Derivation of Itô SDE and Relationship to ODE and CTMC Models

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Euler-Maruyama Method for Numerical Solution of an Itô SDE

$$dX(t) = \alpha(X(t), t)dt + \beta(X(t), t)dW(t)$$

Assume conditions (a) and (b) for existence and uniqueness of an Itô SDE are satisfied and in addition

(c) $|\alpha(x,t_1) - \alpha(x,t_2)| + |\beta(x,t_1) - \beta(x,t_2)| \le K |t_1 - t_2|^{1/2}$, for all $t_1, t_2 \in [0,T]$ and $x \in \mathbf{R}$.

Theorem 1. Assume that the Itô SDE satisfies conditions (a), (b), and (c). Euler-Maruyama method approximates a sample path X(t) at time points t_i , $X(t_i) \approx X_i$, on the interval [0, T]:

$$X_{i+1} = X_i + \alpha(X_i, t_i) \,\Delta t + \beta(X_i, t_i) \sqrt{\Delta t} \,\eta_i \tag{1}$$

for i = 0, 1, ..., k - 1, where $0 = t_0 < t_1 < ... < t_{k-1} < t_k = T$, $\Delta t = t_{i+1} - t_i = T/k$, $X_0 = X(0)$, and $\eta_i \sim N(0, 1)$ with error:

$$E\left(\left|X(t_{i})-X_{i}\right|^{2} \mid X(t_{i-1})=X_{i-1}\right)=O(\left(\Delta t\right)^{2})$$
(2)

and

$$E\left(|X(t_i) - X_i|^2 | X(0) = X_0\right) = O(\Delta t)$$
(3)

Relationship Between a CTMC Model and an SDE Model

Consider a birth and death process. Recall for a CTMC model the infinitesimal transition probabilities are

$$p_{ji}(\Delta t) = \begin{cases} b(i)\Delta t + o(\Delta t), & j = i + 1\\ d(i)\Delta t + o(\Delta t), & j = i - 1\\ 1 - [b(i) + d(i)]\Delta t + o(\Delta t), & j = i\\ o(\Delta t), & \text{otherwise.} \end{cases}$$

The probability mass function $p_i(t) = \text{Prob}\{X(t) = i\}$ satisfies the forward Kolmogorov differential equatons (FKDE):

$$\frac{dp_i}{dt} = p_{i-1}b(i-1) + p_{i+1}d(i+1) - p_i[b(i) + d(i)]$$

for i = 1, 2, ..., N and $dp_0/dt = p_1 d(1)$.

The FKDEs for the CTMC Model lead to the FKDE associated with a Diffusion Process

The FKDEs can be expressed as a finite difference scheme with $\Delta i = 1$.

$$\begin{aligned} \frac{dp_i}{dt} &= p_{i-1}b(i-1) + p_{i+1}d(i+1) - p_i[b(i) + d(i)] \\ &= -\frac{\{p_{i+1}[b(i+1) - d(i+1)] - p_{i-1}[b(i-1) - d(i-1)]\}}{2\Delta i} \\ &+ \frac{1}{2} \frac{\{p_{i+1}[b(i+1) + d(i+1)] - 2p_i[b(i) + d(i)] + p_{i-1}[b(i-1) + d(i-1)]\}}{(\Delta i)^2} \end{aligned}$$

Let i = x, $\Delta i = \Delta x$ and $p_i(t) = p(x, t)$. Then the limiting form of the preceding equation (as $\Delta x \to 0$) is the forward Kolmogorov differential equation for p(x, t):

$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial}{\partial x} \{ [b(x) - d(x)]p(x,t) \} + \frac{1}{2} \frac{\partial^2}{\partial x^2} \{ [b(x) + d(x)]p(x,t) \}.$$

The coefficient of p(x,t) in the first term, [b(x) - d(x)], is the infinitesimal mean and the coefficient of p(x,t) in the second term, [b(x) + d(x)], is the infinitesimal variance.

The FKDE leads to an Itô SDE

In a small period of time, the infinitesimal mean, $\mu\Delta t = [b(x) - d(x)]\Delta t$ and the infinitesimal variance is $\sigma^2\Delta t = [b(x) + d(x)]\Delta t$. Assume there are a large number of changes in a small period of time and we can apply the Central Limit Theorem:

$$\Delta X(t) \sim N(\mu \Delta t, \sigma \sqrt{\Delta t}).$$

Then

$$X(t + \Delta t) = X(t) + \mu \Delta t + \sigma \sqrt{\Delta t} \eta,$$

where $\eta \sim N(0,1)$. Expressed in terms of the birth and death process,

$$X(t + \Delta t) = X(t) + [b(X) - d(X)]\Delta t + \sqrt{[b(X) + d(X)]}\Delta t\eta$$

This latter expression is the Euler-Maruyama method for numerically solving the following Itô SDE:

$$dX(t) = [b(X) - d(X)]\Delta t + \sqrt{[b(X) + d(X)]}dW(t).$$

Logistic SDE

The deterministic model:

$$\frac{dn}{dt} = rn\left(1 - \frac{n}{K}\right),\,$$

where n(t) is the population size at time t. Let X(t) denote the random variable for the total population size.

(a) Suppose the probability of a birth or death in a small time interval is $b(X) = rX \Delta t$ or $d(X) = (rX^2/K) \Delta t$, respectively. The SDE for logistic growth is

$$dX = rX\left(1 - \frac{X}{K}\right)dt + \sqrt{rX\left(1 + \frac{X}{K}\right)dW}, \quad X \in [0, \infty).$$
(4)

(b) Suppose the probability of a birth or a death in a small time interval is $b(X) = rX(1 - X/2K) \Delta t$ or $d(X) = (rX^2/2K) \Delta t$, respectively. The SDE for logistic growth is

$$dX = rX\left(1 - \frac{X}{K}\right)dt + \sqrt{rX}\,dW, \quad X \in [0, 2K].$$
(5)

The forward Kolmogorov differential equations corresponding to the SDEs (4) and (5) are

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x} \left[rx \left(1 - \frac{x}{K} \right) p \right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[rx \left(1 + \frac{x}{K} \right) p \right],$$

 $x \in (0, \infty)$ and

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x} \left[rx \left(1 - \frac{x}{K} \right) p \right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} [rxp],$$

 $x \in (0, 2K)$, respectively. It is easy to see that the infinitesimal variance is larger in case (a) than in case (b).

Euler's method applied to cases (a) and (b) yields the following iterative schemes:

$$X_{i+1} = X_i + rX_i \left(1 - \frac{X_i}{K}\right) \Delta t + \sqrt{rX_i \left(1 + \frac{X_i}{K}\right) \sqrt{\Delta t}} \eta_i, \quad X_i \in [0, \infty)$$

and

$$X_{i+1} = X_i + rX_i \left(1 - \frac{X_i}{K}\right) \Delta t + \sqrt{rX_i} \sqrt{\Delta t} \ \eta_i, \ X_i \in [0, 2K],$$

respectively, for $i = 0, 1, 2, \ldots, k - 1$.

Three samples paths for the SDEs (a) and (b) on the interval [0,10] are graphed (Euler-Maruyama method with with $\Delta t = 0.01$). Note the larger variation in the solutions for (a) than for (b).



Figure 1: Three stochastic realizations of the logistic model for case (a) and case (b) with r = 1, K = 10, and X(0) = 10.

Before Continuing, We Note a Relationship between Stratonovich SDE and Itô SDE.

In general, a Stratonovich SDE,

$$d_S X(t) = \alpha(X(t), t) dt + \beta(X(t), t) dW(t)$$

can be converted into an Itô SDE

$$dX(t) = \left[\alpha + \frac{1}{2}\beta \frac{\partial \beta}{\partial x}\right] (X(t), t) dt + \beta (X(t), t) dW(t)$$

- Itô's Formula only applies to an Itô SDE.
- Our derivation method gives rise to Itô SDEs.

Formulation of Multivariate SDE Processes

For a bivariate diffusion process $\{X_1(t), X_2(t)\}: t \in [0, \infty)\}$, there is an associated joint p.d.f. $p(x_1, x_2, t)$. Let $X(t) = (X_1(t), X_2(t))^T$. Suppose the diffusion process has infinitesimal mean

$$E(\Delta X) = E\begin{pmatrix}\Delta X_1\\\Delta X_2\end{pmatrix} = \begin{pmatrix}f_1(X_1, X_2, t)\\f_2(X_1, X_2, t)\end{pmatrix}\Delta t = \mathbf{f}\Delta t$$

and infinitesimal covariance

$$E(\Delta X (\Delta X)^T) \Delta t = E \begin{pmatrix} (\Delta X_1)^2 & \Delta X_1 \Delta X_2 \\ \Delta X_1 \Delta X_2 & (\Delta X_2)^2 \end{pmatrix} = \begin{pmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{pmatrix} \Delta t = \Sigma \Delta t$$

Matrix Σ is symmetric $\sigma_{ij} = \sigma_{ji}$.

The FKDE for this bivariate diffusion process with associated joint p.d.f. $p(x_1, x_2, t)$ is

$$\frac{\partial p(x_1, x_2, t)}{\partial t} = -\frac{\partial \left[f_1 p\right]}{\partial x_1} - \frac{\partial \left[f_2 p\right]}{\partial x_2} + \frac{1}{2} \left[\frac{\partial^2 [\sigma_{11} p]}{\partial x_1^2} + 2\frac{\partial^2 \sigma_{12} p]}{\partial x_1 \partial x_2} + \frac{\partial^2 [\sigma_{22} p]}{\partial x_2^2}\right]$$

or

$$\frac{\partial p(x_1, x_2, t)}{\partial t} = -\sum_{i=1}^2 \frac{\partial [f_i p]}{\partial x_i} + \frac{1}{2} \sum_{i=1}^2 \sum_{j=1}^2 \frac{\partial^2 [\sigma_{ij} p]}{\partial x_i \partial x_j}$$

It is easy to see how to generalize the FKDE for multivariate processes $\{(X_1, X_2, \ldots, X_n) : t \in [0, \infty)\}$

The Covariance Matrix can be Expressed as $\Sigma = GG^T$ which allows for Different but Equivalent Itô SDEs.

Equivalent Itô SDE formulations is in the sense that the Itô SDEs generate the same sample paths and have the same joint pdf $p(x_1, x_2, t)$.

Suppose $\Sigma = GG^T$, where $G = (g_{ij})$ is a $2 \times m$ matrix:

$$\sigma_{ij} = \sum_{l=1}^{2} g_{il} g_{jl}.$$

Then the FKDE is

$$\frac{\partial p(x_1, x_2, t)}{\partial t} = -\sum_{i=1}^2 \frac{\partial [f_i p]}{\partial x_i} + \frac{1}{2} \sum_{i=1}^2 \sum_{j=1}^2 \frac{\partial^2}{\partial x_i \partial x_j} \left[p \sum_{l=1}^2 g_{il} g_{jl} \right]$$

Thus, the solution $p(x_1, x_2, t)$ to the FKDE depends on f_i and g_{ij} . The corresponding Itô SDE for this bivariate process $\{X(t) : t \in [0, \infty)\}$ is

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

Note that the Itô SDE is a vector SDE:

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

dX(t) is of dimension 2×1 , f(X, t)dt is 2×1 , G(X, t) is $2 \times m$ and dW(t) is $m \times 1$. In particular $dW(t) = (dW_1(t), \ldots, dW_m(t))^T$ is a vector of m independent Wiener processes.

The matrix G can be easily generated directly from the changes that occur in the process, births, deaths, immigration, emigration, transitions, etc. We will give two examples illustrating how to formulate Itô SDEs from first principles and show that the Itô SDE directly relates to the ODE model and to the CTMC model – SIR epidemic Model and Lotka-Volterra Competition.

Consider an SIR Epidemic Model.

ODE model:

$$\frac{dS}{dt} = -\frac{\beta}{N}SI$$
$$\frac{dI}{dt} = \frac{\beta}{N}SI - \gamma I$$
$$\frac{dR}{dt} = \gamma I$$

Basic Reproduction Number:

$$\mathcal{R}_0 = rac{eta}{\gamma}$$

There is an epidemic (an increase in number of infectives) if $\mathcal{R}_0 \frac{S(0)}{N} > 1$, $\lim_{t\to\infty} I(t) = 0$.

CTMC SIR Epidemic Model

S(t) + I(t) + R(t) = N = maximum population size.

Since R = N - S - I, the process is bivariate. Let S(t) and I(t) denote discrete random variables for the number of susceptible and infected individuals, respectively with joint probability function

$$p_{(s,i)}(t) = \operatorname{Prob}\{S(t) = s, I(t) = i\}$$

where R(t) = N - S(t) - I(t). For this stochastic process, we define transition probabilities as follows:

$$p_{(s+k,i+j),(s,i)}(\Delta t) = \text{Prob}\{(\Delta S, \Delta I) = (k,j) | (S(t), I(t)) = (s,i)\}$$

$$= \begin{cases} \beta i(N-i)\Delta t/N + o(\Delta t), & (k,j) = (-1,1) \\ \gamma i\Delta t + o(\Delta t), & (k,j) = (0,-1) \\ 1 - [\beta i(N-i)/N + \gamma i]\Delta t + o(\Delta t), & (k,j) = (0,0) \\ o(\Delta t), & \text{otherwise} \end{cases}$$

Next we Formulate Itô SDEs

We find the infinitesimal mean and infinitesimal variance. for the bivariate process $\{(S(t), I(t)) : t \in [0, \infty)\}$.

Changes $(\Delta S, \Delta I)$	Probability
(-1, 1)	$(\beta SI/N)\Delta t$
(0,-1)	$\gamma I \Delta t$

Let $X(t) = (\Delta S(t), \Delta I(t))^T$. Then

$$E(\Delta X(t)) = \begin{pmatrix} -\beta SI/N \\ \beta SI/N - \gamma I \end{pmatrix} \Delta t = \mathbf{f} \Delta t$$

$$E(\Delta X (\Delta X)^T) = \begin{pmatrix} \beta SI/N & -\beta SI/N \\ -\beta SI/N & \beta SI/N + \gamma I \end{pmatrix} \Delta t = \Sigma \Delta t$$

Consider the specific changes listed in the table, a transmission and a recovery. Define G in terms of those two changes but use square roots so that $GG^T = \Sigma$:

$$G = \begin{pmatrix} -\sqrt{\beta SI/N} & 0\\ \sqrt{\beta SI/N} & -\sqrt{\gamma I} \end{pmatrix}$$

Then the Itô SDE take the following form:

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

$$dS = -[\beta SI/N]dt - \sqrt{\beta SI/N}dW_1$$

$$dI = [\beta SI/N - \gamma I]dt + \sqrt{\beta SI/N}dW_1 - \sqrt{\gamma I}dW_2,$$

where W_1 and W_2 are two independent Wiener processes,

$$G = \begin{pmatrix} -\sqrt{\beta SI/N} & 0\\ \sqrt{\beta SI/N} & -\sqrt{\gamma I} \end{pmatrix}$$

$$GG^{T} = \Sigma = \begin{pmatrix} \beta SI/N & -\beta SI/N \\ -\beta SI/N & \beta SI/N + \gamma I \end{pmatrix}.$$

If the terms associated with the Wiener processes are dropped, then we have the ODE model.

A Lotka-Volterra Competition Model

ODE model:

$$\frac{dx_1}{dt} = x_1(r_1 - a_{11}x_1 - a_{12}x_2)
\frac{dx_2}{dt} = x_2(r_2 - a_{21}x_1 - a_{22}x_2),$$

As in the case of logistic growth, it is necessary to define the contribution to birth and to death. We use the simplest choice for birth and death rates. Assume $b_1 = r_1X_1$, $d_1 = X_1(a_{11}X_1 + a_{12}X_2)$, $b_2 = r_2X_2$, $d_2 = X_2(a_{21}X_1 + a_{22}X_2)$. We can write these in tabular form as follows:

Changes $(\Delta X_1, \Delta X_2)$	Probability
(1,0)	$r_1 X_1 \Delta t$
(-1,0)	$X_1(a_{11}X_1 + a_{12}X_2)\Delta t$
(0,1)	$r_2 X_2 \Delta t$
(0,-1)	$X_2(a_{21}X_1 + a_{22}X_2)\Delta t$

The infinitesimal mean and variance are

$$E(\Delta X) = \begin{pmatrix} r_1 X_1 - X_1 (a_{11} X_1 + a_{12} X_2) \\ r_2 X_2 - X_2 (a_{21} X_1 + a_{22} X_2) \end{pmatrix} \Delta t = \mathbf{f} \Delta t$$

$$E(\Delta X (\Delta X)^T) = \begin{pmatrix} X_1(r_1 + a_{11}X_1 + a_{12}X_2) & 0\\ 0 & X_2(r_2 + a_{21}X_1 + a_{22}X_2) \end{pmatrix} \Delta t = \Sigma \Delta t$$

Matrix G can be chosen as follows:

$$G_1 = \begin{pmatrix} \sqrt{r_1 X_1} & -\sqrt{X_1(a_{11} X_1 + a_{12} X_2)} & 0 & 0\\ 0 & 0 & \sqrt{r_2 X_2} & -\sqrt{X_2(a_{21} X_1 + a_{22} X_2)} \end{pmatrix}$$

or as

$$G_2 = \begin{pmatrix} \sqrt{X_1(r_1 + a_{11}X_1 + a_{12}X_2)} & 0\\ 0 & \sqrt{X_2(r_2 + a_{21}X_1 + a_{22}X_2)} \end{pmatrix}$$

The system of Itô SDEs for Lotka-Volterra competition based matrix G_2 :

$$dX_1 = X_1(r_1 - a_{11}X_1 - a_{12}X_2)dt + \sqrt{X_1(r_1 + a_{11}X_1 + a_{12}X_2)} dW_1$$

$$dX_2 = X_2(r_2 - a_{21}X_1 - a_{22}X_2)dt + \sqrt{X_2(r_2 + a_{21}X_1 + a_{22}X_2)} dW_2,$$

$$X_1(t), X_2(t) \in [0, \infty).$$



Figure 2: A sample path of the Lotka-Volterra competition model over time and in the phase plane with parameter values $a_{10} = 2$, $a_{20} = 1.5$, $a_{11} = 0.03$, $a_{12} = 0.02$, $a_{21} = 0.01$, $a_{22} = 0.04$, $X_1(0) = 50$, and $X_2(0) = 25$.

Last Example: Population Genetics Process.

We shall derive the Kolmogorov differential equations for the allele frequencies X(t) of a population assuming random mating and no selection nor mutation. Assume that the population is diploid; each individual has two copies of the chromosomes. Assume that the gene is determined by a single locus with only two alleles, A and a and three possible genotypes,

AA, Aa, and aa.

In addition, assume the total population size is N. The total number of alleles equals 2N. Let Y(t) denote the number of A alleles in the population in generation t and X(t) denote the proportion or frequency of A alleles in the population, X(t) = Y(t)/(2N). Suppose individuals mate randomly and generations are nonoverlapping. The number of alleles in generation t + 1 is derived by sampling with replacement from the alleles in generation t. Given X(t) = x, then Y(t + 1) has a binomial distribution, b(2N, x); that is,

 $Y(t+1) \sim b(2N, x).$

Based on these assumptions the drift and diffusion coefficients a(x) and b(x) (infinitesimal mean and variance) can be derived.

Let $\Delta Y(t) = Y(t+1) - Y(t)$ and $\Delta X(t) = X(t+1) - X(t)$. Then given X(t) = x, Y(t) = 2Nx and applying the formula for the mean of a binomial distribution:

$$E(Y(t+1)|X(t) = x) = 2Nx$$

$$E(\Delta Y(t)|X(t) = x) = 2Nx - 2Nx = 0.$$

Then $E([\Delta Y(t)]^2 | X(t) = x)$ equals $E(Y^2(t+1) - 2Y(t+1)Y(t) + Y^2(t) | X(t) = x)$ which can be simplified to

$$E([\Delta Y(t)]^2) = E(Y^2(t+1)) - 2(2Nx)(2Nx) + 4N^2x^2$$

= $E(Y^2(t+1)) - 4N^2x^2 = E(Y^2(t+1)) - E(Y(t+1))^2.$

But this is just the variance of Y(t+1) which applying the formula for the variance of the binomial distribution gives

$$E([\Delta Y(t)]^2 | X(t) = x) = Var(Y(t+1) | X(t) = x)$$

= $2Nx(1-x).$

Because X(t) = Y(t)/(2N),

$$E(\Delta X(t)|X(t) = x) = \frac{1}{2N}E(\Delta Y(t)|X(t) = x) = 0 = a(x)$$
$$E([\Delta X(t)]^2|X(t) = x) = \frac{1}{(2N)^2}E([\Delta Y(t)]^2|X(t) = x)$$
$$= \frac{2Nx(1-x)}{(2N)^2} = \frac{x(1-x)}{2N} = b(x).$$

Hence, the pdf p(x, t) for the population genetics process satisfies

$$\frac{\partial p}{\partial t} = \frac{1}{4N} \frac{\partial^2 (x(1-x)p)}{\partial x^2}, \quad 0 < x < 1,$$
(6)

where $p(x,0) = \delta(x - x_0)$. Note that the forward Kolmogorov differential equation is singular at the boundaries, x = 0 and x = 1. Both boundaries are exit boundaries. At the states zero or one, there is fixation of either the allele a or A, respectively. The solution p(x,t) was derived by Kimura (1955), a complicated expression depending on the hypergeometric function. We shall examine the solution behavior of p(x,t) through the corresponding Itô SDE for this process.

The Itô SDE for Population Genetics Process.

The Itô SDE has the form

$$dX(t) = \sqrt{\frac{X(t)(1 - X(t))}{2N}} \, dW(t), \quad X(t) \in [0, 1],$$

where $X(0) = x_0$, $0 < x_0 < 1$. The boundaries 0 and 1 are absorbing [e.g., if X(t) = 0 (or 1), then $X(t + \tau) = 0$ (or 1) for $\tau > 0$]. Euler-Maruyama method is used to numerically solve this SDE. The sample paths illustrate random genetic drift.



Figure 3: Three sample paths, X(0) = 1/2 and N = 100.

Approximation of the p.d.f. of frequency of allele A, t = 10, 50, 200 based on 10,000 sample paths.



Figure 4: X(0) = 1/2 and N = 100. Approximate probability histograms at t = 10, 50, and 200.

The Mean is Constant.

It was shown by Kimura (1955, 1994), for large t, that

 $p(x,t) \approx C e^{-t/(2N)}, \quad 0 < x < 1.$

The pdf is approximately constant and very small when 0 < x < 1 and t is large. The probability of fixation at either x = 0 and x = 1 approaches one as $t \to \infty$, i.e., p(x,t) tends to infinity at x = 0 and x = 1 and to zero for 0 < x < 1 as t approaches infinity. When X(0) = 1/2, fixation at 0 or 1 is equally likely; the probability distribution is symmetric about x = 1/2. It follows from the properties of the Wiener process that the mean equals the initial proportion:

$$E(X(t)) = E\left[X(0) + \int_0^t \sqrt{\frac{X(t)(1 - X(t))}{2N}} \, dW(t)\right] = X(0)$$

In deterministic population genetics, this equilibrium is referred to as a Hardy-Weinberg equilibrium. At Hardy-Weinberg equilibrium there is random mating, no mutation, and no selection; the proportion of alleles stays constant in the population. Thank you.

It has been my pleasure to be your teacher this past academic year.