Brownian motion near a boundary

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A discrete-time dynamical system is purely noise driven if

$$x_{n+1} = x_n + \sigma(x_n) r_n$$

where $\{r_n\}$ are mean 0, i.i.d. random variables.

Definition (Multiplicative Noise)

$\sigma(x)$ is not constant

Note if $\mathbb{E} r_n^2 = \Delta t$ then $\sigma(x) = \sqrt{2D(x)}$, where

Definition (Diffusion constant)

$$D(x) := \frac{1}{2\Delta t} \mathbb{E}\left[(x_{n+1} - x_n)^2 | x_n = x \right]$$

Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

Proof:

$$
\begin{aligned}
2D(x) &= \frac{1}{\Delta t}\mathbb{E}\left[(x_{n+1} - x_n)^2 | x_n = x\right] \\
&= \frac{1}{\Delta t}\mathbb{E}\left[(\sigma(x_n) r_n)^2 | x_n = x\right] \\
&= \frac{1}{\Delta t}\mathbb{E}\left[(\sigma(x) r_n)^2 | x_n = x\right] \\
&= \frac{\big(\sigma(x)\big)^2}{\Delta t}\mathbb{E}\left[r_n^2 | x_n = x\right] \\
&= \frac{\big(\sigma(x)\big)^2}{\Delta t}\mathbb{E}\left[r_n^2\right] \\
&= \frac{\big(\sigma(x)\big)^2}{\Delta t}\Delta t \\
&= \big(\sigma(x)\big)^2
\end{aligned}
$$

$\square$

In homogeneous, isotropic fluid bulk, $D(x)$ is constant.

$$D = \frac{1}{2\Delta t}\mathbb{E}\left[\Delta x^2\right] = \frac{\Delta t}{2}\mathbb{E}v^2$$

Assuming 1D equipartition,

$$\frac{\Delta t}{m}\mathbb{E}\left[\frac{1}{2}mv^2\right] = \frac{\Delta t}{2m}k_B T$$

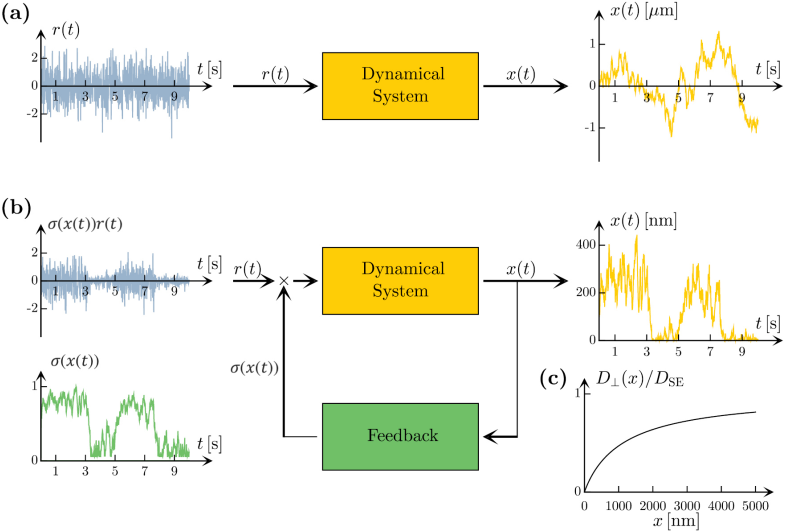
Definition (Einstein relation)

$$D_E = \mu k_B T$$

Mobility $\mu = v_{\text{ter}}(F)/F$ ratio of terminal velocity to applied force:

$$m\mu \approx \frac{m\Delta v}{F} = \frac{1}{F}\int_0^{\Delta t} F_{\text{net}}(s)\mathrm{d}s \approx \frac{1}{F}\int_0^{\Delta t}\left(1 - \frac{s}{\Delta t}\right)F\mathrm{d}s = \frac{\Delta t}{2}.$$

Systems (a) and (b) driven by Gaussian white noise r.



Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

(c) Hydrodynamic effects reduce Brownian motion near a wall.

Let independent $r_i(\Delta t) := \pm\sqrt{\Delta t}$ each with probability 1/2, and partial sum $S_t := \displaystyle\sum_{\{i\,:\,i\Delta t<t\}} r_i$.

Lemma

For any $t \geq 0$, S_t converges **weakly** *to $\mathcal{N}(0,t)$ as $\Delta t \to 0$.*

Sketch of proof: Fix Δt. The r_i i.i.d. so by CLT, as $n \to \infty$:

$$\mathcal{N}(0,1) \longleftarrow \frac{\frac{1}{n}\sum^{n} r_i - \mathbb{E}r_i}{\sqrt{\frac{1}{n}\mathbb{E}[r_i^2]}} = \frac{S_{n\Delta t}/n}{\sqrt{\Delta t}/\sqrt{n}} = \frac{S_{n\Delta t}}{\sqrt{n\Delta t}}$$

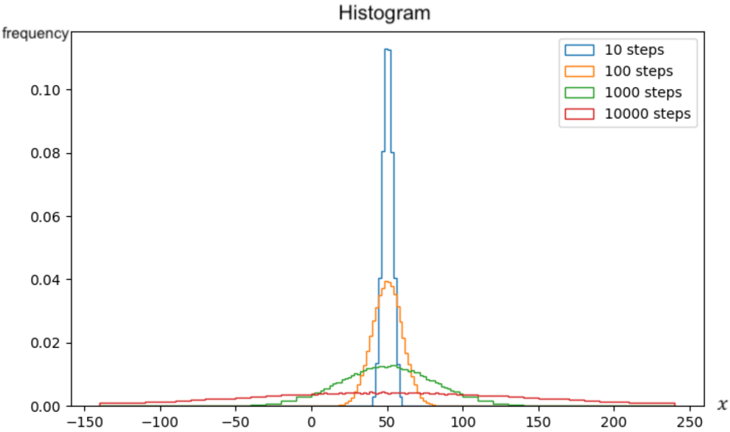
Choose $\Delta t := t/n$ for each n, giving a sequence $\dfrac{S_t^{(n)}}{\sqrt{t}} \to \mathcal{N}(0,1)$.

$\square$

$t = n$ for $\Delta t = 1$, so for constant σ the distribution of

$$x_n = x_{n-1} \pm \sigma = x_0 + \sigma S_n$$

approaches $\mathcal{N}\left(x_0, n\sigma^2\right)$ as $n \to \infty$.

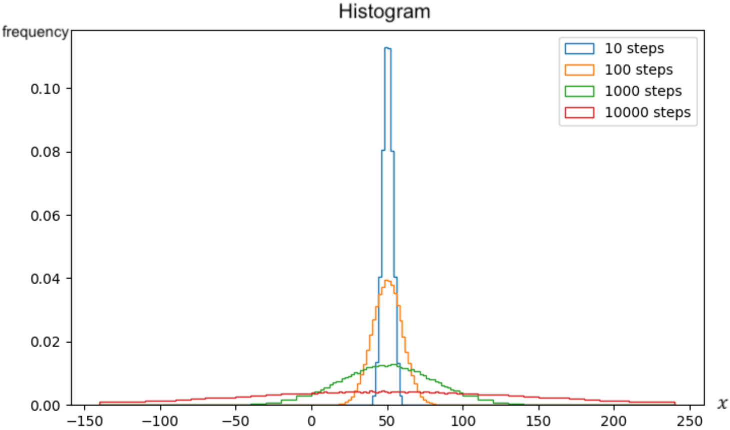


Source: Own simulations of the model for $x_0 = 50,\ \sigma = 1$.

$$x_n = x_{n-1} \pm \sigma = x_{n-1} + \frac{\sigma}{\sqrt{\Delta t}} r_{n-1} = x_0 + \frac{\sigma}{\sqrt{\Delta t}} S_{n\Delta t}$$

As $n \to 0$, distribution approaches:

$$x_0 + \frac{\sigma}{\sqrt{\Delta t}} \mathcal{N}\left(0, n\Delta t\right) = \mathcal{N}\left(x_0, n\sigma^2\right)$$



Source: Own simulations of the model for $x_0 = 50,\ \sigma = 1$.

Set $\Delta t := 1/k$, and interpolate $S_\cdot$ over $t \in [0,1]$.

$$\begin{aligned}\xi_t^k &:= S_{n\Delta t} + \frac{t - n\Delta t}{\Delta t} r_n,\ t \in [n\Delta t, (n+1)\Delta t] \\ &= \frac{1}{\sqrt{k}} \left(\sum_{i=1}^{[kt]} \eta_i + (kt - [kt])\eta_{[kt]+1} \right),\ [kt] = n\end{aligned}$$

where η_i i.i.d. with $\mathbb{E}\eta_i = 0$ and $\mathbb{E}\eta_i^2 = 1$.

Theorem (Donsker's invariance)

The sequence of distributions of $\xi_\cdot^k$ converges weakly to μ, the Wiener measure on $C[0,1]$.

Source: Krylov, N. V. *Introduction to the Theory of Random Processes.* American Mathematical Society; Graduate Studies in Mathematics, Volume 43; 2002; pp 28-32

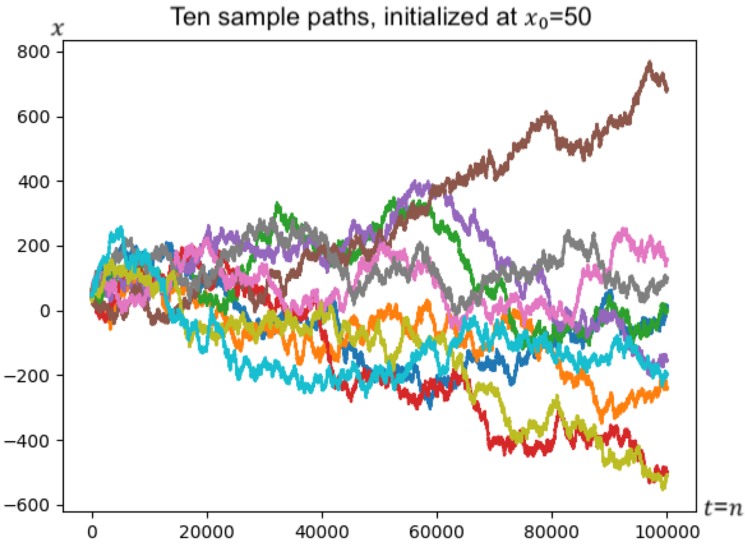
For constant σ,

$$x_{n+1} = x_n + \sigma r_n = x_0 + \sigma S_{(n+1)\Delta t}$$

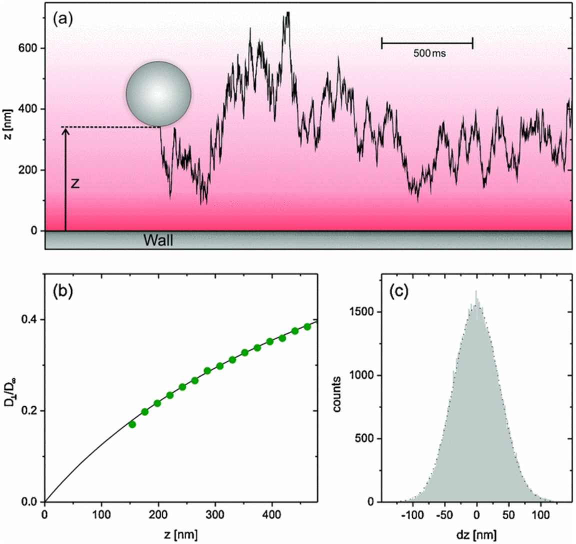
Interpolating model for $r_n = \pm\sqrt{\Delta t}$ yields continuous paths with distributions weakly convergent to the Wiener measure.

$$\begin{aligned} x^{(k)}(t) &:= x_n + \frac{t - n\Delta t}{\Delta t}\sigma r_n \\ &= x_0 + \sigma S_{n\Delta t} + \frac{t - n\Delta t}{\Delta t}\sigma r_n \\ &= x^{(k)}(0) + \sigma \xi_t^k \end{aligned}$$

$$\begin{aligned} (x(t) - x(s))^{(k)} &= \sigma\xi_t^k - \sigma\xi_s^k = \sigma(\xi_t - \xi_s)^k \\ \mathrm{d}x_{\cdot}^{(k)} &= \mathrm{d}\Big(\sigma\xi_{\cdot}^k\Big) = \sigma\mathrm{d}\xi_{\cdot}^k \longrightarrow \sigma\mathrm{d}W_{\cdot} := \sigma\mu(\mathrm{d}x_{\cdot}) \end{aligned}$$



Source: Own simulations, $\Delta t = 1,\ \sigma = 1.$



(a) Experimental setup with sample path. Particle not to scale. Data via Total Internal Reflection Microscopy.

(b) Note $D(0) = 0$ and $D(\mathrm{z}) \to D_\infty$.

(c) Distribution of relative position after 5ms for a fixed distance of z=380nm from the wall.

Source: Giovanni Volpe, Laurent Helden, Thomas Brettschneider, Jan Wehr, and Clemens Bechinger 2010 *Phys. Rev. Lett.* **104**, 170602

Let $D(x) = D_\infty \left(\frac{x}{x+a}\right)^2$ for $a > 0$ (h asymptote, crosses origin)

$$\sigma(x) = \sqrt{2D(x)} = \sqrt{2D_\infty}\frac{x}{x+a}$$

Recall: $$x_{n+1} = x_n + \sigma(\boxed{x_n})r_n$$

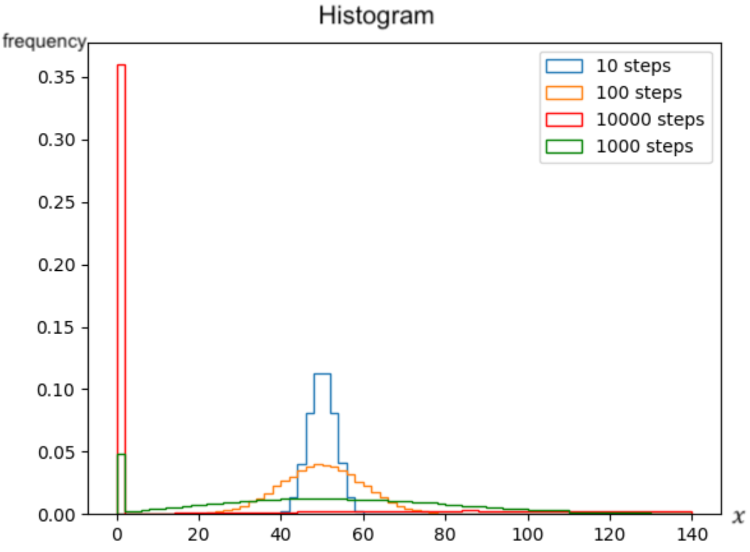
To ensure $x_{n+1} \geq 0$ we need $x_n \geq \sigma(x_n)||r_n||_\infty$ $\forall n$:

$$\begin{aligned}
x \geq \sqrt{2D}\frac{x}{x+a}||r||_\infty &\implies x^2 + ax \geq \sqrt{2D_\infty}||r||_\infty x \\
&\implies x(x + a - \sqrt{2D_\infty}||r||_\infty) \geq 0 \\
(x \geq 0) &\implies a \geq \sqrt{2D_\infty}||r||_\infty - x
\end{aligned}$$

$x \geq 0$ so we need $a \geq \sqrt{2D_\infty}||r||_\infty = \sqrt{2D_\infty \Delta t}$ for our model.
We wouldn't be able to make this guarantee with Gaussian noise.

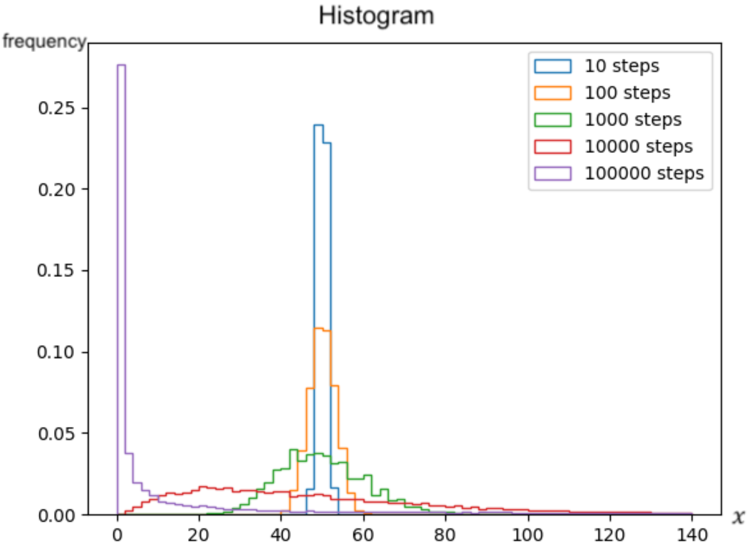
$a > 0$ can be arbitrarily small if we shrink the time step $\Delta t \to 0$.

$$a = \sqrt{2D_\infty \Delta t} = 1$$



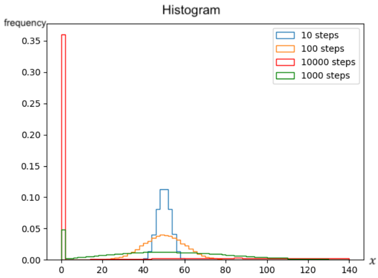
Source: Own simulations, $\Delta t = 1,\ \sigma = 1$.

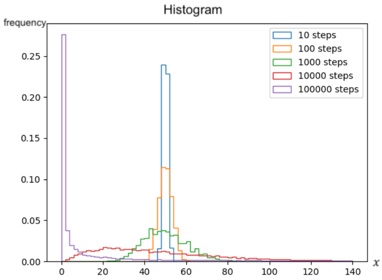
$$a = 100\sqrt{2D_\infty \Delta t} = 100$$



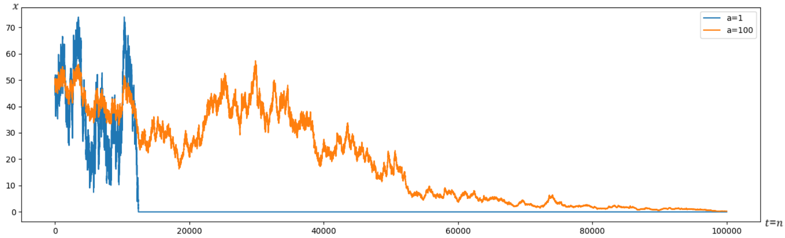
Source: Own simulations, $\Delta t = 1,\ \sigma = 1.$

$a = \sqrt{2D_\infty \Delta t} = 1$ $\qquad$ $a = 100\sqrt{2D_\infty \Delta t} = 100$





Here's a sample path for each a:



Source: Own simulations, $\Delta t = 1,\ \sigma = 1$.

Looks unrealistic. Why does this happen?

Let $\Delta t = 1$, and consider $x > 0$.

σ increasing and $x^+_{n+1} > x_n$ so $\sigma(x^+_{n+1}) > \sigma(x_n)$.

$$\begin{aligned} x^{+-}_{n+2} = x^+_{n+1} - \sigma(x^+_{n+1}) &= \overbrace{x_n + \sigma(x_n)}^{x^+_{n+1}} - \sigma(x^+_{n+1}) \\ &< x_n + \sigma(x_n) - \sigma(x_n) \\ &= x_n \end{aligned}$$

$x^-_{n+1} < x_n$ so by similar argument $x^{-+}_{n+2} < x_n$.

In either case, new position is behind.

$$p = 3/4 \text{ of } x_{n+2} < x_n$$

$\sigma(x_n)$ is bad. Is $\sigma\left(\dfrac{x_n + x_{n+1}}{2}\right)$ or $\sigma(x_{n+1})$ better?

A convex combination of endpoints x_n, x_{n+1} gives $\sigma(x_n + \alpha\Delta x_n)$ where $\alpha \in [0, 1]$ for $\Delta x_n = x_{n+1} - x_n$. Above, $\alpha = 0, \frac{1}{2}, 1$.

$\Delta t \to 0$, these choices lead to the Itô, Stratonovich, and "anti-Itô" interpretations of $\mathrm{d}x_t = \sigma(x_t)\mathrm{d}W_t$.

These interpretations evaluate the integrand σ at different points:

$$\mathbb{E}\left[\sum \sigma(x_{t_i} + \alpha\Delta x_{t_i})\underbrace{(W_{t_{i+1}} - W_{t_i})}_{\sim\mathcal{N}(0,\sqrt{\Delta t})}\right] \xrightarrow{L_2} \int \sigma(x_t) \circ_\alpha \mathrm{d}W_t$$

Itô denoted by $\sigma(x_t)\mathrm{d}W_t := \sigma(x_t) \circ_{\alpha=0} \mathrm{d}W_t$.

Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

Let σ_n denote $\sigma(x_n)$, and Taylor expand σ to "half order" in Δt:

$$\begin{aligned}
\sigma(x_n + \alpha\Delta x_n) &\approx \sigma_n + \alpha\sigma_n'\Delta x_n \\
&= \sigma_n + \alpha\sigma_n'\sigma(x_n + \alpha\Delta x_n)(\pm\sqrt{\Delta t}) \\
&\approx \sigma_n \pm \alpha\sigma_n'\big(\sigma_n + \alpha\sigma_n' \underbrace{\Delta x_n}_{\pm\sigma\sqrt{\Delta t}}\big)\sqrt{\Delta t} \\
&\approx \sigma_n \pm \alpha\sigma_n'\sigma_n\sqrt{\Delta t}
\end{aligned}$$

To first order in Δt,
$$\begin{aligned}
x_{n+1} &= x_n \pm \sigma(x_n + \alpha\Delta x_n)\sqrt{\Delta t} \\
&\approx x_n \pm \left(\sigma_n \pm \alpha\sigma_n'\sigma_n\sqrt{\Delta t}\right)\sqrt{\Delta t} \\
&= x_n \pm \sigma(x_n)\sqrt{\Delta t} + \underbrace{\alpha\sigma(x_n)\sigma'(x_n)\Delta t}_{\text{noise-induced drift}}
\end{aligned}$$

Accordingly, $\mathrm{d}x_t = \sigma(x_t) \circ_\alpha \mathrm{d}W = \sigma(x_t)\mathrm{d}W_t + \overbrace{\alpha\sigma(x_t)\frac{\mathrm{d}\sigma(x_t)}{\mathrm{d}x}\mathrm{d}t}$

Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

$$\sigma(x_t) \circ_\alpha \mathrm{d}W = \sigma(x_t)\mathrm{d}W_t + \alpha\sigma(x_t)\frac{\mathrm{d}\sigma(x_t)}{\mathrm{d}x}\mathrm{d}t$$

Result remains valid with addition of deterministic drift, i.e. still holds for

$$\mathrm{d}X_t = \mu(X_t)\mathrm{d}t + \sigma(X_t) \circ_\alpha \mathrm{d}W_t$$

E.g. Stratonovich ($\alpha = 1/2$) and Itô ($\alpha = 0$) integrals differ by

$$\int \sigma(X_t) \circ_{\alpha=\frac{1}{2}} \mathrm{d}W_t - \int \sigma(X_t)\mathrm{d}W_t = \frac{1}{2}\int \sigma(X_t)\frac{\mathrm{d}\sigma}{\mathrm{d}x}(X_t)\mathrm{d}t$$

Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

Dynamics of a colloid at thermal equilibrium with fluid are anti-Itô.

Equilibrium with heat bath at temp T yields Boltzmann distribution:

$$\rho(x,v) = Z^{-1}\exp\left(-\frac{U(x)}{k_B T} - \frac{mv^2}{2k_B T}\right) = \rho(x)\rho(v)$$

for colloidal particle of mass m at position x and velocity v.

$\rho(v) \sim \mathcal{N}\left(0, \frac{k_B T}{m}\right)$ implies energy equipartition:

$$\mathbb{E}\left[\frac{1}{2}mv^2\right] = \frac{m}{2}\mathbb{E}[v^2] = \frac{m}{2}\frac{k_B T}{m} = \frac{1}{2}k_B T$$

Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

Let F denote net external force (i.e. $F(x) = -\frac{\mathrm{d}U(x)}{\mathrm{d}x}$) and $\gamma(x)$ viscous friction coefficient. Modified Langevin equation:

$$
\begin{aligned}
ma &= F(x) - \gamma(x)(v + v_{\text{noise}}) \\
m\Delta v &= F(x)\Delta t - \gamma(x)v\Delta t - \gamma(x)v_{\text{noise}}\Delta t \\
v_{\text{noise}}\Delta t &= \Delta x_{\text{noise}} \approx \pm\sqrt{\mathbb{E}[(\Delta x)^2]} = \pm\sqrt{2D(x)\Delta t} \\
m\mathrm{d}v_t &= F(x_t)\mathrm{d}t - \gamma(x_t)v_t\mathrm{d}t + \gamma(x_t)\sqrt{2D(x_t)}\mathrm{d}W_t \\
v_t\mathrm{d}t &= \frac{1}{\gamma(x_t)}\Big(-m\mathrm{d}v_t + F(x_t)\mathrm{d}t\Big) + \sqrt{2D(x_t)}\mathrm{d}W_t
\end{aligned}
$$

Near equilibrium, system satisfies the fluctuation-dissipation relation $D(x)\gamma(x) = k_B T$. By definition $\mathrm{d}x_t = v_t\mathrm{d}t$, so

$$
\mathrm{d}x_t = -\frac{\boxed{m}}{k_B T}D(x_t)\mathrm{d}v_t + \frac{1}{k_B T}D(x_t)F(x_t)\mathrm{d}t + \sqrt{2D(x_t)}\mathrm{d}W_t
$$

Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

Only first term depends on $m \to 0$ for microscopic particles.

$$
\begin{aligned}
-\int_0^t \frac{m}{k_B T} D(x_s) \mathrm{d}v_s &= -\int_0^t \frac{m}{k_B T} D(x_s) \frac{\mathrm{d}v_s}{\mathrm{d}s} \mathrm{d}s = (\mathrm{IBP}) \\
&= \frac{1}{k_B T}\Big(m v_0 D(x_0) - m v_t D(x_t)\Big) + \int_0^t \frac{m}{k_B T} \frac{\mathrm{d}D(x_s)}{\mathrm{d}s} v_s \mathrm{d}s
\end{aligned}
$$

Boundary term vanishes by equipartition. Integral term is the "spurious" drift:

$$
\begin{aligned}
\int_0^t \frac{m}{k_B T} \frac{\mathrm{d}D(x_s)}{\mathrm{d}s} v_s \mathrm{d}s &= \int_0^t \frac{m}{k_B T} \frac{\mathrm{d}D(x_s)}{\mathrm{d}x} v_s^2 \mathrm{d}s \\
&\approx \int_0^t \frac{2}{k_B T} \frac{\mathrm{d}D(x_s)}{\mathrm{d}x} \mathbb{E}\left[\frac{1}{2} m v_s^2\right] \mathrm{d}s \\
&= \int_0^t \frac{\mathrm{d}D(x_s)}{\mathrm{d}x} \mathrm{d}s
\end{aligned}
$$

Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

$$\mathrm{d}x_t = \underbrace{\frac{\mathrm{d}D(x_s)}{\mathrm{d}x}\mathrm{d}t}_{\text{spurious drift}} + \frac{1}{k_B T} D(x_t)F(x_t)\mathrm{d}t + \sqrt{2D(x_t)}\mathrm{d}W_t$$

Spurious drift is just anti-Itô noise-induced drift since $\sigma = \sqrt{2D}$:

$$D = \frac{1}{2}\sigma^2 \Longrightarrow \frac{\mathrm{d}D}{\mathrm{d}\sigma} = \sigma \Longrightarrow \frac{\mathrm{d}D}{\mathrm{d}x} = \frac{\mathrm{d}D}{\mathrm{d}\sigma}\frac{\mathrm{d}\sigma}{\mathrm{d}x} = \sigma\frac{\mathrm{d}\sigma}{\mathrm{d}x}$$

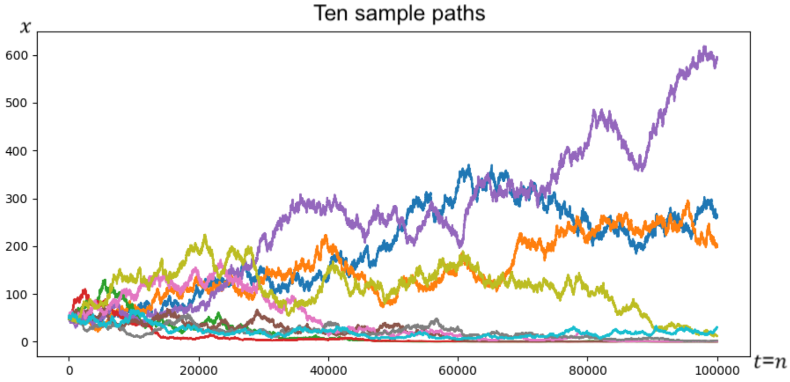
Thus, $\mathrm{d}x_t = \beta D(x_t)F(x_t)\mathrm{d}t + \sqrt{2D(x_t)} \circ_{\alpha=1} \mathrm{d}W_t$.

Source: Giovanni Volpe and Jan Wehr 2016 *Rep. Prog. Phys.* **79** 053901.

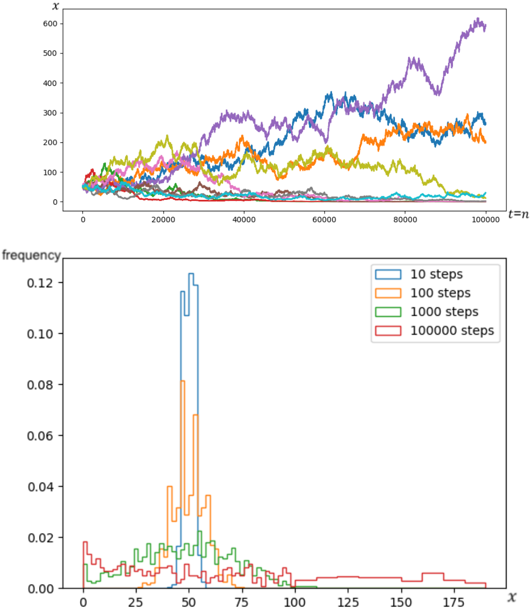
Back to $x_{n+1} = x_n \pm \sigma(x_{n+1})\sqrt{\Delta t}$. How to actually find $\sigma(x_{n+1})$?

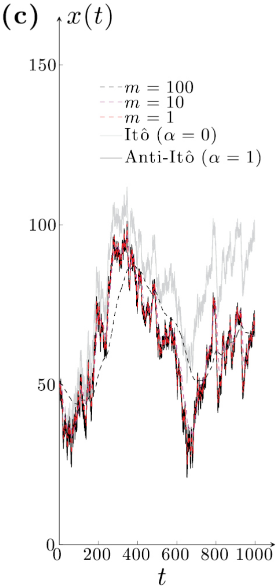
$$\sigma(x) = \sqrt{2D_\infty}\frac{x}{x+a} \Longrightarrow$$

$$x_{n+1} = \frac{x_n - a \pm \sqrt{2D_\infty \Delta t} + \sqrt{(x_n + a)^2 \pm \sqrt{2D_\infty \Delta t}(x_n - a)}}{2}$$



Source: Own simulations, $\alpha = 1, a = \sqrt{2D_\infty \Delta t} = 1$





Source: Own simulations, $\alpha = 1, a = \sqrt{2D_\infty \Delta t} = 1$

Source: Volpe and Wehr

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