2. Langevin dynamics

An example of a stochastic differential equation — SDE.

Add two terms:

- a random force, ζ, adds energy,
- a friction term $-\alpha\mathbf{v}$, dissipates energy.

The equations of motion then become

$$m\dot{\mathbf{v}} = \mathbf{F} - \alpha\mathbf{v} + \zeta.$$

How should the magnitude of ζ be chosen to do a simulation at a desired temperature?

We first need to consider how the noise should be treated.

Properties of the noise

Each component of the noise is an independent random process with...

- Average: $\langle \zeta(t) \rangle = 0$.
- Correlation between noise at different times: $\langle \zeta(t)\zeta(t') \rangle = A\delta(t - t')$.

This "noise process" jumps infinitely quickly between minus and plus infinity—terrible!

Consider the average noise during a time interval Δ:

$$\zeta_\Delta(t) = \frac{1}{\Delta} \int_t^{t+\Delta} dt' \zeta(t'),$$

and calculate the expectation value, $\langle \zeta_\Delta^2 \rangle$. The amplitude of this average noise depends on the time interval Δ in an unusual way:

$$\begin{aligned} \langle \zeta_\Delta^2 \rangle &= \frac{1}{\Delta^2} \int_t^{t+\Delta} dt' \int_t^{t+\Delta} dt'' \langle \zeta(t')\zeta(t'') \rangle \\ &= \frac{1}{\Delta^2} \int_t^{t+\Delta} dt' \int_t^{t+\Delta} dt'' A\delta(t' - t'') = \frac{A}{\Delta}. \end{aligned}$$

SDE—mathematical finance

This is a huge field within mathematics. Two important concepts:

- Itô calculus—rules to extends the methods of calculus to stochastic processes.
- Wiener process—W_t characterized by
  - $W_0 = 0$,
  - W_t has independent increments for all $t > 0$,
  - W has Gaussian increments, $W_{t+u} - W_t \sim \mathcal{N}(0, u)$.
- It seems that $W_{t+u} - W_t \sim \int_t^{t+u} dt' \zeta(t')$, (though this is presumably not the proper way to express things).

Temperature and noise magnitude

From the above: $\langle \zeta^2 \rangle = A/\Delta_t$.

In equilibrium there should be balance between added and dissipated power (energy): Choose the noise such that the expectation value of the kinetic energy doesn't change with time.

Consider one dimension and no external forces:

$$mv(t + \Delta_t) = mv(t) - \alpha \Delta_t v(t) + \Delta_t \zeta.$$

In equilibrium $\langle mv^2 \rangle$ at times $t + \Delta_t$ and t should be the same:

$$m^2 \langle v^2(t + \Delta_t) \rangle = (m - \alpha \Delta_t)^2 \langle v^2(t) \rangle + \Delta_t^2 \langle \zeta^2 \rangle. \tag{1}$$

To first order in Δ_t this leads to the requirement

$$0 = -2m\alpha \Delta_t \langle v^2(t) \rangle + \Delta_t^2 \langle \zeta^2 \rangle.$$

Temperature and noise magnitude...cont'd

Note that "$\Delta_t^2 \langle \zeta^2 \rangle$", is to first order in Δ_t since $\langle \zeta^2 \rangle \sim 1/\Delta_t$.

This tells how to choose the magnitude of the noise,

$$\langle \zeta^2 \rangle = \frac{2m\alpha \langle v^2(t) \rangle}{\Delta_t},$$

and together with $m\langle v^2 \rangle = T$:

$$\langle \zeta^2 \rangle = \frac{2\alpha T}{\Delta_t}. \tag{2}$$

Effects of the damping α

How does a change in α affect the system?

- static, i.e. *time-independent*, quantities remain the same independent of α,
- *time-dependent* quantites are affected.

Time-dependent correlations

The velocity autocorrelation function.
Measures how long a particle moves in the same direction.

$$g_v(t) = \langle \mathbf{v}_i(t' + t) \cdot \mathbf{v}_i(t') \rangle.$$

Here $\langle \cdots \rangle$ is an average over all particles i, and many initial times, t'.

Related to the diffucsion constant: At long times the particles diffuse around with

$$\langle (\mathbf{r}(t' + t) - \mathbf{r}(t'))^2 \rangle = Dt, \tag{3}$$

The diffusion constant, D— related to $g_v(t)$:

$$D = \int_{-\infty}^{\infty} g_v(t) dt. \tag{4}$$

Static quantities

Simple example: the energy.

More detailed information: the pair correlation function, $g(r)$,

> *The probability to find a particle at* $\mathbf{r}$*, granted that there is a particle at the origin.*

To calculate $g(r)$: collect a histogram over particle separations, $h(r)$, with resolution Δr. In two dimensions the relation between $h(r)$ and the pair correlation function is

$$h(r) = 2\pi r\, g(r)\Delta r. \quad \text{Invert to get get } g(r)!$$

- Equal to the density at large distances,
- Displays a peak at $r \approx r_{\min}$ and often more peaks at larger distances.

Time step and damping

One needs to decrease the time step when increasing α to avoid introducing errors in the results.

Keeping terms to second order in Δ_t^2 we find

$$m^2\langle v^2(t+\Delta_t)\rangle = (m^2 - 2m\alpha\Delta_t + \alpha^2\Delta_t^2)\langle v^2(t)\rangle + \Delta_t^2\langle\zeta^2\rangle.$$

Assuming a time-independent kinetic energy, $\langle v^2(t+\Delta_t)\rangle = \langle v^2(t)\rangle$:

$$\langle v^2\rangle(2m\alpha\Delta_t - \alpha^2\Delta_t^2) = 2\alpha T\Delta_t,$$

which gives

$$\langle v^2\rangle = \frac{T}{m - \alpha\Delta_t/2}.$$

The error depends on $\alpha\Delta_t$. Need smaller time step for larger α.

3. Brownian dynamics

The friction term in the Langevin equation introduces a time scale, m/α.

To see this, consider a particle in one dimension with inital velocity $v(0)$. Then $m\dot{v} = -\alpha v$ gives $v(t) = v(0)e^{-t/(m/\alpha)}$ + noise.

Consider the limit of very small time scale. The velocity decays quickly to zero, the dynamics is if there were no inertia—overdamped dynamics.

One way to approach this limit would be to take $m \to 0$ and the dynamics then becomes

$$0 = \mathbf{F} - \alpha \mathbf{v} + \boldsymbol{\zeta}, \quad \Rightarrow \quad \mathbf{v} = \frac{1}{\alpha}\mathbf{F} + \frac{\boldsymbol{\zeta}}{\alpha}.$$

There is now no need to remember the velocity $\Rightarrow$ keep the position coordinates, only:

$$\dot{\mathbf{r}} = \frac{1}{\alpha}\mathbf{F} + \boldsymbol{\eta},$$

where the components of the noise variable are now characterized by

$$\langle \eta^2 \rangle = \frac{2T}{\alpha \Delta_t}.$$

Brownian dynamics. . . cont'd

We are now considering the limit when

$$\frac{m}{\alpha} \ll \Delta_t.$$

However, from the Langevin dynamics and

$$\langle v^2 \rangle = \frac{T}{m - \alpha\Delta_t/2}.$$

we concluded that the dynamics is only valid for small $\alpha\Delta_t/m$, i.e.

$$\frac{m}{\alpha} \gg \Delta_t.$$

$\Rightarrow$ the derivation cannot be trusted.
Brownian dynamics has to be motivated by other means—the Fokker-Planck equation!

The Fokker-Planck equation

We will

1. Derive the Fokker-Planck equation which is an expression for $\partial P / \partial t$.
2. Make use of this to show that Brownian dynamics gives

$$P(x) \propto e^{-U(x)/T},$$

by demonstrating that

$$\frac{\partial P}{\partial t} = 0 \quad \text{if} \quad P(x) \propto e^{-U(x)/T}.$$

Derivation of the Fokker-Planck equation

Consider starting from some probability distribution $P(x,0)$ at time $t=0$. The change to this distribution with time comes from two terms:

$$P(x,\Delta_t) = P(x,0) \; - \; \int d\tilde{x}\; D(x-\tilde{x},\Delta_t|x,0)\; P(x,0) \; + \; \int d\tilde{x}\; D(x,\Delta_t|x-\tilde{x},0)\; P(x-\tilde{x},0). \quad (5)$$

Here $D(x-\tilde{x},\Delta_t|x,0)$ describes the dynamics, it is the probability that the particle which was at x at $t=0$ is at $x-\tilde{x}$ at time Δ_t.
The second integral is the probability that the particle originally at $x-\tilde{x}$ will be found at x at time Δ_t.

The first integral is simplified with the use of

$$\int d\tilde{x}\; D(x-\tilde{x},\Delta_t|x,0) = 1, \quad (6)$$

which is just a statement that the particle originally at x has to be somewhere a time Δ_t later.

Derivation of the Fokker-Planck equation. . . cont'd

With $\partial P(x,0)/\partial t \approx [P(x,\Delta_t) - P(x,0)]/\Delta_t$ one finds

$$\frac{\partial P(x,0)}{\partial t}\Delta_t = -P(x,0) + \int d\tilde{x}\; D(x,\Delta_t|x-\tilde{x},0)\; P(x-\tilde{x},0).$$

With

$$f(x) = D(x+\tilde{x},\Delta_t|x,0)\; P(x,0),$$

this is

$$\frac{\partial P(x,0)}{\partial t}\Delta_t = -P(x,0) + \int d\tilde{x}\; f(x-\tilde{x}).$$

Derivation of the Fokker-Planck equation…cont'd

With $f(x) = D(x+\tilde{x}, \Delta_t | x, 0)\, P(x,0)$ and the expansion

$$f(x-\tilde{x}) = \sum_{n=0}^{\infty} \frac{(-\tilde{x})^n}{n!} \frac{\partial^n}{\partial x^n} f(x), \qquad \text{this gives}$$

$$\begin{aligned}
&\frac{\partial P(x,0)}{\partial t} = \\
= \quad & -\frac{P(x,0)}{\Delta_t} + \sum_n \frac{(-1)^n}{n!} \frac{\partial^n}{\partial x^n} \left[P(x,0) \frac{1}{\Delta_t} \int d\tilde{x}\; \tilde{x}^n D(x+\tilde{x}, \Delta_t | x, 0) \right] \\
\approx \quad & -\frac{\partial}{\partial x} \left[P(x,0) M_1 \right] + \frac{1}{2} \frac{\partial^2}{\partial x^2} \left[P(x,0) M_2 \right],
\end{aligned}$$

where

$$M_n = \frac{1}{\Delta_t} \int d\tilde{x}\; \tilde{x}^n D(x+\tilde{x}, \Delta_t | x, 0),$$

and the $n=0$ term in the sum cancels the $P(x,0)$ term. This is the Fokker-Planck equation.

C programs—simple introduction

The shown code snippets are found at links from
`www.tp.umu.se/modsim/`

- Compiling with `make`.
- Return values from programs.
  - Why they are useful—how they work in a shell script.
- Linking to the math library:
  - Syntax with `cc`.
  - Syntax with `make`.
  - The Makefile.
- Code split into several files—compiling and linking.