Chapter 5

Potential Theory Approach to SDEs

5.1 Introduction

The examples in the previous chapter make it clear that the behavior of individual realizations of a stochastic process are often too variable to give a satisfactory account of the behavior of the physical system that the process is designed to model. Instead, one has to simulate many realizations, and draw conclusions from an appropriate statistical analysis of the results.

This conclusion is reinforced if one considers in more detail the physical interpretation of an individual realization. For example, in the porous flow problem, a single realization of the solution to the SDE that models liquid flow, might give the path followed by a single fluid element through the porous medium starting from a given initial position at a given initial time, such as that illustrated in Figure 1.1. In the case of deterministic stationary laminar flow, all subsequent fluid elements starting from the same position follow the same path and there would be no interest in solving the flow equation for more than one initial time. However, in the case of a stochastic model of the flow, even if the macroscopic conditions are stationary, at a microscopic level the flow path is unstable and fluid elements departing from the same position at different times can follow completely different paths. In this case then, the different realizations can be taken to represent these different paths. Alternatively, referring again to Figure 1.1, one can consider different fluid elements that all start from the same X-coordinate at the same time, but at different positions on the cross section perpendicular to the X-axis of the porous medium. If we track the x- coordinate of each of these fluid element as a function of time, these will clearly develop differently for each fluid element and once more it would be reasonable to consider them each as a different realization of a 1-dimensional flow equation that models flow along the X-direction.

Whether the realizations are distinguished according to starting times or starting positions, the details of the movement of a single fluid element is clearly not of physical interest, but rather the effect of superimposing all the fluid elements. If in the example above a contaminant is introduced into the flow at a certain point, the concentration profile further downstream is determined by adding the contributions from each of the fluid elements that received some contaminant at the injection point, but then followed different paths and are found at different X positions after a given time lapse.

To model the macroscopic behavior of contaminant transport, it would therefore be very desirable to find a direct mathematical description of the temporal behavior of the statistical quantities, such as the mean and standard deviation of the position, rather than having to extract this from multiple simulated individual realizations.

It turns out that there is indeed a way to achieve this improbable goal, and that is the subject of this chapter. It is based on a major development in the theory of stochastic differential equations that was performed over the second half of the 20^{th} century by many of the leading mathematicians of the time, and the discussion here will only aim to convey the essentials of that theory in a way that explains its application to the porous medium flow problem.

The outcome of the theory is that the problem of solving a particular SDE is replaced by that of solving a connected deterministic differential equation, of the sort that is well known in potential theory. The concept of a potential arises in physical problems in many areas, such as electrostatics, hydrodynamics and thermal conduction. A typical problem from the latter area will serve as a straightforward example. Consider a heat conductor in which there is a temperature gradient because it is located between a heat source and a heat sink, but the system is in a steady state so that the temperature everywhere remains constant with time. The basic law of heat conduction states that heat flow is proportional to the gradient of the temperature, which means that temperature T plays the role of a potential for heat flow. It is easily proven from the conduction law that inside the conductor, where there are no heat sources, T must satisfy the partial differential equation

$$\nabla^2 T = 0. \tag{5.1}$$

This is the Laplace equation, that also applies, for example, to the electrostatic potential in a charge-free region. For any point P inside the conductor, it is intuitively plausible that the temperature at P is equal to the average of the

temperature over any spherical surface within the conductor and centered on P. If , for example, the average on this sphere was higher than at P, heat would flow from it towards P, and the temperature would no longer be stationary.

The statement can also be mathematically proven to be a direct consequence of the Laplace equation and is often called the *mean value theorem.* The problem of solving the Laplace equation subject to known values of the potential on an enclosing boundary, is usually referred to as the Dirichlet problem in potential theory.

In a seminal paper, it was pointed out by Shizuo Kakutani (1945) that there is a close connection between the Dirichlet problem and random walks. Let P be any point in a source free region of the potential Φ, and S is an enclosing boundary around P. If one considers all random walks that start at point P, and notes the value of the potential at the first time that each random walk crosses S, the average of these values over all the random walks approaches a statistical expectation value $E[\Phi(S)]$ as the number of walks tends to infinity. It was proven by Kakutani that

$$E[\Phi(S)] = \Phi(P). \tag{5.2}$$

The proof is quite straightforward, and relies on the mean value theorem as well as the Markov property of random walks (i.e., that the subsequent development of a random walk is independent of the way in which a particular point on the path was reached). The proof is discussed on a non-mathematical level by Hersh and Griego (1969).

In the special case that S is chosen to be a sphere, it is easy to see that equation (5.2) merely reduces to the mean value theorem. As the incremental displacements in the random walk are equally likely to be in any direction, all points on a spherical S are equally likely to be the exit point of the random walk. Hence a very large number of random walks sample all parts of the spherical surface equally, and the expectation value is just the ordinary average.

However, for any other shape of the surface, equation (5.2) is a generalisation and may in fact yield a practical method of solving the Dirichlet problem approximately in cases where the shape of surface on which the boundary values are known is too complicated to allow computation directly from the deterministic differential equation of the potential.

In subsequent development of Kakutani's basic idea by many authors, a comprehensive mathematical framework has been established that moves beyond the Laplace equation and random walks. It leads to a well-defined correspondence between a large class of stochastic differential equations and an associated set of deterministic 2nd order partial differential equations. No attempt will be made here to present all the theory and derivations; these are well covered in the books by Øksendal, and Kloeden and Platen. We will restrict ourselves to introducing some definitions and stating the theorems, together with a discussion of simple illustrative examples to demonstrate the applications to the flow problems that is our main concern.

5.2 Ito Diffusions

The theory that follows is restricted to SDE's of the type

$$dX_t = b(X_t)dt + \sigma(X_t)dB_t . \tag{5.3}$$

Note that the so-called *drift coefficient* b and *diffusion coefficient* σ are restricted to be independent of the time variable, unlike the more general case represented e.g. by equation (2.4). Moreover, b and σ must satisfy a continuity condition (the Lipschitz condition):

$$|b(x)-b(y)|+|\sigma(x)-\sigma(y)| \leq D|x-y| \tag{5.4}$$

where D is an arbitrary constant, for all x and y. An SDE that satisfies these restrictions is called an *Ito diffusion* (ID). Note, however, that X_t and B_t are not restricted to be scalars – they can be n- and m-dimensional vectors respectively, and b and σ correspondingly a vector and a matrix respectively, in n x m dimensions. So equation (5.3) really represents a set of first order SDE's rather than a single equation. Moreover, this means that an ID is not restricted to 1st order equations only, since higher order differential equations can be reduced to a set of 1st order equations by introducing derivatives as independent variables.

The term "Ito diffusion" is a mathematical convention that can become confusing in a study of actual flow and transport phenomena, where real physical diffusion is relevant. We therefore prefer to only use the acronym "ID" to identify the mathematical concept. The simplest concrete example of an ID, is the 1-dimensional Brownian motion itself, given trivially by

$$dX_t = dB_t. \tag{5.5}$$

The same formal equation would represent 2-dimensional Brownian motion, provided that we interpret it as an equation for the vectors

$$X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}, \quad B = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}; \qquad b = (0,0), \quad \sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{5.6}$$

Another interesting example of an ID is the pair of SDEs

$$\begin{aligned} dY_1 &= -\tfrac{1}{2}Y_1 dt - Y_2 dB, \\ dY_2 &= -\tfrac{1}{2}Y_2 dt + Y_1 dB, \end{aligned} \tag{5.7}$$

which is the special case of equation (5.3) where

$$b = \begin{pmatrix} -\frac{1}{2}Y_1 \\ -\frac{1}{2}Y_2 \end{pmatrix}, \quad \sigma = \begin{pmatrix} 0 & -Y_2 \\ Y_1 & 0 \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} B \\ B \end{pmatrix} = B\begin{pmatrix} 1 \\ 1 \end{pmatrix}. \tag{5.8}$$

Notice that although B in this equation is a vector, since its components are equal there is only one independent stochastic term. The solution to equation (5.7) satisfies

$$\begin{aligned} dY_1(t) &= -\sin(B)dB - \tfrac{1}{2}\cos(B)dt, \\ dY_2(t) &= \cos(B)dB - \tfrac{1}{2}\sin(B)dt, \end{aligned} \tag{5.9}$$

as is easily proven from the Ito formula by applying it to the vector function $g(t,x) = exp(ix) = (cos\ x,\ sin\ x)$. From equation (5.9) it is clear that if the initial values of the vector $Y = (Y_1, Y_2)$ is chosen to fall on the unit circle, Y will always stay on the unit circle. This ID can be called *Brownian motion on the unit circle* and in this case the B can be interpreted as a stochastically varying angle coordinate.

5.3 The Generator of an ID

The next important step is to define the generator of an ID. The generator A is a special kind of differential operator, defined by the following limit:

$$A f(x) = \lim_{\Delta t \to 0} \frac{E^x\left[f(X_t)\right] - f(x)}{\Delta t} \,. \tag{5.10}$$

Here, f is an arbitrary function of the n-dimensional vector x, and the notation E^x means the expectation value taken over all realizations of the ID X_t that start at $t = 0$ at the particular position x. In words, A gives the expected time rate of change of a function, as its argument undergoes an Ito diffusion away from the starting point at x.

It is proven in Øksendal (1998) (theorem 7.3.3) that for a given ID, the associated A can be expressed in terms of the coefficient matrices of the ID equations as follows, provided that f is twice differentiable:

$$A f(x) = \sum_i b_i(x) \frac{\partial f}{\partial x_i} + \tfrac{1}{2} \sum_{i,j} (\sigma \cdot \sigma^T)_{ij}(x) \frac{\partial^2 f}{\partial x_i \partial x_j} \,. \tag{5.11}$$

Notice the appearance of the second derivative, although equation (5.10) ostensibly defines A as a first derivative. This is a manifestation of the inclusion of 2nd order differentials of the Wiener increment that was discussed in connection with equation (2.5). The proof of equation (5.11) involves using the Ito formula to express the differential of f ; when this is integrated, one term in the result takes the form of an Ito integral, but this term falls away when the expectation value that appears in equation (5.10) is taken and the result is as shown above.

In the literature, a somewhat generalized definition of the generator is sometimes encountered and often referred to as the *characteristic operator* of the ID. However, as shown in Øksendal (1998) wherever the generator exists the two operators are identical and equation (5.11) is a valid representation of both operators.

5.4 The Dynkin Formula

In integrating a deterministic differential equation for some function f in the time domain, one may usually integrate from $t = 0$ to some indefinite final time t. The solution found in this way, will directly answer a question such as about the value(s) of t at which a given value of f will be reached.

In the case of an SDE, the situation is more complex. While one could still integrate the SDE up to a chosen time, each realization of the solution will reach a predetermined value at a different time, so no unique t value corresponds to a particular value of f. To clarify this, the concept of a *stopping time* is introduced. A stopping time τ is defined as a fixed time value for which it is possible to decide on the grounds of a single realization whether τ has been reached. Any specified time value is a valid stopping time, and so is the time at which a specified value of f is reached for the first time. The latter is an example of a *first exit time*; if a subset of realizations is defined by a condition that can be applied to any realization at time t to decide its membership of the subset, the first exit time from this subset is a valid stopping time. By contrast, the expected time for f to reach a specified value is not a valid stopping time, because it is a statistical quantity that requires knowledge about all possible realizations.

Using this concept we can now formulate Dynkin's formula, which reads:

$$E^x[f(X_\tau)] = f(x) + E^x\left[\int_0^\tau A f(X_s)\,ds\right]. \tag{5.12}$$

Here, τ is a stopping time satisfying $E^x[\tau] < \infty$ while f is as before any twice differentiable function.

The derivation of Dynkin's formula is contained in the derivation of equation (5.11) as outlined above. It is also intuitively plausible as essentially the expectation value of an integral of equation (5.10). Despite this apparently straightforward origin, it has profound consequences and is the basis of most of the SDE theory that we have applied in the flow problem. An extended account of this result can be found in Dynkin (1965).

If we consider Dynkin's formula for the case that τ is a fixed time t so that the expectation value on the right hand side of equation (5.12) can be taken inside the integral, and define

$$u(t,x) = E^x[f(X_t)]. \tag{5.13}$$

We may differentiate equation (5.12) to find

$$\frac{\partial u}{\partial t} = Au, \qquad t > 0 \tag{5.14}$$

$$u(0,x) = f(x). \tag{5.15}$$

and moreover, as proved in Øksendal (1998) Chapter 8, the reverse also holds: for any appropriately differentiable function that solves equations (5.14) and (5.15), equation (5.13) also holds. This differential version of Dynkin's equation, sometimes referred to as Kolmogorov's backward equation, is in some cases simpler to apply than the original integral version.

5.5 Applications of the Dynkin Formula

We first illustrate that Dynkin's equation is a generalisation of Kakutani's result that was discussed in the introduction, section 0. Suppose the ID under discussion is simple 3-dimensional Brownian motion, represented by equations such as (5.5) and (5.6). The generator of this ID is found by putting the 3-dimensional equivalents of equation (5.6) into equation (5.11) yielding

$$Af = \nabla^2 f. \tag{5.16}$$

We choose a bounded region S in space surrounding the starting point x of the Brownian motion, and define τ to be the first exit time from this region. Then, if f is chosen as a solution of the Laplace equation inside S, and equation (5.16)(5.16) substituted into Dynkin's equation, the integral on the right vanishes and Kakutani's result follows.

A very interesting result is obtained if we choose S to be an annular region bounded by a small inner sphere of infinitesimal radius ε centered on an arbitrary point b, and an outer concentric sphere of radius $R>>\varepsilon$, chosen big enough that the starting point x is inside the annulus. The stopping time is taken as the first time the Brownian motion exits S across either boundary. Let p be the probability that it leaves S across the inner boundary first, i.e. that

it reaches point b, and $q = 1\text{-}p$ the probability that it leaves S across the outer boundary.

We choose f to be spherically symmetric around point b, i.e. only a function of the radius measured from b. This is a choice allowed by the Laplace equation. The expected value of f at the stopping time is just the probability weighted sum of f values on the two boundaries. If we choose the boundary condition $f(\varepsilon) = 1$ and $f(R) = 0$, it follows that

$$E^x[f(X_\tau)] = p\,. \tag{5.17}$$

We consider this problem for the case of n spatial dimensions. Expressing the Laplace operator in the appropriate radial coordinates according to the number of dimensions, the solution satisfying the stated boundary conditions is easily found by direct integration to be

$$\begin{aligned} f(r) &= \frac{R-r}{R-\varepsilon} && ;n=1 \\ f(r) &= \frac{\ln(R)-\ln(r)}{\ln(R)-\ln(\varepsilon)} && ;n=2 \\ f(r) &= \frac{\frac{1}{R}-\frac{1}{r}}{\frac{1}{R}-\frac{1}{\varepsilon}} && ;n=3 \end{aligned} \tag{5.18}$$

Applying the Kakutani result equation (5.2) to equation (5.17)(5.17), it follows that $p = f(r_0)$ where $r_0 = |x\text{-}b| > \varepsilon$, is the starting radius. Consider now the effect of relaxing the restriction to the finite spatial region enclosed by S, by taking the limit as $R \to \infty$. From equation (5.18) it is seen that in the cases of 1 and 2 dimensions, $p \to 1$, but for 3 (or more) dimensions $p \to 0$ (as $\varepsilon \to 0$). This means that in 1 or 2 dimensions we can be sure, in a probabilistic sense, that starting from an arbitrary spatial point, Brownian motion will eventually reach any other arbitrarily chosen point (in the example, the point b chosen as the centre of the annulus); but in more dimensions, this probability vanishes. The argument is easily extended to say that in less than 3 dimensions, a Brownian motion starting from a given point will eventually return to the point, i.e. it is recurrent; but in 3 or more dimensions it is not recurrent.

This result is known as Polya's theorem. The power of the Dynkin formula is demonstrated by the ease by which this subtle result was obtained, compared to the original proof by Polya (1921).

It is a feature of the application of Dynkin's equation, that we do not usually have a preconceived notion of the function f for which it allows us to calculate the expectation value. Instead, we start by finding the generator from the SDE that describes a problem. Then we construct a differential equation that f should satisfy in order to simplify the integral on the right hand side of Dynkin's equation – such as equation (5.16) above. In this way Dynkin's equation dictates the form of the function for which expectation values are found, and this form is different for different ID's and even for the same ID, different forms are obtained depending on how the right hand side of the generator equation is chosen. That is demonstrated by the example in the next section.

5.6 Extracting Statistical Quantities from Dynkin's Formula

The procedure by which statistical properties of the solutions to an SDE can be extracted from Dynkin's formula, will now be demonstrated by applying it to the population growth problem.

The first step is to find the generator for the SDE, contained e.g. in equation (2.4). Identifying the drift and diffusion coefficients of equation (5.3) (5.3) as $b(x) = r\,x$ and $\sigma(x) = \sigma\,x$ equation (5.11) becomes:

$$A f(x) = rx\frac{\partial f}{\partial x} + \tfrac{1}{2}\sigma^2 x^2 \frac{\partial^2 f}{\partial x^2}. \tag{5.19}$$

In order to be useful in Dynkin's formula, an f is now to be found such that it makes the integral on the right hand side of the equation tractable. The simplest choice is to find f such that $A f = 0$; that was the choice which led to Kakutani's theorem in the previous section. Other possibilities are to make $A f$ = *constant* or $A f = \partial f/\partial t$. Each choice supplies the answer to a different question about the SDE solution and will be discussed separately below.

5.6.1 What is the probability to reach a population value K ?

To answer this, we define the stopping time as the first time the population exits from the bounded set of values defined by the interval [ε,K] or in other words, the open interval (0,K] . The value 0 is excluded because it can never be reached, as is also clear from the explicit solution in equation (2.5). Using the choice $A f = 0$ and equation (5.19) it is easily seen that

$$f(x) = \frac{x^\gamma}{\gamma} \; ; \; \gamma = 1 - \frac{2r}{\sigma^2}, \tag{5.20}$$

where γ is a dimensionless constant. At the stopping time, X_t must either have the value ε or K; define p_ε and p_K respectively as the probabilities for each of these to happen. Dynkin's equation reduces to

$$E^{X_0}[f(X_\tau)] = p_\varepsilon f(\varepsilon) + p_K f(K) = f(X_0) + 0 \tag{5.21}$$

and by using $p_\varepsilon + p_K = 1$ and equation (5.10) it is found that

$$p_K = \frac{X_0{}^\gamma - \varepsilon^\gamma}{K^\gamma - \varepsilon^\gamma}. \tag{5.22}$$

The case of interest is when $\varepsilon \to 0$ for which two expressions are obtained:

$$p_K \xrightarrow[0]{\varepsilon} \begin{cases} \left(X_0 / K \right)^\gamma & , \gamma > 0 \\ 1 & , \gamma \le 0 \end{cases} \tag{5.23}$$

The deterministic limit is when $\sigma = 0$ i.e. when $\gamma \to -\infty$. In this case any finite value $K > X_0$ will always be reached as the population is growing exponentially, and equation (5.23) shows that the same is true for any negative γ. However, for strictly positive γ, there is a finite probability that K will never be reached and this increases as either γ or K increases.

This straightforward result would be quite difficult to obtain from numerical simulations; especially when the probability is low, a very large number of simulations would be needed to obtain reliable statistics. Moreover, the result shows that there is a marked qualitative difference in the behavior below and above the critical value $\gamma = 0$ that separates the regions where the

deterministic and stochastic contributions dominate. This fact is not so clear even from the explicit stochastic solution of equation (2.4).

5.6.2 What is the expected time for the population to reach a value K?

This question is answered by choosing $Af = constant$. The constant must have the dimensions $[T^{-1}]$ because as is clear from equation (5.10), A is essentially a time derivative. We may therefore simplify the calculation by choosing the constant to be r, since it is the only relevant constant in the problem and has the right dimension. Solving the resulting generator equation yields

$$f(x) = \frac{x^{\gamma}}{\gamma} + \frac{\gamma - 1}{\gamma} \ln x . \tag{5.24}$$

Dynkin's equation now becomes

$$E^{X_0}[f(X_\tau)] = f(X_0) + E^{X_0}\left[\int_0^\tau r\, ds\right] = f(X_0) + rE^{X_0}[\tau] = f(X_0) + rT . \tag{5.25}$$

where T is the expected exit time. Once more expressing the expectation value on the left hand side in terms of the probabilities, substituting equations (5.25) and (5.22) and simplifying one obtains

$$rT = \frac{\gamma - 1}{\gamma}[p_K \ln K - \ln X_0 + (1 - p_K) \ln \varepsilon] . \tag{5.26}$$

The deterministic limit of this ($\gamma \rightarrow -\infty$ and $p_K \rightarrow 1$) gives a time that is identical with that solved directly from the deterministic exponential growth solution. However, the behavior of the stochastic solution is most easily interpreted from a numerical plot (see Figure 5.1).

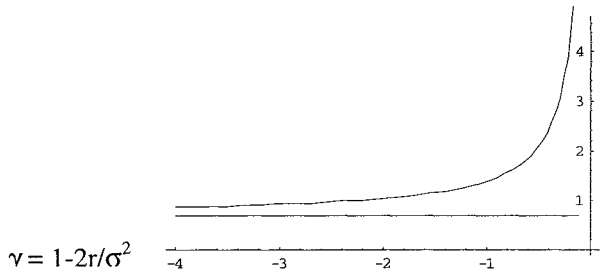

Figure 5.1 The expected time for the population to double as stochastic amplitude increases.

Figure 5.1 shows the expected time for the population to double, i.e $K=2\ X_0$. The straight line is the deterministic time, and as shown this is approached as $\gamma \rightarrow -\infty$. However, for the stochastic solution the expected time is always more than the deterministic value, and it becomes infinite for $\gamma \geq 0$.

To put it in perspective, we note that the realizations explicitly calculated in Chapter 3 represent a value of $\gamma = -2$ for Figure 3.13, and $\gamma = -11$ for Figure 3.14 respectively. In both these cases the behavior remains essentially one of unlimited growth, although an extended time is needed to reach a population doubling. However the implication is that in the region where stochastic contributions dominate, the population of a "typical" realization will never reach the value K.

This result is a stronger one than that of the previous subsection, which was that there is a finite probability that K will never be reached. Here we find that even where there is a finite probability that K will be reached, one may on average have to wait an infinite time for this to happen. These statements may appear contradictory; but before discussing it, we first address the next question since it appears to throw up an even stronger contradiction.

5.6.3 What is the Expected Population at a Time t ?

One possibility to answer this question is to extend the treatment to a 2-dimensional problem, in which time becomes the second variable, represented as a trivial "stochastic" variable regulated by the equation $dX_2 = dt$, i.e. without an actual stochastic variation. The expected population can then be found by taking the stopping "time" as the escape from a rectangular region bounded by the lines $X_1 = K$ and $X_2 = T$ in the (X_1, X_2) plane. An example of this approach is found in Øksendal(1998).

However, we show a more direct technique based on the Kolmogorov backward equation (5.14). This corresponds to the case where we put a partial time derivative on the right hand side of the generator equation, and it becomes a partial differential equation in the two variables x and t. Using the same generator as in the previous subsections and solving the equation by separation of variables introducing a separation constant C, the solution is:

$$u(x,t) = e^{\frac{Ct}{1-\gamma}} x^{\frac{1}{2}[\gamma+\sqrt{\gamma^2-4C}]}. \tag{5.27}$$

This is a solution for all values of the separation constant; we choose C such that the exponent of x becomes an integer N, in terms of which equation (5.27) is expressed as

$$u(x,t) = x^N e^{Nrt+\frac{1}{2}N(N-1)\sigma^2 t}. \tag{5.28}$$

If we now apply equations (5.15) and (5.13) we find that

$$E^{X_0}[X_t^{\,N}] = (X_0 e^{rt})^N e^{\frac{1}{2}N(N-1)\sigma^2 t}. \tag{5.29}$$

A case of particular interest is the mean value μ of the population, i.e. $N = 1$. Using this, the case $N = 2$ yields a value for the standard deviation s as well:

$$\mu = X_0 e^{rt}; \qquad s = X_0 e^{rt}\sqrt{e^{\sigma^2 t} - 1}. \tag{5.30}$$

Notice that the functional form of the function of x for which the expectation value is given by Dynkin's formula, is dictated by the solutions to the generator equation. Different forms were obtained in answering the various questions above. In the first cases examined, individual functions were obtained, namely equations (5.20) and (5.24). In the case of the expected

population, instead, a whole family of functions was found, i.e. integer powers of x, making the extraction of statistical moments particularly simple. For other problems, more mathematical manipulation is usually required to achieve that.

A noteworthy feature of equation (5.30) is that μ is given by exactly the deterministic expression for the population, irrespective of the value of σ. While this behavior would be expected if the stochastic solution merely consisted of a random variation superimposed on the deterministic behavior, the results of the previous subsections showed that in fact the behavior of the stochastic solution is more complex. In fact, the behavior of μ seems difficult to reconcile with that of the probability and the expected time – if the average value grows exponentially with time, how can it take an infinite expected time (for some range of σ values) to reach a fixed value, such as twice the initial population?

The resolution of this paradox lies in the fact that the population value is bound from below, as the exponential growth does not allow it to reach 0, but not from above. At any fixed time, there must be some realizations which have populations far above μ. To balance these and restore the average, there must be many more realizations in the range between 0 and μ. So the majority of realizations actually have populations below average, and this accounts for the fact that the expected time to reach a fixed value is always larger than the deterministic time. When the stochastic term dominates, the probability of reaching the fixed value is less than one according to equation (5.23), meaning that a finite fraction of realizations never reach it. The fraction that does not reach it in a finite time interval must be even bigger.

For the deterministic system, the questions about the population at a given time, and about the time to reach a fixed value, are two sides of the same coin in the sense that their answers can be read off from the same point on a plot of population vs. time.

The stochastic term destroys this relation. In fact, the argument above suggests that the behavior of the population mean, while simple, is not representative of the behavior of a typical realization. Conversely, if a finite number of realizations are generated numerically, the mean value would not give a reliable estimate of the population mean, because the sample would not be likely to include enough of the low probability, high population

realizations. In this case the estimated time to reach a fixed value, would give a more realistic description of the behavior of typical realizations.

This discussion highlights the fact that SDE solutions can be inherently different from the underlying deterministic system, and do not just represent a random variation about a deterministic mean value. This is particularly visible in the population growth example, because of the highly non-linear properties of the exponential growth curve.

The advection-dispersion approach to contaminant transport discussed in Chapter 1 was in fact just such a simplification based on superimposing random variation on a deterministic transport equation. It may be that the solutions to the flow equations have a more moderate behavior than for exponential population growth, giving more practical justification of the a priori splitting of the velocity into a mean drift velocity and fluctuations. However, in principle the objection that stochastic variation needs to be included into the differential equation itself for a valid description remains valid.

5.7 The Probability Distribution of Population Growth Realization

The calculation of the previous section contains far more information than just the mean and standard deviation of the population. In fact, equation (5.29) specifies the value of all statistical moments of the probability distribution, and as is well known this is enough to fully determine the distribution itself. If an explicit expression for the distribution can be derived, this will facilitate the calculation of any other statistical quantities of interest. The problem can be mathematically formulated by rewriting equation (5.29) as:

$$\int_0^\infty dx\, x^N P(x,t) = (X_0 e^{rt})^N e^{\frac{1}{2}N(N-1)\sigma^2 t} \tag{5.31}$$

where $P(x,t)$ is the desired probability density of finding a population x at time t. The appearance of the factor x^N in the integrand is a consequence of the structure of the generator for the population growth SDE. Other problems will yield a similar integral on the left of the equation, but with different factors in the integrand. A common feature, however, is that while the Dynkin equation refers only to a single function $f(x)$ for which the expectation value is calculated, the solution of the time-dependent equation (5.14) in fact yields a family of solutions, indexed by the value of an integration constant such as the separation constant that manifests in equation (5.33) as the integer value N. Such a more general form of the equation could be written as

$$\int f_n(x) P(x,t) = u_n(x_0,t)\,. \tag{5.32}$$

While there is no unique solution for $P(x,t)$ from this integral equation for a single known function $f(x)$ and $u(x,t)$, such a unique solution does exist if the equation is satisfied by each member of a linearly independent set $f_n(x)$. In fact, the solution is facilitated if the $f_n(x)$ form a complete orthonormal set of functions, as is often the case when the set is found as solutions of a differential equation. If so, one may use the completeness relation which is typically of the form

$$\sum_n f_n(x) f_n(x') = \delta(x - x')\,, \tag{5.33}$$

where $\delta(x)$ is the Dirac delta-function, to solve equation (5.32):

$$P(x,t) = \sum_n f_n(x) u_n(x,t) . \tag{5.34}$$

Equation (5.31) cannot be solved in this way directly, because the set of functions x^N are linearly independent but not orthonormal. However, each x^N can be expressed as a linear combination of any of the well-known sets of orthogonal polynomials such as Hermite or Laguerre polynomials, and in this way a similar solution for $P(x,t)$ in the case of the population growth problem can be constructed.

While the problem of calculating the probability distribution is formally solved this way, it turns out that the resulting infinite sum expression suffers from convergence problems in practical numerical calculations. This is closely connected with the fact that the infinitely sharp peak on the right hand side of equation (5.33) cannot be successfully approximated by any finite sum of orthogonal polynomials. Consequently only imperfect representations of the probability density valid for limited ranges of the arguments are obtained. It turns out that in cases of interest in the contaminant flow problem, more elegant but ad hoc solutions for the probability density can be constructed. We will therefore not pursue the details of the solution for the population growth problem any further, beyond pointing out that even for this relatively simple problem, solving for the probability density is in principle possible but in practice quite difficult.