Lecture 4

The Wiener process

1D FP eq'n, no drift, diffusion coefficient = 1: r.v. $W(t)$

$$\frac{\partial p(w,t|w_0,t_0)}{\partial t} = \frac{1}{2}\frac{\partial^2 p(w,t|w_0,t_0)}{\partial w^2}.$$

IC: $p(w,t_0|w_0,t_0) = \delta(w-w_0)$

Characteristic function:

$$\varphi(s,t) = \underbrace{\int dw\, e^{isw}\, p(w,t|w_0,t_0)}_{``\langle e^{isw}\rangle}$$

satisfies $\dfrac{\partial \varphi}{\partial t} = -\dfrac{1}{2}s^2\varphi$, solved by

$$\varphi(s,t) = e^{-\frac{s^2}{2}(t-t_0)}\varphi(s,t_0).$$

Here, $\varphi(s,t_0) = \int dw\, \delta(w-w_0)\, e^{isw} = e^{isw_0}.$

So, $\varphi(s,t) = e^{isw_0 - \frac{s^2}{2}(t-t_0)}$, yielding

$$p(w,t|w_0,t_0) = \frac{1}{\sqrt{2\pi(t-t_0)}}\, e^{-\frac{(w-w_0)^2}{2(t-t_0)}},$$

as expected.

Then $\begin{cases} \langle W(t)\rangle = w_0, \\ \langle [W(t)-w_0]^2\rangle = t-t_0. \end{cases}$

Multi-D Wiener process:

$$\vec{W}(t) = [W_1(t), \ldots, W_n(t)]$$

FP equation:

$$\frac{\partial p(\vec{w}, t \mid \vec{w}_0, t_0)}{\partial t} = \frac{1}{2} \sum_{i=1}^{\overset{\#\text{DoF}}{n}} \frac{\partial^2}{\partial w_i^2} p(\vec{w}, t \mid \vec{w}_0, t_0),$$

solved by

$$p(\vec{w}, t \mid \vec{w}_0, t_0) = \frac{1}{(2\pi(t-t_0))^{n/2}} e^{-\frac{(\vec{w}-\vec{w}_0)^2}{2(t-t_0)}},$$

a product of 1D gaussians.

Note that
$$\begin{cases} \langle \vec{W}(t) \rangle = \vec{w}_0, \\ \langle [W_i(t) - w_{0,i}][W_j(t) - w_{0,j}] \rangle = \\ \qquad = (t - t_0)\,\delta_{ij} \end{cases}$$

__Properties of the Wiener process:__

(1) Irregularity of sample paths:
mean $= 0$ but variance $\uparrow$ as $t \uparrow$.
This results in very variable paths.

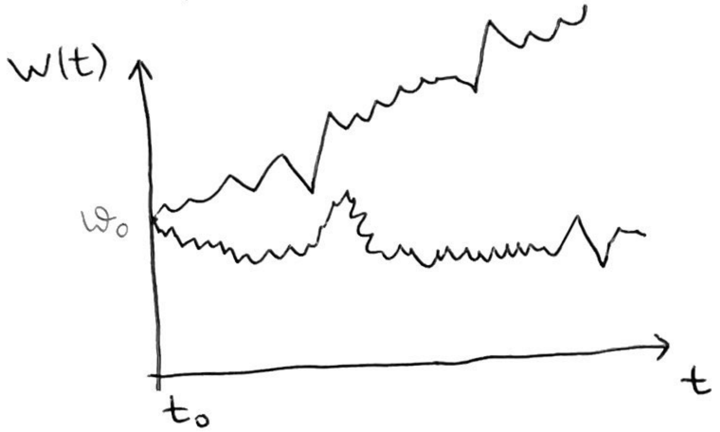
(2) Sample paths of $W(t)$ are continuous but __not__ differentiable.

Consider $\lim_{h \to 0} P\left\{ \left| \frac{W(t+h) - W(t)}{h} \right| > \underset{\substack{\uparrow \\ \text{some const}}}{k} \right\} =$

$$\stackrel{\lim_{h\to 0}}{=} 2\int_{hk}^{\infty} dw \, \frac{1}{\sqrt{2\pi h}} e^{-\frac{w^2}{2h}} = 1$$ for any finite k.

So, $\lim_{h\to 0} \frac{|W(t+h) - W(t)|}{h}$ is guaranteed to be greater than any cutoff k $\Rightarrow$ the derivative of $W(t)$ is 'almost certainly' infinite. This is an idealization of physical Brownian motion.

Sample paths:



substantial variability

(3) Independence of increments:

since the Wiener process is Markovian, we have

$$p(w_n, t_n; w_{n-1}, t_{n-1}; \ldots; w_0, t_0) =$$

$$= \prod_{i=0}^{n-1} p(w_{i+1}, t_{i+1} | w_i, t_i) \times p(w_0, t_0) \;\boxed{=}$$

$$\Leftrightarrow \prod_{i=0}^{n-1} \left\{ \frac{1}{\sqrt{2\pi (t_{i+1} - t_i)}} e^{-\frac{(w_{i+1} - w_i)^2}{2(t_{i+1} - t_i)}} \right\} \times p(w_0, t_0).$$

Define $\begin{cases} \Delta W_i = W(t_i) - W(t_{i-1}), \\ \Delta t_i = t_i - t_{i-1}. \end{cases}$

Then $p(\Delta w_n; \Delta w_{n-1}; \ldots; w_0) =$

$$= \prod_{i=1}^{n} \left\{ \frac{1}{\sqrt{2\pi \Delta t_i}} e^{-\frac{\Delta w_i^2}{2\Delta t_i}} \right\} \times p(w_0, t_0).$$

So, ΔW_i's are indep. of each other and of $W(t_0)$.

(4) Autocorrelation function: [assumed $t > s$]

$$\langle W(t) W(s) \rangle = \int dw_1 \, dw_2 \, w_1 w_2 \, p(w_1, t; w_2, s | w_0, t_0)$$

conditioned on $W(t_0) = w_0$

Then $\langle W(t) W(s) \rangle = \langle [\underbrace{W(t) - W(s)}_{\text{indep. of } W(s),\ \langle\ldots\rangle\langle W(s)\rangle = 0}] W(s) \rangle +$

$$+ \underbrace{\langle W^2(s) \rangle}_{(s - t_0) + w_0^2} \;=$$

$$= (s - t_0) + w_0^2.$$

Likewise, if $t<s$ we have

$$\langle W(s)\, W(t)\rangle = (t-t_0) + w_0^2 .$$

In general,

$$\langle W(t)\, W(s)\rangle = \min(t-t_0,\, s-t_0) + w_0^2 .$$

The Ornstein - Uhlenbeck process

1D FP eq'n, linear drift, diffusion coeff. $= D$: r.v. $X(t)$

$$\frac{\partial p(x,t|x_0,0)}{\partial t} = \frac{\partial}{\partial x}(k x p) + \frac{1}{2} D \frac{\partial^2}{\partial x^2}(p) .$$

Introduce the characteristic function again:

$$\varphi(s,t) = \int_{-\infty}^{\infty} dx\, e^{isx}\, p(x,t|x_0,0) ,$$ then

$$\frac{\partial \varphi}{\partial t} + \underbrace{ks \frac{\partial \varphi}{\partial s}} = -\frac{1}{2} D s^2 \varphi . \qquad (*)$$

Indeed, $k \int_{-\infty}^{\infty} dx\, e^{isx}\, \partial_x (x p) =$

$$\overset{(=)}{=} k\varphi(s,t) + k\int_{-\infty}^{\infty} dx\, \underbrace{e^{isx} x(\partial_x p)}_{\text{by parts}} =$$

$$= k\varphi - k\int_{-\infty}^{\infty} dx\, p\, \partial_x (e^{isx} x) =$$

$$= k\varphi - k\varphi - iks \underbrace{\int_{-\infty}^{\infty} dx\, p\, x\, e^{isx}}_{= \frac{\partial}{\partial (is)} \varphi(s,t)} =$$

$$= -ks\,\partial_s \varphi,$$

as desired.

Eq. (*) can be solved by the <u>method of characteristics</u>.

<u>Method of characteristics</u>

This is a technique for solving first-order PDEs.

Consider
$$a(x,y)\, \underset{}{\overset{\frac{\partial u}{\partial x}}{u_x}} + b(x,y)\, \overset{\frac{\partial u}{\partial y}}{u_y} = c(x,y) \qquad (**)$$
$$u = u(x,y)$$

The goal is to find $u(x,y)$. Consider a 3D surface S given by $(x, y, u(x,y))$. What is a normal to this surface? Well, consider the gradient in the x-dir:
$$\frac{\partial}{\partial x}(x, y, u) = (1, 0, u_x).$$

Likewise, the grad in the y-dir is given by:

$$\frac{\partial}{\partial y}(x, y, u) = (0, 1, u_y).$$

Then the normal to surface S at (x,y) is given by

$$\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ 1 & 0 & u_x \\ 0 & 1 & u_y \end{vmatrix} = (-u_x, -u_y, 1).$$

We will actually use $(u_x, u_y, -1)$ and notice that

$$(a, b, c) \underset{\substack{\uparrow \\ \text{scalar} \\ \text{product}}}{\cdot} (u_x, u_y, -1) = 0.$$

Thus, $(a(x,y), b(x,y), c(x,y))$ lies in the **tangent plane** of S. We need to construct a surface S s.t. at each point $(x, y, z = u(x,y))$ on the surface, vector (a, b, c) lies in the tangent plane.

Let's construct a parametrized curve C (which lies in S): $C = (x(s), y(s), z(s))$ s.t. the vector

$$(a(x(s), y(s)), b(x(s), y(s)), c(x(s), y(s)))$$

is everywhere tangent to the curve C.

This leads to the system of ODEs:

$$\begin{cases} \dfrac{dx}{ds} = a(x(s), y(s)), \\ \dfrac{dy}{ds} = b(x(s), y(s)), \\ \dfrac{dz}{ds} = c(x(s), y(s)). \end{cases}$$

C is called the <u>characteristic</u> <u>curve</u> of the PDE (**). S is a union of the characteristic curves.

<u>Ex.</u> Consider $u_t + a u_x = 0$ (+) transport equation

characteristic equations:

$$\begin{cases} \dfrac{dx}{ds} = a, \\ \dfrac{dt}{ds} = 1, \\ \dfrac{dz}{ds} = 0. \end{cases} \Rightarrow \begin{cases} x(s) = as + C_1, \\ t(s) = s + C_2, \\ z(s) = C_3. \end{cases}$$

Then $\begin{cases} x - at = C_1 - aC_2 \equiv \underbrace{x_0}_{\text{const}}, \\ z = \underbrace{C_3}_{\text{const}}. \end{cases}$

We notice that $z(x,t) = \text{const}$ if

$$\underbrace{z(x,t)}_{\text{"}u(x,y)\text{" from before}} = f(x - at).$$

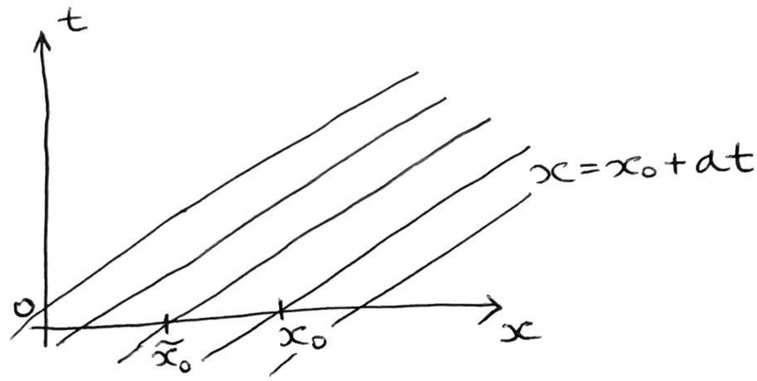
↑ arbitrary function

$f(x-at)$ is in fact the general solution of the transport eq'n (+):

$$u_t + a u_x = -a f'(x-at) + a f'(x-at) = 0.$$

Since $x = x_0 + at$, the initial distribution $f(x_0)$ will propagate in time along the projected characteristic curves:

with s-prm eliminated



Often, the system of ODEs is written as $ds = \dfrac{dx}{a} = \dfrac{dy}{b} = \dfrac{dz}{c}$ and the equations are solved pairwise without introducing s at all.

In our case, we have:

$$a(x,y)\,u_x + b(x,y)\,u_y = c(x,y,u),$$

which leads to

the following system of characteristic ODEs:

$$
\begin{cases}
\dfrac{dx}{ds} = a(x,y), \\[2mm]
\dfrac{dy}{ds} = b(x,y), \\[2mm]
\dfrac{dz}{ds} = c(x,y,\underset{\approx}{z}).
\end{cases}
$$

In the case of Eq. (*) we obtain:

$$
\frac{dt}{1} = \frac{ds}{ks} = -\frac{d\varphi}{\frac{1}{2}Ds^2\varphi}.
$$

In particular,

$$
dt = \frac{ds}{ks} \Rightarrow \frac{ds}{s} = k\,dt, \text{ or}
$$

$$
s = \underbrace{a}_{\text{arbitrary const}} e^{kt}
$$

Then $u(s,t,\varphi) \equiv \underbrace{s e^{-kt}}_{\text{no } \varphi\text{-dependence}} = a.$

Likewise, $\dfrac{d\varphi}{\varphi} = -\dfrac{1}{2}\dfrac{D}{k} s\,ds$, or

$$
\varphi = \underbrace{b}_{\text{arb. const}} e^{-\frac{Ds^2}{4k}}
$$

Then $v(s,t,\varphi) \equiv \underbrace{\varphi e^{\frac{Ds^2}{4k}}}_{\text{no } t\text{-dependence}} = b$

So, $\tilde{f}(u,v) = \tilde{f}(a,b) \equiv \underbrace{A}_{\text{const}}$

But then

$$\underbrace{\tilde{f}(u,v) - A}_{\equiv f(u,v)} = \tilde{f}(a,b) - A = 0 .$$

$f(u,v)=0$ yields $v = g(u)$.

$\uparrow$ some function of u

We do not need $u = \tilde{g}(v)$ because $v \sim \varphi$, and our goal is to find $\varphi(s,t)$.

Thus, $\varphi(s,t) = e^{-\frac{Ds^2}{4k}} \, g(s e^{-kt})$. $\Leftarrow$ general solution

Indeed,

$$\partial_t \varphi + ks\, \partial_s \varphi = e^{-\frac{Ds^2}{4k}} g' \times (-sk) e^{-kt} +$$

$$+ ks \Big[-\frac{Ds}{2k} \underbrace{g\, e^{-\frac{Ds^2}{4k}}}_{\varphi} + e^{-\frac{Ds^2}{4k}} g' \times e^{-kt} \Big] =$$

$$= -\frac{Ds^2}{2}\varphi \text{ , as expected.}$$

IC: $p(x,0 \mid x_0, 0) = \delta(x - x_0)$.

Then $\varphi(s,0) = e^{isx_0}$, yielding at $t=0$:

$$g(s) = \varphi(s,0)\, e^{\frac{Ds^2}{4k}} = e^{\frac{Ds^2}{4k} + isx_0} .$$

$\Leftarrow$ explicit g, fixed by ICs

Finally,

$$\varphi(s,t) = e^{-\frac{Ds^2}{4k}} e^{\frac{D}{4k}s^2 e^{-2kt}} e^{ix_0 s e^{-kt}} =$$

$$= e^{-\frac{Ds^2}{4k}(1-e^{-2kt})} e^{ix_0 s e^{-kt}}.$$

This actually corresponds to a gaussian $p(x,t|x_0,0)$:

if $p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\bar{x})^2}{2\sigma^2}}$,

$$\varphi(s) = \langle e^{isx} \rangle = e^{is\bar{x} - \frac{1}{2}s^2\sigma^2}.$$

In our case,

$$\begin{cases} \overset{\langle X(t)\rangle}{\overset{\parallel}{\bar{x}}} = x_0 e^{-kt}, \\ \underset{\mathrm{Var}\{X(t)\}}{\underset{\parallel}{\sigma^2}} = \frac{D}{2k}(1-e^{-2kt}). \end{cases}$$

<u>Stationary solution</u>:

$$t\to\infty: \begin{cases} \bar{x}\to 0, \\ \sigma^2 \to \frac{D}{2k}. \end{cases}$$

Indeed, if $\partial_t p = 0$,

$$\partial_x [\underbrace{kxp + \frac{D}{2}\partial_x p}_{-J_{ss}\ =\ SS\ \text{current}}] = 0.$$

With DB, $J_{ss} = 0$, yielding

$$\frac{\partial_x p}{p} = -\frac{2kx}{D},$$ solved by

$$p_{ss}(x) = \sqrt{\frac{k}{\pi D}}\, e^{-\frac{kx^2}{D}}.$$ indep. of ICs

Consistent with $\bar{x}$ & σ^2 in the $t \to \infty$ limit.

$U(x) = \frac{\bar{k}x^2}{2}$

Note that $F_{fr} = \zeta \frac{dx}{dt} = F_{ext} = \bar{k}x$ in the overdamped limit, or $\frac{dx}{dt} = \underbrace{\frac{\bar{k}}{\zeta}}_{=k} x$

<u>Time correlation function</u>:

$\frac{D}{2} = \bar{D}$ ← diff'n const. Then $p_{ss}(x) \sim e^{-\frac{\bar{k}x^2}{2\underbrace{\zeta\bar{D}}_{=k_BT}}} = e^{-\beta U(x)}$ Boltzmann equil.

Consider SS correlation f'n:

$$\lim_{t_0 \to -\infty} p(x_2, s \mid x_0, t_0) = p_{ss}(x_2) = \sqrt{\frac{k}{\pi D}}\, e^{-\frac{kx_2^2}{D}}.$$

Then $\langle X(t) X(s) \rangle_{ss} = \int dx_1 dx_2\, x_1 x_2 \times$

$$\times\, p(x_1, t; x_2, s \mid x_0, t_0) =$$

$$= \int dx_1 dx_2\, x_1 x_2\, p(x_1, t \mid x_2, s)\, \underbrace{p(x_2, s \mid x_0, t_0)}_{= p_{ss}(x_2)}.$$

$$t \geq s \geq t_0 = -\infty$$

Here, $$p(x_1, t \mid x_2, s) = \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{(x_1 - \bar{x}_1)^2}{2\sigma^2}},$$

with $$\begin{cases} \bar{x}_1 = x_2\, e^{-k(t-s)}, \\ \sigma^2 = \frac{D}{2k}\left(1 - e^{-2k(t-s)}\right). \end{cases}$$

One can show that

$$\langle X(t)X(s)\rangle_{ss} = \frac{D}{2K} e^{-k|t-s|}.$$

Thus, the correlation time is finite:

$$\tau = \frac{1}{K}.$$