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Prototype Landscape Notes v2

1 Definition of a landscape

Let X be the state space.

Definition. A *global landscape* is a function $L : X \to \mathbb{R}$ satisfying:

- Let $x_1, x_2 \in X$. If $P_{ss}(x_1) > P_{ss}(x_2)$, then $L(x_1) < L(x_2)$.
  If $P_{ss}(x_1) = P_{ss}(x_2)$, then $L(x_1) = L(x_2)$.

Definition. A *local landscape* is a function $L : X \to \mathbb{R}$ and a distinguished point $x_0 \in X$ such that:

- Let $x_1, x_2 \in X$. If there exists a $T' > 0$ such that $P(x_0 \to x_1, T) > P(x_0 \to x_2, T)$ for all $0 < T < T'$, then $L(x_1) < L(x_2)$.
  If there exists a $T' > 0$ such that $P(x_0 \to x_1, T) = P(x_0 \to x_2, T)$ for all $0 < T < T'$, then $L(x_1) = L(x_2)$.

REST OF DOCUMENT NEEDS TO BE UPDATED...

2 General mathematical properties

Lemma 2.1. *Let X be some state space, and $\phi : X \to \mathbb{R}$ be a landscape. Then*

1. *$\phi + c$ is a landscape for any $c \in \mathbb{R}$*
2. *$c\phi$ is a landscape for any $c > 0$*
3. *Let B be an absolute lower bound for ϕ. Then $f(\phi)$ is a landscape for any strictly increasing function $f : [B, \infty)$.*
4. *If ϕ is a global/local landscape, each of the modifications above produces a global/local landscape.*

Proof. (1) Shifting ϕ by a constant does not change its local minima. Since there exists an absolute lower bound B of ϕ_1, clearly $B + c$ is an absolute lower bound of $\phi + c$, so $\phi + c$ is indeed a landscape.

(2) Multiplying ϕ by a constant does not change its local minima. Since there exists an absolute lower bound B of ϕ, clearly $cB \leq c\phi(x)$ for all $x \in X$. Hence, $c\phi$ is a landscape.

(3) If B is an absolute lower bound for ϕ, and f is strictly increasing, then $B \leq \phi(x)$ for all $x \in X$ implies that $f(B) \leq f(\phi(x))$ for all $x \in X$ (since f is strictly increasing, it preserves the inequality). Hence, $f(\phi)$ is bounded from below. Also, since f is strictly increasing, $f(\phi)$ has the same local minima as ϕ. Hence, $f(\phi)$ is a landscape.

(4) Since inequalities are preserved by each of the previous changes, the global/local property is clearly maintained. □

I should note: in general, the sum of two landscapes is not a landscape. In fact, the sum of two landscapes is generally not a landscape even if their local minima exactly coincide.

What is the relationship between global and local landscapes? We will see later on that, in the small symmetric additive noise limit, U^{norm} and P_{ss} (both global landscapes in this regime) are also local landscapes. How general is this?

One has to keep in mind that, in some sense, the properties of Wang's $-\log P_{ss}$ control the properties of every other global landscape; if Wang's landscape is local in some regime, so is *every other global landscape* (given our definition). An example of this is the result below.

Theorem 2.2 (Global landscapes are local landscapes for small noise)**.** *Consider a system with state space X governed by Langevin/Fokker-Planck dynamics with symmetric additive* *noise. In the low noise limit, if $\phi : X \to \mathbb{R}$ is a global landscape, then ϕ is also a local landscape.*

Proof. As we will show below, Huang's U^{norm} is a local landscape in this limit. That can be used to show that Wang's P_{ss} landscape is also a local landscape in this limit. Hence, for any $x_0, x_1, x_2 \in X$,

$$\begin{aligned} P(x_0 \to x_1, T) \geq P(x_0 \to x_2, T) \text{ for all } T > 0 \\ \implies \log P_{ss}(x_1) \leq -\log P_{ss}(x_2) \\ \implies P_{ss}(x_1) \geq P_{ss}(x_2) \\ \implies \phi(x_1) \leq \phi(x_2) \end{aligned}$$

so ϕ is indeed a local landscape. □

3 Examples

3.1 Potential for equilibrium systems

Consider the system with state space $X = \mathbb{R}$ whose dynamics are

$$\dot{x} = -\frac{dV(x)}{dx} + \sigma\eta(t)$$

for some potential function V (which is bounded from below and twice differentiable on $\mathbb{R}$) and additive noise coefficient $\sigma > 0$. We want to show that, given our definitions above, V is a valid landscape.

3.1.1 Showing V is a landscape

By assumption, V is bounded from below, so the first property is trivially satisfied.

Suppose that $-\frac{dV}{dx}\big|_{x=y} = 0$ for some $y \in X$, and that $-\frac{dV}{dx} > 0$ for x a little smaller than y, and $-\frac{dV}{dx} < 0$ for x a little bigger than y. Then $V(y)$ is trivially a local minimum.

Hence, V is a landscape. Is it a global or local landscape?

3.1.2 Showing V is a global landscape

The Fokker-Planck equation (at steady state) reads

$$0 = -\frac{d}{dx}\left[-\frac{dV(x)}{dx}P_{ss}(x) - \frac{\sigma^2}{2}P'_{ss}(x)\right]$$

or equivalently

$$C = \frac{dV(x)}{dx} P_{ss}(x) + \frac{\sigma^2}{2} P'_{ss}(x)$$

for some $C \in \mathbb{R}$. In fact, because the probability flux J should vanish at infinity, this C should generally be zero, so we can write

$$0 = \frac{dV(x)}{dx} P_{ss}(x) + \frac{\sigma^2}{2} P'_{ss}(x)$$

and solve it to find that

$$P_{ss}(x) = N e^{-V(x)/(\sigma^2/2)}$$

where N is a normalization factor.

Let $x_1, x_2 \in X$, and suppose that $P_{ss}(x_1) \geq P_{ss}(x_2)$. Then

$$\begin{aligned} & e^{-V(x_1)/(\sigma^2/2)} \geq e^{-V(x_2)/(\sigma^2/2)} \\ \implies & -V(x_1)/(\sigma^2/2) \geq -V(x_2)/(\sigma^2/2) \\ \implies & V(x_1) \leq V(x_2) \end{aligned}$$

as desired. Hence, V is a global landscape.

3.1.3 Showing V is a local landscape in the low noise limit

The dynamics of our system are controlled by the Lagrangian

$$L(x(t), \dot{x}(t)) = \frac{(\dot{x} + V'(x))^2}{2\sigma^2}$$

Let $x_0 \in X$ be arbitrary. In the low noise limit, transition probabilities can be calculated according to the semiclassical approximation

$$P(x_0 \to x) \sim e^{-S_{cl}}$$

where

$$S_{cl}[x_{cl}(t)] := \int_0^T L(x_{cl}(t), \dot{x}_{cl}(t)) dt$$

and $x_{cl}(t)$ is the classical path starting at x_0 and reaching $x \in X$ at time T according to the Euler-Lagrange equations.

Let $x_1, x_2 \in X$. If $P(x_0 \to x_1, T) \geq P(x_0 \to x_2, T)$ for all $T > 0$, then

$$
\begin{aligned}
& e^{-S_{cl}[x_1(t)]} \geq e^{-S_{cl}[x_2(t)]} \\
\implies & S_{cl}[x_1(t)] \leq S_{cl}[x_2(t)] \\
\implies & \int_0^T L(x_1(t), \dot{x}_1(t))dt \leq \int_0^T L(x_2(t), \dot{x}_2(t))dt \\
\implies & 0 \leq \int_0^T L(x_2(t), \dot{x}_2(t)) - L(x_1(t), \dot{x}_1(t))dt \\
\implies & 0 \leq \int_0^T \frac{(\dot{x_2} + V'(x_2))^2}{2\sigma^2} - \frac{(\dot{x_1} + V'(x_1))^2}{2\sigma^2}dt \\
\implies & 0 \leq \int_0^T \dot{x_2}^2 + 2\dot{x_2}V'(x_2) + (V'(x_2))^2 - \dot{x_1}^2 - 2\dot{x_1}V'(x_1) - (V'(x_1))^2 dt \\
\implies & 0 \leq 2\left[V(x_2) - V(x_1)\right] + \int_0^T \dot{x_2}^2 + (V'(x_2))^2 - \dot{x_1}^2 - (V'(x_1))^2 dt
\end{aligned}
$$

Since this inequality holds *regardless* of T (remember: we are assuming that $P(x_0 \to x_1, T) \geq P(x_0 \to x_2, T)$ for *all* $T > 0$), we can imagine taking T to be very small. For sufficiently small T, the contribution of the integral will be very small; for the overall expression to still be greater than or equal to zero, it must be that

$$0 \leq V(x_2) - V(x_1)$$

which is exactly what we wanted to show. Hence, V is also a *local* landscape. Remarkably, it is a local landscape *independent of the base point chosen*, so long as we are working in the small noise regime.

3.2 Markov model

Consider a discrete time Markov chain: a list of N vertices X together with transition probabilities p_{ij} for each $i, j = 1, ..., N$ (all satisfying $0 \leq p_{ij} \leq 1$). In a given time step, the state either changes or it doesn't, so we have

$$p_{i1} + p_{i2} + \cdots + p_{iN} = 1$$

for each $i = 1, ..., N$.

Calculating P_{ss} for a completely general Markov chain is difficult, so we will wait to discuss a global landscape on X until we look at a specific example. Instead, consider the landscape defined by

$$\phi(j) = -\log(1 + p_{ij})$$

for a fixed $i \in \{1, ..., N\}$. We want to show that this is, as expected, a local landscape with distinguished point i.

First, ϕ is a function $X \to \mathbb{R}$ which is bounded below by $-\log(2)$ (since none of the transition probabilities can be greater than one). Second, since we have a discrete unordered state space, the second condition is trivially satisfied (since all vertices are attractors by definition). So ϕ is a landscape.

Suppose $j_1, j_2 \in X$ satisfy $P(i \to j_1, T) \geq P(i \to j_2, T)$ for all $T > 0$. Let's parse what this means here. Our model has discrete time, so $T > 0$ means $T = 1, 2, ...$ steps. Also, the transition probabilities are all constant and do not change with time, so

$$P(i \to j_1, T) \geq P(i \to j_2, T) \implies p_{ij_1} \geq p_{ij_2}$$

Trivially, then, it is true that

$$-\log(1 + p_{ij_1}) \leq -\log(1 + p_{ij_2})$$

i.e. that $L(j_1) \leq L(j_2)$. Hence, ϕ really is a local landscape.

3.2.1 Two state Markov chain example

Consider the discrete time Markov chain with two states (conservatively labeled 1 and 2). Its transition probabilities (which we leave arbitrary) are p_{11}, p_{12}, p_{21}, and p_{22}.

In one time step, the probabilities $P(1)$ and $P(2)$ of being in state 1 or state 2 change according to:

$$P(1, i+1) = p_{11} P(1, i) + p_{21} P(2, i)$$
$$P(2, i+1) = p_{21} P(1, i) + p_{22} P(2, i)$$

which of course can be rewritten in matrix form as

$$\begin{pmatrix} P(1, i+1) \\ P(2, i+1) \end{pmatrix} = \begin{pmatrix} p_{11} & p_{21} \\ p_{12} & p_{22} \end{pmatrix} \begin{pmatrix} P(1, i) \\ P(2, i) \end{pmatrix}$$

or, more succinctly,

$$P_{i+1} = T P_i$$

The matrix T has eigenvalues $\lambda = 1, p_{11} + p_{22} - 1$, and can be diagonalized:

$$T = \begin{pmatrix} p_{11} & p_{21} \\ p_{12} & p_{22} \end{pmatrix} = \frac{1 - p_{22}}{2 - p_{11} - p_{22}} \begin{pmatrix} 1 & 1 \\ -1 & \frac{1-p_{11}}{1-p_{22}} \end{pmatrix} \begin{pmatrix} p_{11} + p_{22} - 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1-p_{11}}{1-p_{22}} & -1 \\ 1 & 1 \end{pmatrix}$$

where everything has been written in terms of p_{11} and p_{22} since $p_{12} = 1-p_{11}$ and $p_{21} = 1-p_{22}$.

We can calculate that

$$
\begin{aligned}
T^N &= \frac{1-p_{22}}{2-p_{11}-p_{22}} \begin{pmatrix} 1 & 1 \\ -1 & \frac{1-p_{11}}{1-p_{22}} \end{pmatrix} \begin{pmatrix} (p_{11}+p_{22}-1)^N & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1-p_{11}}{1-p_{22}} & -1 \\ 1 & 1 \end{pmatrix} \\
&= \frac{1-p_{22}}{2-p_{11}-p_{22}} \begin{pmatrix} (p_{11}+p_{22}-1)^N \frac{1-p_{11}}{1-p_{22}} + 1 & -(p_{11}+p_{22}-1)^N \frac{1-p_{11}}{1-p_{22}} + 1 \\ -(p_{11}+p_{22}-1)^N \frac{1-p_{11}}{1-p_{22}} + \frac{1-p_{11}}{1-p_{22}} & (p_{11}+p_{22}-1)^N + \frac{1-p_{11}}{1-p_{22}} \end{pmatrix}
\end{aligned}
$$

Taking $N \to \infty$ (keeping in mind that $-1 < p_{11}+p_{22}-1 < 1$) yields

$$
T^\infty = \begin{pmatrix} \frac{1-p_{22}}{2-p_{11}-p_{22}} & \frac{1-p_{22}}{2-p_{11}-p_{22}} \\ \frac{1-p_{11}}{2-p_{11}-p_{22}} & \frac{1-p_{11}}{2-p_{11}-p_{22}} \end{pmatrix}
$$

so that

$$
\begin{aligned}
P(1,\infty) &= \left(\frac{1-p_{22}}{2-p_{11}-p_{22}}\right)[P(1,0)+P(2,0)] = \frac{1-p_{22}}{2-p_{11}-p_{22}} \\
P(2,\infty) &= \left(\frac{1-p_{11}}{2-p_{11}-p_{22}}\right)[P(1,0)+P(2,0)] = \frac{1-p_{11}}{2-p_{11}-p_{22}}
\end{aligned}
$$

since $P(1,0)+P(2,0) = 1$ (i.e. the initial state has to be *somewhere*).

Now we have P_{ss} (although it looks like we probably could've just guessed the answer), so we can think about how to define a global landscape. Rewriting P_{ss} in a more intuitively clear form, we have

$$
\begin{aligned}
P(1,\infty) &= \frac{p_{21}}{p_{12}+p_{21}} \\
P(2,\infty) &= \frac{p_{12}}{p_{12}+p_{21}}
\end{aligned}
$$

We can define a landscape ϕ by

$$
\begin{aligned}
\phi(1) &:= -\log(1+p_{21}) \\
\phi(2) &:= -\log(1+p_{12})
\end{aligned}
$$

It is clearly a landscape, since $\phi : \{1,2\} \to \mathbb{R}$ is bounded below by $-\log(2)$ and the attractor condition is trivially satisfied.

To check that it is a global landscape, we need to verify that, for all $i, j \in \{1,2\}$, $P_{ss}(i) \geq P_{ss}(j) \implies \phi(i) \leq \phi(j)$. This is trivially true for $i = j$, so we only need to check that $P_{ss}(2) \geq P_{ss}(1) \implies \phi(2) \leq \phi(1)$ and $P_{ss}(1) \geq P_{ss}(2) \implies \phi(1) \leq \phi(2)$.

If $P_{ss}(1) \geq P_{ss}(2)$, then $p_{21} \geq p_{12}$, so that $\phi(1) \leq \phi(2)$ as desired. The opposite case is true by the exact same argument. Hence, ϕ is a global landscape.

Is ϕ a *local* landscape? Suppose that $p_{12} \geq p_{11}$. We would need it to be true that $\phi(2) \leq \phi(1)$—or equivalently that $p_{12} \geq p_{21}$, but this is not necessarily true. For example, we can take $p_{21} > p_{12} > p_{11} > p_{22}$. So ϕ is not generally a local landscape with respect to state 1.

Similarly, if $p_{22} \geq p_{21}$, it is not necessarily true that $\phi(2) \leq \phi(1)$ i.e. that $p_{12} \geq p_{21}$, since we can take $p_{11} > p_{22} > p_{21} > p_{12}$. So ϕ is not generally a local landscape with respect to state 2.

But it *is* possible for ϕ to be *both* a local and global landscape. For example, if $p_{12} = p_{22}$, our global landscape ϕ becomes exactly the local landscape discussed in the previous section. But the cases in which local and global landscapes coincide seem to be the exception rather than the rule.

3.3 Sui Huang's normal decomposition for symmetric additive noise Langevin dynamics

Consider a system whose dynamics evolve according to the Langevin equation

$$\frac{dx_i}{dt} = F_{x_i}(\mathbf{x}) + \sigma\eta_i(t)$$

for $i = 1, ..., N$ and $\sigma > 0$. The state space here is $X = \mathbb{R}^N_{\geq 0}$. The normal decomposition quasipotential U^{norm} is defined via the Hamilton-Jacobi equation

$$(\nabla U^{\text{norm}}, \mathbf{F} + \nabla U^{\text{norm}}) = 0$$

which, upon expansion, becomes

$$\frac{\partial U^{\text{norm}}}{\partial x_1}\left(F_{x_1} + \frac{\partial U^{\text{norm}}}{\partial x_1}\right) + \cdots + \frac{\partial U^{\text{norm}}}{\partial x_i}\left(F_{x_i} + \frac{\partial U^{\text{norm}}}{\partial x_i}\right) + \cdots + \frac{\partial U^{\text{norm}}}{\partial x_N}\left(F_{x_N} + \frac{\partial U^{\text{norm}}}{\partial x_N}\right) = 0$$

Let's check that this is really a landscape.

3.3.1 Showing U^{norm} is a landscape

First off, U^{norm} is a function from X to $\mathbb{R}$. Is it bounded from below?

To show this, we have to make a (reasonable) assumption about our function $\mathbf{F}(\mathbf{x})$ which holds true in real biological systems. If some x_i is sufficiently large, it must be that F_{x_i} becomes negative; if this were *not* true, then F_{x_i} would push x_i off to infinity, which is not biologically realistic. Similarly, if some x_i is sufficiently small, it must be that F_{x_i} becomes *positive*; if this were *not* true, then F_{x_i} would push x_i below zero, which is not biologically realistic either.

If some x_i is sufficiently large, F_{x_i} becomes very negative, so our condition above forces

$$F_{x_i} + \frac{\partial U^{\text{norm}}}{\partial x_i} = 0$$

which means that

$$\frac{\partial U^{\text{norm}}}{\partial x_i} > 0$$

when x_i is sufficiently large. In other words, if x_i gets big enough, U^{norm} will increase; in particular, after a certain point, *increasing* x_i *will never make* U^{norm} *smaller.*

Similarly, we can argue that, if some x_i is sufficiently small, F_{x_i} becomes positive, so

$$\frac{\partial U^{\text{norm}}}{\partial x_i} < 0$$

This means that, after a certain point, *decreasing* x_i *will never make* U^{norm} *smaller.* Putting these arguments together, since U^{norm} is continuous and differentiable and *increases* for large and small x_i, there must be some lower bound in the intermediate x_i region. If there was *not* an absolute lower bound, then U^{norm} would have to be singular or discontinuous.

For each stable steady state $\mathbf{y}$, does U^{norm} have a local minimum? We have $F_{x_i}(\mathbf{y}) = 0$ for all $i = 1, ..., N$, so

$$\left(\frac{\partial U^{\text{norm}}}{\partial x_1}\right)^2 + \cdots + \left(\frac{\partial U^{\text{norm}}}{\partial x_i}\right)^2 + \cdots + \left(\frac{\partial U^{\text{norm}}}{\partial x_N}\right)^2 = 0$$

which forces

$$\frac{\partial U^{\text{norm}}}{\partial x_1}(\mathbf{y}) = 0$$

for each $i = 1, ..., N$. Hence, U^{norm} has some sort of extremum at $\mathbf{y}$. If we increase each x_i slightly, we know each $F_{x_i} < 0$. Then

$$\frac{\partial U^{\text{norm}}}{\partial x_1}\left(F_{x_1} + \frac{\partial U^{\text{norm}}}{\partial x_1}\right) + \cdots + \frac{\partial U^{\text{norm}}}{\partial x_i}\left(F_{x_i} + \frac{\partial U^{\text{norm}}}{\partial x_i}\right) + \cdots + \frac{\partial U^{\text{norm}}}{\partial x_N}\left(F_{x_N} + \frac{\partial U^{\text{norm}}}{\partial x_N}\right) = 0$$

Since this is true *independently of how much we increased each* x_i, it must be that

$$F_{x_i} + \frac{\partial U^{\text{norm}}}{\partial x_i} = 0$$

for each $i = 1, ..., N$. Hence,

$$\frac{\partial U^{\text{norm}}}{\partial x_i} > 0$$

for $\mathbf{y} + \epsilon$. Similarly, we can find that

$$\frac{\partial U^{\text{norm}}}{\partial x_i} < 0$$

for $\mathbf{y} - \epsilon$. Hence, U^{norm} has a local minimum at each $\mathbf{y}$, so it is a legitimate landscape.

3.3.2 Showing U^{norm} is a global landscape in the small noise limit

Is U^{norm} a global landscape? Since noise does not contribute to the Hamilton-Jacobi equation defining U^{norm}, we should expect that, in general, the answer is no (especially when noise is not additive). But it is possible that U^{norm} is a global landscape in the small (additive) noise limit, where it doesn't matter much what the noise coefficients are.

In fact, it is not only possible, but true. In the small noise limit, we can use the WKB approximation (I follow Zhou and Li 2016 here) to approximate P_{ss} as

$$P_{ss}(\mathbf{x}) = \exp\left[-\frac{\phi(\mathbf{x})}{D} + \phi_0(\mathbf{x}) + \phi_1(\mathbf{x})D + \cdots\right]$$

where the functions $\phi(\mathbf{x}), \phi_0(\mathbf{x}), \phi_1(\mathbf{x})$... must be determined via consistency with the Fokker-Planck equation, and where I am writing $D := \sigma^2/2$ to ease notation a little.

Substituting this into the Fokker-Planck equation, we find that

$$0 = \sum_{i=1}^{N} \frac{1}{D}\frac{\partial \phi}{\partial x_i}\left(F_{x_i} + \frac{\partial \phi}{\partial x_i}\right) - \frac{\partial F_{x_i}}{\partial x_i} - \frac{\partial^2 \phi}{\partial x_i^2}$$

in the small noise limit, where I can neglect $\phi_0(\mathbf{x})$, $\phi_1(\mathbf{x})$, and so on.

Taking D very small (i.e. taking σ very small), the terms that *don't* go like $1/D$ make negligible contributions, so the Fokker-Planck equation just reads

$$0 = \sum_{i=1}^{N} \frac{1}{D}\frac{\partial \phi}{\partial x_i}\left(F_{x_i} + \frac{\partial \phi}{\partial x_i}\right)$$

or equivalently

$$\frac{\partial \phi}{\partial x_1}\left(F_{x_1} + \frac{\partial \phi}{\partial x_1}\right) + \cdots + \frac{\partial \phi}{\partial x_i}\left(F_{x_i} + \frac{\partial \phi}{\partial x_i}\right) + \cdots + \frac{\partial \phi}{\partial x_N}\left(F_{x_N} + \frac{\partial \phi}{\partial x_N}\right) = 0$$

so that $\phi = U^{\text{norm}}$.

Hence, in the small noise limit, suppose $\mathbf{x_1}, \mathbf{x_2} \in X$ have $P_{ss}(\mathbf{x_1}) \geq P_{ss}(\mathbf{x_2})$. Then

$$\begin{aligned} \exp\left[-\frac{\phi(\mathbf{x_1})}{D}\right] &\geq \exp\left[-\frac{\phi(\mathbf{x_2})}{D}\right] \\ \implies \quad \phi(\mathbf{x_1}) &\leq \phi(\mathbf{x_2}) \\ \implies \quad U^{\text{norm}}(\mathbf{x_1}) &\leq U^{\text{norm}}(\mathbf{x_2}) \end{aligned}$$

which is just what we wanted to verify.

3.3.3 Showing U^{norm} is a local landscape in the small noise limit

Again, since U^{norm} does not depend on noise, if it *is* a local landscape, it is probably only one in the small noise limit.

Our argument here will basically follow the argument from the equilibrium potential section.

Let $\mathbf{x_0}, \mathbf{x_1}, \mathbf{x_2} \in X$. If $P(\mathbf{x_0} \to \mathbf{x_1}, T) \geq P(\mathbf{x_0} \to \mathbf{x_2}, T)$ for all $T > 0$, then

$$\begin{aligned} e^{-S_{cl}[\mathbf{x_1}(t)]} &\geq e^{-S_{cl}[\mathbf{x_2}(t)]} \\ \implies \quad S_{cl}[\mathbf{x_1}(t)] &\leq S_{cl}[\mathbf{x_2}(t)] \\ \implies \quad \int_0^T L(\mathbf{x_1}(t), \dot{\mathbf{x}}_1(t))dt &\leq \int_0^T L(\mathbf{x_2}(t), \dot{\mathbf{x}}_2(t))dt \\ \implies \quad 0 &\leq \int_0^T L(\mathbf{x_2}(t), \dot{\mathbf{x}}_2(t)) - L(\mathbf{x_1}(t), \dot{\mathbf{x}}_1(t))dt \\ \implies \quad 0 &\leq \frac{1}{2\sigma^2}\int_0^T \sum_{i=1}^N \left[\dot{\mathbf{x}}_\mathbf{2} - \mathbf{F}(\mathbf{x_2})\right]^2 - \left[\dot{\mathbf{x}}_\mathbf{1} - \mathbf{F}(\mathbf{x_1})\right]^2 dt \end{aligned}$$

We recall from Huang's 2012 RSIF paper that

$$\mathbf{F}(\mathbf{x}) = -\nabla U^{\text{norm}}(\mathbf{x}) + \mathbf{F}_\perp(\mathbf{x})$$

so we can substitute this in to find

$$0 \leq \int_0^T \sum_{i=1}^N \left[\dot{\mathbf{x}}_\mathbf{2} + \nabla U^{\text{norm}}(\mathbf{x_2}) - \mathbf{F}_\perp(\mathbf{x_2})\right]^2 - \left[\dot{\mathbf{x}}_\mathbf{1} + \nabla U^{\text{norm}}(\mathbf{x_1}) - \mathbf{F}_\perp(\mathbf{x_1})\right]^2 dt$$

If the squares are expanded, one finds terms $2\nabla U^{\text{norm}}(\mathbf{x_2}) \cdot \dot{\mathbf{x}}_\mathbf{2}$ and $2\nabla U^{\text{norm}}(\mathbf{x_1}) \cdot \dot{\mathbf{x}}_\mathbf{1}$, whose sum integrates to

$$2\left[U^{\text{norm}}(\mathbf{x_2}) - U^{\text{norm}}(\mathbf{x_1})\right]$$

So our inequality reads

$$0 \leq 2\left[U^{\text{norm}}(\mathbf{x_2}) - U^{\text{norm}}(\mathbf{x_1})\right] + I(T)$$

where $I(T)$ is the rest of the integral, which depends on T. If we take T to be very small, the integral contribution will become small, so it needs to be true that

$$U^{\text{norm}}(\mathbf{x_2}) - U^{\text{norm}}(\mathbf{x_1}) \geq 0$$

which is exactly what we wanted to show. Hence, U^{norm} is a local landscape in the small noise limit (and its validity does not depend on the choice of base point, as our calculations here show).

3.4 Jin Wang's potential landscape

Consider a single species chemical system governed by Langevin/Fokker-Planck stochastic dynamics, with a state space $X = \mathbb{R}_{\geq 0}$. Define $\phi(x) := -\log P_{ss}(x)$ for all $x \in X$. Let's check that, given our definitions above, this is really a landscape.

Let $x \in X$. Since $0 \leq P_{ss}(x) \leq 1$, $-\log(2) \leq -\log P_{ss}(x) \leq \infty$, so our function is bounded below. (Also, we note here that it is all right if our landscape takes values of infinity. The proper thing to do, though, would be to not include impossible states as part of your state space.)

Do the minima of ϕ correspond to the system's attractors? I am pretty sure that this is true, although I am not sure how to prove it in general. For a 1D system with additive noise, the proof is simple.

The Fokker-Planck equation reads

$$0 = -\frac{d}{dx}\left[f(x)P_{ss}(x)\right] + \frac{\sigma^2}{2}P''_{ss}(x)$$

and it can be integrated to find

$$C = f(x)P_{ss}(x) - \frac{\sigma^2}{2}P'_{ss}(x)$$

where it must be that $C = 0$ since $P_{ss}(x) \to 0$ and $P'_{ss}(x) \to 0$ as $x \to \infty$. Hence,

$$f(x)P_{ss}(x) = \frac{\sigma^2}{2}P'_{ss}(x)$$

For each $y \in X$ such that $f(y) = 0$, this equation tells us that $P'_{ss}(y) = 0$. If y corresponds to an attractor (meaning that $f(y + \epsilon) < 0$ and $f(y - \epsilon) > 0$), this relationship also tells us that $P'_{ss}(y+\epsilon) < 0$ and $P'_{ss}(y-\epsilon) > 0$. This means:

$$\begin{aligned} \phi(y) &= 0 \\ \phi(y+\epsilon) &> 0 \\ \phi(y-\epsilon) &< 0 \end{aligned}$$

i.e. y is a local minimum for ϕ, as desired. Hence, ϕ is definitely a landscape (at least in this case).

3.4.1 Showing ϕ is a global landscape

This is almost trivial given our definition. Let $x_1, x_2 \in X$, and suppose that $P_{ss}(x_1) \geq P_{ss}(x_2)$. Easily, we see that

$$\begin{aligned} & \log P_{ss}(x_1) \geq \log P_{ss}(x_2) \\ \implies & -\log P_{ss}(x_1) \leq -\log P_{ss}(x_2) \end{aligned}$$

i.e. $\phi(x_1) \leq \phi(x_2)$. Incidentally, defining ϕ via as the logarithm of P_{ss} is not particularly special; any monotonic function of P_{ss} will do.

3.4.2 Showing ϕ is a local landscape in the small additive noise limit

ϕ is clearly the archetypal global landscape. Is it a local landscape? The answer, of course, is *no* in general; however, the answer (surprisingly, perhaps) turns out to be *yes* in the small additive noise limit.

In the small additive noise limit, as we showed in the previous example,

$$P_{ss}(x) = \exp\left(-U^{\text{norm}}/(\sigma^2/2)\right)$$

Hence,

$$\phi(x) = -\log P_{ss}(x) = U^{\text{norm}}/(\sigma^2/2)$$

so that U^{norm} is just a rescaling of ϕ. Since U^{norm} is a local landscape in this limit, ϕ must also be a local landscape.

3.5 Freidlin-Wentzell/Stochastic path integral local quasipotential