

STOCHASTIC EQUATIONS

We consider the equation

$$\frac{dr}{dt} = \lambda F(r) + \alpha \eta(t) \quad r(t=0) = r_0$$

where $\eta(t)$ is a random variable [noise]

We assume Gaussian uncorrelated noise

$$\langle \eta(t) \rangle = 0 \quad \langle \eta(t) \eta(s) \rangle = \delta(t-s)$$

↑
NOTE: DIRAC DELTA FUNC

We wish to define a numerical algorithm for this equation.

The verlet idea

$$r(t+\Delta t) = r(t) + v(t)\Delta t$$

$$r(t+\Delta t) = r(t) + \Delta t (\lambda F(t) + \alpha(\eta(t)))$$

UNFORTUNATELY: THIS SCHEME IS WRONG

IN The Verlet approach one assumes that all quantities in the equation are SMOOTH in t .

THE NOISE IS NOT SMOOTH

THE WAY OUT

We integrate the equation between t and $t + \Delta t$

$$\int_t^{t+\Delta t} \frac{dr}{dt} dt = \lambda \int_t^{t+\Delta t} F(r(t)) dt + \alpha \int_t^{t+\Delta t} \eta(t) dt$$

$$r(t + \Delta t) - r(t) = \lambda \int_t^{t+\Delta t} F(r(t)) dt + \alpha \int_t^{t+\Delta t} \eta(t) dt$$

Now, the force $F(r)$ depends smoothly on r :

$$\int_t^{t+\Delta t} F(r(s)) ds \approx F(r(t)) \Delta t$$

For the noise term we define $\xi(t) = \int_t^{t+\Delta t} \eta(s) ds$

$\xi(t)$ is a "sum" (integral) of Gaussian variables of zero mean.

Therefore $\xi(t)$ is a Gaussian variable of zero mean

$$\langle \xi(t) \rangle = 0$$

VARIANCE:

$$\begin{aligned} \langle \xi(t)^2 \rangle &= \left\langle \int_t^{t+\Delta t} \eta(s_1) ds_1 \int_t^{t+\Delta t} \eta(s_2) ds_2 \right\rangle \\ &= \int_t^{t+\Delta t} ds_1 \int_t^{t+\Delta t} ds_2 \langle \eta(s_1) \eta(s_2) \rangle \end{aligned}$$

$$= \int\limits_t^{t+\Delta t} ds_1 \int\limits_t^{t+\Delta t} ds_2 \delta(s_1 - s_2) = \int\limits_t^{t+\Delta t} ds_1 = \Delta t \quad (3)$$

$$\text{Thus: } \langle \xi(t) \rangle = 0 \quad \langle \xi^2(t) \rangle = \Delta t$$

We thus define $p(t) = \frac{1}{\sqrt{\Delta t}} \xi(t)$

$$r(t+\Delta t) = r(t) + \lambda F(t) \Delta t + \alpha \sqrt{\Delta t} p(t)$$

$p(t)$: Gaussian variable with variance = 1

Note the $\sqrt{\Delta t}$ DEPENDENCE

The equation can be seen as a Markov process, in which the probability of arriving in a given point $r(t+\Delta t)$ depends on the probability distribution of $p(t)$

IMPLEMENTATION

Given $r(t)$

- a) compute $F(r(t)) = F(t)$
- b) extract Gaussian variable with variance 1
- c) $r(t+\Delta t) = r(t) + \lambda F(t) \Delta t + \alpha \sqrt{\Delta t} p(t)$

