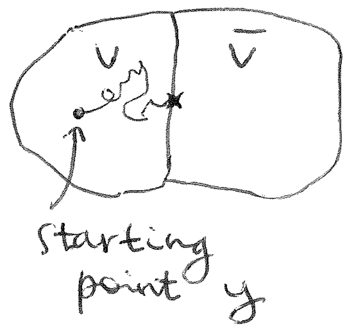
Consider random var. $X(t)$ [scalar or vector] ; define $p(x,t|y,0)$ as before.

Consider



1st passage (FPT) time: time needed to reach $\bar{V}$ for the 1st time. For ex.: a chemical reaction which need activation energy E_c to occur:

$$V = \{E < E_c\}, \quad \bar{V} = \{E \geq E_c\}$$

Prob. that $X(t)$ is still in V at time t is given by $p_V(y,t) = \int_V dx\, p(x,t|y,0)$

Define $\eta(y,t)$ to be prob. density for FPT: if $\tilde{t}$ is the 1st time $X(t)$ reaches $\bar{V}$, given $X(0) = y \in V$, $\eta(y,t)dt$ is the prob. that $t < \tilde{t} < t+dt$.

Note that if $X(t)$ is in V @ time t, @ $t+dt$ it either stays in V or makes 1st passage.

So, $p_v(y,t) - p_v(y,t+dt) = \eta(y,t)\,dt$, or

$$\boxed{\eta(y,t) = -\frac{\partial p_v(y,t)}{\partial t}}$$

FPT moments:

$$\langle t^n(y)\rangle = \int_0^\infty dt\, t^n \eta(y,t) \overset{\text{by parts}}{=}$$

$$= n\int_0^\infty dt\, t^{n-1} p_v(y,t). \qquad n = 1, 2, \ldots$$

Now, 1D case: $0 \;\text{———}\; A$ — $X(t)$ takes these values; endpoints are absorbing

Theoretically, could solve the FP eq'n w/ absorbing boundary conditions; however, it's easier to define $\psi(x,t)$ - the prob. that FPT is $<t$, given $X(0) = x$.

Define $p(y,dt\,|\,x,0)dy$ - the prob. that $y \le X(dt) \le y+dy$, given that $X(0) = x$. [homogeneous process, $p(y,t+dt\,|\,x,t) = p(y,dt\,|\,x,0)$]

Then

$$\psi(x,t+dt) = \int_0^A dy\, \underbrace{p(y,dt\,|\,x,0)}_{\substack{x\to y \text{ transition}\\ \text{for } \forall y\in(0,A);\\ \text{this transition}\\ \text{does not lead to}\\ \text{1st passage}}}\, \underbrace{\psi(y,t)}_{\substack{\text{prob. that}\\ \text{FPT is } <t}}$$

Expand $\varphi(y,t)$ around x:

$$\varphi(y,t) \simeq \varphi(x,t) + \frac{\partial \varphi(x,t)}{\partial x} + \frac{1}{2}\frac{\partial^2 \varphi(x,t)}{\partial x^2}$$

Then

$$\varphi(x,t+dt) = \varphi(x,t) \underbrace{\int_0^A dy\, p(y,dt|x,0)}_{=1} +$$

$$+ \frac{\partial \varphi(x,t)}{\partial x} \int_0^A dy\,(y-x)\, p(y,dt|x,0) +$$

$$+ \frac{1}{2}\frac{\partial^2 \varphi(x,t)}{\partial x^2} \int_0^A dy\,(y-x)^2\, p(y,dt|x,0) + \ldots,$$

$$\lim_{dt\to 0} \frac{\varphi(x,t+dt)-\varphi(x,t)}{dt} = \frac{\partial \varphi(x,t)}{\partial t} =$$

$$= A(x)\frac{\partial \varphi(x,t)}{\partial x} + \frac{B(x)}{2}\frac{\partial^2 \varphi(x,t)}{\partial x^2}. \qquad (*)$$

$$\begin{cases} A(x) = \lim\limits_{dt\to 0} \frac{1}{dt}\int_0^A dy\,(y-x)\,p(y,dt|x,0), \\ B(x) = \lim\limits_{dt\to 0} \frac{1}{dt}\int_0^A dy\,(y-x)^2\,p(y,dt|x,0). \end{cases}$$

"another" backward eq'n in 1D

No t-dependence in $A(x)$ & $B(x)$ b/c the process is homogeneous.

BCs: $\varphi(0,t) = 1$, $\varphi(A,t) = 1$.

absorbing ends

Compute moments of $\varphi(x,t)$ [easier than solving $(*)$ directly]

Define $\mu_j(x) = \int_0^\infty dt\, t^j \underbrace{\frac{\partial \varphi(x,t)}{\partial t}}$

$$\varphi(x,t+dt) - \varphi(x,t) = \tilde{\eta}(x,t)\,dt, \text{ or}$$

$$\tilde{\eta}(x,t) = \frac{\partial \varphi(x,t)}{\partial t}$$

Now, apply $\int_0^\infty dt\, t^j \frac{\partial}{\partial t}$ to (*):

<u>j=1</u>: $\int_0^\infty dt \underbrace{t}_{u} \underbrace{\frac{\partial}{\partial t}\left(\frac{\partial \varphi}{\partial t}\right)}_{\frac{dv}{dt}} \overset{\text{by parts}}{=} \frac{\partial \varphi}{\partial t} t \Big|_0^\infty - \int_0^\infty dt \frac{\partial \varphi}{\partial t} =$

$= -\underbrace{\varphi(x,+\infty)}_{1} + \underbrace{\varphi(x,0)}_{0} =$

$\mu_1(0) = \mu_1(A) = 0$
[absorbing]

$= -1$

So, $A(x)\frac{d\mu_1(x)}{dx} + \frac{B(x)}{2}\frac{d^2\mu_1(x)}{dx^2} = -1,$

Likewise, <u>j=2</u>:

$\int_0^\infty dt\, t^2 \frac{\partial}{\partial t}\left(\frac{\partial \varphi}{\partial t}\right) = \frac{\partial \varphi}{\partial t}(t^2)\Big|_0^\infty - 2\int_0^\infty dt\, t \frac{\partial \varphi}{\partial t} =$

$= -2\mu_1(x).$

So, $A(x)\frac{d\mu_2}{dx} + \frac{B(x)}{2}\frac{d^2\mu_2}{dx^2} = -2\mu_1.$

In general,

$A(x)\frac{d\mu_j}{dx} + \frac{B(x)}{2}\frac{d^2\mu_j}{dx^2} = -j\mu_{j-1}.$

$j = 2, 3, \ldots$

BCs: $\mu_j(0) = \mu_j(A) = 0.$

These are <u>ordinary</u> differential eq's,
can be solved (!)

For example, for $\mu_1(x)$:

$$\mu_1(x) = 2\underbrace{\frac{\int_0^A e^{-u(y)}dy\int_0^y dz\left[e^{u(z)}/B(z)\right]}{\int_0^A e^{-u(y)}dy}}_{C_1\ (=\text{const})}\int_0^x e^{-u(y)}dy\ -$$

$$-2\int_0^x e^{-u(y)}dy\int_0^y dz\left[e^{u(z)}/B(z)\right]$$

$[B]=\frac{L^2}{T}$

$[C_1]=L/D=\frac{T}{L}$ $\quad {}''L^2/T$

$[\mu_1]=T$

$$\boxed{u(x)=2\int_0^x dy\,\frac{A(y)}{B(y)}}$$

$[\frac{A}{B}]=\frac{1}{L}$, $[u]$ dim'less

$\mu_1(0)=0$ (obviously)

$$\mu_1(A) = 2\int_0^A e^{-u(y)}dy\int_0^y dz\ldots\ -$$

$$-2\int_0^A e^{-u(y)}dy\int_0^y dz\ldots = 0 \quad \text{as well.}$$

Finally,

$$\frac{d\mu_1}{dx} = \cancel{2}\,C_1 e^{-u(x)} - 2e^{-u(x)}\int_0^x dz\,\frac{e^{u(z)}}{B(z)},$$

$$\frac{d^2\mu_1}{dx^2} = -C_1 e^{-u(x)}\Big[\underbrace{2\frac{A(x)}{B(x)}}_{u'(x)}\Big] + 2e^{-u(x)}\Big[\underbrace{2\frac{A(x)}{B(x)}}_{u'(x)}\Big]\times$$

$$\times\int_0^x dz\,\frac{e^{u(z)}}{B(z)} - 2e^{-u(x)}\frac{e^{u(x)}}{B(x)} =$$

$$= 2\frac{A(x)}{B(x)}e^{-u(x)}\left[2\int_0^x dz\,\frac{e^{u(z)}}{B(z)} - C_1\right] -$$

$$-\frac{2}{B(x)}.$$

Now, $$\frac{B(x)}{2}\frac{d^2\mu_1}{dx^2} + A(x)\frac{d\mu_1}{dx} = A(x)e^{-u(x)}\left[2\int_0^x dz\,\frac{e^{u(z)}}{B(z)} - \right.$$

$$\left.-C_1\right] - 1 + A(x)C_1 e^{-u(x)} - 2A(x)\times$$

$$\times e^{-u(x)}\int_0^x dz\,\frac{e^{u(z)}}{B(z)} = \underline{\underline{-1}}.$$

So, the sol'n is valid.

Finally, consider $A(x)=0$ & $B(x)=2D$,
D - diff'n const

Then $\frac{d^2\mu_1}{dx^2} = -\frac{1}{D}$.

at both 0 & A

With absorbing BCs,

$$\mu_1(x) = \frac{1}{2D}\, x(A-x) \quad \text{is the sol'n.}$$

MFPT (!)

Now consider diffusion with drift:

$A(x) = -v$, $B = 2D$ Note: only $x=0$ is absorbing here

From above,
$$\mu_1(x) = C_1 \int_0^x dy\, e^{\frac{vy}{D}} - 2\int_0^x dy\, e^{\frac{vy}{D}} \int_0^y dz\, \frac{e^{-\frac{vz}{D}}}{2D} \;\ominus$$

$U(x) = -\frac{vx}{D} \Rightarrow$

$$\ominus\; C_1 \frac{D}{v}\left[e^{\frac{vx}{D}} - 1\right] - \frac{1}{D}\int_0^x dy\, e^{\frac{vy}{D}}\left(-\frac{D}{v}\right)\left[e^{-\frac{vy}{D}} - 1\right]$$

$$= C_1 \frac{D}{v}\left[e^{\frac{vx}{D}} - 1\right] + \frac{1}{v}\int_0^x dy\left[1 - e^{\frac{vy}{D}}\right] =$$

$$= C_1 \frac{D}{v}\left[e^{\frac{vx}{D}} - 1\right] + \frac{1}{v}\left\{x - \frac{D}{v}\left[e^{\frac{vx}{D}} - 1\right]\right\}$$

$\mu_1(0) = 0$ is satisfied for $\forall C_1$.

~~$\mu_1(A)$~~ Now, consider $\frac{vA}{D} \gg 1$ ← for some sufficiently large A, then

$$\cancel{\mu_1(A) \simeq C_1 \frac{D}{v} e^{\frac{vA}{D}} + \frac{A}{v} - \frac{D}{v^2} e^{\frac{vA}{D}} = 0, \text{or}}$$

$$C_1 \approx \cancel{\frac{D e^{\frac{vA}{D}} - A}{D e^{\frac{vA}{D}}}} \approx \frac{1}{v}$$ (see below)

Now, $$\mu_1(x) \approx \frac{D}{v^2}\left[\cancel{e^{\frac{vx}{D}}} - 1\right] + \frac{x}{v} - \frac{D}{v^2}\left[\cancel{e^{\frac{vx}{D}}} - 1\right] =$$

$$= \frac{x}{v}$$ indep. of D (!)

Indeed,

$$C_1 = 2\,\frac{\int_0^A dy\, e^{\frac{vy}{D}} \int_0^y dz\, \frac{e^{-\frac{vz}{D}}}{2D}}{\int_0^A dy\, e^{\frac{vy}{D}}} =$$

$$= \frac{1}{D}\,\frac{\int_0^A dy\, e^{\frac{vy}{D}} \left(-\frac{D}{v}\right)\left[e^{-\frac{vy}{D}} - 1\right]}{\left(\frac{D}{v}\right)\left[e^{\frac{vA}{D}} - 1\right]} =$$

$$= -\frac{1}{D}\,\frac{\int_0^A dy\left[1 - e^{\frac{vy}{D}}\right]}{e^{\frac{vA}{D}} - 1} = \frac{1}{D}\,\frac{\left(\frac{D}{v}\right)\left[e^{\frac{vA}{D}} - 1\right] - A}{e^{\frac{vA}{D}} - 1} \underset{\frac{vA}{D} \gg 1}{\approx}$$

$$\approx \frac{1}{v}.$$