(Lesson 4b of 21/10/19) Compiled: November 11, 2019

0.1 Wiener's integral

From the previously derived results we know how to compute the probability for a Brownian particle, starting in x_0 at t_0 , to be inside an interval [A, B] at a certain time t:

$$\mathbb{P}\{x(t) \in [A, B]\} = \int_{A}^{B} dx \, W(x, t | x_0, t_0)$$

We are now interested in computing the expected value of functionals of the trajectories, i.e. of quantities that depend on several (or all) points of the trajectory $x(\tau)$ of a Brownian particle. The simplest example is the *correlation function*, which involves only the position at two different times $t_1 < t_2$:

$$f(t_1, t_2) = x(t_1)x(t_2)$$
 $t_1 < t_2$

A more general (and difficult) case is given by a function of the *entire* trajectory, such as:

$$F(\lbrace x(\tau) \colon 0 < \tau \le \tau \rbrace) = f\left(\int_0^t x(\tau)a(\tau) d\tau\right) \qquad a, f \colon \mathbb{R} \to \mathbb{R}$$

How to compute $\langle F \rangle$?

As always, we start from the simplest case, and then work our way up to the most complex one. So, let's start with the two points case: $f(x(t_1), x(t_2))$. For the average $\langle f \rangle$ we need to weight every possible value of f with the probability that f assumes that value, which will depend on the likelihood of the inputs $x(t_1)$ and $x(t_2)$. Thus, this becomes a problem of computing probabilities of compound events - that is, of the particle passing through a specific sets of points at certain times. As $x(\tau) \in \mathbb{R}$, any kind of $\mathbb{P}\{x(t_1) = x_1, x(t_2) \in x_2\}$ for certain t_1, t_2 and t_1, t_2 will be 0. We need, in general, to consider instead a range of possibilities, i.e. that the particle passes through a set of gates, so that $t_1, t_2 \in [A_1, B_1]$ and $t_2, t_3 \in [A_2, B_2]$.

In general, if we consider N gates $[A_i, B_i]_{i=1,\dots,N}$ the probability of a particle passing through all of them will be:

$$\mathbb{P}\{x(t_1) \in [A_1, B_1], x(t_2) \in [A_2, B_2], \dots, x(t_N) \in [A_N, B_N]\} =$$

$$= \int_{A_1}^{B_1} dx_1 W(x_1, t_1 | x_0, t_0) \int_{A_2}^{B_2} dx_2 W(x_2, t_2 | x_1, t_1) \cdots \int_{A_N}^{B_N} dx_N W(x_N, t_N | x_{N-1}, t_{N-1}) =$$

$$= \int_{A_1}^{B_1} \frac{dx_1}{\sqrt{4\pi D(t_1 - t_0)}} \exp\left(-\frac{(x_1 - x_0)^2}{4D(t_1 - t_0)}\right) \cdots \int_{A_N}^{B_N} \frac{dx_N}{\sqrt{4\pi D(t_N - t_{N-1})}} \exp\left(-\frac{(x_N - x_{N-1})^2}{4D(t_N - t_{N-1})}\right)$$

This is because the events of passing through two different gates are always *independent*: the transition probability between two gates depends only on their

distance, and not on the *history* of the particle¹.

However, for computing expected values of functions we are interested in *tiny* gates, so that the value of f at a gate is well defined (otherwise we would not know which value of f we are weighting with the trajectories probability). So, we diminish the size of gates, and instead of integrating the transition probabilities over sets $[A_i, B_i]$, we consider just their differentials:

$$W(x_t, t | x_0, t_0) dx_t \equiv \mathbb{P}\{x(t) \in [x_t, x_t + dx_t, x(t_0) = x_0]\}$$

So, we can now compute the (infinitesimal) probability that a Brownian particle will be very close to x_1 at $t = t_1$, and to x_2 at $t = t_2$:

$$\mathbb{P}\{x(t_1) \in [x_1, x_1 + \mathrm{d}x_1], x(t_2) \in [x_2, x_2 + \mathrm{d}x_2]\} =$$

$$= W(x_2, t_2 | x_1, t_1) W(x_1, t_1 | x_0, t_0) \, \mathrm{d}x_1 \, \mathrm{d}x_2$$

$$\equiv dP_{t_2, t_1}(x_2, x_1 | x_0, t_0)$$

And then we can compute the expected value of f:

$$\langle f(x(t_1), x(t_2)) \rangle = \iint_{\mathbb{R}^2} x_1 x_2 f(x_1, x_2) dP_{t_2, t_1}(x_2, x_1 | x_0, t_0)$$

$$\begin{split} \langle x(t_1)x(t_2)\rangle &= \iint_{\mathbb{R}^2} x_1 x_2 dP_{t_2,t_1}(x_2,x_1|x_0,t_0) = \\ &= \int_{\mathcal{C}\{x_0,t_0;t\}} x(t_1)x(t_2) \,\mathrm{d}_W x(\tau) = \\ &= \iint_{\mathbb{R}^2} \mathrm{d}x_1 \,\mathrm{d}x_2 \, x_1 x_2 \int_{\mathcal{C}\{x_0,t_0;x_1,t_1\}} \mathrm{d}_W x(\tau) \int_{\mathcal{C}\{x_1,t_1;x_2,t_2\}} \mathrm{d}_W x(\tau) \int_{\mathcal{C}\{x_2,t_2;t\}} \mathrm{d}_W x(\tau) \end{split}$$

In a certain (probabilistic) sense, dP_{t_2,t_1} measures the *volume* of all trajectories passing "really close" to x_1 at t_1 and x_2 at t_2 . The power of this idea becomes clear when we extend the number of gates N to infinity, while decreasing the interval $\Delta t_i = t_i - t_{i-1}$ between them:

$$\lim_{\substack{\Delta t_{i} \to 0 \\ N \to \infty}} \mathbb{P}\{x(t_{1}) \in dx_{1}, \dots, x(t_{N}) \in dx_{N}\} = \lim_{\substack{\Delta t_{i} \to 0 \\ N \to \infty}} \exp\left(-\sum_{i=1}^{N} \frac{(x_{i} - x_{i-1})^{2}}{4D(t_{i} - t_{i-1})}\right) \prod_{i=1}^{N} \frac{dx_{i}}{\sqrt{4\pi D(t_{i} - t_{i-1})}} = \lim_{\substack{\Delta t_{i} \to 0 \\ N \to \infty}} \exp\left(-\frac{1}{4D} \sum_{i=1}^{N} \frac{(x_{i} - x_{i-1})^{2}}{(t_{i} - t_{i-1})^{2}} \Delta t_{i}\right) \prod_{i=1}^{N} \frac{dx_{i}}{\sqrt{4\pi D \Delta t_{i}}} = \lim_{\substack{\Delta t_{i} \to 0 \\ N \to \infty}} \exp\left(-\frac{1}{4D} \int_{0}^{t} d\tau \, \dot{x}^{2}(\tau)\right) \prod_{\tau=0}^{t} \frac{dx(\tau)}{\sqrt{4\pi D d\tau}}$$

where in (a) we replaced the infinite "dense" sum with a formal integral (Riemann sum) of $(dx/dt)^2 = \dot{x}^2(\tau)$.

 $^{^{1} \}wedge \text{For example}$, the fact that a particle has travelled to the right for $0 < t < t_1$ tells nothing on the motion after t_1 .

0.2 Notes 1

Recall that W(x,t) dx is the probability of finding the Brownian particle in the interval [x, x + dx] at time t.

Then, letting the initial condition be $W(x, t_0|x_0, t_0) = \delta(x - x_0)$ (particle located in x_0 at t_0), the following holds (prove it explicitly as exercise):

$$\int dx' W(x, t|x', t') W(x', t'|x_0, t_0) = W(x, t|x_0, t_0) =$$

$$= \frac{1}{\sqrt{4\pi D(t - t_0)}} \exp\left(-\frac{(x - x_0)^2}{4D(t - t_0)}\right)$$

Define:

$$dP_{t,t'}(x, x'|x_0, t_0) = W(x, t|x', t')W(x', t'|x_0, t_0) dx dx'$$

with $t_0 < t' < t$ as the probability of finding a particle in [x, x + dx] at time t, and then in [x', x' + dx'] at time t'. Then:

$$\langle x'(t)x(t)\rangle = \int dP_{t,t'}(x,x'|x_0,t_0)x_0x'$$

Consider a function g of n points of the trajectory, sampled at times t_1, t_2, \ldots, t_n :

$$g(x(t_1), x(t_2), \ldots, x(t_n))$$

To compute $\langle g \rangle$, we need to extend the joint pdf:

$$dP_{t_n,t_{n-1},\dots,t_1}(x_n,\dots,x_1,x_0,t_0) \equiv W(x_n,t_n|x_{n-1}t_{n-1})\cdots W(x_1,t_1|x_0,t_0) \prod_{i=1}^n dx_i$$
(1)

leading to:

$$\langle g(x(t_1), x(t_2), \dots, x(t_n)) \rangle = \int dP_{t_n, t_{n-1}, \dots, t_2, t_1}(x_n, \dots, x_1 | x_0, t_0) g(x_1, \dots, x_n)$$

Expanding (1):

$$dP_{t_n, t_{n-1}, \dots, t_2, t_1} = \int \prod_{i=1}^{n} \frac{\mathrm{d}x_i}{\sqrt{4\pi D\Delta t_i}} \exp\left(-\sum_{i=1}^{n} \frac{(x_i - x_{i-1})^2}{4D\Delta t_i}\right)$$

Consider now a function of the *whole* trajectory:

$$F(\{x(\tau)\colon 0<\tau\leq t\})$$

For example:

$$F = f\left(\int_0^t x(\tau)a(\tau)\,\mathrm{d}\tau\right)$$

with a given function $a(\tau)$, such as $a(\tau) = 1$ or $a(\tau) = e^{-\tau/\tau_0}$. To compute the average of F we introduce the Wiener measure $d_W x$, i.e. a generalization of (1) to the continuum, so that:

$$\langle F \rangle = \int d_W x F(\{x(\tau) \colon 0 < \tau \le \tau\})$$

and the integral is over a *space of trajectories* $x: T \to R$, with $R \subseteq \mathbb{R}$, denoted with \mathbb{R}^T (generalizing the common notation). For example: $T = [0, \infty]$.

We have to define a sigma algebra in this space \mathbb{R}^T in order to define a measure $d_W x$, i.e. a domain of measurable sets for which a probability measure makes sense.

We start by defining a set of intervals $H_i \subset \mathbb{R}$ (for example $H_i = (x_i, x_i + \Delta x_i)$). We then consider the set of functions having values inside these H_i : $\mathbb{R}^T : \{x(t_i) \in H_i\}_{i=1,\dots,n}$. In other words, this is the set of trajectories that pass through each H_i at instant t_i . Then we define the measure:

$$\mu_W(\{x(t_1) \in H_1, x(t_2) \in H_2, \dots, x(t_n) \in H_n\}) =$$

$$= \int dP_{t_n, \dots, t_1}(x_n, \dots, x_1 | x_0, t_0) \mathbb{I}_{H_1}(x_1) \cdots \mathbb{I}_{H_n}(x_n)$$

where \mathbb{I}_{H_i} are characteristic sets:

$$\mathbb{I}_{H_i}(x) = \begin{cases} 1 & x \in H_i \\ 0 & x \notin H_i \end{cases}$$

Thanks to the **Kolomogorov theorem** we can *extend* this measure, defined in the "tube that passes through all gates" $\{x(t_i) \in H_i\}$ to the entire \mathbb{R}^T .

Knowing that this measure exists in the *continuous case*, we can give meaning to a *continuum limit* of the *discrete case*. More precisely, in order to compute a function of the entire trajectory:

$$F(\{x(\tau) \colon 0 < \tau < t\})$$

we start with a discretization $t_1 < t_2 < \cdots < t_N < t \equiv t_{N+1}$, evaluate a discretized function $F_N(x(t_1), \dots, x(t_N))$ and then consider the limit $N \to \infty$:

$$\lim_{N\to\infty} \langle F_N(x(t_1),\ldots,x(t_N)) \rangle$$

meaning that $\Delta t_i \to 0$, where $\Delta t_i = t_i - t_{i-1}$. We know how to compute the average of a function that depends on a *finite* set of trajectory points:

$$\lim_{N \to \infty} \int \prod_{i=1}^{N+1} \frac{\mathrm{d}x_i}{\sqrt{4\pi D\Delta t_i}} \exp\left(-\sum_{i=1}^{N+1} \frac{(x_i - x_{i-1})^2}{4D\Delta t_i}\right) F_N(x_1, \dots, x_N)$$

The normalization condition:

$$\begin{split} 1 &= \int dP_{t_1,\dots,t_N}(x_1,\dots,x_N|x_0,t_0) = \\ &= \int \prod_{i=1}^{N+1} \frac{\mathrm{d}x_i}{\sqrt{4\pi D\Delta t_i}} \exp\left(-\sum_{i=1}^N \frac{(x_i-x_{i-1})^2}{4D\Delta t_i}\right) = \\ &= \int \frac{\mathrm{d}x_N}{(4\pi D\Delta t_N)} \exp\left(-\frac{(x_N-x_{N-1})^2}{4D\Delta t_N}\right) \end{split}$$

Example 1 (Correlator function):

$$\langle x(t_1')x(t_2')\rangle = \int dx_1' dx_2' W(x_2', t_2'|x_1', t_1')W(x_1', t_1'|0, 0)x_1'x_2'$$

The same result can be obtained by using Wiener's measure:

$$\langle x(t_1')x(t_2')\rangle = \int d_W x \, x_1(t_1')x_2(t_2') = \int d\mathbb{P}_{t_1,\dots,t_N}(x_1,\dots,x_N|0,0)x(t_k)x(t_n) =$$

$$= \int dx_1 \dots dx_N \, W(x_N,t_N|x_{N-1},t_{N-1}) \dots W(x_1,t_1|0,0)x_k x_n =$$

$$= \int dx_k \, dx_n \, W(x_n,t_n|x_k|t_k)W(x_k,t_k|0,0)x_k x_n$$

Note that:

$$W(x,t|0,0) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x^2}{4Dt}\right) = \int d_W x \,\delta(x(t) - x)$$

0.3 Change of random variables

Consider a random variable $X \sim q(x)$, with q(x) being a generic distribution (e.g. $q(x) = \mu e^{-\mu x}$). Now consider a function y(x), e.g. $y(x) = x^2$. Y is then a new random variable, with a certain distribution p(y). We now want to compute p(y) starting from q(x) and y(x).

Suppose that y(x) is invertible. Then, if we extract a value from X, it will be inside [x, x + dx] with a probability q(x) dx. Knowing X, we can use y(x) to uniquely determine Y, that will be in [y, y + dy] with the same probability. So, the following holds:

$$q(x) dx = p(y) dy (2)$$

We can compute dy by nudging y(x), and expanding in Taylor series:

$$y(x + dx) \equiv y + dy + O(dy^{2}) = y(x) + \underbrace{dx \, y'(x)}_{dy} + O(dx^{2})$$

and so dy = dx y'(x). Substituting in (2) we get:

$$q(x) dx = p(y) dy = p(y(x))y'(x) dx \Rightarrow p(y) = q(x(y))\frac{dx}{dy}(x(y))$$

For a more general y(x), $x \sim q(x)$ and y = y(x), the expected value of a function f is:

$$\langle f(y) \rangle = \int dx \, f(y(x)) q(x) = \int dy \, f(y) p(y) =$$

$$= \int dx \, f(y(x)) q(x) \underbrace{\int dz \, \delta(z - y(x))}_{=1} =$$

$$= \int dz \, f(z) \underbrace{\int dx \, q(x) \delta(z - y(x))}_{\langle \delta(z - y(x)) \rangle}$$

and so:

$$p(z) = \int dx \, q(x) \delta(z - y(x)) = \langle \delta(z - y(x)) \rangle$$

which, in general, is not:

$$p(z) \neq q(x(z)) \frac{\mathrm{d}x(z)}{\mathrm{d}z}$$

However, if y(x) is invertible, i.e. $\operatorname{sgn} y'(x) = \operatorname{constant} (y'(x) \neq 0 \text{ always})$, then:

$$\delta(z - y(x)) = \frac{\delta(x - x(z))}{|y'(x)|}$$

leading to:

$$p(z) = \langle \frac{\delta(x - x(z))}{|y'(x)|} \rangle_q = \int dx \, q(x) \frac{\delta(x - x(z))}{|y'(x)|} = q(x(z))|y'(x(z))|^{-1} = q(x(z)) \frac{dx}{dy}$$

and we recover the previous formula.

0.4 The 1st integral

So we can now write:

$$W(x,t|0,0) = \int d_W x \, \delta(x(t) - x) =$$

$$= \lim_{N \to \infty} \int \prod_{i=1}^{N+1} \frac{dx_i}{\sqrt{4\pi D\Delta t_i}} \exp\left(-\sum_{i=1}^{N} \frac{(x_i - x_{i-1})^2}{4D\Delta t_i}\right) \delta(x_{N+1} - x)$$

where $t_n = t$, $x(t_n) = x_{N+1}$.

Recall that:

$$W(x_t, t|0, 0) = \frac{1}{\sqrt{4\pi Dt}} \exp\left(-\frac{x_t^2}{4Dt}\right)$$

If we set $x_t = 0$ (for simplicity), we get:

$$W(0,t|0,0) = \frac{1}{\sqrt{4\pi Dt}}$$
 (3)

As an exercise to get some familiarity with Wiener integrals, we want now to re-derive this result, by instead solving a path integral:

$$W(0, t|0, 0) = \int_{\mathcal{C}\{0,0;0,t\}} d_W x(\tau) = \langle \delta(0-x) \rangle = \langle \delta(x) \rangle \equiv I_1????$$

Here we are computing the *fraction* of Brownian paths that start in x = 0 at t = 0 and return in x = 0 after a fixed interval t.

The standard way to compute a Wiener integral is to discretize it, and then take a continuum limit. So, consider a uniform time discretization $\{t_i\}_{i=1,\dots,N+1}$, ϵ apart from each other, so that:

$$t_i - t_{i-1} = \epsilon = \frac{t}{N+1} \quad \forall i = 1, \dots, N+1$$

Note that the end-points are $x_0 = x_{N+1} = 0$.

Then:

$$I_1 \equiv \lim_{\substack{\epsilon \to 0 \\ N \to \infty}} I_1^{(N)} \tag{4}$$

$$I_1^{(N)} \equiv \frac{1}{(\sqrt{4\pi D\epsilon})^{N+1}} \int_{-\infty}^{+\infty} \mathrm{d}x_1 \int_{-\infty}^{+\infty} \mathrm{d}x_2 \cdots \int_{-\infty}^{+\infty} \mathrm{d}x_N \exp\left(-\frac{1}{4D\epsilon} \sum_{i=0}^{N} (x_{i+1} - x_i)^2\right)$$
(5)

Let's focus on the summation in the exponential:

$$\sum_{i=0}^{N} (x_{i+1} - x_i)^2 = x_1^2 + x_0^2 - 2x_0 x_1 + x_2^2 + x_1^2 - 2x_1 x_2 + \dots + x_{N+1}^2 + x_N^2 - 2x_N x_{N+1} =$$

$$= 2(x_1^2 + \dots + x_N^2) - 2(x_1 x_2 + x_2 x_3 + \dots + x_{N-1} x_N) =$$

$$= 2\left(\sum_{i=1}^{N} x_i^2\right) - 2\left(\sum_{i=1}^{N-1} x_i x_{i+1}\right)$$

This is a *quadratic form*, i.e. a polynomial with all terms of order 2. So, it can be written in *matrix form*:

$$= \sum_{k,l=1}^{N} x_k A_{kl} x_l = \boldsymbol{x}^T A_N \boldsymbol{x}$$

for an appropriate choice of entries A_{kl} of the $N \times N$ matrix A_N :

$$A_{kk} = 2; \ A_{kl} = -(\delta k, l+1+\delta_{k+1,l}) \Rightarrow A_N = \begin{pmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{pmatrix}$$

Substituting back in (5):

$$I_1^{(N)} = \frac{1}{(\sqrt{4\pi D\epsilon})^{N+1}} \int_{-\infty}^{+\infty} \mathrm{d}x_1 \cdots \int_{-\infty}^{+\infty} \mathrm{d}x_N \exp\left(-\frac{\boldsymbol{x}^T A_N \boldsymbol{x}}{4D\epsilon}\right)$$

Recall the multivariate Gaussian integral:

$$\int_{-\infty}^{+\infty} dx_1 \cdots dx_N \exp\left(-\sum_{ij}^N B_{ij} x_i x_j\right) = \frac{(\sqrt{\pi})^N}{\sqrt{\det B}}$$

leading to:

$$I_{1}^{(N)} = \frac{1}{(\sqrt{4\pi D\epsilon})^{N+1}} \sqrt{\frac{\pi^{N}}{\det\left(A_{N} \left[\frac{1}{4D\epsilon}\right]^{N}\right)}} \stackrel{=}{=} \frac{1}{(\sqrt{4\pi D\epsilon})^{N+1}} \frac{\sqrt{4\pi D\epsilon}^{N}}{\sqrt{\det A_{N}}} = \frac{1}{\sqrt{4\pi D\epsilon}} \frac{1}{\sqrt{\det A_{N}}}$$

$$(6)$$

where in (a) we used the property of the determinant $\det(cA) = c^n \det(A) \, \forall c \in \mathbb{R}$. Now, all that's left is to compute the determinant of A_N . Fortunately, as A_N is a tri-diagonal matrix, there is a recurrence relation in terms of the leading principal minors of A_N , which turns out to be multiples of the determinants of A_{N-1} and A_{N-2} .

Explicitly, consider A_N :

$$\det A_N \equiv \begin{vmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{vmatrix}_{N \times N}$$

and start computing the determinant following the last column. The only non-zero

contributions are:

$$\det A_{N} = \underbrace{(-1)^{(N-1)+N}(-1)}_{+1} \begin{vmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & -1 & 2 & -1 \\ 0 & \cdots & 0 & 0 & -1 \end{vmatrix}_{(N-1)\times(N-1)} + (-1)^{2N}(2) \det A_{N-1} =$$

$$= (-1)^{2(N-1)}(-1) \det A_{N-2} + 2 \det A_{N-1} = 2 \det A_{N-1} - \det A_{N-2}$$
 (7)

where the terms in blue are just the alternating signs from the determinant expansion, and the other colours identify the matrix entries that are being used. Then, it is just a matter of computing the first two terms of the succession ($|A_N|$ = det A_N for brevity):

$$|A_1| = 2$$
 $|A_2| = \begin{vmatrix} 2 & -1 \\ -1 & 2 \end{vmatrix} = 4 - 1 = 3$

And now we can use (7) to iteratively compute all $|A_N|$, e.g. $|A_3| = 2 \cdot 3 - 2 = 4$. To find $|A_N|$ for a *generic* N, we need to make an hypothesis, and then verify that it is compatible with (7). In this case, note that $|A_N| = N + 1$ (*) for all the examples we explicitly computed. Then, by induction:

$$|A_{N+1}| = 2 \cdot |A_N| - |A_{N-1}| = 2 \cdot (N+1) - (N-1+1) = 2N + 2 - N = (N+1) + 1$$

which is indeed compatible with (*). So, substituting back in (6) we get:

$$I_1^{(N)} = \frac{1}{\sqrt{4\pi D\epsilon}} \frac{1}{\sqrt{N+1}} \stackrel{=}{=} \frac{1}{\sqrt{4\pi Dt}}$$

where in (a) we used $\epsilon = t/(N+1) \Rightarrow N+1 = t/\epsilon$ from the discretization. Note that this result is *constant* with respect to ϵ or N (recall that t is fixed beforehand) and so taking the *continuum* limit leads immediately to I_1 (4):

$$I_1 \equiv \lim_{\substack{\epsilon \to 0 \\ N \to \infty}} \frac{1}{\sqrt{4\pi Dt}} = \frac{1}{\sqrt{4\pi Dt}}$$

which is coherent with the result we previously computed (3).