Stochastic Processes:
Data Analysis and Computer Simulation

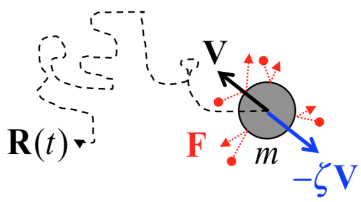
Brownian motion 2: computer simulation

1. Random force in the Langevin equation

1.1. Langevin equation

Model for a Brownian particle in 3-D

Particle radius:	a
Particle mass:	m
Solvent viscosity:	η
Friction constant:	$\zeta = 6\pi\eta a$
Particle position:	$\mathbf{R}(t)$
Particle velocity:	$\mathbf{V}(t) = d\mathbf{R}/dt$
Friction force:	$-\zeta\mathbf{V}(t)$
Random force:	$\mathbf{F}(t)$



$$m\frac{d\mathbf{V}(t)}{dt} = -\zeta\mathbf{V}(t) + \mathbf{F}(t) \tag{21}$$

1.2. Time evolution equations

$$\frac{d\mathbf{R}(t)}{dt} = \mathbf{V}(t) \tag{F1}$$

$$m\frac{d\mathbf{V}(t)}{dt} = -\zeta\mathbf{V}(t) + \mathbf{F}(t) \tag{F2}$$

Random force

$$\langle\mathbf{F}(t)\rangle = \mathbf{0} \tag{F3}$$

$$\langle\mathbf{F}(t)\mathbf{F}(0)\rangle = 2k_BT\zeta\mathbf{I}\delta(t) \tag{F4}$$

1.3. Cf. Euler method for a damped harmonic oscillator

$$\frac{d\mathbf{R}(t)}{dt} = \mathbf{V}(t) \tag{B1}$$

$$m\frac{d\mathbf{V}(t)}{dt} = -\zeta\mathbf{V}(t) - k\mathbf{R}(t) \tag{B2}$$

$$\mathbf{R}_{i+1} = \mathbf{R}_i + \int_{t_i}^{t_{i+1}} dt\mathbf{V}(t) \simeq \mathbf{R}_i + \mathbf{V}_i\Delta t \tag{B3}$$

$$\begin{aligned}\mathbf{V}_{i+1} &= \mathbf{V}_i - \frac{\zeta}{m}\int_{t_i}^{t_{i+1}} dt\mathbf{V}(t) - \frac{k}{m}\int_{t_i}^{t_{i+1}} dt\mathbf{R}(t) \\ &\simeq \left(1 - \frac{\zeta}{m}\Delta t\right)\mathbf{V}_i - \frac{k}{m}\mathbf{R}_i\Delta t \end{aligned} \tag{B4}$$

1.4. Application of Euler method to Eqs.(F1) and (F2)

$$\mathbf{R}_{i+1} = \mathbf{R}_i + \int_{t_i}^{t_{i+1}} dt\mathbf{V}(t) \simeq \mathbf{R}_i + \mathbf{V}_i\Delta t \tag{F5}$$

$$\begin{aligned}\mathbf{V}_{i+1} &= \mathbf{V}_i - \frac{\zeta}{m}\int_{t_i}^{t_{i+1}} dt\mathbf{V}(t) + \frac{1}{m}\int_{t_i}^{t_{i+1}} dt\mathbf{F}(t) \\ &\neq \left(1 - \frac{\zeta}{m}\Delta t\right)\mathbf{V}_i + \frac{1}{m}\mathbf{F}_i\Delta t \end{aligned} \tag{F6}$$

$$\because \int_{t_i}^{t_{i+1}} dt\mathbf{F}(t) \neq \mathbf{F}_i\Delta t \tag{F7}$$

1.5. Cumulative impulse $\Delta\mathbf{W}_i$: the Wiener process

$$\int_{t_i}^{t_{i+1}} dt\mathbf{F}(t) \equiv \Delta\mathbf{W}_i \tag{F8}$$

- $F_\alpha(t)$ → A series of random numbers drawn from some distribution with an average and variance equal to zero and $2k_BT\zeta$, respectively.
- $\Delta W_{\alpha,i}$ → A series of random numbers drawn from a "Gaussian distribution", with an average and variance equal to zero and $2k_BT\zeta\Delta t$, respectively. This is a consequence of the central limit theorem (see the supplemental note for details).

1.6. Modified velocity update equation (Eq.(F6)→(F9))

$$\begin{aligned}\mathbf{V}_{i+1} &= \mathbf{V}_i - \frac{\zeta}{m}\int_{t_i}^{t_{i+1}} dt\mathbf{V}(t) + \frac{1}{m}\int_{t_i}^{t_{i+1}} dt\mathbf{F}(t) \\ &\simeq \left(1 - \frac{\zeta}{m}\Delta t\right)\mathbf{V}_i + \frac{1}{m}\Delta\mathbf{W}_i \end{aligned} \tag{F9}$$

$$\langle\Delta\mathbf{W}_i\rangle = \mathbf{0} \tag{F10}$$

$$\langle\Delta\mathbf{W}_i\Delta\mathbf{W}_j\rangle = 2k_BT\zeta\Delta t\mathbf{I}\delta_{ij} \tag{F11}$$