P1 8.2

Consider the operator $\mathcal{L}$ associated with the process. Let $n=3$.
$x \in S^2$

$$\mathcal{L} f(\bar{x}) = -\bar{x} \cdot \nabla f(\bar{x}) + \frac{1}{2} \Delta f(\bar{x}) + \frac{1}{2} (\bar{x} \otimes \bar{x}) : \nabla^2 f(\bar{x}).$$

For the adj. operator, $(\mathcal{L} f, g) = (f, \mathcal{L}^* g)$. Then, the PDE is given by

$$\partial_t p(\bar{x}, t \mid \bar{y}, t) = (\mathcal{L}^* p)(\bar{x}, t \mid \bar{y}, t).$$

First, we compute $(\mathcal{L}^* f)$.

$$\mathcal{L}^* f(\bar{x}) = -\nabla \cdot (\bar{x} f(\bar{x})) + \frac{1}{2} \Delta f(\bar{x}) + \frac{1}{2} \nabla^2 : [(\bar{x} \otimes \bar{x}) \cdot f(\bar{x})]$$

$$= -\nabla \cdot (\bar{x} f(\bar{x})) + \frac{1}{2} \Delta f(\bar{x}) + \frac{1}{2} \Sigma_{ij} \partial_{ij} [(\bar{x} \otimes \bar{x})_{ij} f(\bar{x})]$$

$$= 0 + \frac{1}{2} \Delta f(\bar{x}) + 0$$

Evaluate the last term

$$\partial_{ij} [(\bar{x} \otimes \bar{x})_{ij} f(\bar{x})] = \partial_{ij} [x_i x_j \cdot f]$$

Since $\bar{x} \otimes \bar{x}$ is a symmetric matrix, the last term in the above equ. must be zero.

Moreover, the first term

$-\nabla \cdot (\bar{x} f(\bar{x}))$ also disappears.

Then, $\mathcal{L}^* f = \frac{1}{2} \Delta f(\bar{x})$

— This is the Laplace-Bertrami operator.

Then, let $\bar{x} = \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} \in S^1$. for $\theta \in [0, 2\pi)$.

The Laplace-Beltrami operator yields. ($\Delta f = \nabla \cdot \nabla f$).

$$R_\alpha^2 = \Delta_{S^1} = \nabla \cdot \nabla = \frac{d^2}{d\theta^2}$$ if parameterized by θ.

P2 8.5 (Reference Gardiner's hand book)

Consider the probability current

$j(\bar{x},t) = B(\bar{x},t)\, p(\bar{x},t) - \frac{1}{2}\nabla\cdot(A\cdot p(\bar{x},t))$

where $A = \sigma\sigma^T$

Assume $j_s(\bar{x}) = 0$ and invariant distribution

$$p(\bar{x},t) = \frac{1}{Z}\exp\{-x^T\Sigma^{-1}x/2\}.$$

Substitute this into forward equation.

$$B\cdot\frac{1}{Z}e^{-x^T\Sigma^{-1}x/2} = \frac{1}{2}\nabla\cdot\left(\sigma\sigma^T\frac{1}{Z}e^{-x^T\Sigma^{-1}x/2}\right).$$

$$-\sum_i B_{ii} - \frac{1}{2}A_{ij}\Sigma^{-1}_{ij} + \sum_{kj}\left(\sum_i \Sigma^{-1}_{ki}B_{ij} + \frac{1}{2}\sum_{il}\Sigma^{-1}_{ij}A_{il}\Sigma^{-1}_{lj}\right)x_k x_j = 0.$$

Use the symmety of Σ. The quadratic term vanishes.

Then,

$$\Sigma^{-1}B + B^T\Sigma = -\Sigma^{-1}B\Sigma^{-1}$$

since the constant vanishes

Substitute $B \to -B$.

Using detailed balanced condition

w/ $s = \mathrm{diag}(s_1, \cdots)$. $s^2 = I$,

we get

$$\begin{cases} sBs + B = -A\Sigma^{-1} \\ \varepsilon A \varepsilon = A. \end{cases}$$

The detailed balance requires $s\Sigma = \Sigma s$.

Then,

$$B\Sigma + \Sigma B^T = -A.$$

$$\Rightarrow \quad sBs\Sigma + Bs = -A$$

$$\Rightarrow \quad sBs\Sigma = sB^T$$

$$\Rightarrow \quad s(B\Sigma) = (B\Sigma)^T s \quad \Rightarrow \quad B\Sigma = B\Sigma^T.$$

P3.8.8

Consider the linear Langevin equ.

$$\begin{cases} dX_t = V_t\, dt \\ dV_t = (-\gamma V_t - X_t)\, dt + \sqrt{2\gamma}\, dW_t . \end{cases}$$

The corresponding Fokker - Plank equation is

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}[V_t p] + \frac{\partial}{\partial v}[(-\gamma V_t - X_t)p] + \gamma \frac{\partial^2 p}{\partial v^2}$$

First, we solve for the invariant probability.

$$y = \begin{bmatrix} x \\ v \end{bmatrix}, \quad b = \begin{bmatrix} v \\ -\gamma v - x \end{bmatrix}, \quad A = \begin{bmatrix} 0 & 0 \\ 0 & 2\gamma \end{bmatrix}$$

Check the detailed balance condition

(a) $s \cdot b(sy)\, p_s(y) = -b(y)\, p_s(y) + \nabla \cdot (A(y)\, p_s(y))$.

(b) $s \cdot A(sy) = A(y) \cdot s$

where s is the sign matrix s.t. $sy = \begin{bmatrix} x \\ -v \end{bmatrix}$

It's easy to check that

$$s \cdot A(sy) = s \cdot A(y) = A(y) \cdot s . \qquad (b)$$

since A is indep. of y.

Then, we apply condition (a).

$$\frac{1}{p_s(y)} \nabla_v\, p_s(y) = -v$$

$$\Rightarrow \quad p_s(y) = \frac{1}{Z_v} \exp\left(-\frac{v^2}{2}\right) f(x)$$

Substitute the above into $\nabla \cdot j_s = 0$.

$$f(x) = \frac{1}{Z_x} \exp\left(-\frac{x^2}{2}\right)$$

$\Rightarrow$ Invariant Distribution of Linear Langevin is

(1)

$$\boxed{P_s(y) = \frac{1}{Z} \exp\left(-\frac{|v|^2}{2} + \frac{x^2}{2}\right)}$$

Here, Z is a normalization coefficient.

We still need to solve for the diff. equ. to get the transition PDF $p(x,t \mid y,s)$ for $t > s$, with

$$p(x,t \mid y,s)|_{t=s} = \delta(x-y).$$

Forward Equ.

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}[V_t p] + \frac{\partial}{\partial v}[(-\gamma V_t - X_t) p] + \gamma \frac{\partial^2 p}{\partial v^2}$$

OR in the matrix form

Forward

$$\boxed{\frac{\partial p(x,t \mid x_0,t_0)}{\partial t} = \frac{\partial (b(x,t) p(x,t \mid x_0,t_0))}{\partial x} + \frac{1}{2} \frac{\partial^2 (A(x,t) p(x,t \mid x_0,t_0))}{\partial x^2}}$$

Moreover, $p(x,t \mid x_0,t_0)$ should also satisfy the backward equ. given by

Backward

$$\boxed{\frac{\partial p(x,t \mid x_0,t_0)}{\partial t_0} = -b(x_0,t_0) \frac{\partial p(x,t \mid x_0,t_0)}{\partial x_0} - \frac{1}{2} A(x_0,t_0) \frac{\partial^2 p(x,t \mid x_0,t_0)}{\partial x_0^2}}$$

Notice that the derivatives are w.r.t. x_0, t_0.
So, let's try to solve the backward equ.

It's reasonable to take a guess of the transition pdf. Then, show it actually satisfies the backward equation above.

In 1d case,

$$\boxed{p(x,t \mid x_0,t_0) = \frac{e^{-\lambda(t-t_0)}}{\sqrt{4\pi D(t-t_0)}} \exp\left\{-(x-x_0)^2/4D(t-t_0)\right\}}$$

where D is the diffusion coe. & λ is decaying of the particles.

For the process w/o decaying,

$$\boxed{p(x,t \mid x_0,t_0) = \frac{1}{\sqrt{4\pi D(t-t_0)}} \exp\left\{-(x-x_0)^2/4D(t-t_0)\right\}}.$$

with initial condition

$$p(x,t_0 \mid x_0,t_0) = \delta(x-x_0)$$

With the invariant probability given by (1), let's take a reasonable guess.

$$\boxed{p(x,t \mid x_0,t_0) = \frac{1}{\sqrt{4\pi b(t-t_0)}} \exp\left\{-\left(|v-v_0|^2-(x-x_0)^2\right)/4b(t-t_0)\right\}}$$

We can also add the decaying term $e^{-\lambda(t-t_0)}$.

References: [1] Textbook
[2] https://www.scirp.org/pdf/JMP_2017102315173123.pdf

P4. 8.10 (Reference Gardiner's hand book).

(a) Consider the SDE w/ $b(x)=0$ and $\sigma(x)=1$

$$dX_t = dW_t \quad , \quad X_0 = x_0 \in [0,1].$$

The reflecting boundary condition gives

$$n \cdot j(x,t) = 0.$$

The forward yields, for $t \le s \le t'$

$$0 = \frac{\partial}{\partial s} p(x,t \mid x',t') = \frac{\partial}{\partial s} \int p(x,t \mid y,s)\, p(y,s \mid x',t')\, dy$$

Then, in higher dimension, $b(x,t)=0$, $\sigma(x)=1$,

$$0 = \int_U \frac{\partial^2}{\partial y^2} p(y,s \mid x',t') \cdot p(x,t \mid y,s)\, dy$$

$$+ \int_U \frac{\partial^2}{\partial y^2} p(x,t \mid y,s)\, p(y,s \mid x',t')\, dy$$

$$= \int_U \frac{\partial}{\partial y} \frac{1}{2} \left[p(x,t \mid y,s) \frac{\partial}{\partial y} p(x,t \mid x',t') - p(x,t \mid x',t') \frac{\partial}{\partial y} p(x,t \mid y,s) \right] dy$$

$$= \int_{\partial U} p(x,t \mid y,s) \cdot \frac{1}{2} \frac{\partial}{\partial y} p(x,t \mid x',t')\, ds - \frac{1}{2} \int_{\partial U} p(x,t \mid x,t') \frac{\partial}{\partial y} p(x,t \mid y,s)\, ds.$$

Then, the reflecting boundary implies

$$\frac{\partial}{\partial y} p(x,t \mid y,s) = 0.$$

$$\frac{\partial}{\partial x_0} p(x,t \mid x_0,s) = 0$$

$$\Rightarrow \quad p(x,t \mid x_0,s) = \frac{1}{\sqrt{2\pi t}} e^{-(x-x_0)^2/2t}$$

(b) Consider

$$\partial_t p = \frac{1}{2} \Delta p \quad w/ \quad p(x,0) = \delta(x - x_0).$$

Then, solve for $p(x,t)$

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

The stationary dist. is

$$p(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2} \right)$$

P5. 8.12

Consider the operator in (8.50) in $L^2_{\mu^{-1}}$

$$\begin{cases} \mathcal{L} f(x) = -\nabla U(x) \cdot \nabla f(x) + \Delta f(x) \\ \mathcal{L}^* f(x) = \nabla \cdot (\nabla U(x) f(x)) + \Delta f(x). \end{cases}$$

$\mu^{-1} = Z \exp(U(x)) > 0$.

Follow the procedure in the textbook. We get

$$\mathcal{L}^*(g\mu^{-1}) = \mathcal{L}^*\left(\frac{g}{\mu}\right)$$

$$= \nabla \cdot \left(\nabla U \cdot \frac{g}{\mu}\right) + \Delta\left(\frac{g}{\mu}\right)$$

$$= \nabla \cdot \left(\frac{\nabla U}{\mu}\right) g + \nabla U \cdot \frac{\nabla g}{\mu} + [\Delta g \mu^{-1} + \Delta(\mu^{-1}) g + 2 \nabla g \cdot \nabla(\mu^{-1})]$$

$$= \mu^{-1} \mathcal{L} g$$

Then,

$$(\mathcal{L}f, g)_{\mu^{-1}} = \int \mathcal{L} f(x) g(x) \mu^{-1}(x) dx$$

$$= \int f(x) \mathcal{L}^*(g\mu^{-1}) dx = (f, \mathcal{L}g)_{\mu^{-1}}$$

This shows $\mathcal{L}$ is selfadjoint. Moreover,

$$(-\mathcal{L}f, f)_{\mu^{-1}} = -\int (-\nabla U \cdot \nabla f f \mu^{-1} - \nabla f \cdot \nabla f \mu^{-1} - \nabla f \cdot \nabla(\mu^{-1}) f) dx$$

$$= \|\nabla f\|^2_{\mu^{-1}} \geq 0.$$

This implies $\mathcal{L}$ is nonpositive.

$\Rightarrow$ The eigenvalues are real and nonpositive

$\downarrow$ Next Page

Let $Q_\lambda(x)$ be the eigenfunctions of $\mathcal{L}$ with eigenvalue λ and normalization $(Q_\lambda, Q_{\lambda'})_{\mu^{-1}} = \delta_{\lambda\lambda'}$.

Then, by the above relation $\mathcal{L}^*(\mu^{-1} g) = \mu^{-1} \mathcal{L} g$,

$$\mu^{-1} \mathcal{L}(Q_\lambda) = \mu^{-1} \lambda Q_\lambda = \lambda \mu^{-1} Q_\lambda = \mathcal{L}^*(\mu^{-1} Q_\lambda).$$

This shows that the eigenfunctions of $\mathcal{L}^*$ are

$$P_\lambda(x) = \mu^{-1}(x)\, Q_\lambda(x).$$

P6.

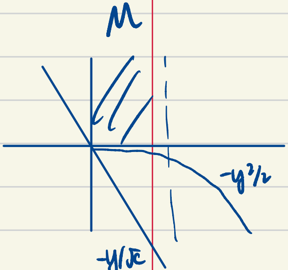
Let $X_t = \sqrt{c}\, W_t$ for $c > 0$.

(a) (Reference: Stochastic Calc. I took in Fall.)

Compute
$$p(c) = p(\sqrt{c}\, W_1 > 1)$$
$$= \int_1^\infty \frac{1}{\sqrt{2\pi c}} e^{-x^2/2c}\, dx.$$

let $x = 1 + \sqrt{c}\, y$, $dx = \sqrt{c}\, dy$.

$$= \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{-(1+\sqrt{c}\, y)^2/2c}\, dy$$
$$= \frac{1}{\sqrt{2\pi}} \int_0^\infty e^{-(1+2\sqrt{c}\, y + cy^2)/2c}\, dy$$
$$= \frac{1}{\sqrt{2\pi}} e^{-1/2c} \int_0^\infty e^{-y/\sqrt{c}}\, e^{-y^2/2}\, dy$$



In the shaded area M, $-y^2/2$ is very small.

$$\approx \frac{1}{\sqrt{2\pi}} e^{-1/2c} \int_0^\infty e^{-y/\sqrt{c}}\, dy$$

Then, we have

$\log(\sqrt{c})$.

$$\lim_{c\to 0} -c \log p(c) = \lim_{c\to 0} -c\left[-\frac{1}{2\cancel{c}} - \log(\sqrt{2\pi}) + \log \cancel{\int_0^\infty e^{-y/\sqrt{c}} dy}\right]$$
$$= \lim_{c\to 0} \left(\frac{1}{2} + c\log\sqrt{2\pi} - \frac{c}{2}\log c\right)$$
$$= \frac{1}{2}$$

(b)

1 Problem 6 Experimental Results

We use the formula from part (a) to evaluate $p(c)$.

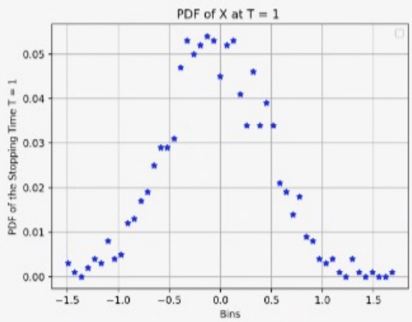
$$p(c) = \frac{1}{\sqrt{2\pi}} e^{-1/2c} \int_{\infty}^{0} e^{-y/\sqrt{c}}\, dy$$

Here, M is the number of samples. $p(c)$ is evaluated by the above formula. $A(c, M)$ is produced by the algorithm.
Relative error is $|(v_{actual} - v_{expected})/v_{expected}|$.

$M \approx 500$ would be a good choice as we decrease c.

c	M	p(c)	A(c,M)	relative error (%)
0.5	2000	0.1038	0.0795	23
0.5	500	0.1038	0.082	21
0.5	100	0.1038	0.11	6
1	2000	0.242	0.1677	31
1	500	0.242	0.184	24
1	100	0.242	0.27	11

M = 1000



(c) Reference: my HW from Stoch. Calc. last semester taught by Goodman.

In part (b), we were sampling in the p-world. According to p-measure,

$$p(x) = \frac{1}{\sqrt{2\pi c}} e^{-x^2/2c}$$

Now, we want to change the measure in q.

$$q(x) = \frac{1}{\sqrt{2\pi c}} e^{-(x-\mu)^2/2c}.$$

we want a good μ.

$$L(x) = \frac{p(x)}{q(x)} = \exp\{(-x^2 + (x-\mu)^2)/2c\}$$

$\cancel{x^2} - 2\mu + \mu^2$.

$$= \exp\left\{\frac{1}{2c}(-2\mu x + \mu^2)\right\}$$

$$= \exp\left\{\frac{1}{c}\left(-\mu x + \frac{1}{2}\mu^2\right)\right\}$$

The goal here is to minimize Var_q.

$$\mathrm{Var}_q = E_q[L^2(x)\, V^2(x)] - E_q[L(x)V(x)]^2$$

$$= E_q[L^2(x)\, V^2(x)] - A^2$$

where $V(x) = \begin{cases} 1 & \text{if } x > a \\ 0 & \text{if } x < a \end{cases}$ is indicator fct.

and $A = E_p[V(x)] = E_q[L(x)V(x)] = Pr_p(x > a)$.

Since A^2 is known, we want to minimize the 1st term.

$$E_q[\mathcal{L}^2(x)\, V^2(x)] = E_q[\mathcal{L}^2(x)\, V(x)]$$

$$= E_q[\, e^{-2\mu x/c + \mu^2/c}\; V(x)]$$

$$= \frac{e^{\mu^2/c}}{\sqrt{2\pi}} \underbrace{\int_a^\infty e^{-2\mu x/c}\, e^{-(x-\mu)^2/2c}\, dx}_{B}.$$

Let's evaluate B. Consider the intergrand.

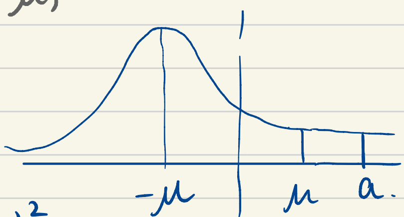
$$e^{-2\mu x/c - (x-\mu)^2/2c} : \quad -\frac{2\mu x}{c} - \frac{(x-\mu)^2}{2c}$$

$$= \frac{1}{c}\left[-2\mu x - \frac{1}{2}x^2 + \mu x - \frac{1}{2}\mu^2\right]$$

$$= -\frac{1}{c}\left[\frac{1}{2}x^2 + \mu x + \frac{1}{2}\mu^2\right]$$

$$= -\frac{1}{2c}(x+\mu)^2$$

$$B = \int_a^\infty e^{-\frac{1}{2c}(x+\mu)^2}\, dx$$



Let $a=1$, $x = 1 + \sqrt{c}\, y$

$$(x+\mu)^2 = (1+\sqrt{c}\,y+\mu)^2 = (1+\mu+\sqrt{c}\,y)^2$$
$$= (1+\mu)^2 + 2(1+\mu)\sqrt{c}\,y + c y^2$$

Then, B yields

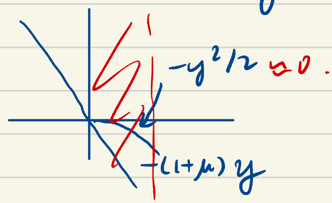
$$B = \int_0^\infty e^{-(1+\mu)^2/2c}\, e^{-(1+\mu)y/\sqrt{c}}\, e^{-y^2/2}$$

$$= e^{-(1+\mu)^2/2c} \int_0^\infty e^{-(1+\mu)y/\sqrt{c}} \, e^{-y^2/2} \, dy$$

$$\approx e^{-(1+\mu)^2/2c} \int_0^\infty e^{-(1+\mu)y/\sqrt{c}} \, dy$$

$\uparrow$

SAME REASON



$$\boxed{B = e^{-(a+\mu)^2/2c} \frac{\sqrt{c}}{1+\mu}}$$

Then, substitute B into the above.

(1) $$E_q[L^2(x)\,V(x)] = \frac{1}{\sqrt{2\pi}} \frac{\sqrt{c}}{1+\mu} e^{-(a+\mu)^2/2c} \, e^{\mu^2/c}$$

We want to minimize (1) for some μ.

The trick here is to ignore $\frac{1}{1+\mu}$ b/c $a=1$ is large relative to other values in $p(x)$.
Hence, $\frac{1}{1+\mu}$ is small for $\mu>0$.

Hence, $\min_{\mu} e^{\mu^2/c - (a+\mu)^2/2c}$

$$\Rightarrow \min_{\mu} e \;\; \mu^2/c - (a+\mu)^2/2c = \min_{\mu} F(\mu).$$

$$\frac{d}{d\mu} F(\mu) = \frac{d}{d\mu}\left[\mu^2 - \tfrac{1}{2}a^2 - a\mu - \tfrac{1}{2}\mu^2\right]$$

$$= -a + \mu = 0. \quad \Rightarrow \boxed{\mu = a}$$

Hence, $\mu = a = 1$ will minimize $E_q[L^2 V]$.

$$\mathrm{Var}_q = \frac{c}{\sqrt{2\pi}(a+\mu)} e^{-a^2/c} - p^2$$

where $p = \Pr_p(x > a)$

Let $a = 1$ in our case $p = \Pr_p(x > 1)$

$$\mathrm{Var}_q = \frac{c}{\sqrt{2\pi}(1+\mu)} e^{-1/c} - p^2 \text{ is minimized!}$$

Hence, the optimal importance sampling est. should have dist.

$$\boxed{q(x) = \frac{1}{\sqrt{2\pi c}} e^{-(x-1)^2/2c}}$$

This is $\boxed{X_t = \sqrt{c}\, W_t - 1}$