8.808/8.308 IAP 2026 Recitation 1-2: Numerical stochastic integration

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1 Introduction

First, make sure you have Julia installed (see `julialang.org/install`) along with an IDE. I simply use the free Sublime text editor (`https://www.sublimetext.com/`) and run the code from the command line as `julia script.jl arg1 arg2 ...`.

The following theory follows a simplified version of the calculation in R. Mannella, *Integration of Stochastic Differential Equations on a Computer*, Int. J. Mod. Phys. C (2002). This recitation is adapted from Sunghan Ro's recitation from the 2024 iteration of this class.

2 Theory: additive noise

We will integrate the stochastic differential equation (SDE) for an overdamped Langevin equation of the form

$$\dot{x}(t) = f(x(t)) + \sqrt{2D}\eta(t)\ . \tag{1}$$

Consider a timestep h. In going from time t to time $t+h$, the system explicitly evolves as

$$x(t+h) = x(t) + \int_0^h \dot{x}(t+s)ds = x(t) + \int_0^h f(x(t+s))ds + \sqrt{2D}\int_0^h \eta(t+s)ds\ . \tag{2}$$

We will derive, and then implement, two different approximations for this equation, which will be used for numerical integration. First, let's define the random variable

$$Z_1(h) \equiv \int_0^h \eta(t+s)ds\ . \tag{3}$$

Clearly it is a Gaussian random variable with zero mean. We can furthermore see that its variance is

$$\langle Z_1(h)^2\rangle = \int_0^h ds_1 \int_0^h ds_2 \langle \eta(t+s_1)\eta(t+s_2)\rangle = \int_0^h ds_1 \int_0^h ds_2 \delta(s_1-s_2) = h\ . \tag{4}$$

So, we can replace $Z_1(h)$ with the random variable $\sqrt{h}\xi$, where ξ is a centered, unit-variance Gaussian random variable. We thus have

$$x(t+h) = x(t) + \int_0^h ds f(x(t+s)) + \sqrt{2Dh}\xi \ . \tag{5}$$

The force term remains to be simplified.

2.1 Lowest-order (Euler/Maruyama) scheme

First, let's find an integration scheme that is correct to order h. One option is to replace

$$f(x(s)) = f(x(t)) + \mathcal{O}(\sqrt{h}) \ . \tag{6}$$

Then, we can see that the force integral is

$$\int_0^h ds f(x(t+s)) = hf(x(t)) + \mathcal{O}(h^{3/2}) \ . \tag{7}$$

The result is the integration scheme

$$x(t+h) = x(t) + hf(x(t)) + \sqrt{2Dh}\xi \ . \tag{8}$$

This is known as the **Euler(/Maruyama)** integration scheme, and is the most common.

2.2 Higher-order (Mannella) scheme

What if we want to go to order h^2? One such scheme was derived by Mannella in 2002. In this case, we should replace the force with

$$f(x(s)) = \underbrace{f(x(t))}_{\equiv f_t} + [x(s)-x(t)] \underbrace{f'(x(t))}_{\equiv f'_t} + \frac{1}{2}[x(s)-x(t)]^2 \underbrace{f''(x(t))}_{\equiv f''_t} + \mathcal{O}(h^{3/2}) \ . \tag{9}$$

Integrating this gives

$$\int_0^h ds f(x(t+s)) \approx hf_t + f'_t \underbrace{\int_0^h ds[x(t+s)-x(t)]}_{\equiv ①} + \frac{1}{2}f''_t \underbrace{\int_0^h ds[x(t+s)-x(t)]^2}_{\equiv ②} \ . \tag{10}$$

We can calculate

$$① = \int_0^h ds[x(t+s)-x(t)] = \int_0^h ds \int_0^s ds' \left[f(x(t+s')) + \sqrt{2D}\eta(t+s')\right] = f_t\frac{h^2}{2} + \sqrt{2D}\int_0^h ds Z_1(s) + \mathcal{O}(h^{5/2}) \ . \tag{11}$$

We have substituted $f(x(t+s')) \to f_t$ because we know that each integral contributes a factor of h^2, thus the only relevant term is f_t. For the other term, we have

$$② = \int_0^h ds\left[x(t+s)-x(t)\right]^2 = \int_0^h ds \int_0^s ds_1\left[f(x(t+s_1)) + \sqrt{2D}\eta(t+s_1)\right] \int_0^s ds_2\left[f(x(t+s_2)) + \sqrt{2D}\eta(t+s_2)\right] \tag{12}$$

$$= \int_0^h ds\left[2\int_0^s ds_1 f(x(t+s_1))\sqrt{2D}Z_1(s) + Z_1(s)^2 + \mathcal{O}(h^{5/2})\right] \ . \tag{13}$$

Recall that $Z_1(s)$ is $\mathcal{O}(\sqrt{h})$ when $s \sim \mathcal{O}(h)$. Then, because again each integral contributes $\sim \mathcal{O}(h)$, the first term disappears and we find

$$② = \int_0^h ds Z_1(s)^2 + \mathcal{O}(h^{5/2}) \ . \tag{14}$$

All in all, we find

$$x(t+h) = x(t) + f_t h + \sqrt{2D}Z_1(h) + f'_t f_t \frac{h^2}{2} + f'_t\sqrt{2D}\int_0^h ds Z_1(s) + f''_t \int_0^h ds Z_1(s)^2 \ , \tag{15}$$

where we recall that

$$Z_1(h) = \int_0^h \eta(t+s)ds \sim \sqrt{h}\xi \ . \tag{16}$$

2.3 Error: explicit computation

We will now explicitly calculate the error of our integration schemes for an overdamped harmonic oscillator with mobility μ, spring constant $\tilde{k}$, and diffusivity $\mu k_B T$:

$$\dot{x}(t) = -\mu\tilde{k}x(t) + \sqrt{2\mu k_B T}\eta(t) \tag{17}$$

where $\eta(t)$ is a standard Gaussian white noise, which satisfies

$$\langle\eta(t)\rangle = 0 \ , \qquad \langle\eta(t)\eta(s)\rangle = \delta(t-s) \ . \tag{18}$$

Define the scaled spring constant $k \equiv \mu\tilde{k}$, along with the diffusivity $D = \mu k_B T$. Then, we have the Langevin equation

$$\dot{x}(t) = -kx(t) + \sqrt{2D}\eta(t) \ . \tag{19}$$

2.3.1 Analytical solution

We can explicitly calculate the steady-state probability distribuion for x using Itō's formula. We can write the dynamics of each moment

$$\frac{d}{dt}\langle x(t)^n\rangle = n\langle x(t)^{n-1}\dot{x}(t)\rangle + n(n-1)D\langle x(t)^{n-2}\rangle \tag{20}$$

$$= -kn\langle x(t)^n\rangle + n(n-1)D\langle x(t)^{n-2}\rangle \ . \tag{21}$$

Using causality, we have replaced $\langle x(t)^{n-1}\eta(t)\rangle = \langle x(t)^{n-1}\rangle\langle\eta(t)\rangle = 0$. In the steady state, this then gives us the nth moment in terms of the $(n-2)$nd one:

$$\langle x^n\rangle = (n-1)\frac{D}{k}\langle x^{n-2}\rangle \ . \tag{22}$$

Clearly only the even moments $n = 2m$ are nonzero. These are given by

$$\langle x^{2m}\rangle = (2m-1)(2m-3)\dots 1\left(\frac{D}{k}\right)^m = (2m-1)!!\left(\frac{D}{k}\right)^m \ . \tag{23}$$

But these are the moments of the Gaussian distribution with variance D/k. Thus, because a probability distribution is uniquely characterized by its moments, the steady-state probability distribution for x is given by

$$P_{\text{th}}(x) = \frac{\exp\left(-\frac{k}{2D}x^2\right)}{\sqrt{2\pi D/k}} = \mathcal{N}\left(0, \frac{D}{k}\right) \ . \tag{24}$$

Luckily for us, in the harmonic oscillator model, we can explicitly calculate the steady-state probability distributions resulting from our (approximate) simulation schemes, and thus explicitly calculate their error.

2.3.2 Euler/Maruyama scheme error

For the harmonic oscillator, the Euler scheme is defined by the recursion relation

$$x(t+h) = x(t) - hkx(t) + \sqrt{2Dh}\xi \tag{25}$$

where now ξ is a centered Gaussian random variable of unit variance.

We are interested in the probability distribution of $x(t)$ as $t \to \infty$. We can compute the following recursion relation for the mean:

$$\langle x(t+h)\rangle = \langle x(t)\rangle(1-hk) + \sqrt{2Dh}\langle\xi(t)\rangle = \langle x(t)\rangle(1-hk) \ . \tag{26}$$

As long as $h < 1/k$, this converges to zero. Likewise, the variance satisfies the recursion relation

$$\langle x(t+h)^2\rangle = \langle x(t)^2\rangle(1-hk)^2 + 2\sqrt{2Dh}(1-hk)\langle x(t)\xi(t)\rangle + 2Dh\langle\xi(t)^2\rangle = \langle x(t)^2\rangle(1-hk)^2 + 2Dh \ . \tag{27}$$

In the steady state, i.e. at long times, we find

$$\langle x(t\to\infty)^2\rangle = \frac{2Dh}{1-(1-hk)^2} = \frac{D}{k}\frac{1}{1-hk/2} \ . \tag{28}$$

Let's moreover suppose that the initial distribution for x is Gaussian. Then, because the recursion relation simply scales x then adds another Gaussian random variable to it, we see that the distribution remains a Gaussian. (It is also possible to prove that if it doesn't start as a Gaussian, it becomes one, using the Central Limit Theorem.) Thus, we can conclude the the steady-state probability distribution for the Euler scheme is

$$P_{\text{Euler}}(x) = \mathcal{N}\left(0, \frac{D}{k}\frac{1}{1-hk/2}\right) . \tag{29}$$

The error is evidently $\mathcal{O}(h)$.

2.3.3 Mannella scheme error

For the harmonic oscillator, the Mannella scheme is defined by the recursion relation

$$x(t+h) = x(t) - hkx(t) + \frac{h^2k^2}{2}x(t) + \sqrt{2D}Z_1(h) - k\sqrt{2D}\int_0^h dsZ_1(s) \tag{30}$$

$$\equiv x(t)\left[1 - hk + \frac{h^2k^2}{2}\right] + \sqrt{2D}\zeta . \tag{31}$$

We have defined the Gaussian white noise ζ. Clearly ζ has mean zero. The variance is given by

$$\langle\zeta^2\rangle = \left\langle\left[Z_1(h) - k\int_0^h dsZ_1(s)\right]^2\right\rangle \tag{32}$$

$$= h - 2k\int_0^h ds_2 \underbrace{\int_0^h ds_1\int_0^{s_2} ds_2'\langle\eta(t+s_1)\eta(t+s_2')\rangle}_{=s_2} + k^2\int_0^h ds_1\int_0^h ds_2 \underbrace{\int_0^{s_1} ds_1'\int_0^{s_2} ds_2'\langle\eta(t+s_1')\eta(t+s_2')\rangle}_{=\min(s_1,s_2)} \tag{33}$$

$$= h - kh^2 + k^2\int_0^h ds_1\left(\int_0^{s_1} ds_2 s_2 + \int_{s_1}^h s_1\right) \tag{34}$$

$$= h - kh^2 + \int_0^h ds_1\left(hs_1 - \frac{s_1^2}{2}\right) \tag{35}$$

$$= h\left[1 - hk + \frac{h^2k^2}{3}\right] . \tag{36}$$

Thus, the noise is equivalent to a single Gaussian random variable

$$\sqrt{2D}Z_1(h) - k\sqrt{2D}\int_0^h dsZ_1(s) \sim \sqrt{2Dh\left[1 - hk + \frac{h^2k^2}{3}\right]}\,\xi \tag{37}$$

where ξ is now a centered Gaussian random variable of unit variance. Thus, our integration scheme is equivalent to

$$x(t+h) = x(t) - hkx(t) + \frac{h^2k^2}{2}x(t) + \sqrt{2Dh\left[1 - hk + \frac{h^2k^2}{3}\right]}\,\xi . \tag{38}$$

Again, for small enough h, the mean of x decays to zero. The variance now satisfies the recursion relation

$$\langle x(t+h)^2\rangle = \langle x(t)^2\rangle\left[1 - hk + \frac{h^2k^2}{2}\right]^2 + 2Dh\left[1 - hk + \frac{h^2k^2}{3}\right] \tag{39}$$

so that in steady state

$$\langle x(t\to\infty)^2\rangle = \frac{2Dh[1 - hk + h^2k^2/3]}{1 - (1 - hk + h^2k^2/2)^2} = \frac{D}{k}\frac{1 - hk + h^2k^2/3}{[1 - hk/2][1 - hk/2 + h^2k^2/4]} = \frac{D}{k}\left[1 - \frac{h^2k^2}{6} + \mathcal{O}(h^3)\right] . \tag{40}$$

Again, the steady-state probability distribution is a Gaussian

$$P_{\text{Mannella}}(x) = \mathcal{N}\left(0, \frac{D}{k}\frac{1 - hk + h^2k^2/3}{[1 - hk/2][1 - hk/2 + h^2k^2/4]}\right) \tag{41}$$

but now the error is $\mathcal{O}(h^2)$.

3 Theory: multiplicative noise

What if the strength of the noise in our Langevin equation is spatially-varying? This is called **multiplicative noise**. In 1 dimension, the most general such system is described by the Langevin dynamics

$$\dot{x}(t) = f(x(t)) + g(x(t))\eta(t) \; . \tag{42}$$

However, Eq. (42) is ill-defined without the specification of a discretization. For instance, the average velocity of a particle $\langle \dot{x}(t)\rangle$ is given by

$$\langle \dot{x}(t)\rangle = \langle f(x(t))\rangle + \langle g(x(t))\eta(t)\rangle \; . \tag{43}$$

If we are using the Itō convention, then

$$\langle x(t)\eta(t)\rangle = \langle x(t)\rangle\langle \eta(t)\rangle = 0 \qquad \Longrightarrow \qquad \langle g(x(t))\eta(t)\rangle = \langle g(x(t))\rangle\langle \eta(t)\rangle = 0 \; . \tag{44}$$

However, if we are using the Stratonovich convention,

$$\langle x(t)\eta(t)\rangle \neq \langle x(t)\rangle\langle \eta(t)\rangle \qquad \Longrightarrow \qquad \langle g(x(t))\eta(t)\rangle \neq \langle g(x(t))\rangle\langle \eta(t)\rangle \; . \tag{45}$$

Thus even tangible physical quantities such as the particle velocity are sensitive to the choice of discretization.

To remedy the ambiguity of Eq. (42), we will explicitly discretize it. Construct a lattice of times $\{t_0, t_1, \ldots, t_N\}$ such that $t_{k+1} - t_k = \Delta t$, and define $x_k \equiv x(t_k)$ and $\Delta x_k \equiv x_{k+1} - x_k$. Let $\alpha \in [0,1]$ be a number that specifies the discretization convention[1], and define $x_k^\alpha \equiv x_k + \alpha \Delta x_k$. Then, we write

$$\Delta x_k = \Delta t f(x_k^\alpha) + \sqrt{\Delta t} g(x_k^\alpha)\eta_k \; , \tag{46}$$

where η_k is a unit-variance centered Gaussian random variable. Now, Eq. (42) is understood as the $\Delta t \to 0$ limit of Eq. (46). We should always keep in mind that different α lead to different physics.

Now, we will figure out how to build a numerical integrator for this system that is accurate to $\mathcal{O}(h)$ for some *finite* timestep h.

3.1 Euler integration scheme

As before, we will build an "Euler" integration scheme that is accurate to $\mathcal{O}(h)$, where h is the timestep used in the numerical simulation. We will thus consider a lattice of times that starts at $t_0 = t$ and ends at $t_N = t + h$, so that $\Delta t = h/N$. We will take the fine-lattice limit $N \to \infty$. Note, then, that we must have

$$\Delta t \;\ll h \;\ll\; \text{all other timescales} \; . \tag{47}$$

We would like to know $x(t+h)$. It is exactly given by the $\Delta t \to 0$ limit of

$$x(t+h) - x(t) = \sum_{k=0}^{N-1} \Delta x_k = \sum_{k=0}^{N-1} \Big[\Delta t f(x_k^\alpha) + \sqrt{\Delta t} g(x_k^\alpha)\eta_k\Big] \; . \tag{48}$$

As before, we expand f and g in powers of h around $x(t) = x_0$:

$$x(t+h) - x(t) = \sum_{k=0}^{N-1} \Big\{ \Delta t \Big[f(x_0) + \mathcal{O}(\sqrt{h})\Big] + \sqrt{\Delta t}\Big[g(x_0) + (x_k^\alpha - x_0)g'(x_0) + \mathcal{O}(h)\Big]\eta_k \Big\} \; . \tag{49}$$

This is because, as before, increments in x for timesteps of order h are of order $\sqrt{h}$. Note that $\sum_{k=0}^{N-1} \Delta t = h$. Also,

$$\left\langle \sum_{k=0}^{N-1} \sqrt{\Delta t}\eta_k \right\rangle = 0 \; , \quad \left\langle \left(\sum_{k=0}^{N-1} \sqrt{\Delta t}\eta_k \right)^2 \right\rangle = \sum_{k=0}^{N-1}\sum_{\ell=0}^{N-1} \Delta t \delta_{k\ell} = N\Delta t = h \tag{50}$$

so that we can define

$$\eta = \frac{1}{\sqrt{h}} \sum_{k=0}^{N-1} \sqrt{\Delta t}\eta_k \; , \quad \langle \eta \rangle = 0 \; , \quad \langle \eta^2 \rangle = 1 \; . \tag{51}$$

[1]The Itō convention is given by $\alpha = 0$ and the Stratonovich convention is given by $\alpha = 1/2$. $\alpha = 1$ is sometimes called the "Hänggi" or "anti-Itō" convention.

Then, we have

$$x(t+h) - x(t) = hf(x(t)) + \sqrt{h}g(x(t))\eta + g'(x(t)) \underbrace{\sum_{k=0}^{N-1} \left(x_k^\alpha - x_0\right)\sqrt{\Delta t}\eta_k}_{\equiv \circledast} \ . \tag{52}$$

We only have to simplify the term $\circledast$. Expanding x_k and Δx_k gives

$$\circledast = \sum_{k=0}^{N-1} \left[\sum_{\ell=0}^{k-1} \left(\Delta t f(x_\ell^\alpha) + \sqrt{\Delta t} g(x_\ell^\alpha)\eta_\ell \right) + \alpha\left(\Delta t f(x_k^\alpha) + \sqrt{\Delta t} g(x_k^\alpha)\eta_k \right) \right] \sqrt{\Delta t}\eta_k \tag{53}$$

$$= \Delta t \sum_{k=0}^{N-1} \left[\sum_{\ell=0}^{N-1} g(x_\ell^\alpha)\eta_\ell + \alpha g(x_k^\alpha)\eta_k \right] \eta_k + \mathcal{O}(h^{3/2}) \tag{54}$$

$$= \Delta t g(x(t)) \sum_{k=0}^{N-1} \left[\sum_{\ell=0}^{N-1} \eta_\ell + \alpha\eta_k \right] \eta_k + \mathcal{O}(h^{3/2}) \ . \tag{55}$$

Because $\langle \eta_\ell \eta_k \rangle = 0$ for all $\ell \neq k$, $\circledast$ has mean

$$\langle \circledast \rangle = \alpha \Delta t g(x(t)) \ . \tag{56}$$

In principle, it also has some fluctuations. However, it can be shown that these are subleading in the $\Delta t \to 0$ limit. One proves this rigorously by showing that the L^2 difference between $\circledast$ and its mean to converge to 0 as $\Delta t \to 0$.[2] Thus, we have our $\mathcal{O}(h)$ discretization scheme

$$x(t+h) = hf(x(t)) + h\alpha g'(x(t))g(x(t)) + \sqrt{h}g(x(t))\eta \ , \quad \langle \eta \rangle = 0 \ , \quad \langle \eta^2 \rangle = 0 \ . \tag{57}$$

In the numerical section, you will simulate a Brownian particle in the absence of any forces, i.e. $f(x(t)) = 0$, but with spatially-varying temperature. Letting $\mu = k_B = 1$, the Langevin dynamics are

$$\dot{x}(t) \stackrel{\alpha}{=} \sqrt{2T(x(t))}\eta(t) \tag{58}$$

where $\stackrel{\alpha}{=}$ indicates the discretization specification of α. You will show that different α indeed leads to different density distributions, and thus the discretization "convention" is actually physically relevant.

4 Numerics

4.1 Additive noise & h convergence

In the file `Rec1-2_Langevin_Harmonic.jl`, you'll find partial code to simulate the harmonic oscillator. It takes one argument, "1" or "2", indicating the Euler/Maruyama and Mannella algorithms respectively. You will fill in the algorithms inside the `runHarmonicOscillator` function. For simplicity, we take $k = D = 1$. See the code comments for more information about what it does.

One important thing: to generate a unit-variance, zero-mean Gaussian random number using the random number generator `rng`, you can call `randn(rng)`.

4.2 Multiplicative noise: $T(x)$

In the file `Rec2_Brownian_Tofx.jl`, you will simulate a Brownian particle in a spatially-varying temperature, and plot the density distribution alongside the theoretical prediction.

[2] see Sec. 2.1.3 and the beginning of Sec. 2.2 of de Pirey et al. 2022 (arXiv:2211.09470) for a more in-depth explanation.