Brownian motion equation for neurotransmitters

1 From Brownian motion to the diffusion equation

We consider a particle moving around inside a fluid in $\mathbb{R}^3$ undergoing Brownian motion. Let $X(t)$ be the position of the particle at time $t \geq 0$, and let $f(t, \mathbf{x})$ be the probability density function of the position of the particle, so that

$$\mathbb{P}[X(t) \in S] = \int_S f(t, \mathbf{x}) \mathrm{d}\mathbf{x}$$

for measurable $S \subset \Omega$. For a partition $\mathcal{P} = \{S_i\}_{i=1}^N$ of $\mathbb{R}^3$ and a time interval $\Delta t > 0$, we may associate a transition function

$$\phi_{\Delta t}(S_i, S_j) = \mathbb{P}[X(t + \Delta t) \in S_i \mid X(t) \in S_j].$$

Thus, from the law of total probability:

$$\begin{aligned}
\mathbb{P}[X(t+\Delta t) \in S_i] &= \sum_{j=1}^N \mathbb{P}[X(t+\Delta t) \in S_i \mid X(t) \in S_j]\, \mathbb{P}[X(t) \in S_j] \\
&= \sum_{j=1}^N \phi_{\Delta t}(S_i, S_j) \int_{S_j} f(t, \mathbf{y}) \mathrm{d}\mathbf{y} \\
&= \sum_{j=1}^N \int_{S_j} \phi_{\Delta t}(S_i, S_j) f(t, \mathbf{y}) \mathrm{d}\mathbf{y}.
\end{aligned}$$

In the limit as $\#\mathcal{P} = N \to +\infty$ and $\mathrm{mesh}(\mathcal{P}) = \max\limits_{1 \leq j \leq N} \mathrm{diam}(S_j) \to 0^+$, we obtain

$$f(t + \Delta t, \mathbf{x}) = \int_{\mathbb{R}^3} \phi_{\Delta t}(\mathbf{x}, \mathbf{y}) f(t, \mathbf{y}) \mathrm{d}\mathbf{y}. \tag{1}$$

1.1 Assumptions on the transition function

We first assume that

$$\phi_{\Delta t}(\mathbf{x}, \mathbf{y}) = \Phi_{\Delta t}(\mathbf{y} - \mathbf{x}) \tag{2}$$

for some radial function $\Phi_{\Delta t}$ that is highly localized around $\mathbf{0}$ for small Δt.

Also, $\phi_{\Delta t}$ being a transition function implies $\int_{\mathbb{R}^3} \phi_{\Delta t}(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y} = 1$ (a particle located somewhere must end up somewhere). This gives us

$$\int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{z}) \mathrm{d}\mathbf{z} = 1. \tag{3}$$

Finally, since $\Phi_{\Delta t}$ is radial for Δt fixed, we can write

$$\Phi_{\Delta t}(\mathbf{z}) = (\Delta t)^{-3/2} \widehat{\Phi}\left(\tfrac{1}{\sqrt{\Delta t}} \mathbf{z}\right). \tag{4}$$

for some function $\widehat{\Phi}$. Under the substitution $\mathbf{y} = \frac{1}{\sqrt{\Delta t}}\mathbf{z},\ \mathrm{d}\mathbf{y} = (\Delta t)^{-3/2}\mathrm{d}\mathbf{z}$, this yields

$$\int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{z})\|\mathbf{z}\|_2^2 \mathrm{d}\mathbf{z} = (\Delta t)^{-3/2} \int_{\mathbb{R}^3} \widehat{\Phi}(\tfrac{1}{\sqrt{\Delta t}}\mathbf{z})\|\mathbf{z}\|_2^2 \mathrm{d}\mathbf{z} = \Delta t \int_{\mathbb{R}^3} \widehat{\Phi}(\mathbf{y})\|\mathbf{y}\|_2^2 \mathrm{d}\mathbf{y}. \tag{5}$$

1.2 Obtaining the diffusion equation

In this section, we assume that f is sufficiently smooth that the Taylor expansions can be justified.

On one hand, we have

$$f(t+\Delta t, \mathbf{x}) = f(t,\mathbf{x}) + \frac{\partial f}{\partial t}(t,\mathbf{x})\Delta t + \frac{1}{2}\frac{\partial^2 f}{\partial t^2}(t,\mathbf{x})(\Delta t)^2 + \cdots \ .$$

On the other hand, if we Taylor expand the spatial variable, then we get from (1) and (2):

$$\begin{aligned} f(t+\Delta t, \mathbf{x}) &= \int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{x}-\mathbf{y}) f(t,\mathbf{y})\mathrm{d}\mathbf{y} = \int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y}) f(t,\mathbf{x}-\mathbf{y})\mathrm{d}\mathbf{y} \\ &= \int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y}) \left(f(t,\mathbf{x}) - \mathbf{y}^\intercal \nabla^{\mathrm{sp}} f(t,\mathbf{x}) + \tfrac{1}{2}\mathbf{y}^\intercal H_f^{\mathrm{sp}}(t,\mathbf{x})\mathbf{y} + \cdots \right) \mathrm{d}\mathbf{y} \\ &= f(t,\mathbf{x}) \underbrace{\int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y})\mathrm{d}\mathbf{y}}_{I_1} - \underbrace{\int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y})\mathbf{y}^\intercal \nabla^{\mathrm{sp}} f(t,\mathbf{x})\mathrm{d}\mathbf{y}}_{I_2} + \frac{1}{2} \underbrace{\int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y})\mathbf{y}^\intercal H_f^{\mathrm{sp}}(t,\mathbf{x})\mathbf{y}\mathrm{d}\mathbf{y}}_{I_3} + \cdots, \end{aligned} \tag{6}$$

where $\nabla^{\mathrm{sp}} f$ and H_f^{sp} denote the gradient and Hessian matrix of the function f with respect to the spatial variables, respectively. By (3), the integral $I_1 = 1$. Furthermore, we have

$$I_2 = \int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y}) \sum_{i=1}^{3} \frac{\partial f}{\partial x_i}(t,\mathbf{x}) y_i \mathrm{d}\mathbf{y} = \sum_{i=1}^{3} \frac{\partial f}{\partial x_i}(t,\mathbf{x}) \int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y}) y_i \mathrm{d}\mathbf{y} = 0,$$

which follows from the fact that $\Phi_{\Delta t}$ is a quickly vanishing radial function, and the fact that y_i is odd in the i-th variable. For the third integral, we have

$$\begin{aligned} I_3 &= \int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y}) \sum_{1\le i,j\le 3} \frac{\partial^2 f}{\partial x_i \partial x_j}(t,\mathbf{x}) y_i y_j \mathrm{d}\mathbf{y} \\ &= \sum_{i=1}^{3} \frac{\partial^2 f}{\partial x_i^2}(t,\mathbf{x}) \underbrace{\int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y}) y_i^2 \mathrm{d}\mathbf{y}}_{\substack{\text{Same for all } i \\ \text{by symmetry}}} + \sum_{\substack{1\le i,j\le 3 \\ i\ne j}} \frac{\partial^2 f}{\partial x_i \partial x_j}(t,\mathbf{x}) \underbrace{\int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y}) y_i y_j \mathrm{d}\mathbf{y}}_{0} \\ &= \Delta^{\mathrm{sp}} f(t,\mathbf{x}) \int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y}) \|\mathbf{y}\|_2^2 \mathrm{d}\mathbf{y} \\ &= \Delta t \ \Delta^{\mathrm{sp}} f(t,\mathbf{x}) \int_{\mathbb{R}^3} \widehat{\Phi}(\mathbf{y}) \|\mathbf{y}\|_2^2 \mathrm{d}\mathbf{y}. \end{aligned}$$

If we now compare the two Taylor expansions just obtained, then we get

$$\frac{\partial f}{\partial t}(t,\mathbf{x}) = \underbrace{\left(\frac{1}{2} \int_{\mathbb{R}^3} \widehat{\Phi}(\mathbf{y}) \|\mathbf{y}\|_2^2 \mathrm{d}\mathbf{y} \right)}_{\alpha} \Delta^{\mathrm{sp}} f(t,\mathbf{x}) + O(|\Delta t|^2). \tag{7}$$

For concreteness, let us assume that $\Phi_{\Delta t}$ is approximately a trivariate normal distribution $\mathcal{N}(\mathbf{0}, \boldsymbol{\Sigma})$ with all components of equal standard deviation. That is, with 3×3 covariance matrix

$$\boldsymbol{\Sigma} = \sigma^2 I_{3\times 3},$$

with $I_{3\times 3}$ the identity matrix. The function $\Phi_{\Delta t}$ should then be given by

$$\Phi_{\Delta t}(\mathbf{y}) = \frac{\exp\left(-\frac{1}{2}\mathbf{y}^\intercal \mathbf{\Sigma}^{-1}\mathbf{y}\right)}{\sqrt{(2\pi)^3 \det(\mathbf{\Sigma})}} = \frac{\exp\left(-\frac{\|\mathbf{y}\|_2^2}{2\sigma^2}\right)}{\sqrt{(2\pi)^3 \cdot (\sigma^2)^3}}.$$

Keeping (5) in mind and letting $C(\sigma) = 1/\sqrt{(2\pi)^3 \cdot (\sigma^2)^3}$, we get by symmetry:

$$\begin{aligned}
\int_{\mathbb{R}^3} \Phi_{\Delta t}(\mathbf{y})\|\mathbf{y}\|_2^2 \mathrm{d}\mathbf{y} &= 3C(\sigma) \iiint_{\mathbb{R}^3} y_1^2 e^{-\frac{y_1^2}{2\sigma^2}} e^{-\frac{y_2^2}{2\sigma^2}} e^{-\frac{y_3^2}{2\sigma^2}} \mathrm{d}y_1 \mathrm{d}y_2 \mathrm{d}y_3 \\
&= 3C(\sigma) \left(\int_{\mathbb{R}} e^{-\frac{y^2}{2\sigma^2}} \mathrm{d}y\right)^2 \int_{\mathbb{R}} y_1^2 e^{-y_1^2/2\sigma^2} \mathrm{d}y_1 \\
&= 3C(\sigma) \cdot 2\pi\sigma^2 \cdot \sqrt{2\pi}\sigma^3 \\
&= 3\sigma^2.
\end{aligned}$$

Thus, if the diffusivity α is known and the time step Δt is specified, then we can recover σ from (5) and (7). This yields

$$\sigma = \sqrt{\tfrac{2}{3}\alpha\Delta t},$$

and hence

$$\Phi_{\Delta t}(\mathbf{y}) = \frac{\exp\left(-\frac{\|\mathbf{y}\|_2^2}{2\cdot\frac{2}{3}\alpha\Delta t}\right)}{\sqrt{(2\pi)^3 \cdot (\frac{2}{3}\alpha\Delta t)^3}}.$$

When we now apply the scaling $\mathbf{y} = h\mathbf{z}$, assuming that $\mathbf{y}$ and $\mathbf{z}$ are the random variables corresponding to a dimensional and dimensionless Brownian “jump” from the origin, respectively, then we get then we get $\mathrm{d}\mathbf{y} = h^3 \mathrm{d}\mathbf{z}$, and hence

$$\mathbb{P}[\mathbf{z} \in S] = \mathbb{P}[\tfrac{1}{h}\mathbf{y} \in S] = \mathbb{P}[\mathbf{y} \in hS] = \int_{hS} \Phi_{\Delta t}(\mathbf{y})\mathrm{d}\mathbf{y} = h^3 \int_S \Phi_{\Delta t}(h\mathbf{z})\mathrm{d}\mathbf{z}.$$

Thus, the transition function corresponding to a Brownian jump of a “dimensionless particle” is given by the normal distribution

$$\Omega_{\Delta t}(\mathbf{z}) = h^3 \Phi_{\Delta t}(h\mathbf{z}) = h^3 \frac{\exp\left(-\frac{h^2\|\mathbf{z}\|_2^2}{2\cdot\frac{2}{3}\alpha\Delta t}\right)}{\sqrt{(2\pi)^3 \cdot (\frac{2}{3}\alpha\Delta t)^3}} = \frac{\exp\left(-\frac{\|\mathbf{z}\|_2^2}{2\cdot\frac{2}{3}\alpha\Delta t h^{-2}}\right)}{\sqrt{(2\pi)^3 \cdot (\frac{2}{3}\alpha\Delta t h^{-2})^3}},$$

whose standard deviation is

$$\sigma^* = \frac{1}{h}\sqrt{\tfrac{2}{3}\alpha\Delta t}.$$

References

[1] The derivation is modified from Xavier Raynaud’s problem description at `https://www.math.ntnu.no/emner/TMA4195/2022h/public/project/matmodproject-2022.pdf`