These notes draw from the following sources:

- Nils Berglund, Kramer's Law: Validity, derivations, and generalisations; Markov Processes Relat. Fields 19 (2013) pg. 459-90.

- BJ Matkowsky & Z. Schuss, Eigenvalues of the Fokker-Planck operator and the approach to equilibrium for diffusions in potential fields; SIAM J. Applied Math 40 (1981), no. 2.

- Z. Schuss & BJ Matkowsky, The exit problem: a new approach to diffusion across potential barriers; SIAM J. Applied Math 36 (1979), no. 3.

- AP Ghosh, Backward and forward equations for diffusion processes. Wiley Encyclopedia of Operations Research and Management Science, (2011).

- Bernt Øksendal, Stochastic differential equations: An introduction with applications (3rd edition). Berlin: Springer. (1995)

* Peter Glynn's course notes were originally used for Page 4, derivation of the $w_A(x)$ ODE, but have since been taken offline, so this page is in flux and will be updated with a new proof.

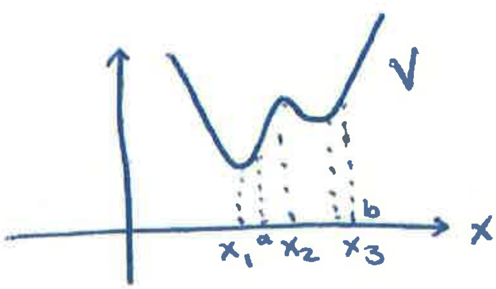
We will consider the stochastic differential equation

$$dX_t = -\underbrace{\nabla V(X_t)}_{\substack{\uparrow \\ \text{non-negative} \\ \text{potential with} \\ \text{two wells}}} dt + \underbrace{\sqrt{2\varepsilon}}_{\substack{\uparrow \\ \varepsilon \ll 1}} \underbrace{dW_t}_{\substack{\uparrow \\ \text{Brownian motion}}} \qquad (*)$$

In order for X_t to be a solution to $(*)$, X_t must satisfy

$$\begin{aligned} X_t &= X_0 + \int_0^t dX_t \\ &= X_0 - \int_0^t \nabla V(X_s)\, ds + \sqrt{2\varepsilon} \int_0^t dW_s \quad \text{a.s.} \end{aligned}$$

Our set-up is:



- V has 2 wells
- V has a local max at x_2 and local mins at x_1, x_3
- The well at x_1 is deeper than the well at x_3, so $V(x_1) < V(x_2)$.

Define $A = (-\infty, a)$ and $B = (b, \infty)$ where $a < b$.

Suppose the maximum of V in $[a, b]$ occurs at x_2 (not at the endpoints). Let $x \in (a, b)$.

Then we are interested in:

① $w_A(x) = \mathbb{E}^x[\tau_A]$

= expected first hitting time of A given we start at x

② $h_{A,B}(x) = \mathbb{P}^x(\tau_A < \tau_B)$

= probability that we hit A before B assuming we start at x.

③ $p(x,t)$ = probability density of X_t

It turns out w_A, $h_{A,B}$, and p satisfy deterministic diff. eqns. involving the generator of the diffusion $\mathcal{L}$. The generator $\mathcal{L}$ encodes a lot of info about the process. It's a measure of the infinitessimal change.

<u>Definition</u>:

The infinitessimal generator of the diffusion is the operator $\mathcal{L}$ given by

$$(\mathcal{L}f)(x) = \lim_{t \to 0} \frac{\mathbb{E}^x[f(X_t)] - f(x)}{t}$$

where we will consider $f \in C_b^2(\mathbb{R}^d)$.

Note that when $\mathcal{L}$ operates on a deterministic function the result is just the time derivative.

Now we will calculate $\mathcal{L}$ for our problem.

Let $d=1$. Then for the diffusion $(*)$ with $f \in C_b^2(\mathbb{R})$, we have

$$f(X_t) = f(x) + \int_0^t f'(X_s)\,dX_s + \varepsilon \int_0^t f''(X_s)\,ds,$$

where the second term is the "Ito correction".

Using $(*)$ we then obtain:

$$f(X_t) = f(x) - \int_0^t f'(X_s)V'(X_s)\,ds + \sqrt{2\varepsilon}\int_0^t f'(X_s)\,dW_s$$
$$+ \varepsilon \int_0^t f''(X_s)\,ds$$

Then

$$\mathcal{L}f(x) = \lim_{t \to 0} \frac{1}{t}\left[\mathbb{E}^x[f(X_t)] - f(x)\right]$$
$$= \lim_{t \to 0} \mathbb{E}^x\left[\frac{1}{t}\left(-\int_0^t f'(X_s)V'(X_s)\,ds + \sqrt{2\varepsilon}\int_0^t f'(X_s)\,dW_s + \varepsilon \int_0^t f''(X_s)\,ds\right)\right]$$
$$= -f'(x)V'(x) + \varepsilon f''(x)$$

(or in higher dimensions, as discussed in Berglund 2011, $\mathcal{L} = \varepsilon\Delta - \nabla V \cdot \nabla$).

Now we will sketch an argument for finding the differential equation satisfied by $w_A(x) = \mathbb{E}^x \tau_A$. First note that $w_A(x) = 0$ if $x \in A$, so we will consider $x \in A^c$.

Furthermore, let $t \ll 1$ be small. Then

$$\frac{\mathbb{E}^x[w_A(X_t)] - w_A(x)}{t} = \frac{1}{t}\left(\mathbb{E}^x\left[\mathbb{E}^{X_t}[\tau_A]\right] - w_A(x)\right).$$

Taking the limit as $t \to 0$, we obtain

$$\lim_{t\to 0} \frac{\mathbb{E}^x[w_A(X_t)] - w_A(x)}{t} = \lim_{t \to 0} \frac{1}{t}\left(\mathbb{E}^x\left[\mathbb{E}^{X_t}\tau_A\right] - \mathbb{E}^x \tau_A\right)$$

$$= \lim_{t\to 0} \frac{1}{t}\left(\mathbb{E}^x\tau_A - t - \mathbb{E}^x \tau_A\right)$$

$$= -1.$$

This motivates why $\mathcal{L} w_A(x) = -1$ for $x \in A^c$, and a more careful explanation can be found in Bernt Øksendal's book. Nils Berglund derives this equation for the problem of a symmetric random walk on the integers.

We conclude that

$$\begin{cases} \mathcal{L} w_A(x) = -1 & x \in A^c \\ w_A(x) = 0 & x \in A \end{cases}$$

Similarly,

$$\begin{cases} \mathcal{L} h_{A,B}(x) = 0 & x \in (A \cup B)^c \\ h_{A,B}(x) = 1 & x \in A \\ h_{A,B}(x) = 0 & x \in B \end{cases}$$

Lastly, we will find the diff. eqn. satisfied by p: for fixed $T>0$, consider

$$\mathbb{E}[f(X_T)] = \mathbb{E}[\mathbb{E}^{x,t}[f(X_T)]]$$

$$= \int \mathbb{E}^{x,t}[f(X_T)]\, p(x,t)\, dx$$

$$= \int u(x,t) \quad p(x,t)\, dx,$$

where $u(x,t) = \mathbb{E}^x[f(X_T)]$, so u is deterministic. There is no t dependence on the LHS of the above equation, so taking the derivative we obtain:

$$0 = -\int p \frac{\partial u}{\partial t}\, dx + \int u \frac{\partial p}{\partial x}\, dx$$

$$= -\int p \mathcal{L} u\, dx + \int u \frac{\partial p}{\partial t}\, dx.$$

After integrating by parts and replacing derivatives of u with those of p, we find

$$\frac{\partial p}{\partial t} = \varepsilon p_{xx} - \frac{\partial}{\partial x}(V_x p),$$ the Fokker-Planck eqn.

Now that we have diff. eqns. for ω_A, $h_{A,B}$, (6)
and p_1 we will solve them in turn.

Solving for $h_{A,B}$

$$\varepsilon h''_{A,B} - V' h'_{A,B} = 0$$

Integrating factor, integration and the requirements that $h_{A,B}(x) = 1$ for $x \in A$ & $h_{A,B}(x) = 0$ for $x \in B$ imply

$$h_{A,B}(x) = \frac{\int_x^b e^{V(y)/\varepsilon}\,dy}{\int_a^b e^{V(y)/\varepsilon}\,dy}$$

We apply Laplace's method to the denominator first.

Nonlocal Contribution:

Given δ small enough, by the continuity of V $\exists \eta > 0$ so that $V(x) \le V(x_2 - \delta) \le V(x_2) - \eta$ $\forall x \in [a, x_2 - \delta]$ and $V(x) \le V(x_2 + \delta) \le V(x_2) - \eta$ $\forall x \in [x_2 + \delta, b]$. Then:

$$\left| \int_a^{x_2-\delta} e^{V(y)/\varepsilon}\,dy + \int_{x_2+\delta}^b e^{V(y)/\varepsilon}\,dy \right| \le e^{V(x_2)/\varepsilon}(b-a)e^{-\eta/\varepsilon}.$$

Local Contribution:

$$\int_{x_2-\delta}^{x_2+\delta} e^{V(y)/\varepsilon}\,dy = e^{V(x_2)/\varepsilon} \int_{x_2-\delta}^{x_2+\delta} e^{-(V(x_2)-V(y))/\varepsilon}\,dy$$

Let $\tilde{V}(y) = V(x_2) - V(y)$. Notice $\tilde{V}(y) \ge 0$ $\forall y \in [a,b]$.

$\tilde{V}(y)$ has its minimum at $y = x_2$. Then

$$e^{V(x_2)/\varepsilon}\int_{x_2-\delta}^{x_2+\delta} e^{-(V(x_2)-V(y))/\varepsilon}\,dy = e^{V(x_2)/\varepsilon}\int_{x_2-\delta}^{x_2+\delta} e^{-\tilde{V}(y)/\varepsilon}\,dy.$$

Now make the change of variables defined by $\tilde{V}(r(s)s + x_2) = s^2$. Taylor expanding around $s=0$, we have:

$$\begin{aligned}\tilde{V}(r(s)s + x_2) &= V(x_2) - V(r(s)s + x_2)\\ &= \cancel{V(x_2)} - \cancel{V(x_2)} - \cancel{V'(x_2)}\,r(0)\,s\\ &\qquad - \tfrac{1}{2}V''(x_2)\,r(0)^2 s^2 + O(s^3 r^3).\end{aligned}$$

Setting this $= s^2$, we conclude that $r(0) = \sqrt{\dfrac{2}{|V''(x_2)|}}$.

Then our integral becomes:

$$\int_{x_2-\delta}^{x_2+\delta} e^{V(y)/\varepsilon}\,dy \approx e^{V(x_2)/\varepsilon}\int_{-\infty}^{\infty} e^{-s^2/\varepsilon}\left(r'(s)s + r(s)\right)ds.$$

Applying Watson's Lemma, at leading order, we obtain

$$\int_a^b e^{V(y)/\varepsilon}\,dy \approx \sqrt{\frac{2\pi\varepsilon}{|V''(x_2)|}}\; e^{V(x_2)/\varepsilon}$$

After approximating the numerator as well, we end up with

$$h_{A,B}(x) \approx e^{-\frac{1}{\varepsilon}\left[\sup_{y\in[a,b]} V(y) - \sup_{y\in[x,b]} V(y)\right]}$$

as Berglund discusses. Thus, the probability of hitting A before B is nearly 1 when x lies in the basin of attraction of a and is exponentially small otherwise.

Now we turn our attention to $w_A(x)$:

$w_A(x) = \mathbb{E}^x \tau_A$ satisfies

$$\begin{cases} \mathcal{L} w_A(x) = -1 & \text{for } x \in A^c \\ w_A(x) = 0 & \text{for } x \in A. \end{cases}$$

That is, $\varepsilon w_A'' - V' w_A' = -1$. Solving via integrating factor & integration, we obtain

$$w_A(x) = \frac{1}{\varepsilon} \int_a^x \int_z^\infty e^{[V(z)-V(y)]/\varepsilon} \, dy \, dz.$$

Assuming $x > x_3 > x_2 > a$, we note $V(z) - V(y)$ is maximal when $z = x_2$ and $y = x_3$. Then by Laplace's method, we will obtain

$$\mathbb{E}^x \tau_A = w_A(x) \simeq \frac{1}{\varepsilon} \left[\frac{2\pi\varepsilon}{\sqrt{|V''(x_2)||V''(x_3)|}} e^{(V(x_2)-V(x_3))/\varepsilon} + O(\varepsilon^{3/2}) \right]$$

$$\approx \frac{2\pi}{\sqrt{|V''(x_2)||V''(x_3)|}} e^{(V(x_2)-V(x_3))/\varepsilon} \quad \text{at leading order.}$$

This is precisely Kramer's Law in 1D. It tells us that the mean time to get to A depends on the curvatures at x_2 & x_3 and the height difference in the potential from the max to the second well.

Now we will determine the first nonzero eigenvalue of the Fokker-Planck equation. This is related to the time required to overcome the potential barrier at x_2.

As discussed earlier, $p(x, x_0, t)$ = probability density of X_t satisfies the Fokker-Planck equation:

$$\begin{cases} \varepsilon p_{xx} - (V_x p)_x = p_t = \lambda p \\ p(x, x_0, t) \longrightarrow \delta(x - x_0) \text{ as } t \to 0. \end{cases}$$

As Bjorn discussed before, the unique nontrivial stationary distribution is

$$p^0 = C e^{-V/\varepsilon},$$

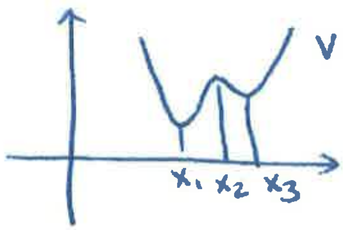
where $C = \int_{-\infty}^{\infty} e^{-V(y)/\varepsilon} dy$ is a normalization constant.

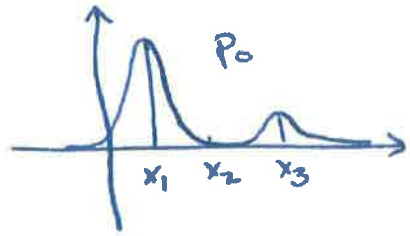
p^0 is the probability density of a random variable X^0, and we are interested in the rate at which $X_t \to X^0$ in distribution.

Expanding p in an eigenfunction expansion, we have:

$$p(x, x_0, t) = p^0(x) + \sum_{n=1}^{\infty} p_n(x) p_n(x_0) e^{-V(x)/\varepsilon} e^{\lambda_n t}$$

where $p^0(x)$ corresponds to the $\lambda_0 = 0$ eigenvalue. (See Matkowsky & Schuss). The rate of approach of X_t to X^0 in distribution is controlled by λ_1.





We expect that the rate of approach to the equilibrium distribution will be controlled by the time required to overcome the potential barrier at x_2. We showed $\omega_A \approx Ce^{(V(x_2)-V(x_3))/\varepsilon}$ earlier, so we expect λ_1 will be exponentially small. With this in mind we set $p_1(x) = e^{-V(x)/\varepsilon}\, u(x)$ wher u is $O(1)$. We obtain:

$$\varepsilon u_{xx} - V_x u_x = \lambda_1 u.$$

Since λ_1 is exponentially small, the leading term u^0 in this expansion as $\varepsilon \to 0$ satisfies

$$V_x u_x^0 = 0.$$

Thus, except when $V_x(x) = 0$, we need $u^0 = $ constant.

Thus,
$$u^0 = \begin{cases} C_1 & x < x_2 \\ C_2 & x > x_2. \end{cases}$$

As $\varepsilon \to 0$, an internal layer in which the solution change rapidly can develop. To investigate this region about x_2, we use the stretching transform

$$\xi = \frac{x - x_2}{\varepsilon^\alpha}.$$

We obtain

$$\varepsilon^{1-2\alpha} u^0_{\xi\xi} - \left[V''(x_2)(x-x_2) + O((x-x_2)^2)\right]\varepsilon^{-\alpha} u^0_\xi = 0.$$

Setting $\alpha = \frac{1}{2}$ gives us

$$u^0_{\xi\xi} - V''(x_2)\frac{x-x_2}{\varepsilon^{1/2}} u^0_\xi = 0$$

$$\Rightarrow \quad u^0_{\xi\xi} - V''(x_2)\,\xi\, u^0_\xi = 0$$

$$\Rightarrow \quad u^0 = C\int_0^\xi e^{V''(x_2)s^2}\,ds + B.$$

In order to satisfy the matching conditions

$$u^0(\xi) \longrightarrow \begin{cases} C_1 & \text{as } \xi \to -\infty \\ C_2 & \text{as } \xi \to +\infty, \end{cases}$$

we require

$$u^0(\xi) = \frac{C_2 - C_1}{\sqrt{2\pi}}\sqrt{|V''(x_2)|}\int_0^\xi e^{-|V''(x_2)|s^2}\,ds + \frac{C_1 + C_2}{2}.$$

In conclusion, for $\varepsilon \ll 1$,

$$u(x) = u^0\left(\frac{x-x_2}{\varepsilon^{1/2}}\right) + o(1) \quad \text{as } \varepsilon \to 0.$$

Matkowsky & Schuss show that, in fact,

$$u(x) \approx \frac{\sqrt{|V''(x_2)|}}{\sqrt{2\pi}}\int_0^{(x-x_2)/\varepsilon^{1/2}} e^{V''(x_2)s^2}\,ds + \frac{1}{2}.$$

Then we find λ_1 by multiplying

$$\varepsilon u_{xx} - V_x u_x = \lambda_1 u$$

by $e^{-V(x)/\varepsilon}$ and integrating from x_2 to ∞:

$$\int_{x_2}^{\infty} e^{-V(x)/\varepsilon}\left[\varepsilon u_{xx} - V_x u_x\right] dx = \lambda_1 \int_{x_2}^{\infty} e^{-V(x)/\varepsilon} u(x)\, dx .$$

<u>LHS:</u>

$$LHS = \int_{x_2}^{\infty} \varepsilon \frac{d}{dx}\left[e^{-V(x)/\varepsilon} u_x\right] dx = -\varepsilon e^{-V(x_2)/\varepsilon} u_x(x_2)$$

since we assume $V \to +\infty$ as $x \to +\infty$.

But $$u_x(x_2) \sim \frac{d}{dx}\left[\frac{\sqrt{|V''(x_2)|}}{\sqrt{2\pi}} \int_0^{(x-x_2)/\varepsilon^{1/2}} e^{V''(x_2)s^2}\, ds + \frac{1}{2}\right]\Bigg|_{x=x_2}$$

$$\sim \frac{\sqrt{|V''(x_2)|}}{\sqrt{2\pi}} \frac{1}{\sqrt{\varepsilon}} .$$

Thus, $$LHS = -\sqrt{\varepsilon}\, e^{-V(x_2)/\varepsilon} \frac{\sqrt{|V''(x_2)|}}{\sqrt{2\pi}} .$$

<u>RHS:</u>

$$RHS = \lambda_1 \int_{x_2}^{\infty} e^{-V(x)/\varepsilon} u(x)\, dx = \lambda_1 e^{-V(x_3)/\varepsilon} u(x_3) \sqrt{\frac{2\pi\varepsilon}{V''(x_3)}}$$

by Laplace Method.

Thus,
$$\lambda_1 \sim \frac{\int_{x_2}^{\infty} e^{-V(x)/\varepsilon}\left[\varepsilon u_{xx} - V_x u_x\right] dx}{\int_{x_2}^{\infty} e^{-V(x)/\varepsilon} u(x)\, dx}$$

$$\lambda_1 \approx -\frac{e^{-V(x_2)/\varepsilon}\, e^{V(x_3)/\varepsilon}}{2\pi}\, u(x_3) \sqrt{V''(x_3)\, |V''(x_2)|}$$

$$\approx -\frac{\sqrt{V''(x_3)\,|V''(x_2)|}}{2\pi}\, e^{-(V(x_2)-V(x_3))/\varepsilon}$$

$$= \frac{1}{\mathbb{E}^x[\tau_A]} = \frac{1}{w_A(x)}.$$