The Fokker-Planck Equation (FPE)

Plan
- Introduction: – some background
  - The equation.
  - some applications
- Derivations of the FPE
- Some Properties: – connections to other equations: Liouville's equation.
  - special cases
    Kramers eq. Smoluchowski eq.
  - relation to the PNP system.

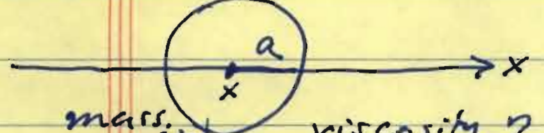
(?)

- A variational principle
  - the Wasserstein metric
  - The FPE is the steepest descent of a free-energy functional w.r.t. the W-metric

Style: Heuristic description + ~~some~~ rigorous statements + Questions for research

1. Introduction.

Example: The one-dimensional motion of a Brownian (spherical) partical in a fluid medium.



mass: m viscosity: η

velocity: v

position: x

Newton's law of motion

$$m \frac{dv}{dt} = F_{total}(t)$$

$\uparrow$ instaneous force on the particle at time t.

What is F_{total}?

Assume F_{total} = a friction force $= -\zeta v$

v ... velocity

ζ ... friction coefficient.

Stokes' law: $\zeta = 6\pi\eta a$

η = viscosity of the surrounding fluid.

Then, $m\frac{dv}{dt} = -\zeta v$

$\Longrightarrow \quad v(t) = e^{-\zeta t/m}\, v(0)$.

$\lim_{t\to\infty} v(t) = 0$.

But: thermal equilibrium ~~fluctuations~~ $\Rightarrow \langle v^2\rangle_{eq} = k_B T/m$.

T — temperature, k_B — Boltzmann's constant.

So, $\boxed{F_{total} = -\zeta v + \delta F(t)}$

$\delta F(t)$ = random or fluctuating force (or stochastic)

This is the ~~Eq~~ Langevin equation for a Brownian particle.

Reasonable assumptions — due to nature of fluctuations

$\langle \delta F(t)\rangle = 0$, $\langle \delta F(t)\delta F(t')\rangle = 2B\,\delta(t-t')$

(vanishing average)

strength of the fluctuation

Formal calculations

$$m\frac{dv}{dt} = -\zeta v + \delta F(t)$$

$$v(t) = e^{-\zeta t/m} v(0) + \int_0^t dt'\, e^{-\zeta(t-t')/m}\, \delta F(t')/m$$

$$\langle v(t)^2\rangle = e^{-2\zeta t/m} v(0)^2 + \frac{B}{\zeta m}\left(1 - e^{-2\zeta t/m}\right)$$

But $\langle v^2\rangle_{eq} = \frac{k_B T}{m} := \lim_{t\to\infty}\langle v(t)^2\rangle$

Hence $\frac{k_B T}{m} = \frac{B}{\zeta m}$

$$\Longrightarrow \quad \boxed{B = \zeta k_B T}$$

The Fluctuation - Dissipation Theorem.
(for the underlying system.)

⊙ Example: The Langevin equation for the motion of a ~~system~~ fluctuating system $X = X(t)$ in a potential $U = U(X)$

motion law:
$$m \ddot{X}(t) = -\nabla U(X) - \zeta \dot{X} + \delta F(t)$$

~~De~~ Coupled system
$$\begin{cases} \dot{x} = \frac{p}{m} \\ \boxed{\dot{p} = -\nabla U - \frac{\zeta p}{m} + \delta F.} \end{cases}$$

⊙ Stochastic Differential Equations (SDE)

$$dX_t = f(X_t, t)\, dt + \sigma(X_t, t)\, dW(t) \qquad X_0 = \xi.$$

$X = X_t$ ... stochastic process
$W = W(t)$ ... Wiener ~~process~~ or Brownian motion ~~process~~
$f = f(X,t)$, $\sigma = \sigma(X,t)$: ... given stochastic process.

Interpreted as stochastic integral equation
$$X_t = \xi + \int_0^t \sigma(s, X_s)\, dW(s) + \int_0^t f(s, X_s)\, ds.$$

<u>Definition</u> (Brownian motion / Wiener process)

A stochastic process $B(t,\omega)$ [with respect to a probability space $(\Omega, \mathcal{F}, P)$] is called a Brownia motion (or Wiener process) if the following conditions are satisfied:

A continuous-path, stochastic process...

(1) $P\{\omega \in \Omega : B(0,\omega)=0\}=1$; (or just $B_0=0$)

(2) For any $0 \le s < t$, the random variable $B(t)-B(s)$ is normally distributed with mean 0 and variance $t-s$. i.e. for any $a<b$.

$$P\{a \le B(t)-B(s) \le b\} = \frac{1}{\sqrt{2\pi(t-s)}}\int_a^b e^{-x^2/2(t-s)}dx.$$

(3) $B(t,\omega)$ has independent increments, i.e. for any $0 \le t_1 < t_2 < \cdots < t_n$, the random variables

$$B(t_1),\ B(t_2)-B(t_1),\ \cdots,\ B(t_n)-B(t_{n-1})$$

are independent.

$\Rightarrow$ ① $\mathbb{E}(B(t))=0$. $\mathbb{E}(B^2(t)) = t \quad \forall t \ge 0$

① $B(t,\omega)$ is Markovian.

Wiener Integral

$$I[f] = \int_a^b f(t)\, dB(t,\omega)$$

$f=f(t)$ ... a given function (a deterministic function)

$B=B(t,\omega)$ ... a Brownian motion.

<u>Definition</u> <u>Step 1</u> If $f(t) = \sum_{i=1}^n a_i \chi_{[t_{i-1},t_i]}$ a ~~the~~ step function. then

$$I[f] = \sum_{i=1}^n a_i\left[B(t_i)-B(t_{i-1})\right]$$

Step 2. $\forall f \in L^2[a,b]$. Let $\{f_k\}$ be a seq. of step functions such that $f_k \to f$ in $L^2(a,b)$.

Define $I[f] = \int_a^b f(t)\,dB(t,\omega) = \lim_{k\to\infty} I[f_k]$.

Proved that this is well-defined.

Stochastic integrals

$$\int_a^b f(t,\omega)\,dB(t,\omega)$$

$B = B(t,\omega)$ ... Brownian motion
$f = f(t,\omega)$ ... stochastic process.

See some of the references.

Itô's Formula. (chain rule)

$$dX = F\,dt + G\,dB \qquad F, G: \text{nice}$$

$$Y(t) = u(X(t),t). \qquad u: \text{smooth}$$

$$\Longrightarrow dY = \frac{\partial u}{\partial t}dt + \frac{\partial u}{\partial x}dX + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}G^2 dt$$

Examples. $d(B^m) = mB^{m-1}dB + \frac{1}{2}m(m-1)B^{m-2}dt$

$m=2$: $d(B^2) = 2B\,dB + dt$.

Hence. $\int_s^r B\,dB = \frac{B^2(r) - B^2(s)}{2} - \frac{r-s}{2}$.

The Fokker-Planck Equation

$f = f(x) = f(x_1, \ldots, x_n)$: probability density function.

$$\frac{\partial f}{\partial t} = -\sum_{i=1}^{n} \frac{\partial}{\partial x_i}\left(D_i^1(x) f\right) + \sum_{i,j=1}^{n} \frac{\partial^2}{\partial x_i \partial x_j}\left(D_{ij}^2(x) f\right)$$

$D^1 = D^1(x)$ ... drift vector

$D^2 = D^2(x)$ ... diffusion tension.

<u>Example</u>. Heat equation. $\frac{\partial f}{\partial t} = \Delta f$.

$D^1 \equiv 0$. $D^2 = I$.

<u>Example</u> $D^1 = -D\nabla\psi$, ψ: a given (scalar) function, representing a potential.

$D^2 = D\beta^{-1} I$.

$$\frac{\partial f}{\partial t} = D\left[\nabla \cdot (f \nabla \psi) + \beta^{-1} \Delta f\right].$$

<u>Brownian motion with drift</u>

Or: Begin w/ X_t.
Then $Y_t = X_{\sigma^2 t} + x + \mu t$.
$\mathbb{E}[Y_t] - x] = \mu t$.

Let X_t be a Brownian motion on the real line $\mathbb{R}$ that has mean 0 and variance σ^2, and that starts at some point $x \in \mathbb{R}$. Let $\mu \in \mathbb{R}$.

[If B_t starts from 0 then $x + B_t$ ~~set~~ starts from x.
If B_t is ~~the~~ a standard Brownian motion ~~thence the mean is variance is 1~~. then $B_{\sigma^2 t}$ is a Brownian motion w/ the variance σ^2.]

Define $Y_t = X_t + t\mu$.
Call it a Brownian motion with drift μ.

<u>Example</u> A particle (of mass 1) is in motion
$$\frac{dv}{dt} = -\mu + \text{stochastic force}$$

The drift is, e.g., due to an applied field.
So
$$dv = -\mu\,dt + 2B\,dW$$
with $W = W_t$ a Brownian motion. Hence
$$d(v + t\mu) = 2B\,dW.$$
$v + t\mu$ is a (shifted) Brownian motion.

Note: ① $X_0 = x$.
② $\mathbb{E}(Y_t) = \mathbb{E}(X_t + t\mu) = t\mu$

Let $p_t(x,y)$ denote the density of Y_t. We have
$$p_t(x,y) = \frac{1}{\sqrt{2\pi\sigma^2 t}}\, e^{-|y-x-t\mu|^2/2t\sigma^2}$$

This satisfies the Chapman-Kolmogorov equation:
$$p_{s+t}(x,y) = \int_{-\infty}^{\infty} p_s(x,z)\, p_t(z,y)\,dz$$

This is the density at time $t=0$

Now, given $u_0 = u_0(x) \in L^1(\mathbb{R})$, smooth. Let
$$u(t,x) = \mathbb{E}^x[f(Y_t)] = \int_{-\infty}^{\infty} u_0(y)\, p_t(y,x)\,dy$$
Taylor's expansion:
$$u_0(y) = u_0(x) + u_0'(x)(y-x) + \tfrac{1}{2}u_0''(x)(y-x)^2 + o\left((y-x)^2\right)$$
$$\mathbb{E}^x[f(Y_t)] = u_0(x) + u_0'(x)\,\mathbb{E}^x[Y_t - x] + \tfrac{1}{2}u_0''(x)\,\mathbb{E}^x[(Y_t-x)^2] + o\left(\mathbb{E}^x[(Y_t-x)^2]\right)$$

$Y_t = X_t + \mu t, \qquad X_t = X_t^\circ + x$

$\mathbb{E}^x[Y_t - x] = \mathbb{E}[X_t^\circ + \mu t] = \mathbb{E}[X_t^\circ] + \mathbb{E}[\mu t]$
$= 0 + \mu t.$

$\mathbb{E}^x[(Y_t - x)^2] = \mathbb{E}^x[(X_t^\circ + t\mu)^2]$
$= [\mathbb{E}^x(X_t^\circ + t\mu)]^2 + Var(X_t^\circ + t\mu)$
$= (t\mu)^2 + \sigma^2 t$

Also, $(Y_t - x)^2 = o(t)$.
$o((Y_t - x)^2) = o(t)$.

Hence $\left.\frac{\partial u}{\partial t}\right|_{t=0} = \lim_{t\to 0} \frac{\mathbb{E}^x[f(Y_t)] - \mathbb{E}^x[f(Y_0)]}{t}$
$= \mu u_0'(x) + \frac{\sigma^2}{2} u_0''(x).$

The same argument applies to any $t > 0$. Hence

$$\boxed{\frac{\partial u}{\partial t} = \mu \frac{\partial u}{\partial x} + \frac{\sigma^2}{2} \frac{\partial^2 u}{\partial x^2}}$$

A Markov process: w/ density $p(x,t)$.

conditional prob:
$p_{1,n-1}(x_1, t_1 | x_2, t_2; \cdots; x_n, t_n)$
$= p_{1,1}(x_1, t_1 | x_2, t_2) \qquad \forall\, t_1 > t_2 > \cdots > t_n.$

$p_{1,1}(x_1, t_1 | x_2, t_2)$ — transition probabilities

Now. The Chapman-Kolmogorov equation is

$p_{1,1}(x_1, t_1 | x_3, t_3) = \int p_{1,1}(x_1, t_1 | x_2, t_2)\, p_{1,1}(x_2, t_2 | x_3, t_3)\, dx_2$

Consider $\{X_t\}$ a stochastic process.

Notation:

$p_1(x_1, t_1)$ ... density (or prob. density) of the prob. distribution of X_{t_1} at x_1.

$p_2(x_1, t_1; x_2, t_2)$ ... density of the joint distribution of X_{t_1}, X_{t_2} at x_1, x_2.

- - - - -

$p_n(x_1, t_1; x_2, t_2; \cdots; x_n, t_n)$ ... prob. density of the joint dist. of $X_{t_1} \cdots X_{t_n}$ at $x_1 \cdots x_n$.

Assume:

(i) Markov:

$$p_{1,n-1}(x_1, t_1 \mid x_2, t_2; \cdots; x_n, t_n) = p_{1,1}(x_1, t_1 \mid x_2, t_2)$$

$$\forall t_1 > \cdots > t_n, \quad \forall x_1 \cdots x_n.$$

Call $p_{1,1}(x_1, t_1 \mid x_2, t_2)$ the transition prob. density

(ii) Time homogeneous

$$p_{1,1}(x_1, t_1 \mid x_2, t_2) = p_{1,1}(x_1, t_1 - t_2 \mid x_2, 0)$$

$$\forall t_1 > t_2, \quad \forall x_1, x_2.$$

The Chapman-Kolmogorov Equation.

$$\boxed{p_{1,1}(x_1, t_1 \mid x_3, t_3) = \int p_{1,1}(x_1, t_1 \mid x_2, t_2)\, p_{1,1}(x_2, t_2 \mid x_3, t_3)\, dx_2}$$

Derivation of the Fokker-Planck equation for
$\underline{u(x,t) = p_{1,1}(x,t \mid y,0)}$ for a fixed y.
$\underline{= p_{1,1}(x, t+s \mid y, s)}$

Result:

$$\boxed{\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}(A(x)u) + \frac{1}{2}\frac{\partial^2}{\partial x^2}(B(x)u)}$$

$$A(z) = \lim_{s\to 0}\frac{1}{s}\int (x-z)\, p_{1,1}(x,s \mid z,0)\,dx$$

$$B(z) = \lim_{s\to 0}\frac{1}{s}\int (x-z)^2 p_{1,1}(x,s \mid z,0)\,dx.$$

Derivation

By the CKE,

$$p_{1,1}(x, t+s \mid y,0) = \int p_{1,1}(x,t+s \mid z,t)\, p_{1,1}(z,t \mid y,0)\,dz$$

Let $\phi \in C_c^\infty$

$$\int \phi(x)\, p_{1,1}(x,t+s \mid y,0)\,dx$$

$$= \int \left[\phi(x)\int \underbrace{p_{1,1}(x, t+s \mid z,t)}_{\text{time-homogeneity}}\, p_{1,1}(z,t \mid y,0)\,dz\right]dx$$

$$= \int \left[\phi(x)\int p_{1,1}(x,s \mid z,0)\, p_{1,1}(z,t \mid y,0)\,dz\right]dx$$

$$\overset{dx \rightleftarrows dz}{=} \int p_{1,1}(z,t \mid y,0)\left[\int \phi(x)\, p_{1,1}(x,s \mid z,0)\,dx\right]dz$$

$$= \int p_{1,1}(z,t \mid y,0)\left[\int \left\{\phi(z) + \phi'(z)(x-z) + \tfrac{1}{2}\phi''(z)(x-z)^2 + \cdots\right\} \cdot p_{1,1}(x,s \mid z,0)\,dx\right]dz.$$

$$= \int p_{1,1}(z,t \mid y,0)\left\{\int \phi(z)\, p_{1,1}(x,s \mid z,0)\,dx \right.$$
$$+ \int \phi'(z)(x-z)\, p_{1,1}(x,s \mid z,0)\,dx$$
$$\left. + \int \tfrac{1}{2}\phi''(z)(x-z)\, p_{1,1}(x,s \mid z,0)\,dx + \cdots\right]dz$$

$$= \int p_{1,1}(z,t\,|\,y,0)\Big\{\phi(z) + \phi'(z)\underbrace{\int (x-z)\,p_{1,1}(x,s\,|\,z,0)\,dx}_{=A(z)s+o(s)}$$
$$+ \frac{1}{2}\phi''(z)\underbrace{\int (x-z)^2 p_{1,1}(x,s\,|\,z,0)\,dx}_{=B(z)s+o(s)} + \cdots\Big\}\,dz$$

$$= \int p_{1,1}(z,t\,|\,y,0)\Big\{\phi(z) + \phi'(z)\big[A(z)s + o(s)\big]$$
$$+ \frac{1}{2}\phi''(z)\big[B(z)s + o(s)\big]\Big\}\,dz.$$

change z to x in $\int \cdots dz$.

$$\frac{1}{s}\Big[\int \phi(x)\,p_{1,1}(x,t+s\,|\,y,0)\,dx - \int \phi(x)\,p_{1,1}(x,t\,|\,y,0)\,dx\Big]$$
$$= \int p_{1,1}(x,t\,|\,y,0)\Big[\phi'(x)A(x) + \frac{1}{2}\phi''(x)B(x)\Big]dx + o(1)$$

Let $s \to 0$, $\displaystyle\int \frac{\partial}{\partial t} p_{1,1}(x,t\,|\,y,0)\,\phi(x)\,dx$

$$= \int p_{1,1}(x,t\,|\,y,0)\Big[\phi'(x)A(x) + \frac{1}{2}\phi''(x)B(x)\Big]dx$$

$$\int \phi(x)\frac{\partial u}{\partial t}\,dx = \int u(x,t)\Big[\phi'(x)A(x) + \frac{1}{2}\phi''(x)B(x)\Big]dx$$

Integration by parts: [Recall $\phi \in C_c^\infty$]

$$\int \phi(x)\frac{\partial u}{\partial t}\,dx = \int \phi(x)\Big[-\frac{\partial}{\partial x}\big(A(x)u\big) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\big(B(x)u\big)\Big]dx$$

Hence $$\boxed{\frac{\partial u}{\partial t} = -\frac{\partial}{\partial x}\big(A(x)u\big) + \frac{1}{2}\frac{\partial^2}{\partial x^2}\big(B(x)u\big)}$$

where $u(x,t) = p_{1,1}(x,t\,|\,y,0) = p_{1,1}(x,t+s\,|\,y,s)$

Remark

① Starting from the CKE for $p_{1,1}(x,t \mid y, t-s) = p_{1,1}(x, 0 \mid y, -s)$,
we obtain by the same procedure the following equation

$$\frac{\partial p_{1,1}(x,t \mid y,s)}{\partial s} = -A(y)\frac{\partial p_{1,1}(x,t \mid y,s)}{\partial y} - \frac{1}{2}B(y)\frac{\partial^2 p_{1,1}(x,t \mid y,s)}{\partial y^2}$$

This is called the Kolmogorov's backward equation.

② Assumptions used: $\begin{cases} \text{- Markov} \\ \text{- time homogeneity} \\ \text{- } A, B \text{ are proportional to time difference} \end{cases}$

$\Longrightarrow$ These are diffusion processes.