A stochastic differential equation is a particular type of noisy dynamical system. Applications call for generating SDE sample paths subject to a variety of constraints.

## 1 Multivariate normal

Let $X \in R^{n}$ be an $n$ component normal with covariance matrix $C$. Choose an orthonormal family of vectors $v_{k}$ and eigenvalues $\lambda_{k}$ so that $C v_{k}=\lambda_{k} v_{k}$. The $\lambda_{k}$ are the principle components of $X$ (or of $C$ ) and the $v_{k}$ the corresponding principle components (the terminology differs slightly from place to place). The random numbers $Y_{k}=v_{k}^{t} X$ are independent mean zero Gaussians with mean zero and variance $\lambda_{j}$. Said another way, if $V$ is the orthogonal matrix whose columns are the $v_{k}$, then $Y=V^{t} X$ is a multivariate normal with mean zero and covariance $\Lambda$, the diagonal matrix with $\lambda_{k}$ in the $(k, k)$ position. The $Y_{k}$ also may be called principle components, or possibly components in the principle directions. To summarize, the eigenvalue/eigenvector decomposition of $C$ is the principle component analysis of $X$. When using PCE, we usually order the principle values from largest to smallest: $\lambda_{k} \geq \lambda_{k+1}$ for all $k$.

On the other hand, suppose we know the $v_{k}$ and $\lambda_{k}$. We can construct a sample $Y_{k}$ as $Y_{k}=\sigma_{k} Z_{k}$, where $\sigma_{k}=\sqrt{\lambda_{k}}$ and the $Z_{k}$ are independent standard normals. Therefore, the formula $X=\sum_{k=1}^{n} \sigma_{k} Z_{k}$ provides a sample of $X$ from independent standard normals. This kind of PCA is helpful in many ways in Monte Carlo practice. If we want to know $A=E[f(X)]$, it is likely that the larger principle components are more important than the smaller ones. For example, the quantity $B=\int f\left(\sigma_{1} v_{1} z_{1}\right) e^{-z_{1}^{2} / 2} d z / \sqrt{2 \pi}$ may be a helpful control variate for evaluating $A$.

## 2 Brownian motion

A standard univariate Brownian motion path is a continuous random function $X(t)$ with $X(0)=0$ and increments, $\Delta X_{k}=X\left(t_{k+1}\right)-X\left(t_{k}\right)$ independent Gaussian random variables with mean zero and variance $t_{k+1}-t_{k}$. Here $t_{k}$ is any sequence of positive numbers with $t_{k+1}>t_{k}$. Many problems involve expected values of functions of Brownian motion and the intuitions gained by studying Brownian motion help design methods for related problems.

We start with the PCA of standard Brownian motion. Since Brownian motion is infinite dimensional, we start with finite dimensional approximations then get the PCA of Brownian motion itself as a limit. Suppose we fix a $T>0$. For any integer $n>0$, we divide the interval $[0, T]$ into $n$ equal subintervals using the notation $h=T / n$ and $t_{k}=k h$. The multivariate normal $X^{h} \in R^{n}$ has components $X_{k}^{h}=X\left(t_{k}\right)$, for $1 \leq k \leq n$. We showed before that the covariance matrix for $X^{h}$ has $H=C^{-1}$ that is tri-diagonal of the form .... . Clearly the eigenvalues of $C$ are the inverses of the eigenvalues of $H$ while the eigenvectors are the same. It happens (we will get more insight into this later)
that the eigenvectors of $H$ have the form $v_{k, j}^{h}=\sin \left(\omega_{k}^{h} t_{j}^{h}\right)$, where ... . If we take the limit $h \rightarrow 0$ and $n \rightarrow \infty$ with $T=n h$ fixed, the sequence of eigenvalues of $H$ converges to $\mu_{k}=(k+1)^{2} \pi^{2} / T^{2}$, as we verify by direct computation.

The PCA representation of a Brownian motion path is

$$
\begin{equation*}
X(t)=\frac{T}{\pi} \sum_{k=1}^{\infty} \frac{Z_{k}}{k+\frac{1}{2}} \sin \left(\frac{\left.k+\frac{1}{2}\right) \pi}{T} t\right) \tag{1}
\end{equation*}
$$

This representation is valid only for $t$ in the range $0 \leq t \leq T$. Moreover, it presents serious mathematical challenges. It is not straightforward to see that the sum converges. Indeed, the $Z_{k}$ and the sine factors are of the order of unity, so the terms in the sum seem to have the order of magnitude $1 / k$, which would not by itself lead to a convergent sum. The series does converge in the $L^{2}$ sense because

$$
E\left[\sum_{k=1}^{\infty} \frac{Z_{k}^{2}}{\left(k+\frac{1}{2}\right)^{2}}\right]=\sum_{k=1}^{\infty} \frac{1}{\left(k+\frac{1}{2}\right)^{2}}<\infty .
$$

However, this kind of convergence does not even imply that $X(t)$ is continuous. Many discontinuous are represented by $L^{2}$ convergence Fourier series. If we wish to generate a Brownian motion path using (1), we can use the FFT to calculate the sums on the right efficiently.

The Brownian Bridge construction is another good way to generate Brownian motion paths. For this, we consider a diadic collection of times. On level $k$, the interval $[0, T]$ is divided into $2^{k}$ equal subintervals. At the top is level zero with a single interval $[0, T]$ whose endpoints may be written $t_{0,0}=0$ and $t_{0,1}=T$. At the next level $[0, T]$ is broken into two halves bounded by the points $t_{1,0}=0$, $t_{1,1}=T / 2$, and $t_{1,2}=T$. The diadic points at level $k$ are $t_{k, j}=j 2^{-k} T$, for integers $j$ in the range $0 \leq j \leq 2^{k}$.

The construction itself is an algorithm that generates values for $X_{k, j}=$ $X\left(t_{k, j}\right)$ recursively proceeding from $k$ to $k+1$. At the top level we already have $X_{0,0}=X(0)=0$ and we need $X_{0,1}=X(T)$. But $X(T)$ is a mean zero Gaussian with variance $T$, so we can take $X_{0,1}=\sqrt{T} Z_{0,1}$, where $Z_{0 l, 1}$ is a standard normal. Things get interesting at the next level. From the properties of Brownian motion, we know that the values $\left(X\left(t_{1,1}\right), X\left(t_{1,2}\right)\right)=\left(X_{1,1}, X_{1,2}\right)$ is a bivariate normal. Therefore, conditional on the value of $X_{1,2}$, which already is known from the previous level, the value of $X_{1,1}$ is a univariate normal. Simple calculations show that $E\left[X_{1,1} \mid X_{1,2}\right]=\frac{1}{2} X_{1,2}$, and $\operatorname{var}\left[X_{1,1} \mid X_{1,2}\right]=\frac{1}{4} T$. The first result is very natural, that the expected value of the midpoint value should be the average of the two end values. The second result may be surprising, since the variance of $X_{1,1}$ without information about $X_{1,2}$ is $T / 2$ instead of $T / 4$. Specifying both endpoint values constrains $X_{1,1}$ to have a smaller variance. With this information the sampling can be done using $X_{1,1}=\frac{1}{2} X_{0,1}+\frac{\sqrt{t}}{2} Z_{1,1}$. As usual, $Z_{1,1}$ is a standard normal independent of all others.

The step of going from level $k-1$ to level $k$ is clear. We already have values $X_{k, 2 j}=X_{k-1, j}$ from the previous levels. We need to generate values for the new points $t_{k, 2 j+1}$. The Markov property (which is the main thing that makes this
construction work) implies that the conditional distribution of $X_{k, 2 j+1}$ given all the values on level $k-1$ is the same as the distribution given the level $k-1$ endpoints $X_{k, 2 j}=X_{k-1, j}$, and $X_{k, 2 j+2}=X_{k-1, j+1}$. As above, the conditional expectation of $X_{k, 2 j+1}$ is $\frac{1}{2}\left(X_{k-1, j}+X_{k-1, j+1}\right)$. Let $\Delta t_{k}=2^{-k} T$ be the length of the diadic intervals at level $k$. The conditional variance of $X_{k, 2 j+1}$ is $\Delta t_{k} / 2$ (which again is half the conditional variance if only the left value $X_{k, 2 j}$ were specified). Therefore, the sampling may be done by

$$
X_{k-2 j+1}=\frac{1}{2}\left(X_{k-1, j}+X_{k-1, j+1}\right)+\sqrt{\frac{\Delta t_{k}}{2}} Z_{k, 2 j+1}
$$

One use of this Brownian bridge construction is similar to the PCA construction, to have a way to separate random variables that have a large impact on $X$ from others that have a smaller impact.

## 3 The Ornstein Uhlenbeck Process

The Ornstein Uhlenbeck process is a simple modification of Brownian motion to add mean reversion. Starting here, we refer to the proces of interest as $X(t)$ while $W(t)$ will be Brownian motion. The general Ornstein Uhlenbeck process satisfies the SDE

$$
\begin{equation*}
d X=-\mu X d t+\sigma d W \tag{2}
\end{equation*}
$$

This means that we can write

$$
\begin{equation*}
X(T)=e^{-\mu T} X(0)+\sigma \int_{0}^{T} e^{-\mu(T-t)} d W(t) \tag{3}
\end{equation*}
$$

We see from this that $X$ is a linear transformation of the Gaussian $W$ so it is Gaussian. This is contingent on $X(0)$ being Gaussian if it is random. From this we can calculate that $X(T)$ is a gaussian with mean $e^{-\mu T} X(0)$, and variance

$$
\begin{equation*}
\sigma^{2} \int_{0}^{T} e^{-2 \mu(T-t)} d t=\frac{\sigma^{2}}{2 \mu}\left(1-e^{2 \mu T}\right) \rightarrow \frac{\sigma^{2}}{2 \mu} \text { as } T \rightarrow \infty \tag{4}
\end{equation*}
$$

As $T \rightarrow \infty$, the distribution of $X(T)$ converges to a gaussian that is independent of the initial condition (if the mean and variance converge and if it's Gaussian, the distribution converges).

Much Monte Carlo depends on time dependent random processes like this so we analyze this in more detail, focusing on features that have analogues in many Monte Carlo applications. Suppose $u(x, t)$ is the probability density function for $X(t)$. This satisfies the Kolmogorov forward equation (other names include, but are not limited to, the forward equation, the Fokker Planck equation, and the Chapman Kolmogorov equation)

$$
\begin{equation*}
\partial_{t} u=\frac{\sigma^{2}}{2} \partial_{x}^{2} u+\mu \partial_{x}(x u) \tag{5}
\end{equation*}
$$

We write this as

$$
\begin{equation*}
\partial_{t} u=L^{*} u, \quad \text { where } L^{*} u=\frac{\sigma^{2}}{2} \partial_{x}^{2} u+\mu \partial_{x}(x u) \tag{6}
\end{equation*}
$$

It is traditional to call the operator in (6) $L^{*}$ so that it's adjoint that appears in the backward equation can be called $L$.

If the distribution of $X(t)$ has a limit as $t \rightarrow \infty$, then we expect $u(x, t) \rightarrow$ $u_{0}(x)$ as $t \rightarrow \infty$. From the equation (5), this suggests that $u_{0}$ is a solution with $L^{*} u_{0}=0$. This gives

$$
\frac{\sigma^{2}}{2} \partial_{x}^{2} u+\mu \partial_{x}(x u)=0
$$

If $u_{0} \rightarrow 0$ as $x \rightarrow \infty$ together with its derivatives, this may be integrated to

$$
\frac{\sigma^{2}}{2} \partial_{x} u_{0}+\mu x u_{0}=0
$$

The solution takes the form $u_{0}(x)=C e^{-x^{2} / 2 \rho}$, with $\rho=\sigma^{2} / 2 \mu$.
We are interested in the rate of convergence $u(\cdot, t) \rightarrow u_{0}$, which depends on the other eigenvalues of the operator $L^{*}$. That is, we seek functions

$$
\begin{equation*}
L^{*} u_{k}=\frac{\sigma^{2}}{2} \partial_{x}^{2} u_{k}(x)+\mu \partial_{x}\left(x u_{k}\right)=-\lambda_{k} u_{k} \tag{7}
\end{equation*}
$$

It turns out that the solutions have the form $u_{k}(x)=\partial_{x}^{k} u_{0}$. We verify this by induction on $k$, the case $k=0$ having been done above. The trick for doing the calculation is the "differentiation by parts" formula $f \partial_{x} g=\partial_{x}(f g)-\left(\partial_{x} f\right) g$. If $f=\partial_{x}^{k-1} u_{0}$ and $g=x$, the result is

$$
x \partial_{x}^{k} u_{0}=\partial_{x}\left(x \partial_{x}^{k-1} u_{0}\right)-\partial_{x}^{k-1} u_{0}
$$

Therefore, using $L^{*} u_{k-1}=-\lambda_{k-1} u_{k-1}$,

$$
\begin{aligned}
L^{*} u_{k}=L^{*} \partial_{x} u_{k-1} & =\frac{\sigma^{2}}{2} \partial_{x}^{2} \partial_{x} u_{k-1}+\mu \partial_{x}\left(x \partial_{x} u_{k-1}\right) \\
& =\partial_{x}\left(\frac{\sigma^{2}}{2} \partial_{x}^{2} u_{k-1}\right)+\partial_{x}\left(\mu \partial_{x}\left(x u_{k-1}\right)\right)-\mu \partial_{x} u_{k-1} \\
& =\partial_{x}\left(L^{*} u_{k-1}\right)-\mu u_{k}=-\left(\lambda_{k-1}+\mu\right) u_{k}
\end{aligned}
$$

This shows that $L^{*} u_{k}=-\lambda_{k} u_{k}$ with $\lambda_{k}=\lambda_{k-1}+\mu$. To conclude, the eigenvalues are 0 (the steady state), $-\mu,-2 \mu$, etc. The corresponding eigenfunctions are derivatives of Gaussians, which is to say, given by Hermite polynomials (more on this below).

We use the above information to describe the behavior of the probability density $u(x, t)$. The solution of the evolution equation (5) is a linear combination of eigenfunctions:

$$
\begin{equation*}
u(x, t)=\sum_{k=0}^{\infty} a_{k} e^{-k \mu t} u_{k}(x) \tag{8}
\end{equation*}
$$

where the coefficients are determined by the initial data $u(x, 0)$. The $k=0$ term corresponds to the steady state solution $a_{0} u_{0}(x)$. All the other terms decay with various exponential rates. Slowest to decay is the $k=1$ term, which will make up most of the difference between $u(x, t)$ and $a_{0} u_{0}(x)$ for large $t$ :

$$
u(x, t)-a_{0} u_{0}(x) \approx a_{1} e^{-\mu t} u_{1}(x), \quad \text { for large } t
$$

It may not be surprising that the exponential decay rate $\mu$ in (2) results in the same exponential decay rate for $u(x, t)-a_{0} u_{0}(x)$. What is new in the PDE solution is the family of faster decay rates $2 \mu, 3 \mu$, etc. We will find versions of this phenomenon in any linear Gaussian process.

There are many practical applications for this kind of analysis. One concerns dynamic sampling methods, also called Markov Chain Monte Carlo. A complicated probability distribution may not have an efficient simple sampler, but there may be a dynamic process, a Markov Chain, that preservers the distribution. Here, the dynamical process (2) preserves the Gaussian $C e^{-x^{2} / 2 \rho}$. A major issue for dynamic samplers is the rate of convergence: How long do you have to run the process before the distribution of $X(t)$ closely approximates $u_{0}(x)$. In this simple problem, the convergence time is of the order of $1 / \mu$, which also is the decay rate for the linear Gaussian process (2).

### 3.1 Hermite polynomials

Hermite polynomials have many applications in Monte Carlo and other parts of applied probability. The $n^{t h}$ Hermite polynomial, $H_{n}(x)$, is defined by

$$
\begin{equation*}
H_{n}(x) e^{-x^{2} / 2}= \pm \partial_{x}^{n} e^{-x^{2} / 2} \tag{9}
\end{equation*}
$$

The calculations $\partial_{x} e^{-x^{2} / 2}=-x e^{-x^{2} / 2}$ and $\partial_{x}^{2} e^{-x^{2} / 2}=\left(x^{2}-1\right) e^{-x^{2} / 2}$, and $\partial_{x}^{3} e^{-x^{2} / 2}=\left(-x^{3}-3 x\right) e^{-x^{2} / 2}$ imply that the first few polynomials are $H_{0}(x)=1$, $H_{1}(x)=x, H_{2}(x)=x^{2}-1$ and $H_{3}(x)=x^{3}-3 x$. It is common to choose the sign so that the leading term is positive and also to choose the sign itself always to be positive (which would give $H_{1}(x)=-x$ ). It is easy to verify by induction that (9) defines polynomials of degree $n$ with leading coefficient equal to $\pm 1$.

The $H_{n}$ have the orthogonality property that

$$
\begin{equation*}
\int_{-\infty}^{\infty} H_{n}(x) H_{m}(x) e^{-x^{2} / 2} d x=0, \quad \text { for } n \neq m \tag{10}
\end{equation*}
$$

We briefly indicate a proof of this by induction on $m$, assuming $m<n$, since a better proof will come shortly. Actually, we prove (10) holds for a given $m$ and all $n>m$ by induction on $m$. It clearly is true for $m=0$, because then it just is $\int \partial_{x}^{n} e^{-x^{2} / 2} d x=0$. Now assume it is true for $m-1$ and try to prove it for $m$. The rewrite of (9) as $H_{m}(x)=e^{x^{2} / 2} \partial_{x}^{m} e^{-x^{2} / 2}$ puts (10) in the form

$$
\int_{-\infty}^{\infty} e^{x^{2} / 2}\left(\partial_{x}^{n} e^{-x^{2} / 2}\right)\left(\partial_{x}^{m} e^{-x^{2} / 2}\right) d x=0
$$

Write $\partial_{x}^{m}=\partial_{x} \partial_{x}^{m-1}$ and integrate by parts, and we get the two terms

$$
\begin{aligned}
& -\int_{-\infty}^{\infty} e^{x^{2} / 2}\left(\partial_{x}^{n+1} e^{-x^{2} / 2}\right)\left(\partial_{x}^{m-1} e^{-x^{2} / 2}\right) d x \\
& \quad-\int_{-\infty}^{\infty} e^{x^{2} / 2}\left(x \partial_{x}^{n} e^{-x^{2} / 2}\right)\left(\partial_{x}^{m-1} e^{-x^{2} / 2}\right) d x
\end{aligned}
$$

The top term is zero by the induction hypothesis, which is why we used a more complex induction hypothesis. We study the bottom term using something similar to the differentiation by parts idea above, namely the formula $x \partial_{x}^{n} f=$ $\partial_{x}^{n}(x f)-n \partial_{x}^{n-1} f$. This implies that the bottom term is

$$
\begin{aligned}
& \int_{-\infty}^{\infty} e^{x^{2} / 2} \partial_{x}^{n}\left(x e^{-x^{2} / 2}\right)\left(\partial_{x}^{m-1} e^{-x^{2} / 2}\right) d x \\
& \quad-n \int_{-\infty}^{\infty} e^{x^{2} / 2}\left(\partial_{x}^{n-1} e^{-x^{2} / 2}\right)\left(\partial_{x}^{m-1} e^{-x^{2} / 2}\right) d x
\end{aligned}
$$

The bottom term is zero because $m-1<n-1$. The top term is zero because $x e^{-x^{2} / 2}=-\partial_{x} e^{-x^{2} / 2}$, so it is equal to

$$
-\int_{-\infty}^{\infty} e^{x^{2} / 2}\left(\partial_{x}^{n+1} e^{-x^{2} / 2}\right)\left(\partial_{x}^{m-1} e^{-x^{2} / 2}\right) d x=0
$$

again by induction.
The orthogonality property of Hermite polynomials gives a different way to find them. This is because of the fact that if $p(x)$ is a polynomial of degree $n$ if and only if it may be written as a sum of Hermite polynomials of order not more than $n$ :

$$
p(x)=\sum_{m=0}^{n} a_{m} H_{m}(x)
$$

Therefore, (10) is true for a given $n$ and all $m<n$ if and only if

$$
\int H_{n}(x) x^{m} e^{-x^{2} / 2} d x=0
$$

for all $m<n$. This is the same as saying that $E\left[H_{n}(X) X^{m}\right]=0$ for all $m<n$, where $X$ is a standard normal random variable. We compute the first few that way. Of course, $H_{0}(x)=1 . H_{1}(x)$ is the polynomial of degree 1 that is orthogonal to $X^{0}=1$, which is to say $H_{1}(x)=x$. Next, $H_{2}(x)$ is the quadratic that is orthogonal to $x$ and 1 . We achieve $E\left[H_{2}(X) X\right]=0$ if $H$ has the form $x^{2}-a$. We achieve $E\left[H_{2}(X) X^{0}\right]=E\left[H_{2}(X)\right]=0$ if $a=E\left[X^{2}\right]=1$, i.e. if $H_{2}(x)=x^{2}-1$. Finally, we want $H_{3}(x)=x^{3}-a x^{2}-b x-c$ to make $H_{3}$ orthogonal to $1, x$, and $x^{2}$. The even powers are automatic if $H_{3}(x)$ is odd, i.e. if $H_{3}(x)=x^{3}-b x$. The remaining orthogonality condition $E\left[H_{3}(X) X\right]=$ 0 is $E\left[X^{4}\right]-b E\left[X^{2}\right]=0$, which gives $b=3$, as claimed above. It is the orthogonality properties of Hermite polynomials that makes them handy, for
example, in finding kernel functions for density estimation that satisfy several moment conditions.

In the slightly more general situation of $e^{-x^{2} / 2 \rho}$, we can define $H_{n}(x, \rho)=$ $e^{x^{2} / 2 \rho} \partial_{x}^{n} e^{-x^{2} / 2 \rho}$. These polynomials are orthogonal in the natural sense

$$
\int_{-\infty}^{\infty} H_{n}(x, \rho) H_{m}(x, \rho) e^{-x^{2} / 2 \rho} d x=0
$$

for $m \neq n$. The proof is the same as above.

### 3.2 Adjoint eigenfunctions

The operator $L^{*}$ has an adjoint operator, $L$. The eigenvalues of $L^{*}$ and $L$ are the same but the eigenfunctions are different. The eigenfunctions of $L$ are used to determine the expansion coefficients $a_{k}$ in (8). Later we will find a way to derive the adjoint eigenfunctions directly from the $u_{n}$ using the principle of detailed balance.

We explain the ideas in a finite dimensional setting. Suppose $A$ is an $n \times$ $n$ matrix. The right eigenvectors of $A$ are $v_{k}$ with $A v_{k}=\lambda_{k} v_{k}$. The left eigenvectors are row vectors $u_{k}$ with $u_{k} A=\lambda_{k} u_{k}$. This is the same as $A^{*} u_{k}^{*}=$ $\lambda_{k} u_{k}^{*}$. That is, the left eigenvectors of $A$ (when written as column vectors) are the right eigenvectors of the adjoint (transpose) of $A$. The eigenvalues $\lambda_{k}$ are the same. The right and left eigenvectors satisfy biorthogonality relations $u_{k} v_{l}=0$ if $\lambda_{k} \neq \lambda_{l}$.

For column vectors $f$ and $g$, let $(f, g)$ be the $l^{2}$ inner product $(f, g)=f^{*} g=$ $\sum_{k=1}^{n} f_{k} g_{k}$. The adjoint of the $n \times n$ matrix $A$ is defined by the property that it should satisfy $\left(A^{*} f, g\right)=(f, A g)$ for all vectors $f$ and $g$ (check this). It is possible to define other inner products. The one that will be useful for us is the weighted $l^{2}$ inner product $\langle f, g\rangle_{w}=\sum_{k=1}^{n} f_{k} g_{k} w_{k}$, where the $w_{k}$ are $n$ positive weights. Each weighted norm determines a different $A^{*}$ through the property $\left\langle A^{*} f, g\right\rangle_{w}=\langle f, A g\rangle_{w}$ for all $f$ and $g$. In this case, the elements of $A^{*}$ are given by $A_{j k}^{*}=A_{k j} w_{k} / w_{j}$ (check this). The eigenvalues of $A^{*}$ are the same as the eigenvalues of $A$ (for example, because $A^{*}$ is similar to the transpose of $A$ ). The eigenvectors satisfy the natural biorthogonality relation: If $A v_{j}=\lambda_{j} v_{j}$ and $A^{*} u_{k}=\lambda_{k} u_{k}$ with $\lambda_{j} \neq \lambda_{k}$, then $\left\langle u_{k}, v_{j}\right\rangle_{w}=0$ (check this).

Back to $L^{*}$, we compute the adjoint in the $L^{2}$ inner product $(f, g)=$ $\int_{-\infty}^{\infty} f(x) g(x) d x$. This adjoint is defined by the requirement that for all functions for which the computation makes sense: $\left(L^{*} f, g\right)=(f, L g)$. This is done by integration by parts:

$$
\begin{aligned}
\left(L^{*} f, g\right) & =\int_{-\infty}^{\infty}\left(L^{*} f(x)\right) g(x) d x \\
& =\int_{-\infty}^{\infty}\left(\frac{\sigma^{2}}{2} \partial_{x}^{2} f(x)+\mu \partial_{x}(x f(x))\right) g(x) d x \\
& =\int_{-\infty}^{\infty} f(x)\left(\frac{\sigma^{2}}{2} \partial_{x}^{2} g(x)-\mu x \partial_{x} g(x)\right) d x
\end{aligned}
$$

$$
=\int_{-\infty}^{\infty} f(x)(L g(x)) d x,
$$

with

$$
\begin{equation*}
L g(x)=\frac{\sigma^{2}}{2} \partial_{x}^{2} g(x)-\mu x \partial_{x} g(x) \tag{11}
\end{equation*}
$$

Note that the second derivative terms in $L^{*}$ and $L$ are the same while the first derivative terms change sign. Also, the $x$ is inside the differentiation in $L^{*}$ but outside in $L$.

It turns out that the eigenfunctions of $L$ are Hermite polynomials $v_{k}(x)=$ $H_{k}(x, \rho)=e^{x^{2} / 2 \rho} \partial_{x}^{k} e^{-x^{2} / 2 \rho}$. The biorthogonality relation $\left(u_{j}, v_{k}\right)=0$ for $j \neq k$ is the orthogonality relation for Hermite polynomials, given that $u_{j}=$ $\partial_{x}^{j} e^{-x^{2} / 2 \rho}=H_{j}(x, \rho) e^{-x^{2} / 2 \rho}$. The eigenvalue relation $L v_{k}=-k \mu v_{k}$ can be verified by induction on $k$ using the recurrence relation (one of many) $v_{k+1}(x)=$ $\frac{-x}{\rho} v_{x}(x)+\partial_{x} v_{k}(x)$.

### 3.3 Detailed balance

So, the eigenfunctions of $L^{*}$ and those of $L$ differ only by the exponential factor $e^{-x^{2} / 2 \rho}$. The $L^{*}$ eigenfunctions have it and the $L$ eigenfunctions do not. This suggests that is a relationship between $L$ and $L^{*}$ that goes beyond one being the adjoint of the other. This relation is that in a suitable inner product, the adjoint of $L$ is equal to $L$ itself. This implies that $L$ is similar to $L^{*}$ with the similarity given by the weight used for the inner product. All of this is related to the ${ }^{1}$ "principle" detailed balance.

There are many formulations of the detailed balance condition. One of them (which is not the origin of the name) is that $L$ should be self adjoint in the inner product given by the steady state $u_{0}$. If $w(x)$ is a non negative weight function, the weighted $L^{2}$ inner product is

$$
\langle f, g\rangle_{w}=\int_{-\infty}^{\infty} f(x) g(x) w(x) d x
$$

$L$ is self adjoint in this inner product if $\langle L f, g\rangle_{w}=\langle f, L g\rangle_{w}$, for all sufficiently regular functions $f$ and $g$. A direct calculation shows that the $L$ in (11) is self-adjoint in the weighted norm with $w(x)=u_{0}(x)=e^{-x^{2} / 2 \rho}$.

Detailed balance implies a relation between the eigenfunctions of $L$ and those of $L^{*}$. We can see this from a formula relating $L$ to $L^{*}$ derived as follows:

$$
\begin{aligned}
\langle f, L g\rangle_{u_{0}} & =\int_{-\infty}^{\infty} f(x)(L g(x)) u_{0}(x) d x \\
& =\int_{-\infty}^{\infty}\left(L^{*}\left(u_{0} f\right)(x)\right) g(x) d x \\
& =\int_{-\infty}^{\infty}\left(\frac{1}{u_{0}(x)} L^{*}\left(u_{0} f\right)(x)\right) g(x) u_{0}(x) d x
\end{aligned}
$$

[^0]$$
\langle f, L g\rangle_{u_{0}}=\left\langle\frac{1}{u_{0}} L^{*}\left(u_{0} f\right), g\right\rangle_{u_{0}}
$$

This, together with the detailed balance condition $\langle f, L g\rangle_{u_{0}}=\langle L f, g\rangle_{u_{0}}$, implies (because it holds for every $g$ ) that

$$
\begin{equation*}
u_{0} L f=L^{*}\left(u_{0} f\right) \tag{12}
\end{equation*}
$$

Applying this with $f=v_{j}$ and $L v_{j}=\lambda_{j} v_{j}$ shows that $u_{j}=u_{0} v_{j}$ satisfies

$$
L^{*} u_{j}=L^{*} u_{0} v_{j}=u_{0} L v_{j}=u_{0} \lambda_{j} v_{j}=\lambda_{j} u_{j}
$$

which is to say that $u_{j}$ is an eigenfunction of $L^{*}$ with eigenvalue $\lambda_{j}$. This is the eigenfunction relation we found above.

The detailed balance condition has a reformulation in terms of transition probabilities. The transition probability density is the probability density for $X(t)$ given that $X(0)=x_{0}$. We write this as $u\left(x_{0}, x, t\right)$, the probability (density) of going from $x_{0}$ to $x$ in time $t$. From (3) and (4), we see that the conditional distribution of $X(t)$ is that of a Gaussian with mean $x_{0} e^{-\mu t}$ and variance $\rho(t)=$ $\frac{\sigma^{2}}{2 \mu}\left(1-e^{-2 \mu t}\right)$. This implies that

$$
u\left(x_{0}, x, t\right)=\frac{1}{\sqrt{2 \pi \rho(t)}} \exp \left(-\left(x-x_{0} e^{-\mu t}\right)^{2} / 2 \rho(t)\right)
$$

Now suppose we sample $x_{0}$ from the steady state density $u_{0}\left(x_{0}\right)=C e^{-x_{0}^{2} / 2 \rho}$. The probability density to observe a transition from $x_{0}$ to $x$ is the probability of first choosing $X(0)=x_{0}$, then making a transition from that $x_{0}$ to $x$ :

$$
\begin{aligned}
r\left(x_{0}, x, t\right) & =u_{0}\left(x_{0}\right) u\left(x_{0}, x, t\right) \\
& =C e^{-x_{0}^{2} / 2 \rho} \frac{1}{\sqrt{2 \pi \rho(t)}} \exp \left(-\left(x-x_{0} e^{-\mu t}\right)^{2} / 2 \rho(t)\right)
\end{aligned}
$$

Calculating the exponents shows that

$$
r\left(x_{0}, x, t\right)=C e^{-x_{0}^{2} / 2 \rho} \frac{1}{\sqrt{2 \pi \rho(t)}} \exp \left\{\frac{-1}{2 \rho}\left(\frac{x_{0}^{2}+x^{2}}{1-e^{-2 \mu t}}-\frac{2 x_{0} x e^{-\mu t}}{1-e^{-2 \mu t}}\right)\right\}
$$

The interesting thing about this formula is that it symmetric in $x$ and $x_{0}$. In other words, the probability of observing an $x_{0} \rightarrow x$ transition is the same as the probability of observing an $x \rightarrow x_{0}$ transition.

This is the principle of detailed balance: In steady state, the probability of observing the transition $y \rightarrow x$ is the same as the probability of observing $x \rightarrow y$. It is called "detailed" balance because it is a more restrictive than the simple balance condition required for $u_{0}$ to be the steady state. Suppose $u\left(x_{0}, x, t\right)$ is any transition density, not necessarily related to the Ornstein Uhlenbeck process. A probability density $u_{0}(x)$ is a steady state for $u$ if it satisfies the balance condition

$$
u_{0}(x)=\int u_{0}\left(x_{0}\right) u\left(x_{0}, x, t\right) d x_{0}
$$

for all $x$. If $u_{0}\left(x_{0}\right) u\left(x_{0}, x, t\right)=u_{0}(x) u\left(x, x_{0}, t\right)$ for all $x_{0}$ and $x$, then we can integrate with respect to $x_{0}$ using the fact that $\int u\left(x, x_{0}, t\right) d x_{0}=1$ for all $x$ (because $u$ is a transition density) and see that $u_{0}$ satisfies the balance condition to be a steady state. It will turn out that detailed balance is a particularly useful way to satisfy the balance condition, even though it is not necessary for balance.

These two forms of the detailed balance condition, $\langle f, L g\rangle_{u_{0}}=\langle L f, g\rangle_{u_{0}}$ and the symmetry of $r$, are closely related. In finite dimensional space and without weights, this relation is that if $A$ is a symmetric matrix, then $S(t)=e^{t A}$ also is symmetric.

### 3.4 Multidimensional processes

A multidimensional Ornstein Uhlenbeck process is a linear process with linear constant intensity random forcing. If $\mu$ is an $n \times n$ matrix and $\sigma$ is an $n \times$ $m$ matrix (neither needs to be symmetric), and $W(t)=\left(W_{1}(t), \ldots, W_{m}(t)\right)$ is an $m$ dimensional standard Brownian motion whose components $W_{k}(t)$ are independent, then we can interpret (2) as an equation for the evolution of $X(t)=$ $\left(X_{1}(t), \ldots, X_{n}(t)\right)$. The case $m<n$ is common. In this case, $\sigma$ has more rows than columns. The case $m>n$ is pointless and we never consider it.

The solution formula (3) is almost correct, provided that we interpret $e^{\mu t}$ as the matrix exponential that satisfies $\partial_{t} e^{\mu t}=\mu e^{\mu t}$. The only modification is that $\sigma e^{\mu(T-t)}$ does not make sense because it is not compatible for matrix multiplication if $m<n$. The correct form is (check this)

$$
\begin{equation*}
X(T)=e^{-\mu t} X(0)+\int_{0}^{T} e^{\mu(T-t)} \sigma d W(t) \tag{13}
\end{equation*}
$$

This formula shows that if $X(0)$ is Gaussian or deterministic, then $X(T)$ also is Gaussian for all $T>0$. Therefore, we can identify the limiting density of $X(T)$ as $T \rightarrow \infty$ by figuring out the limiting mean and covariance matrix. The limit will exist if the ODE $\dot{x}=-\mu x$ is strongly stable, which is the same as the eigenvalues of $\mu$ having positive real parts ${ }^{2}$. The mean $m(t)=E[X(t)]$ satisfies the simple differential equation

$$
d m=d E[X(t)]=E[d X]=E[-\mu X d t]+\sigma E[d W]=-\mu m d t
$$

This shows that $m(t) \rightarrow 0$ as $t \rightarrow \infty$ as expected.
The covariance matrix calculation is similar. Let $\rho(x)=E\left[X(t) X^{*}(t)\right]$ be the covariance matrix at time $t$. Using the Ito calculus and the fact that $E[Q(t) d W(t)]=0$ for any $Q(t)$ defined by time $t$, we have

$$
\begin{aligned}
d \rho & =d E\left[X(t) X^{*}(t)\right] \\
& =E\left[(d X) X^{*}\right]+E\left[X\left(d X^{*}\right)\right]+E\left[(d X)\left(d X^{*}\right)\right] \\
& =E\left[-\mu X d t X^{*}\right]+E\left[X\left(-X^{*} \mu^{*} d t\right)\right]
\end{aligned}
$$

[^1]\[

$$
\begin{aligned}
& =-\mu E\left[X X^{*}\right] d t-E\left[X X^{*}\right] \mu^{*} d t+E\left[\sigma d W d W^{*} \sigma^{*}\right] \\
& =\left\{-\left(\mu \rho+\rho \mu^{*}\right)+\sigma \sigma^{*}\right\} d t
\end{aligned}
$$
\]

The matrix differential equation

$$
\begin{equation*}
\dot{\rho}=-\left(\mu \rho+\rho \mu^{*}\right)+\sigma \sigma^{*} \tag{14}
\end{equation*}
$$

is an example of a class of equations called Liapounov equations or Ricatti equations, though Ricatti equations usually are quadratically nonlinear instead of linear as (14). The limit $\rho=\lim _{t \rightarrow \infty} \rho(t)$ is found by setting $\dot{\rho}=0$ and solving the resulting algebraic equations.

The correct multicomponent generalization of (4) is (check this)

$$
\rho(t)=\int_{0}^{t} e^{-(t-s) \mu} \sigma \sigma^{*} e^{-(t-s) \mu^{*}} d s
$$

It is easy to check that this satisfies (14) and that the integral is positive (as a matrix) for all $t$. Even if $\sigma$ does not have full rank, $\rho(t)$ will be positive definite if the matrix with many columns

$$
K=\left(\sigma|\mu \sigma| \mu^{2} \sigma|\cdots| \mu^{n}\right)
$$

has rank $n$. This is a theorem of R. Kalman (proof omitted but not that difficult). The limit value is

$$
\rho=\lim _{t \rightarrow \infty} \rho(t)=\int_{0}^{\infty} e^{-t \mu} \sigma \sigma^{*} e^{-t \mu^{*}} d t
$$

Techniques of numerical linear algebra give a way to calculate, and show it is unique, $\rho$ without doing the integral. As for any square matrix, $\mu$ may be put in upper Schur form using an orthogonal change of coordinates. That is, there is an $n \times n$ matrix, $Q$ with $Q Q^{*}=I$ so that $\mu=Q L Q^{*}$, where $L$ is upper triangular with the eigenvalues of $\mu$ on the diagonal. Writing $\sigma \sigma^{*}=D$, this puts $\mu \rho+\rho \mu^{*}=\sigma \sigma^{*}$ in the form

$$
Q L Q^{*} \rho+\rho Q^{*} L^{*} Q=D
$$

Note that the elements of $L$ and $Q$ may be complex, particularly if the eigenvalues of $\mu$ are not real. Now multiply from the left by $Q^{*}$ and from the right by $Q$ to get

$$
L \widetilde{\rho}+\widetilde{\rho} L^{*}=\widetilde{D}
$$

where $\widetilde{\rho}=Q^{*} \rho Q$ and $\widetilde{D}=Q^{*} D Q$. This allows us to calculate the elements of $\widetilde{\rho}$ one by one as is done in back substitution. First, $L_{11} \widetilde{\rho}_{11}+\widetilde{\rho}_{11} \bar{L}_{11}=\widetilde{D}_{11}\left(A_{j k}\right.$ is the $(j, k)$ entry of $A, \bar{z}$ is the complex conjugate of $z)$. So, since $\operatorname{Re}\left(L_{11}\right)>0>0$ (by hypothesis on $\mu$ ), $\widetilde{\rho}_{11}=\widetilde{D}_{11} / 2 \operatorname{Re}\left(L_{11}\right)>0$ is determined. The rest of the elements of $\widetilde{\rho}$ can be computed one by one in a similar way. Finally, we have $\rho=Q \widetilde{\rho} Q^{*}$.

Now that we know the multidimensional process has a steady state, we can look for eigenfunctions that describe the rate of convergence to steady state. The probability density for $X(t)$ satisfies the forward equation

$$
\partial_{t} u=L^{*} u=\frac{1}{2} \sum_{i j} D_{i j} \partial_{x_{i}} \partial_{x_{j}} u+\sum_{i} \partial_{x_{i}}\left(\sum_{j} \mu_{i j} x_{j} u\right)
$$

again with $D=\sigma \sigma^{*}$. A calculation shows that if $u_{0}(x)=C e^{-x^{*} H x / 2}$ with $H=\rho^{-1}$ (so that $\mu \rho+\rho \mu^{*}=D$ is equivalent to $H \mu+\mu^{*} H=H D H$ ), then $L^{*} u_{0}=0$. This is the steady state density, which we already knew from the covariance calculations above.

Finding the rest of the eigenfunctions is simpler if we assume that $\mu$ has $n$ real eigenvalues and linearly independent eigenvectors. The construction is an induction as in the one dimensional case. Suppose $w$ is an eigenvector of $\mu$ and satisfies $\mu w=\alpha w$. Suppose that $L^{*} u=\lambda u$. Then $v=(w \cdot \nabla) u$ satisfies $L^{*} v=\lambda v-\alpha v$, as we now verify. These calculations are simpler using the summation convention, which allows formulas such as $(w \cdot \nabla) u=w_{k} \partial_{x_{k}} u$. The calculation concerns only the second term

$$
\begin{aligned}
\partial_{x_{i}}\left(\mu_{i j} x_{j} w_{k} \partial_{x_{k}} u\right) & =w_{k} \partial_{x_{k}}\left\{\partial_{x_{i}}\left(\mu_{i j} x_{j} u\right)\right\}-\partial_{x_{i}}\left(\mu_{i j} \delta_{j k} w_{k} u\right) \\
& =w_{k} \partial_{x_{k}}\left\{\partial_{x_{i}}\left(\mu_{i j} x_{j} u\right)\right\}-\partial_{x_{i}}\left(\mu_{i j} w_{j} u\right) \\
& =w_{k} \partial_{x_{k}}\left\{\partial_{x_{i}}\left(\mu_{i j} x_{j} u\right)\right\}-\alpha w_{i} \partial_{x_{i}} u \\
& =w_{k} \partial_{x_{k}}\left\{\partial_{x_{i}}\left(\mu_{i j} x_{j} u\right)\right\}-\alpha v
\end{aligned}
$$

Therefore,

$$
L^{*} v=L^{*}\{(w \cdot \nabla) u\}=(w \cdot \nabla) L^{*} u-\alpha v=\lambda v-\alpha v
$$

as claimed. Therefore, if $\alpha_{1}, \ldots, \alpha_{n}$ are the eigenvalues of $\mu$ with corresponding eigenvectors $w_{k}$, and if $p=\left(p_{1}, \ldots, p_{n}\right)$ is a sequence of non-negative integers, then

$$
u_{p}=\left(w_{1} \cdot \nabla\right)^{p_{1}} \cdots\left(w_{n} \cdot \nabla\right)^{p_{n}} u_{u}
$$

satisfies

$$
L^{*} u_{p}=-\left(p_{1} \alpha_{1}+\cdots+p_{n} \alpha_{n}\right) u_{p} .
$$

The rest of the structure of the one dimensional problem also generalizes. Let $d=p_{1}+\cdots+p_{n}$ be the degree of $u_{p}$, then $u_{p}=H_{p}(x, \rho) u_{0}$, where $H_{p}$ is a polynomial of degree $d$. These are eigenfunctions of $L: L H_{p}=$ $-\left(p_{1} \alpha_{1}+\cdots+p_{n} \alpha_{n}\right) H_{p}$. They satisfy the orthogonality relation $\left\langle H_{p}, H_{q}\right\rangle_{u_{0}}=$ 0 if $p \neq q$. Let $\mathcal{S}_{d}$ be the space of all polynomials of degree at most $d$. Then the polynomials $H_{p}$ with the degree of $p$ not more than $d$ is a basis for $\mathcal{S}_{d}$. Moreover, let $\mathcal{T}_{d}$ be the orthogonal complement of $\mathcal{S}_{d-1}$ in $\mathcal{S}_{d}$ in the $u_{0}$ weighted inner product. Then the $H_{p}$ with the order of $p$ equal to $d$ form a basis of $\mathcal{T}_{d}$.

### 3.5 Example

We consider a discrete approximation to the heat equation in notation adapted to the above discussion. Let $x(r, t)$ be the temperature at location $r$ at time $t$. Suppose this satisfies

$$
\partial_{t} x=\frac{1}{2} \partial_{r}^{2} x
$$

with boundary conditions $x(0, t)=x(1, t)=0$. Approximate the heat equation using $n$ equally spaced points $r_{j}=j \Delta r$. Let $x_{j}(t)$ be the approximation to $x\left(r_{j}, t\right)$. The approximation to the heat equation is

$$
\dot{x}_{j}=\frac{1}{2} \frac{x_{j+1}-2 x_{j}+x_{j-1}}{\Delta r^{2}} .
$$

This can be written as $\dot{x}=-\mu x$, where $\mu$ (up to a constant multiple) is the $(n-1) \times(n-1)$ matrix we encountered earlier as the inverse of the covariance matrix for Brownian motion constrained to have $X(0)=X(1)=0$.

If we add noise, the dynamics become

$$
\begin{equation*}
d X_{j}=\frac{1}{2 \Delta r^{2}}\left(X_{j+1}-2 X_{j}+X_{j-1}\right)+\sigma d W_{j} \tag{15}
\end{equation*}
$$

The steady state covariance satisfies ( $\mu$ being symmetric) $\mu \rho+\rho \mu=\sigma I$, so $\rho=\frac{1}{2 \sigma} \mu^{-1}$. We have seen that the eigenvalues of $\mu$ are

$$
\alpha_{k}=\frac{1-\cos (k \pi \Delta r)}{\Delta r^{2}}
$$

For small $k$, these are approximately $\alpha_{k}=\pi^{2} k^{2} / 2$. Therefore, the smallest eigenvalues of $L^{*}$ for (15) are $\lambda=-\alpha_{1} \approx-\pi^{2} / 2, \lambda=-\alpha_{2} \approx-2 \pi^{2}, \lambda=$ $-2 \alpha_{1} \approx-\pi^{2}, \lambda=-\alpha_{1}-\alpha_{2} \approx \frac{5}{2} \pi^{2}$, etc. Note that the slowest mode is a linear mode, but the second slowest is quadratic and the third slowest is cubic $\left(-3 \alpha_{3}\right)$.

The fastest linear mode is $-\alpha_{n} \approx 2 / \Delta r^{2}$. The matrix $\mu$ is ill conditioned for large $n$, which means that it has a wide range of eigenvalues: $\alpha_{1} / \alpha_{n}=O\left(n^{2}\right)$. This causes significant difficulties for Markov Chain Monte Carlo algorithms that use dynamics like (15).

## 4 Stochastic Differential Equations

A stochastic differential equation takes the form

$$
\begin{equation*}
d X=a(X(t), t) d t+b(X(t), t) d W(t) \tag{16}
\end{equation*}
$$

The solution, $X(t)$, is a continuous but random function of $t$. It in the multicomponent case, $X(t)=\left(X_{1}(t), \ldots, X_{n}(t)\right)$. In this case the drift "coefficient", $a(x, t)$, has $n$ components and the noise coefficient, $\sigma(x, t)$, is an $n \times m$ matrix with $m \leq n$. The source of noise is $m$ independent Brownian motion components $W(t)=\left(W_{1}(t), \ldots, W_{m}(t)\right)$.

The interpretation of (16) is subtle in ways we will not explore completely here. However, one way to define the solution is as the limit of forward Euler approximations. Choose a time step $h$ and times $t_{k}=k h$. The approximation solution, $X^{h}(t)$, is defined by

$$
\begin{equation*}
X^{h}\left(t_{n+1}\right)=X^{h}\left(t_{n}\right)+a\left(X^{h}\left(t_{n}\right), t_{n}\right) h+b\left(X^{h}\left(t_{n}\right), t\right)\left(W\left(t_{n+1}\right)-W\left(t_{n}\right)\right) . \tag{17}
\end{equation*}
$$

According to this formula, to generate a forward Euler path, we must generate a Brownian motion path, then use (17) to generate the corresponding approximate sample path of (16) from it. More precisely, for fixed $W$ and $T$, we imagine a sequence of $h$ values converging to zero and define

$$
X(W[0, T], T)=\lim _{h \rightarrow 0} X^{h}(W[0, T], T)
$$

Writing $f(W[0, T])$ means that $f$ depends on the values of $W(t)$ for all $t$ in the range $0 \leq t \leq T$. It is convenient for theoretical discussion to consider $X^{h}$ to be defined for all $t$, not just the discrete times $t_{n}$. We do this using piecewise linear interpolation.

The strong accuracy of the Euler method (17) measures the expected difference between $X^{h}$ and $X$. Here and everywhere below we do not indicate the dependence of $X$ or $X^{h}$ on $W$, though it still does. Strong accuracy of order $p$ means that

$$
\begin{equation*}
E\left[\left|X^{h}(T)-X(T)\right|\right]=O\left(h^{p}\right) \tag{18}
\end{equation*}
$$

The Euler method (17) satisfies this with $p=1 / 2$. We will see in examples that this is sharp in the sense that the expected error is of the order of $h^{1 / 2}$ and not smaller. The relation (18) is an $L^{1}$ estimate, which is hard to approach by direct computation. The standard way to approach it is with the $L^{2}$ estimate

$$
\begin{equation*}
E\left[\left|X^{h}(T)-X(T)\right|^{2}\right]=O\left(h^{2 p}\right) \tag{19}
\end{equation*}
$$

This implies the $L^{1}$ estimate because of the Cauchy Schwarz inequality: If $Y$ and $Z$ are any random variables, then

$$
E[|Y Z|] \leq\left(E\left[Y^{2}\right] E\left[Z^{2}\right]\right)^{1 / 2}
$$

In particular, if $Z=1$, then $E[|Y|] \leq E\left[Y^{2}\right]^{1 / 2}$, which is how (18) follows from (19). Some people prefer to cite Jensen's inequality, which states that if $\phi(y)$ is a a convex function of $y$, then

$$
\phi(E[Y]) \leq E[\phi(Y)]
$$

Taking $\phi(y)=y^{2}$ then gives (18) from (19). Finally, versions of Doob's inequality from the theory of martingales allows us to strengthen either (18) or (19) to a statement about the path up to time $T$ :

$$
\begin{equation*}
E\left[\sup _{0 \leq t \leq T}\left|X^{h}(t)-X(t)\right|^{r}\right]=O\left(h^{r p}\right) \tag{20}
\end{equation*}
$$

for $r=1$ and $r=2$.
The main point is the proof of the single time $L^{2}$ bound (19). The basic reason for this is the reasoning behind the Euler scheme in the first place. The SDE (16) implies that

$$
\begin{equation*}
X(t+h)-X(t)=\int_{0}^{h} a(X(t+s)) d s+\int_{0}^{h} b\left(X\left(t_{s}\right)\right) d W(s) \tag{21}
\end{equation*}
$$

For small $h$, we assume that $X(t+s) \approx X(t)$. Using this in (21) gives

$$
\begin{equation*}
X(t+h)-X(t) \approx a(X(t)) h+b(X(t))(W(t+h)-W(t)) \tag{22}
\end{equation*}
$$

The first step here is to find bounds on how far $X$ can go in time $h$. For this we need assumptions on the coefficients $a$ and $b$. We simply assume they both are globally Lipschitz:

$$
\begin{equation*}
|a(x)-a(y)| \leq C|x-y| \quad, \quad|b(x)-b(y)| \leq C|x-y| \tag{23}
\end{equation*}
$$

We assume for simplicity of notation that $t=0$ and $X(0)=0$. The calculation illustrates the simplicity of $L^{2}$ estimates. To estimate $E\left[|X(t)|^{2}\right]$, we calculate

$$
\begin{aligned}
d|X(t)|^{2} & =2 X \cdot d X+d X^{*} d X \\
& =2 X a(X) d t+2 X b(X) d W+|b|^{2} d t
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\frac{d}{d t} E\left[|X|^{2}\right] & =2 E[X a(X)]+E\left[|b(X)|^{2}\right] \\
& \leq C\left(1+E\left[|X(t)|^{2}\right]\right)
\end{aligned}
$$

Now Gronwall's inequality (with $E\left[|X(0)|^{2}\right]=0$ ) implies that if $h<1$ then $E\left[|X(t)|^{2}\right] \leq C t$ for $0 \leq t \leq h$. More generally,

$$
\begin{equation*}
E\left[|X(t+s)-X(t)|^{2} \mid \mathcal{F}_{t}\right] \leq C\left(|X(t)|^{2}+1\right) s \tag{24}
\end{equation*}
$$

whenever $0 \leq s \leq h$.
With this, we can bound the error in approximating the terms in (21) by those in (22), again by estimating squares starting with the drift term

$$
R_{1}=E\left[\left(\int_{0}^{h}\{a(X(t+s))-a(X(t))\} d t\right)^{2}\right]
$$

The first step is to put the square inside the integral, which can be done using the Cauchy Schwarz inequality:

$$
\begin{aligned}
& \left(\int_{0}^{h} f(s) d s\right)^{2}=\left(\int_{0}^{h} f(s) \cdot 1 d s\right)^{2} \\
& \leq \int_{0}^{h} f(s)^{2} d s \cdot \int_{0}^{h} 1 d s=h \int_{0}^{h} f(s)^{2} d s
\end{aligned}
$$

With this, and (23) and (24), we find

$$
R_{1} \leq h C \int_{0}^{h} E\left[(X(t+s)-X(t))^{2} d s\right] \leq C h \int_{0}^{h} s d s=C h^{3}
$$

The noise term may be handled using the Ito isometry formula: If $f(t)$ is adapted to the Brownian motion $W(t)$, then

$$
E\left[\left(\int_{0}^{h} f(s) d W(s)\right)^{2}\right]=\int_{0}^{h} E\left[f(s)^{2}\right] d s
$$

This applies to the noise term in (21) as follows (with (23) and (24)):

$$
\begin{aligned}
R_{2} & =E\left[\left|\int_{0}^{h}(b(X(t+s))-b(X(t))) d W(s)\right|^{2}\right] \\
& =\int_{0}^{h} E\left[|b(X(t+s))-b(X(t))|^{2}\right] d s \\
& \leq C \int_{0}^{h} E\left[|X(t+s)-X(t)|^{2}\right] d s \\
& \leq C \int_{0}^{h} s d s=C h^{2}
\end{aligned}
$$

A little bit of formalism expresses the above analysis in a form that is helpful for the convergence proof. Let $\Psi(x, W[0, h], h)$ denote the solution to the SDE (16) with initial data $X(0)=x$ and noise path $W$. Then (21) may be written as

$$
X(t+h)=X(t)+\Psi(X(t), W[t, t+h], h),
$$

and the right side of (21) gives a formula for $\Psi$. Similarly, let $\Phi(x, W[0, h], h)$ denote the Euler approximation (17), so that

$$
X^{h}(t+h)=X^{h}(t)+\Phi\left(X^{h}(t), W[t, t+h], h\right) .
$$

The above analysis is a proof of the estimate

$$
\begin{equation*}
E\left[|\Psi(x, W[0, h], h)-\Phi(x, W[0, h], h)|^{2}\right] \leq C h^{2} \tag{25}
\end{equation*}
$$

Convergence proofs of computational methods often take the form of consistency and stability arguments. Roughly speaking, consistency is the fact that the computational method is consistent with the formulation of the limit problem. In the present case, the estimate (25) states that at least for one time step, the Euler method is consistent with the SDE. More technically, we might call $\Psi-\Phi$ truncation error. It is the ultimate source of the deviation between the paths $X(t)$ and $X^{h}(t)$. The size of the error is determined by the size of the right side of (25). Stability is the statement that small deviations between
$X$ and $X^{h}$ caused by truncation error are not amplified too much during the simulation process. Stability usually is the harder part, though here it is more complicated than hard. We do the stability argument only for the case with zero drift. Even though drift is the smaller source of error it is the larger source of technical complexity of a not very interesting kind.

To treat the error, we put the two recurrence relations together:

$$
\begin{align*}
X\left(t_{n+1}\right)- & X^{h}\left(t_{n+1}\right)=X\left(t_{n}\right)-X^{h}\left(t_{n}\right)  \tag{26}\\
& +\Psi\left(X\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right)-\Phi\left(X\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right) \\
& +\Phi\left(X\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right)-\Phi\left(X^{h}\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right) .
\end{align*}
$$

In the absence of drift,

$$
E\left[\Psi\left(x, W\left[t_{n}, t_{n+1}\right], h\right) \mid \mathcal{F}_{t_{n}}\right]=0
$$

and the same for the other three terms on the right side. Therefore we may calculate (using the inequality $(a+b)^{2} \leq 2 a^{2}+2 b^{2}$ ):

$$
E\left[\left|X\left(t_{n+1}\right)-X^{h}\left(t_{n+1}\right)\right|^{2}\right] \leq E\left[\left|X\left(t_{n}\right)-X^{h}\left(t_{n}\right)\right|^{2}\right]+2 u_{n}+2 v_{n}
$$

where

$$
u_{n}=E\left[\left|\Psi\left(X\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right)-\Phi\left(X\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right)\right|^{2}\right]
$$

and

$$
v_{n}=E\left[\left|\Phi\left(X\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right)-\Phi\left(X^{h}\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right)\right|^{2}\right]
$$

The inequality (25) says that $u_{n} \leq C h^{2}$. For $v_{n}$, write $W\left(t_{n+1}\right)-W\left(t_{n}\right)=\Delta W_{n}$, so that

$$
\begin{aligned}
\Phi\left(X\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right) & -\Phi\left(X^{h}\left(t_{n}\right), W\left[t_{n}, t_{n+1}\right], h\right) \\
= & \left(b\left(X\left(t_{n}\right)\right)-b\left(X^{h}\left(t_{n}\right)\right)\right) \Delta W
\end{aligned}
$$

The crucial fact now is that $\Delta W$ is independent of everything up to time $t_{n}$, so the expected square is (again using (23))

$$
\begin{aligned}
v_{n} & \leq E\left[\left|b\left(X\left(t_{n}\right)\right)-b\left(X^{h}\left(t_{n}\right)\right)\right|^{2}\right] \cdot E\left[|\Delta W|^{2}\right] \\
& \leq C h E\left[\left|X\left(t_{n}\right)-X^{h}\left(t_{n}\right)\right|^{2}\right]
\end{aligned}
$$

This finally is enough estimates. Defining $e_{n}=E\left[\left|X\left(t_{n}\right)-X^{h}\left(t_{n}\right)\right|^{2}\right]$, we have shown that

$$
e_{n+1} \leq e_{n}+C h^{2}+C h e_{n}
$$

Of course, we start with $e_{0}=0$, so we get (using $t_{n}=n h$ )

$$
e_{n} \leq C e^{C t_{n}} n h^{2}=C e^{C t_{n}} t_{n} h
$$

This implies that if we fix $T$ and let $n$ go to infinity while $h \rightarrow 0$ with $t_{n} \leq T$ always, then there is a $C(T)$ so that (19) is satisfied.


[^0]:    ${ }^{1}$ The principle of detailed balance is that certain physical processes satisfy detailed balance.

[^1]:    ${ }^{2}$ An eigenvalue with real part equal to zero would make the system neutrally stable or "weakly stable". The randomly forced neutrally stable system does not have a steady state.

