t^2 + X^2(t)\right] dt + 2tX(t)\, dW_1(t) + 2X^2(t)\, dW_2(t) \\ X^2(0) = 1. \end{cases}$$

The Euler-Maruyama And Milstein Methods Extend To Systems

Euler's method for systems has the form

$$\vec{X}_{n+1}(\omega) = \vec{X}_n(\omega) + \vec{f}(t_n, \vec{X}_n(\omega))\Delta t + g(t_n, \vec{X}_n(\omega))\Delta\vec{W}_n(\omega)$$

for $n = 0, 1, 2, \ldots, N$**, where** $\vec{X}_n(\omega) \approx \vec{X}(t_n, \omega)$**,** $\Delta t = T/N$**,** $\Delta\vec{W}_n = \vec{W}(t_{n+1}) - \vec{W}(t_n)$**.**

In component form, Euler's method is:

$$X_{i,n+1}(\omega) = X_{i,n}(\omega) + f_i(t_n, \vec{X}_n(\omega))\Delta t + \sum_{j=1}^{m} g_{i,j}(t_n, \vec{X}_n(\omega))\Delta W_{j,n}(\omega)$$

for $i = 1, 2, \ldots, d$**, where** $\Delta W_{j,n} \sim N(0, \Delta t)$**.**

Milstein's method for multidimensional SDEs involves the double stochastic integral

$$I_n(j_1, j_2) = \int_{t_n}^{t_n+\Delta t} \int_{t_n}^{s} dW_{j_1}(r)\, dW_{j_2}(s).$$

Milstein's method has the componentwise form

$$\begin{aligned} X_{i,n+1}(\omega) \; &= \; X_{i,n}(\omega) + f_i(t_n, \vec{X}_n(\omega))\Delta t + \sum_{j=1}^{m} g_{i,j}(t_n, \vec{X}_n(\omega))\Delta W_{j,n}(\omega) \\ &+ \sum_{j_1=1}^{m} \sum_{j_2=1}^{m} \sum_{l=1}^{d} g_{l,j_1} \frac{\partial g_{i,j_2}}{\partial x_l} I_n(j_1, j_2) \end{aligned}$$

for $i = 1, 2, \ldots, d$.

An Example Of Approximation Of An SDE With $d = 1$ And $m = 2$

Consider the SDE;

$$\begin{cases} dX(t) = t^2 X(t)dt + t dW_1(t) + X(t)dW_2(t), & 0 \le t \le T \\ X(0) = 1, \end{cases}$$

where $d = 1$ **and** $m = 2$**.**

For this problem, Euler's method has the form

$$\begin{cases} X_{n+1} = X_n + t_n^2 X_n \Delta t + t_n \Delta W_{1,n} + X_n \Delta W_{2,n} \\ X_0 = 1, \end{cases}$$

for $n = 0, 1, 2, \ldots$**, where** $\Delta W_{1,n}, \Delta W_{2,n} \sim N(0, \Delta t)$ **and** $t_n = n\Delta t$**.**

Milstein's method has the form

$$\begin{cases} X_{n+1} = X_n + t_n^2 X_n \Delta t + t_n \Delta W_{1,n} + X_n \Delta W_{2,n} + t_n I_n(1,2) + X_n I_n(2,2) \\ X_0 = 1, \end{cases}$$

for $n = 0, 1, 2, \ldots$**.**

It is useful to note that

$$I_n(j_1, j_1) = \int_{t_n}^{t_n+\Delta t} \int_{t_n}^{s} dW_{j_1}(r)\, dW_{j_1}(s) = \frac{1}{2}\big((\Delta W_{j_1,n})^2 - \Delta t\big)$$

but $I_n(j_1, j_2)$ **for** $j_1 \neq j_2$ **does not have an analytical form and must be approximated.**

This multiple integral can be approximated by a Fourier series expansion. Also, if $[t_n, t_{n+1}]$ **is divided into** M **equal intervals with** $t_{j,n} = t_n + j\Delta t/M$ **for** $j = 0, 1, \ldots, M$**, then**

$$I_n(j_1, j_2) \approx \tilde{I}_n(j_1, j_2) = \sum_{j=0}^{M-1} [W_{j_1}(t_{j,n}) - W_{j_1}(t_{0,n})][W_{j_2}(t_{j+1,n}) - W_{j_2}(t_{j,n})].$$

It can be shown that $E|I_n - \tilde{I}_n|^2 = (\Delta t)^2/(2M)$.

A Procedure For Deriving Accurate SDE Models Is Useful

The derivation procedure is analogous to that used for many ODEs models. Basically,

(1) The process is studied for a small time interval Δt.

(2) The changes in the process leads to a differential equation model.

For example, consider deriving an ODE model for the temperature of an object immersed in a liquid held at temperature T_L. Suppose for interval Δt, the change in the temperature is proportional to the difference between the object's temperature $T(t)$ and the liquid's temperature T_L.

Based on this, $\Delta T = \alpha(T_L - T(t))\Delta t$ where α is a constant.

Setting $\Delta T = T(t + \Delta t) - T(t)$ and letting $\Delta t \to 0$, one obtains Newton's Law of Cooling:

$$\frac{dT}{dt} = \alpha(T_L - T).$$

The Procedure For Deriving Accurate SDE Models Is Useful

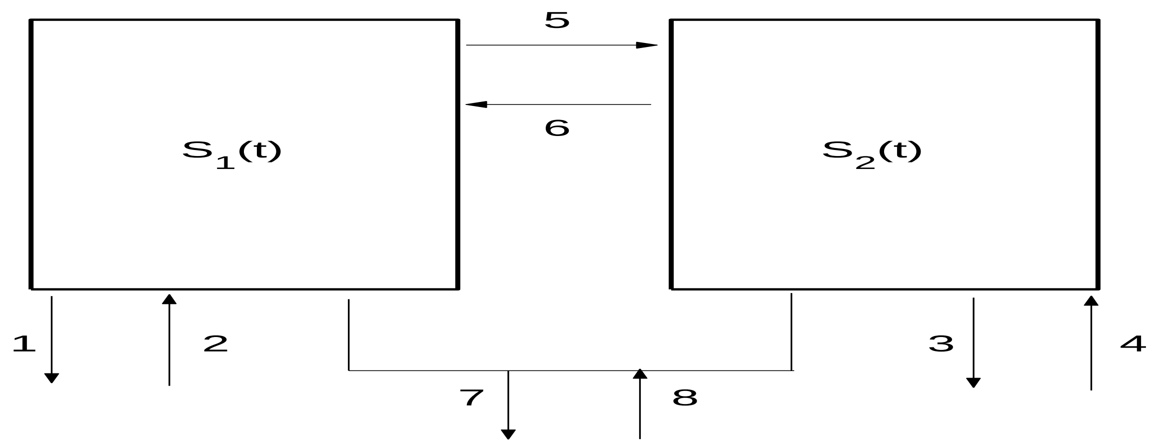
The derivation procedure can be applied to randomly varying dynamical systems in physics, engineering, and biology and is similar to stochastic modeling procedures used in chemistry.

In the procedure, a finite Δt produces a discrete stochastic model. The discrete stochastic model then leads to a stochastic differential equation model as $\Delta t \to 0$. Specifically:

(1) A discrete stochastic model is developed for the random dynamical system. In particular, for a small time interval Δt, the possible changes with their corresponding transition probabilities are determined.

(2) The expected changes and the covariance matrix for the changes are determined for the discrete stochastic process.

(3) A stochastic differential equation model is inferred by similarities in the forward Kolmogorov equations between the discrete and continuous stochastic processes.



THE PROCEDURE IS ILLUSTRATED FOR A TWO-STATE PROBLEM

Let $S_1(t)$ and $S_2(t)$ represent the values of two states at time t.

It is assumed that in a small time interval Δt, state S_1 can change by $-\lambda_1, 0,$ or $+\lambda_1$ and state S_2 can change by $-\lambda_2, 0,$ or $+\lambda_2$ where $\lambda_1, \lambda_2 \geq 0$. Let $\Delta\vec{S} = [S_1, S_2]^T$ be the change in a small time interval Δt.

The changes and probabilities are listed in the table.

For example, change 1 represents a loss of λ_1 in $S_1(t)$ with probability $d_1 \Delta t$.

Change 5 represents a transfer of λ_1 out of state S_1 with a corresponding transfer of λ_2 into state S_2 with probability $m_{12}\Delta t$.

Change 7 represents a simultaneous reduction in both states S_1 and S_2.

Change	**Probability**
$\Delta\vec{S}^{(1)} = [-\lambda_1, 0]^T$	$p_1 = d_1(t, S_1, S_2)\Delta t$
$\Delta\vec{S}^{(2)} = [\lambda_1, 0]^T$	$p_2 = b_1(t, S_1, S_2)\Delta t$
$\Delta\vec{S}^{(3)} = [0, -\lambda_2]^T$	$p_3 = d_2(t, S_1, S_2)\Delta t$
$\Delta\vec{S}^{(4)} = [0, \lambda_2]^T$	$p_4 = b_2(t, S_1, S_2)\Delta t$
$\Delta\vec{S}^{(5)} = [-\lambda_1, \lambda_2]^T$	$p_5 = m_{12}(t, S_1, S_2)\Delta t$
$\Delta\vec{S}^{(6)} = [\lambda_1, -\lambda_2]^T$	$p_6 = m_{21}(t, S_1, S_2)\Delta t$
$\Delta\vec{S}^{(7)} = [-\lambda_1, -\lambda_2]^T$	$p_7 = m_{11}(t, S_1, S_2)\Delta t$
$\Delta\vec{S}^{(8)} = [\lambda_1, \lambda_2]^T$	$p_8 = m_{22}(t, S_1, S_2)\Delta t$
$\Delta\vec{S}^{(9)} = [0, 0]^T$	$p_9 = 1 - \sum_{i=1}^{8} p_i$

Derivation Of An SDE For A Two-State Problem Continues

We calculate the expected change and the covariance matrix for the change $\Delta\vec{S} = [\Delta S_1, \Delta S_2]^T$. Using the table,

$$E(\Delta\vec{S}) = \sum_{j=1}^{9} p_j \Delta\vec{S}^{(j)} = \begin{bmatrix} (-d_1 + b_1 - m_{12} + m_{21} + m_{22} - m_{11})\lambda_1 \\ \\ (-d_2 + b_2 + m_{12} - m_{21} + m_{22} - m_{11})\lambda_2 \end{bmatrix} \Delta t$$

and

$$E(\Delta\vec{S}(\Delta\vec{S})^T) = \sum_{j=1}^{9} p_j (\Delta\vec{S}^{(j)})(\Delta\vec{S}^{(j)})^T =$$

$$= \begin{bmatrix} (d_1 + b_1 + m_a)\lambda_1^2 & (-m_{12} - m_{21} + m_{22} + m_{11})\lambda_1\lambda_2 \\ \\ (-m_{12} - m_{21} + m_{22} + m_{11})\lambda_1\lambda_2 & (d_2 + b_2 + m_a)\lambda_2^2 \end{bmatrix} \Delta t$$

where $m_a = m_{12} + m_{21} + m_{22} + m_{11}$.

Let $\vec{\mu}(t, S_1, S_2) = E(\Delta\vec{S})/\Delta t$ and $V(t, S_1, S_2) = E(\Delta\vec{S}(\Delta\vec{S})^T)/\Delta t$. As Δt is small and $E(\Delta\vec{S})(E(\Delta\vec{S}))^T = O((\Delta t)^2)$, the covariance matrix V is set equal to $E(\Delta\vec{S}(\Delta\vec{S})^T)/\Delta t$. Finally, define the square root of the covariance matrix V as B:

$$B(t, S_1, S_2) = (V(t, S_1, S_2))^{1/2} \text{ and thus, } B^2(t, S_1, S_2) = V(t, S_1, S_2).$$

Derivation Of An SDE For A Two-State Problem Continues

Now, a forward Kolmogorov equation can be determined for the probability distribution at time $t + \Delta t$ in terms of the distribution at time t. Letting $p(t, x_1, x_2)$ be the probability that $S_1 = x_1$ and $S_2 = x_2$ at time t, then

$$(*) \qquad p(t + \Delta t, x_1, x_2) = p(t, x_1, x_2) + \Delta t \sum_{i=1}^{10} T_i$$

where

$$\begin{aligned}
T_1 &= p(t, x_1, x_2)(-d_1(t, x_1, x_2) - b_1(t, x_1, x_2) - d_2(t, x_1, x_2) - b_2(t, x_1, x_2)) \\
T_2 &= p(t, x_1, x_2)(-m_a(t, x_1, x_2)) \\
T_3 &= p(t, x_1 + \lambda_1, x_2)d_1(t, x_1 + \lambda_1, x_2) \\
T_4 &= p(t, x_1 - \lambda_1, x_2)b_1(t, x_1 - \lambda_1, x_2) \\
T_5 &= p(t, x_1, x_2 - \lambda_2)b_2(t, x_1, x_2 - \lambda_2) \\
T_6 &= p(t, x_1, x_2 + \lambda_2)d_2(t, x_1, x_2 + \lambda_2) \\
T_7 &= p(t, x_1 + \lambda_1, x_2 - \lambda_2)m_{12}(t, x_1 + \lambda_1, x_2 - \lambda_2) \\
T_8 &= p(t, x_1 - \lambda_1, x_2 + \lambda_2)m_{21}(t, x_1 - \lambda_1, x_2 + \lambda_2) \\
T_9 &= p(t, x_1 + \lambda_1, x_2 + \lambda_2)m_{11}(t, x_1 + \lambda_1, x_2 + \lambda_2) \\
T_{10} &= p(t, x_1 - \lambda_1, x_2 - \lambda_2)m_{22}(t, x_1 - \lambda_1, x_2 - \lambda_2).
\end{aligned}$$

Expanding out the terms T_3 through T_{10} in Taylor series about the point (t, x_1, x_2), it follows that

$$T_3 \approx pd_1 + \frac{\partial(pd_1)}{\partial x_1}\lambda_1 + \frac{1}{2}\frac{\partial^2(pd_1)}{\partial x_1^2}\lambda_1^2$$

$$T_4 \approx pb_1 - \frac{\partial(pb_1)}{\partial x_1}\lambda_1 + \frac{1}{2}\frac{\partial^2(pb_1)}{\partial x_1^2}\lambda_1^2$$

$$T_5 \approx pb_2 - \frac{\partial(pb_2)}{\partial x_2}\lambda_2 + \frac{1}{2}\frac{\partial^2(pb_2)}{\partial x_2^2}\lambda_2^2$$

$$T_6 \approx pd_2 + \frac{\partial(pd_2)}{\partial x_2}\lambda_2 + \frac{1}{2}\frac{\partial^2(pd_2)}{\partial x_2^2}\lambda_2^2$$

$$T_7 \approx pm_{12} + \frac{\partial(pm_{12})}{\partial x_1}\lambda_1 - \frac{\partial(pm_{12})}{\partial x_2}\lambda_2 + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}(-1)^{i+j}\frac{\partial^2(pm_{12})}{\partial x_i \partial x_j}\lambda_i\lambda_j$$

$$T_8 \approx pm_{21} - \frac{\partial(pm_{21})}{\partial x_1}\lambda_1 + \frac{\partial(pm_{21})}{\partial x_2}\lambda_2 + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}(-1)^{i+j}\frac{\partial^2(pm_{21})}{\partial x_i \partial x_j}\lambda_i\lambda_j$$

$$T_9 \approx pm_{11} + \frac{\partial(pm_{11})}{\partial x_1}\lambda_1 + \frac{\partial(pm_{11})}{\partial x_2}\lambda_2 + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{\partial^2(pm_{11})}{\partial x_i \partial x_j}\lambda_i\lambda_j$$

$$T_{10} \approx pm_{22} - \frac{\partial(pm_{22})}{\partial x_1}\lambda_1 - \frac{\partial(pm_{22})}{\partial x_2}\lambda_2 + \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{\partial^2(pm_{22})}{\partial x_i \partial x_j}\lambda_i\lambda_j.$$

Substituting these expressions into $(*)$ **and assuming that** $\Delta t, \lambda_1,$ **and** λ_2 **are small, then** $p(t, x_1, x_2)$ **approximately solves the Fokker-Planck equation**

$$\begin{aligned} \frac{\partial p(t,x_1,x_2)}{\partial t} &= -\sum_{i=1}^{2} \frac{\partial}{\partial x_i}\left[\mu_i(t,x_1,x_2)p(t,x_1,x_2)\right] \\ &+ \frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{2}\frac{\partial^2}{\partial x_i \partial x_j}\left[\sum_{k=1}^{2} b_{i,k}(t,x_1,x_2)b_{j,k}(t,x_1,x_2)p(t,x_1,x_2)\right], \end{aligned}$$

where μ_i **is the** i**th component of** $\vec{\mu}$ **and** $b_{i,j} = (B)_{i,j}$ **for** $1 \le i, j \le 2$**.**

However, the probability distribution $p(t, x_1, x_2)$ **that exactly satisfies this PDE is identical to the distribution of solutions to the SDE system**

$$\begin{cases} d\vec{S}(t) = \vec{\mu}(t, S_1, S_2)\, dt + B(t, S_1, S_2)\, d\vec{W}(t) \\ \vec{S}(0) = \vec{S}_0, \end{cases}$$

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

Therefore, the discrete stochastic model is closely related to an SDE. In particular, the drift and diffusion terms, $\vec{\mu}$ **and** B**, of the SDE are equal to the expected change divided by** Δt **and the square root of the covariance matrix divided by** Δt **from the discrete stochastic model.**

DERIVATION OF ACCURATE SDE MODELS

In summary, the derivation procedure in deriving an SDE requires three steps:

First, a discrete stochastic model for the process is developed by carefully listing the possible changes along with the corresponding probabilities for a short time step Δt.

Second, the expected change and covariance matrix for the change is calculated for the discrete stochastic process.

Third, the stochastic differential equation system is obtained by letting the expected change divided by Δt be the drift coefficient and the square root of the covariance matrix divided by Δt be the diffusion coefficient.

Note that the derivation procedure provides an Itô SDE rather than, for example, a Stratonovich SDE.

AN ITÔ OR A STRATONOVICH SDE

There have been discussions regarding whether an Itô or a Stratonovich SDE is most appropriate for a given random dynamical system. Whether the SDE is regarded as Itô or Stratonovich is important. For example, if

$$dX(t) = \lambda X(t)\,dt + \mu X(t)\,dW(t)$$

is regarded as Itô, then $X(t) \to X(0)\exp((\lambda - \mu^2/2)t)$ w.p.1 as $t \to \infty$ and, thus, $X(t) \to 0$ with probability 1 if $\lambda < \mu^2/2$. On the other hand, if this SDE is Stratonovich, then the equivalent Itô SDE is

$$dX(t) = (\lambda + \mu^2/2)X(t)\,dt + \mu X(t)\,dW(t).$$

In this case, $X(t) \to X(0)\exp(\lambda t)$ w.p.1 as $t \to \infty$ and, thus, $X(t) \to 0$ with probability 1 if $\lambda < 0$. Thus, specification of the SDE model as Itô or Stratonovich is important.

In the derivation procedure, a discrete stochastic model is first developed. An Itô SDE is then inferred by the similarities between the forward Kolmogorov equations of the discrete-time and the continuous-time models. However, if desired, the Itô SDE can be transformed into a Stratonovich SDE.

CALCULATING SQUARE ROOTS OF MATRICES

The derivation procedure produces a term in the SDE system that involves the square root of a symmetric positive definite matrix, that is, $B = V^{1/2}$. Solution of the stochastic system involves computation of square roots of matrices.

For a 2×2 matrix, the 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 $d = \sqrt{a + c + 2w}$. However, for a general $n \times n$ symmetric positive definite matrix V with $n \geq 3$, there is no formula for $V^{1/2}$ and it must be calculated numerically.

If V is put in the canonical form $V = P^T D P$, where $P^T P = I$ and $d_{ii} > 0$ 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. Fortunately, there are available many numerical procedures for computing $V^{1/2}$ directly.

AN ALTERNATIVE TO SQUARE ROOTS OF MATRICES

Often, the square root of the covariance matrix $B = V^{1/2}$ can be avoided by including additional Wiener processes in the stochastic system.

Consider a stochastic problem that involves N states $S_1, S_2, \ldots, S_N$ with a total of $M \geq N$ possible random changes to these states at each time step Δt. Suppose that the probabilities of the changes are $p_j \Delta t = p_j(t, \vec{S})\Delta t$ for $j = 1, 2, \ldots, M$ where the jth change alters the ith state by the amount λ_{ji} for $i = 1, 2, \ldots, N$. The ith element of vector $\vec{\mu}$ for this problem is then

$$\mu_i = \sum_{j=1}^{M} p_j \lambda_{ji} \ \ \textbf{for} \ \ i = 1, 2, \ldots, N.$$

The covariance matrix, V, can also be computed and the i, l entry of V has the form

$$v_{il} = \sum_{j=1}^{M} p_j \lambda_{ji} \lambda_{jl} \ \ \textbf{for} \ \ 1 \leq i, l \leq N.$$

However, it is generally difficult to compute the $N \times N$ matrix $V^{1/2}$ in the SDE system

$$d\vec{S} = \vec{\mu}\, dt + V^{1/2}\, d\vec{W}(t),$$

where $\vec{W}(t)$ is a vector consisting of N independent Wiener processes.

AN ALTERNATIVE TO SQUARE ROOTS OF MATRICES

However, an $N \times M$ matrix C can be found such that $V = CC^T$ and the SDE system can be modified to:

$$d\vec{S} = \vec{\mu}\, dt + C\, d\vec{W}^*(t),$$

where $\vec{W}^*(t)$ is a vector consisting M independent Wiener processes.

Indeed, Itô's formula and the forward Kolmogorov equation are identical for both SDE systems. The entries of matrix C have the form:

$$c_{ij} = \lambda_{ji} p_j^{1/2} \text{ for } 1 \le i \le N, 1 \le j \le M.$$

To verify this formula, notice that

$$(CC^T)_{il} = \sum_{j=1}^{M} c_{ij} c_{lj} = \sum_{j=1}^{M} \lambda_{ji} p_j^{1/2} \lambda_{jl} p_j^{1/2} = v_{il} \text{ for } 1 \le i, l \le N.$$

For chemically reacting systems, the SDE system with $Cd\vec{W}^*(t)$ replacing $V^{1/2} d\vec{W}(t)$ is referred to as the chemical Langevin equation.

Alternate SDE models are studied more later.

REVIEW OF SDE MODEL OF TWO INTERACTING POPULATIONS

Consider two interacting populations.

The populations may be of the same species or they may be different species.

Populations of the same species may differ, for example, by geographic location or by status in an epidemic such as infective or susceptible. Populations of the same species may interact, respectively, by migration or by transmitting and recovering from a disease.

Let the sizes of the two populations be $x_1(t)$ **and** $x_2(t)$**. Important parameters are** $b_1, d_1, b_2, d_2, m_{12}$**, and** m_{21}**.**

b_i **and** d_i **are per capita birth and death rates for population** i**.**

m_{ij} **is the rate population** i **is transformed to population** j**. (For geographically isolated populations,** m_{ij} **may represent the migration rate of population** i **to** j**.)**

Each parameter may depend on population sizes x_1 **and** x_2 **and time** t**, i.e.,** $b_i = b_i(t, x_1, x_2),\ d_i = d_i(t, x_1, x_2)$**, and** $m_{ij} = m_{ij}(t, x_1, x_2)$**.**

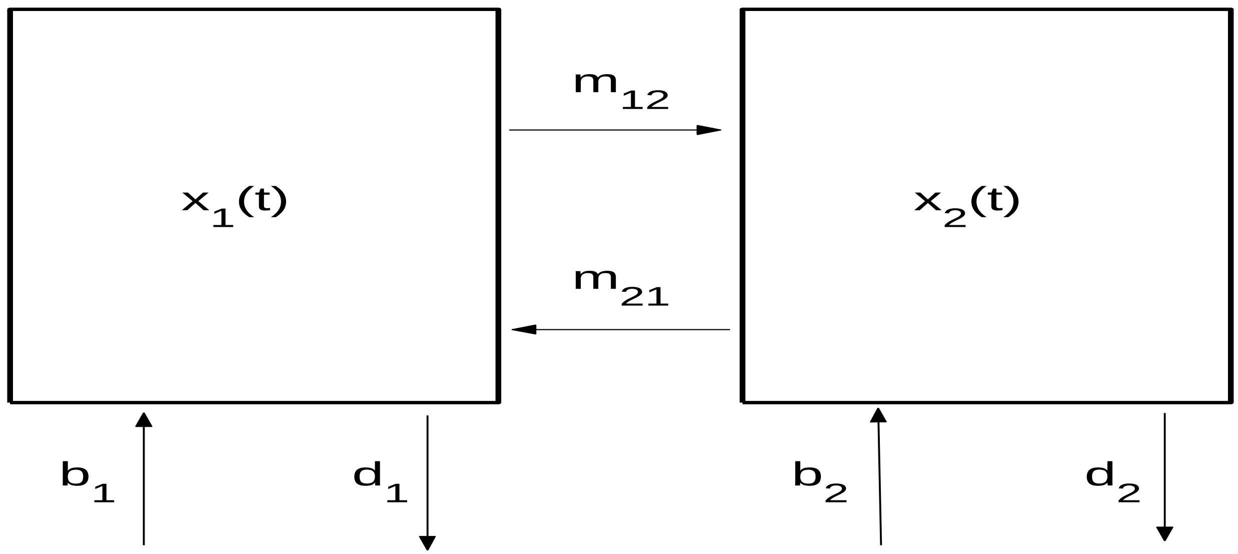


Figure 4: **A diagram of two interacting populations**

REVIEW OF SDE MODEL OF TWO INTERACTING POPULATIONS

The dynamics of two interacting populations is illustrated in the figure. In a small time interval Δt, there are seven possibilities for a population change $\Delta \vec{x}$.

REVIEW OF SDE MODEL OF TWO INTERACTING POPULATIONS

For small Δt, there are seven possibilities for a population change $\Delta\vec{x}$. These possibilities are listed the table along with their corresponding probabilities.

For example, $\Delta\vec{x}_2 = [-1, 1]^T$ represents the movement of one individual from population x_1 to population x_2 during time interval Δt and the probability of this event is proportional to the size of population x_1 and the time interval Δt, that is, $p_2 = m_{12}x_1\Delta t$.

As a second example, $\Delta\vec{x}_4 = [0, 1]^T$ represents a birth in population x_2 with probability $p_4 = b_2x_2\Delta t$.

Notice that $\sum_{i=1}^{7} p_i = 1$.

Change	**Probability**
$\Delta\vec{x}_1 = [-1, 0]^T$	$p_1 = d_1x_1\Delta t$
$\Delta\vec{x}_2 = [-1, 1]^T$	$p_2 = m_{12}x_1\Delta t$
$\Delta\vec{x}_3 = [0, -1]^T$	$p_3 = d_2x_2\Delta t$
$\Delta\vec{x}_4 = [0, 1]^T$	$p_4 = b_2x_2\Delta t$
$\Delta\vec{x}_5 = [1, -1]^T$	$p_5 = m_{21}x_2\Delta t$
$\Delta\vec{x}_6 = [1, 0]^T$	$p_6 = b_1x_1\Delta t$
$\Delta\vec{x}_7 = [0, 0]^T$	$p_7 = 1 - \sum_{i=1}^{6} p_i$

REVIEW OF SDE MODEL OF TWO INTERACTING POPULATIONS

The mean change $E(\Delta\vec{x})$ and the covariance matrix $E(\Delta\vec{x}(\Delta\vec{x})^T)$ are determined as:

$$E(\Delta\vec{x}) = \sum_{j=1}^{7} p_j \Delta\vec{x}_j = \begin{bmatrix} b_1x_1 - d_1x_1 - m_{12}x_1 + m_{21}x_2 \\ \\ b_2x_2 - d_2x_2 - m_{21}x_2 + m_{12}x_1 \end{bmatrix} \Delta t$$

and

$$E(\Delta\vec{x}(\Delta\vec{x})^T) = \sum_{j=1}^{7} p_j \Delta\vec{x}_j (\Delta\vec{x}_j)^T$$
$$= \begin{bmatrix} b_1x_1 + d_1x_1 + m_{12}x_1 + m_{21}x_2 & -m_{12}x_1 - m_{21}x_2 \\ \\ -m_{12}x_1 - m_{21}x_2 & b_2x_2 + d_2x_2 + m_{12}x_1 + m_{21}x_2 \end{bmatrix} \Delta t.$$

The vector $\vec{\mu}$ and the matrix V are defined as

$$\vec{\mu} = E(\Delta\vec{x})/\Delta t = \begin{bmatrix} b_1x_1 - d_1x_1 - m_{12}x_1 + m_{21}x_2 \\ \\ b_2x_2 - d_2x_2 - m_{21}x_2 + m_{12}x_1 \end{bmatrix}$$

and

$$V = \begin{bmatrix} b_1x_1 + d_1x_1 + m_{12}x_1 + m_{21}x_2 & -m_{12}x_1 - m_{21}x_2 \\ \\ -m_{12}x_1 - m_{21}x_2 & b_2x_2 + d_2x_2 + m_{12}x_1 + m_{21}x_2 \end{bmatrix}.$$

REVIEW OF SDE MODEL OF TWO INTERACTING POPULATIONS

Matrix V is positive definite and hence has a positive definite square root $B = V^{1/2}$. For this two-dimensional system, $B = V^{1/2}$ is given by

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

where $w = \sqrt{ac - b^2}$ and $d = \sqrt{a + c + 2w}$ with

$$\begin{aligned} a &= d_1 x_1 + m_{12} x_1 + m_{21} x_2 + b_1 x_1, \\ b &= -m_{12} x_1 - m_{21} x_2, \\ c &= m_{12} x_1 + d_2 x_2 + b_2 x_2 + m_{21} x_2. \end{aligned}$$

Therefore, the SDE for the dynamics of two interacting populations is:

$$d\vec{x} = \vec{\mu}(t, x_1, x_2)\, dt + B(t, x_1, x_2)\, d\vec{W}(t)$$

where $\vec{W}(t)$ is the two-dimensional Wiener process, i.e. $\vec{W}(t) = [W_1(t), W_2(t)]^T$.

This is an SDE system that describes the population dynamics. Notice that if matrix B is set equal to zero, then this system reduces to a standard deterministic model for the population dynamics. Of course, $\vec{\mu} = \vec{\mu}(x_1, x_2, t)$ and $B = B(x_1, x_2, t)$ as the parameters b_i, d_i, m_{ij} may all depend on x_1, x_2, and t.

For a single population, this system reduces to

$$dx_1 = (b_1 x_1 - d_1 x_1)\ dt + \sqrt{b_1 x_1 + d_1 x_1}\ dW_1(t)$$

which is commonly seen in population dynamics.

SPECIAL CASE: EPIDEMIC MODEL

Consider an epidemic consisting of susceptible and infected sub-populations. Consider an SIS epidemic model for a single species. In this model, susceptible individuals become infected, recover, and become susceptible again. There is no immunity to the disease.

A deterministic form of the SIS model is:

$$\begin{aligned}\frac{dS}{dt} &= \gamma I - \alpha IS/N \\ \frac{dI}{dt} &= -\gamma I + \alpha IS/N,\end{aligned}$$

where $S(0) + I(0) = N$ **and therefore** $S(t) + I(t) = N$ **for** $t \geq 0$**.**

In this model, $S(t)$ **is the susceptible population size,** $I(t)$ **is the infected population size,** α **is the contact rate, and** γ **is the removal rate.**

SPECIAL CASE: EPIDEMIC MODEL

In terms of previous parameters,

$$x_1(t) = S(t), \;\; x_2(t) = I(t), \;\; d_1 = d_2 = b_1 = b_2 = 0,$$

$$m_{12} = \alpha I/(I+S) = \alpha x_2/(x_1+x_2), \;\; \textbf{and} \;\; m_{21} = \gamma.$$

Therefore, the stochastic SIS model has the form

$$dx_1 = (-m_{12}x_1 + m_{21}x_2)dt + \sqrt{\frac{m_{12}x_1 + m_{21}x_2}{2}}\big(dW_1 - dW_2\big)$$

$$dx_2 = (m_{12}x_1 - m_{21}x_2)dt + \sqrt{\frac{m_{12}x_1 + m_{21}x_2}{2}}\big(-dW_1 + dW_2\big)$$

and thus, for this problem,

$$B = \begin{bmatrix} m_{12}x_1 + m_{21}x_2 & -m_{12}x_1 - m_{21}x_2 \\ -m_{12}x_1 - m_{21}x_2 & m_{12}x_1 + m_{21}x_2 \end{bmatrix} \Big/ \sqrt{2(m_{12}x_1 + m_{21}x_2)}.$$

Note that the sum $x_1(t) + x_2(t)$ is constant for $t \geq 0$ in the stochastic model as well as in the deterministic model.

SPECIAL CASE: EPIDEMIC MODEL

For a computational example, let $\alpha = 0.04$, $\gamma = 0.01$, with $S(0) = 950$, and $I(0) = 50$. Let the final time be $t = 100$.

In the table, some calculational results are given in solving the SDE system using 10,000 sample paths.

Also listed in the table are values calculated using a Monte Carlo approach. In the Monte Carlo procedure, each individual in the population is checked after each time step of $\Delta t = 1/5$ to determine whether a susceptible individual contracts the disease or if an infected individual recovers. These calculations continue until time $t = 100$ for 10,000 sample paths.

As can be seen in the table, close agreement is obtained between the SDE and Monte Carlo.

Estimate	SDE Model Results	Monte Carlo Results
$E(S(100))$	**561.7**	**562.2**
$E(I(100))$	**438.7**	**437.8**
$\sigma((S(100)))$	**41.5**	**41.0**
$\sigma((I(100)))$	**41.5**	**41.0**

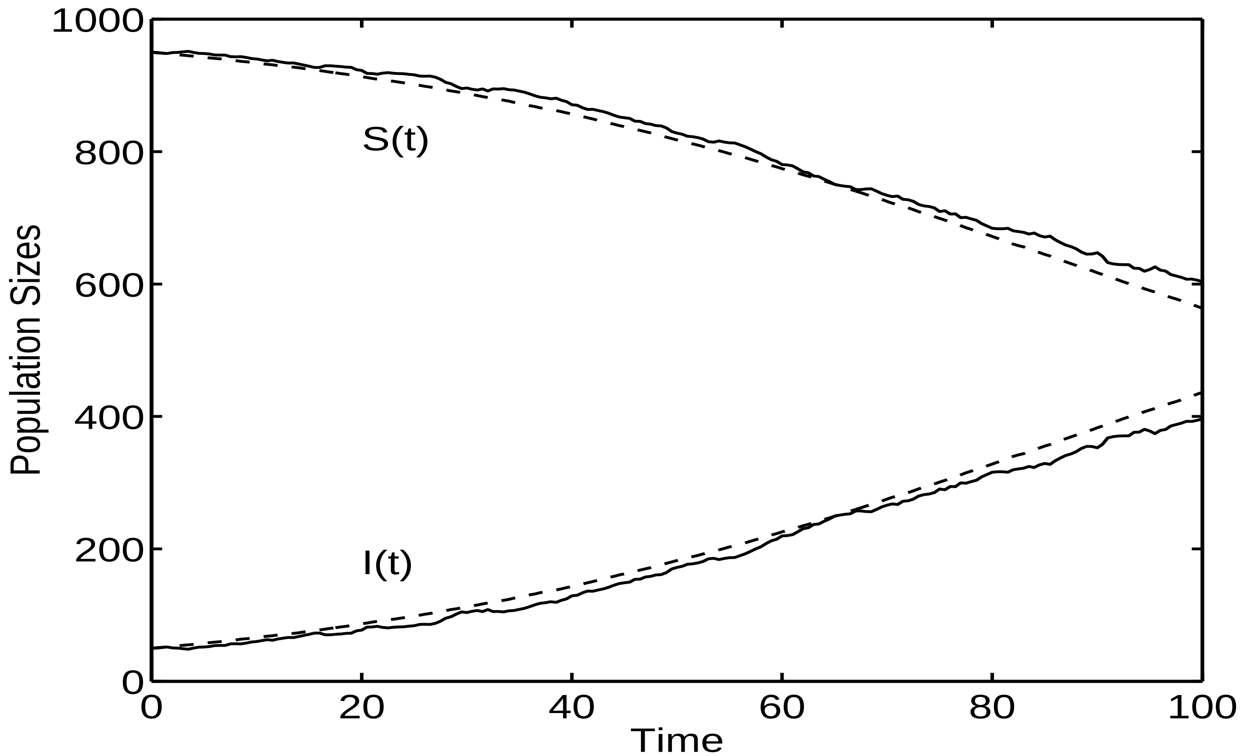


Figure 5: **Expected population sizes (dashed lines) and one sample path for susceptible and infected**

For this example, one sample path and the average of 100 sample paths for the SIS stochastic differential equation model are displayed.

SPECIAL CASE: PREDATOR-PREY MODEL

As a second example of two interacting populations, consider the two species predator-prey system. A deterministic model for the predator and prey populations takes the form:

$$\begin{aligned} dx_1(t) &= \big(b_1(x_1,x_2)x_1(t) - d_1(x_1,x_2)x_1(t)\big)dt \\ dx_2(t) &= \big(b_2(x_1,x_2)x_2(t) - d_2(x_1,x_2)x_2(t)\big)dt, \end{aligned}$$

where $x_1(t)$ **is the population size of the prey and** $x_2(t)$ **is the population size of the predator.**

For example, in the standard Lotka-Volterra model:

$$b_1(x_1,x_2) = b_1, \quad d_1(x_1,x_2) = c_1x_2,$$

$$b_2(x_1,x_2) = c_2x_1, \quad \textbf{and} \quad d_2(x_1,x_2) = d_2.$$

In this case, the predator-prey equations have the equilibrium solution $x_1(t) = d_2/c_2$ **and** $x_2(t) = b_1/c_1$**. The solutions form closed curves in the** x_1x_2**-plane about the equilibrium point** $(d_2/c_2,\ b_1/c_1)$**.**

SPECIAL CASE: PREDATOR-PREY MODEL

Now, consider the SDE model of the predator-prey system. For this problem, as $m_{12} = 0 = m_{21}$, the covariance matrix V is diagonal and the square root matrix B is then also diagonal. Therefore, the stochastic predator-prey equations have the form:

$$dx_1 = (b_1(x_1, x_2) - d_1(x_1, x_2))x_1 dt + \sqrt{(b_1(x_1, x_2) + d_1(x_1, x_2))x_1} dW_1$$

$$dx_2 = (b_2(x_1, x_2) - d_2(x_1, x_2))x_2 dt + \sqrt{(b_2(x_1, x_2) + d_2(x_1, x_2))x_2} dW_2$$

for either the Lotka-Volterra model or a Lotka-Volterra model with logistic growth.

A Few Comments On The SDE Project: Persistence Time Calculations For Biological Systems

Persistence times for several biological problems are studied computationally.

A computer code is given that performs exit time calculations for two-species biological systems such as predator-prey and competition systems.

In the program, Euler's method is used to solve the SDE system for many sample paths.

For each sample path, the populations start at specified initial sizes. The calculations continue until either population size is less than unity or a specified maximum time is reached.

Competition Between Two Species Is Studied First

Consider the competition model with per capita birth and death rates:

$$b_1 = .84,\ d_1 = .40 + .01y_1(t) + .022y_2(t),\ b_2 = .90,\ d_2 = .75 + .0067y_2(t) + .005y_1(t).$$

The resulting deterministic model is:

$$\frac{dy_1(t)}{dt} = (b_1(t) - d_1(t))y_1(t) = .44y_1(t) - .01y_1^2(t) - .022y_1(t)y_2(t)$$

$$\frac{dy_2(t)}{dt} = (b_2(t) - d_2(t))y_2(t) = .15y_2(t) - .0067y_2^2(t) - .005y_1(t)y_2(t).$$

The corresponding SDE model is:

$$\frac{dy_1(t)}{dt} = (b_1(t) - d_1(t))y_1(t) + \sqrt{(b_1(t) + d_1(t))y_1(t)}\,\frac{dW_1(t)}{dt}$$

$$\frac{dy_2(t)}{dt} = (b_2(t) - d_2(t))y_2(t) + \sqrt{(b_2(t) + d_2(t))y_2(t)}\,\frac{dW_2(t)}{dt}.$$

where $W_1(t)$ and $W_2(t)$ are two independent Wiener processes.

The SDE model is solved numerically using Euler's method:

$$y_{1,k+1} = (b_{1,k} - d_{1,k})y_{1,k}h + \sqrt{(b_{1,k} + d_{1,k})y_{1,k}h}\,\eta_{1,k}$$

$$y_{2,k+1} = (b_{2,k} - d_{2,k})y_{2,k}h + \sqrt{(b_{2,k} + d_{2,k})y_{2,k}h}\,\eta_{2,k}$$

for $k = 0, 1, 2, \ldots$ until either $y_{1,k+1}$ or $y_{2,k+1}$ is less than unity or a maximum time is exceeded. This is performed for many sample paths.

Calculational Results Illustrate A Difference Between Deterministic And Stochastic Models

For the deterministic model, the first species always out-competes the second species.

For the stochastic model, the second species out-competes the first species about 44% of the time.

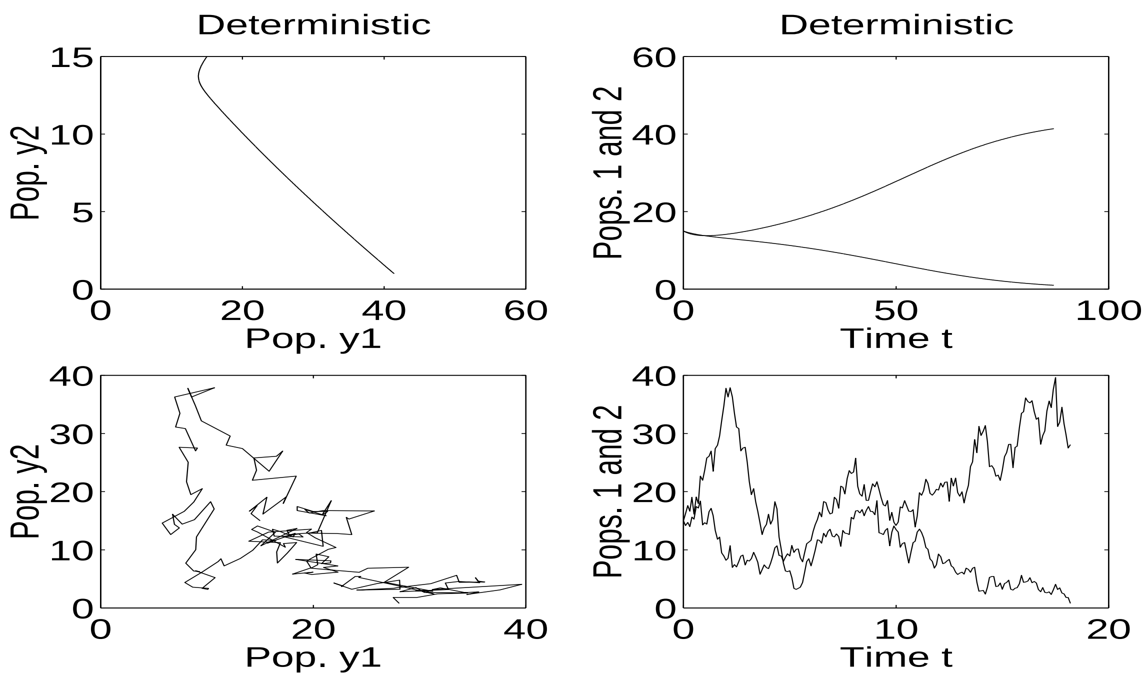


Figure 6: Calculational Results For The Deterministic And Stochastic Models For A Competition System

In The Project, Five Systems Are Studied

Two Competition Systems

A Predator-Prey System

An Epidemic System (SIS)

A System of Your Choice