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Large deviations in noise-perturbed dynamical systems

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Contents

Introduction

- Dynamical system:

$$\dot{x}(t) = F(x(t)) \tag{1}$$

- Random perturbation or disturbance (noise):

$$\dot{x}(t) = \underbrace{F(x(t))}_{\text{deterministic}} + \underbrace{\varepsilon\xi(t)}_{\text{noise}} \qquad \varepsilon \ll 1 \tag{2}$$

- **Questions:**
    - How is the noise affecting the dynamics?
    - What is the probability to go away from an attractor?
    - What is the probability of reaching a point y from a point x?
    - What is the most probable way to reach a point away from an attractor?
    - What is the most probable trajectory going from x to y?
- Applications:
    - Physics: Noise-perturbed systems, diffusion, microscopic transport, nucleation, hydrodynamic fluctuation theory, etc.
    - Chemistry: Stability of chemical reactions, spontaneous transformations;
    - Engineering: Stability of structures, control under noisy conditions, queueing theory, etc.
    - Biology: Molecular transport, molecular motors, chemical networks, etc.
    - Sources: [vK92], [Gar85], [Jac10].
- Plan:
    - Learn about dynamical systems (ODEs) and noisy dynamical systems (SDEs);
    - Study low-noise perturbations of dynamical systems (low-noise large deviation theory);
    - Compare properties of reversible and non-reversible systems.
    - Learn about climbing mountains and swimming rivers.
- Some historical sources:
    - Mathematics: Wiener (Wikipage), Freidlin and Wentzell [FW84].
    - Physics: Einstein [Ein56], Langevin (Wikipage) [LG97], Onsager and Machlup [OM53], Graham [Gra89], Zwanzig [Zwa01].

1. From ordinary to stochastic differential equations

1.1. Ordinary differential equations (ODEs)

- First-order ODE:

$$\dot{x}(t) = F(x,t) \tag{3}$$

  - Initial condition: $x(0) = x_0$
  - Force: $F(x,t)$
  - Homogeneous: $F(x,t) = F(x)$ (no explicit time dependence).
  - Non-homogeneous: $F(x,t)$

- Vector first-order ODE:

$$\dot{\mathbf{x}}(t) = \mathbf{F}(\mathbf{x},t), \qquad \mathbf{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \quad \mathbf{F} = \begin{pmatrix} F_1 \\ \vdots \\ F_n \end{pmatrix} \tag{4}$$

- **Remark:** Bold letters are not used thereafter for vectors; it will be clear from the context whether x is a vector or a scalar.

- **Example:** Newton's equation for the pendulum of length ℓ with friction:

$$\ddot{\theta} + \gamma\dot{\theta} + \frac{g}{\ell}\sin\theta = 0. \tag{5}$$

  Define $x_1 = \theta$ and $x_2 = \dot{\theta}$. Then

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -\gamma x_2 - \frac{g}{\ell}\sin x_1. \end{aligned} \tag{6}$$

- ***Example:** Driven pendulum:

$$\ddot{\theta} + \gamma\dot{\theta} + \frac{g}{\ell}\sin\theta = A(t). \tag{7}$$

  Define $x_1 = \theta$, $x_2 = \dot{\theta}$, and $x_3 = t$. Then

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -\gamma x_2 - \frac{g}{\ell}\sin x_1 + A(x_3) \\ \dot{x}_3 &= 1. \end{aligned} \tag{8}$$

- **Remarks:**
  - An nth order ODE can be written as an n-component first-order ODE.
  - An n-component first-order non-homogeneous ODE can be written as a $(n+1)$-component ODE using $x_{n+1} = t$ so that $\dot{x}_{n+1} = 1$.

- **Example:** Linear ODE:
$$\dot{x} = Ax. \tag{9}$$
General solution:
$$x(t) = x(0)e^{At}. \tag{10}$$
Express the initial condition $x(0)$ in the eigenbasis $\{\lambda_i, v_i\}$ of A:
$$x(0) = \sum_i a_i v_i. \tag{11}$$
Then
$$x(t) = \sum_i a_i e^{\lambda_i t} v_i. \tag{12}$$
Classification of solutions (assuming $a_i > 0$ for all i):
  - Exponentially decaying: $\mathrm{Re}\,\lambda_i < 0$
  - Exponentially exploding: $\mathrm{Re}\,\lambda_i > 0$
  - Pure oscillations: $\mathrm{Re}\,\lambda_i = 0$ but $\mathrm{Im}\,\lambda_i \neq 0$.
- Potential ODE:
$$\dot{x}(t) = -\nabla U(x(t)) \tag{13}$$
  - Potential function: $U(x)$
  - Gradient descending dynamics:
$$\dot{V}(t) = -\nabla U(x(t))^2 \leq 0 \tag{14}$$
  - $\dot{x} = 0$ on critical points of U (minima, maxima, saddles) defined by $\nabla U(x) = 0$.
- Fixed (equilibrium) points: x^* such that $F(x^*) = 0$.
  - Asymptotically stable: $x(t) \to x^*$ as $t \to \infty$
  - Locally stable: $x(t) \to x^*$ for $x(t) = x^* + \delta x$
  - Locally unstable: $x(t) \not\to x^*$ for $x(t) = x^* + \delta x$.
- Linear stability around fixed point x^*:
$$\dot{x} = F(x) = J(x^*)(x - x^*) + O(|x - x^*|^2) \tag{15}$$
  - Jacobian matrix:
$$J(x^*)_{ij} = \frac{\partial F_i}{\partial x_j} \tag{16}$$
  - Stability determined as for linear systems above.
- Euler scheme:
$$x(t + \Delta t) = x(t) + F(x(t), t)\Delta t \tag{17}$$
with $x(0) = x_0$. The force can be evaluated at any other point $x(t')$, $t' \in [t, t + \Delta t]$ if F is continuous.

1.2. Stochastic differential equations (SDEs)

- Noisy ODE:

$$\dot{x}(t) = \underbrace{F(x(t))}_{\text{deterministic}} + \underbrace{\xi(t)}_{\text{noise}} \tag{18}$$

- Gaussian random walk:

$$S_n = \sum_{i=1}^{n} X_i, \qquad X_i \sim \mathcal{N}(0, \sigma^2) \text{ iid.} \tag{19}$$

Then

$$\langle S_n \rangle = 0 \tag{20}$$

$$\text{var}(S_n) = \langle (S_n - \langle S_n \rangle)^2 \rangle = n\sigma^2. \tag{21}$$

- **Brownian motion (BM):** Partition the time interval $[0, t]$ into $n = t/\Delta t$ sub-intervals of size Δt. Assign a Gaussian increment

$$\Delta W(i\Delta t) \sim \mathcal{N}(0, \Delta t) \tag{22}$$

to each sub-interval $i = 1, \ldots, n$ and define

$$W(t) = \lim_{n\to\infty} \sum_{i=1}^{n} \Delta W(i\Delta t). \tag{23}$$

Properties:

  - Initial value: $W(0) = 0$
  - Mean: $\langle W(t) \rangle = 0$ for all t
  - Variance: var $W(t) = t$
  - Independent increments:

$$dW(t) = W(t + dt) - W(t) \sim \mathcal{N}(0, dt) \tag{24}$$

  are independent Gaussian random variables.

  - Integral of increments:

$$W(t) = \int_0^t dW(t). \tag{25}$$

  This gives meaning to (23) above.

- Gaussian white noise: Formally,

$$\xi(t) = \frac{dW(t)}{dt}. \tag{26}$$

The problem is that $W(t)$ is not differentiable for any t. Hence the derivative above does not make sense, but the increments

$$dW(t) = \xi(t)dt \tag{27}$$

do; see properties above.

- **SDE:**

$$dX(t) = F(X(t), t)dt + \sigma(X_t, t)dW(t) \tag{28}$$

In mathematics, the time variable is usually put as a subscript:

$$dX_t = F(X_t, t)dt + \sigma(X_t, t)dW_t \tag{29}$$

  - Force: $F(x, t)$
  - Diffusion coefficient: $\sigma(x, t)$
  - X_t is also called a **diffusion**.

- Euler-Maruyama scheme:

$$X_{t+\Delta t} = X_t + F(X_t, t)\Delta t + \sigma(X_t, t)\Delta W_t, \tag{30}$$

where $\Delta W_t \sim \mathcal{N}(0, \Delta t) = \sqrt{\Delta t}\,\mathcal{N}(0, 1)$.

- Vector SDE:

$$d\mathbf{X}_t = \mathbf{F}(\mathbf{X}, t)dt + \sigma(\mathbf{X}_t, t)d\mathbf{W}_t, \tag{31}$$

where

$$\mathbf{X} = \begin{pmatrix} X_1 \\ \vdots \\ X_n \end{pmatrix}, \quad \mathbf{F} = \begin{pmatrix} F_1 \\ \vdots \\ F_n \end{pmatrix}, \quad \mathbf{W} = \begin{pmatrix} W_1 \\ \vdots \\ W_n \end{pmatrix}. \tag{32}$$

The W_i's are independent BMs. σ is an $n \times n$ diffusion matrix.

- **Remark:** F and σ are mostly assumed here time-independent (homogeneous). For simplicity, we will also often assume σ constant.

- **Example:** Langevin equation or Ornstein-Uhlenbeck (OU) process:

$$dX_t = -\gamma X_t dt + \sigma dW_t, \quad X_t \in \mathbb{R}. \tag{33}$$

Linear, gradient system with $U(x) = \gamma x^2/2$.

- SDE convention:

  - Itō or left-point rule:

$$X_{t+dt} = X_t + F(X_t)dt + \sigma(X_t)dW_t \tag{34}$$

  - *Stratonovich or mid-point rule:

$$X_{t+dt} = X_t + F(\bar{X}_t)dt + \sigma(\bar{X}_t)dW_t, \qquad \bar{X}_t = \frac{X_t + X_{t+dt}}{2} \tag{35}$$

  - ***Remark:** Each convention defines a Markov process to which are associated special calculus rules. For example, in the Itō convention,

$$df(X_t) = f'(X_t)dX_t + \frac{\sigma^2}{2} f''(X_t)dt \tag{36}$$

    for σ constant, whereas in the Stratonovich convention,

$$df(X_t) = f'(X_t)dX_t. \tag{37}$$

    Thus Itō leads to a modified chain rule of calculus, which is part of Itō's stochastic calculus, whereas Stratonovich retains the normal chain rule of calculus. The different calculus rules come from the fact that $W(t)$ is non-differentiable.

- Propagator:
$$P(x,t|x_0,0) = P(X_t = x|X_0 = x_0). \tag{38}$$
Also written as $P_t(x_0, x)$ for a homogeneous process in the mathematical literature.
- Fokker-Planck equation:
$$\frac{\partial}{\partial t}P(x,t|x_0,0) = -\frac{\partial}{\partial x}F(x)P(x,t|x_0,0) + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}P(x,t|x_0,0) \tag{39}$$
  - Linear partial differential equation
  - Operator form:
$$\frac{\partial}{\partial t}P(x,t|x_0,0) = L^\dagger P(x,t|x_0,0) \tag{40}$$
  - Fokker-Planck operator:
$$L^\dagger = -\frac{\partial}{\partial x}F(x) + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2} \tag{41}$$
  - Current form in $\mathbb{R}^d$:
$$\frac{\partial P}{\partial t} + \nabla \cdot J = 0 \tag{42}$$
  - Fokker-Planck current:
$$J = FP - \frac{D}{2}\nabla P, \qquad D = \sigma\sigma^T \tag{43}$$
- Marginal distribution: $P(x,t) = P(X_t = x)$
- **Remark:** $P(x,t) = P(x,t|x_0,0)$ for the initial condition $P(x,0) = \delta(x - x_0)$.
- Stationary distribution:
$$\frac{\partial}{\partial t}P^*(x) = L^\dagger P^*(x) = 0 \tag{44}$$
- Ergodic systems:
$$\lim_{t\to\infty} P(x,t) = P^*(x) \tag{45}$$
for all initial condition.
- *Evolution of observables:
$$\frac{\partial}{\partial t}\langle f(X_t)\rangle = \langle Lf(X_t)\rangle \tag{46}$$
  - Generator:
$$L = F(x)\frac{\partial}{\partial x} + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2} \tag{47}$$
  - Adjoint generator: $L = (L^\dagger)^\dagger$ in the sense of integration by parts; see Exercise 11.
- Infinitesimal propagator:
$$P(y, t + dt|x,t) = P(X_{t+dt} = y|X_t = x) = P_{dt}(x,y) \tag{48}$$

- **Example:** Infinitesimal propagator for BM: From (23),

$$\begin{aligned}P_{dt}(w'|w) &= P(W_{t+dt}=w'|W_t=w)\\ &= \frac{1}{\sqrt{2\pi dt}}e^{-(w'-w)^2/(2dt)}\\ &= \frac{1}{\sqrt{2\pi dt}}e^{-dw^2/(2dt)}\\ &= \frac{1}{\sqrt{2\pi dt}}e^{-\dot{w}^2 dt/2}\end{aligned} \tag{49}$$

- **Example:** Infinitesimal propagator for general Itō SDE:

$$\begin{aligned}P_{dt}(x'|x) &= P(X_{t+dt}=x'|X_t=x)\\ &= \frac{1}{\sqrt{2\pi\sigma^2 dt}}e^{-[x'-x-F(x)dt]^2/(2\sigma^2 dt)}\\ &= \frac{1}{\sqrt{2\pi\sigma^2 dt}}e^{-[\dot{x}-F(x)]^2 dt/(2\sigma^2)}\end{aligned} \tag{50}$$

- **Remark:** The stationary behavior of an SDE is determined by its stationary distribution $P^*(x)$ and its stationary Fokker-Planck current. If a system has zero current (reversible system with gradient force, for example), then the stationary distribution $P^*(x)$ is sufficient.

1.3. Exercises

1. (Lyapunov stability) Prove the inequality in (14); that is, show that, for a gradient descent, $U(x(t))$ decreases or stays the same with time. Discuss the consequence of this result for the stability of $x(t)$.

2. (Normal system) Consider the linear systems $\dot{x} = Bx$. Show that $x(t) \to 0$ exponentially fast if (i) $[B, B^T] = 0$ (we then say that B is a normal matrix) and (ii) $B + B^T$ is negative definite. [Note: These are sufficient but non-necessary conditions for $x(t)$ to be asymptotically stable. Can you state necessary and sufficient conditions?]

3. (Van der Pol oscillator) Consider the nonlinear dynamical system defined by the 2nd-order ODE

$$\ddot{x} + \mu(x^2-1)\dot{x} + x = 0. \tag{51}$$

(a) Write this ODE as a vector system of two first-order ODEs.

(b) Solve this system for $\mu = -1$ using a Euler scheme or some ODE solver available, for example, in Matlab, Maple or Mathematica. Try different initial conditions. Plot a solution for a given initial condition as a function of time t. Then plot it as a phase space plot (i.e., $\dot{x}$ vs x). What is the fixed point or attractor of the system?

(c) Repeat Part (b) for $\mu = 1$.

4. (Time-delayed ODE) Obtain a numerical solution of the following ODE:

$$\dot{x}(t) = \sin\big(x(t-2\pi)\big) \tag{52}$$

for $t \in [0, 200]$ and $\{x(t)\}_{t=-2\pi}^{0} = 0.1$ as the initial (function) condition. Use Euler's scheme or the delayed ODE solver available in Matlab or Mathematica. Repeat for $\{x(t)\}_{t=-2\pi}^{0} = 0.11$ and display your two solutions on the same plot. Can you solve (52) by specifying only the initial point $x(0)$? [Note: $x(t-2\pi)$ is $x(t')$ evaluated at the time $t' = t - 2\pi$.]

5. **(Convergence of Euler scheme)** Consider the simple linear ODE

$$\dot{x}(t) = -x(t).$$

Implement Euler's scheme for this equation and study the convergence of this scheme with the integration time-step Δt by plotting on a log-log plot the maximum difference

$$\max_{t\in[0,T]} \left| x_{\text{euler}}(t) - x_{\text{exact}}(t) \right|$$

between Euler's solution and the exact solution $x_{\text{exact}}(t) = x(0)\, e^{-t}$ as a function of Δt. Use sensible values for T and Δt.

6. **(Brownian motion)** Prove all the properties of BM listed after (23). Show moreover that

$$\langle W(t)W(t')\rangle = \min\{t, t'\}, \tag{53}$$

and

$$\langle \xi(t)\xi(t')\rangle = \delta(t - t'), \tag{54}$$

where $\xi(t)$ is defined formally as in (27).

7. **(Langevin equation)** Consider the Langevin equation of (33).
   (a) Use the Euler-Maruyama scheme to obtain and plot a few sample paths of this SDE.
   (b) Derive the full propagator $P(x, t|x_0, 0)$ of this SDE analytically by solving the associated time-dependent Fokker-Planck equation (39). [Solution in [Gar85].]
   (c) Derive the stationary distribution of this SDE.

8. **(Infinitesimal propagator)** Derive the infinitesimal generator (50) in both the Itō and Stratonovich conventions.

9. **(Gradient SDE)** Prove that the stationary distribution of a gradient SDE,

$$dX_t = -\nabla U(X_t)dt + \sigma dW_t, \tag{55}$$

has the form

$$P(x) = C\, e^{-2U(x)/\sigma^2}, \tag{56}$$

where C is a normalization constant. What conditions on $U(x)$ must be imposed to have this solution?

10. **(Noisy Van der Pol oscillator)** Use the Euler-Maruyama scheme to simulate the following SDE:

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= -x + v(\alpha - x^2 - v^2) + \sqrt{\varepsilon}\, \xi(t). \end{aligned} \tag{57}$$

This system is slightly different from (51): the bifurcation is now at $\alpha = 0$.

11. **(Generator)** Show that the Fokker-Planck generator $L^\dagger$ of (41) is the adjoint of the generator L of (47) with respect to the following inner product:

$$\langle f, g\rangle = \int_{-\infty}^{\infty} f(x)g(x)\, dx. \tag{58}$$

[Hint: Use integration by parts.]

1.4. Further reading

- Bifurcations, limit cycles, chaos and applications of ODEs: [Str94].
- ODE solvers in Matlab and Mathematica.
- SDEs and Markov processes: [vK92], [Gar85], [Ris96], [Jac10].
- Stochastic calculus: [Gar85], [Jac10], [BZ99].
- Itō vs Stratonovich convention: [vK81], [Gar85].
- Numerical integration of SDEs: [Hig01].
- Non-white or colored noises: see Wikipage.

2. Low-noise large deviations of SDEs

2.1. Path distribution

- Noise-perturbed dynamical system (SDE):

$$dX_t = F(X_t)dt + \sqrt{\varepsilon}\,\sigma\, dW_t, \qquad X_t \in \mathbb{R} \tag{59}$$

- **Remark:** We will deal with one-dimensional SDEs throughout the lectures; the generalization to $\mathbb{R}^d$ is the subject of Exercise 6.

- Trajectory: $\{x(t)\}_{t=0}^T$

- Discrete-time (sampled) trajectory: $\{x_i\}_{i=1}^n$ with $x_i = x(i\Delta t)$ and $n = T/\Delta t$; see Fig. 1.

- Joint distribution:

$$P(x_0, x_1, \ldots, x_n) = P(x_0)\prod_{i=1}^{n-1} P_{\Delta t}(x_{i+1}|x_i) \tag{60}$$

- **Path distribution (or density):**

$$P[x] = P(\{X_t = x_t\}_{t=0}^T) = \lim_{\Delta t \to 0} P(x_0, \ldots, x_n) \tag{61}$$

- **Low-noise approximation:**

$$P[x] \asymp e^{-I[x]/\varepsilon} \tag{62}$$

- **Action:**

$$I[x] = \frac{1}{2\sigma^2}\int_0^T [\dot{x}(t) - F(x(t))]^2 dt \tag{63}$$

  - Also called the dynamical action or path rate function.
  - Non-negativity: $I[x] \geq 0$
  - Zero: $I[x] = 0$ iff $\dot{x} = F(x)$
  - Called the deterministic, noiseless, relaxation or natural path.

- **Large deviation principle (LDP):**

$$\lim_{\varepsilon \to 0} -\varepsilon \ln P[x] = I[x]. \tag{64}$$

  This limit gives meaning to the approximation (62).

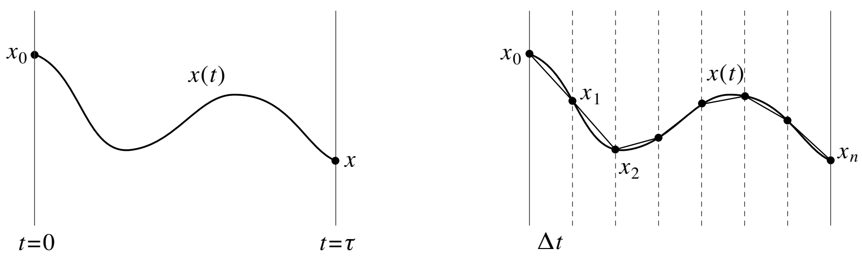


Figure 1: Sampled path.

- ***Remark:** The path density (61) does not exist rigorously speaking. Moreover, it is known that paths of SDEs driven by BM are non-differentiable everywhere, so the $\dot{x}$ in the action (63) seems dubious.

  The proper and rigorous interpretation of the LDP was given by Freidlin and Wentzell [FW84] and goes as follows:

$$\lim_{\delta\to 0}\lim_{\varepsilon\to 0} -\varepsilon \ln P\left\{\sup_{0\le t\le T}|X_t - x_t| < \delta\right\} = I[x]. \tag{65}$$

  This means that the probability of a family of paths $\{X_t\}_{t=0}^T$ of the SDE enclosed in a cylinder or tube of width δ around the deterministic and smooth path $\{x_t\}_{t=0}^T$ is given by $I[x]$ in the low-noise limit and the limit of smaller and smaller tube. Here there is no problem with $\dot{x}$ because $\{x_t\}_{t=0}^T$ is continuous – it is the path followed by the tube enclosing the random paths of the SDE considered. Sources: [Tou09, Sec. 6.1], [FW84].

2.2. Laplace's principle

- Laplace sums:

$$\lim_{n\to\infty}\frac{1}{n}\ln\sum_i e^{na_i} = \max_i a_i \tag{66}$$

- Asymptotic notation:

$$\sum_i e^{na_i} \asymp e^{n\max_i a_i} \tag{67}$$

  Also called the principle of largest term.

- Laplace integrals:

$$\lim_{n\to\infty}\frac{1}{n}\ln\int_\Omega e^{nf(x)}dx = \max_{x\in\Omega} f(x) \tag{68}$$

- Asymptotic notation:

$$\int_\Omega e^{nf(a)}dx \asymp e^{\max_{x\in\Omega} f(x)} \tag{69}$$

  Also called the Laplace or saddle-point approximation.

2.3. Propagator large deviations

- Path LDP:

$$P[x] \asymp e^{-I[x]/\varepsilon} \tag{70}$$

- Path integral representation of the propagator:

$$P(x,t|x_0,0) = \int_{x(0)=x_0}^{x(t)=x}\mathcal{D}[x]\,P[x] \tag{71}$$

- Laplace principle:

$$\begin{aligned} P(x,t|x_0,0) &= \int_{x(0)=x_0}^{x(t)=x}\mathcal{D}[x]\,P[x] \\ &\asymp \int_{x(0)=x_0}^{x(t)=x}\mathcal{D}[x]\,e^{-I[x]/\varepsilon} \\ &\asymp e^{-I[x^*]/\varepsilon} \end{aligned} \tag{72}$$

    - Also called a WKB or semi-classical approximation.
    - Contraction principle: general derivation of an LDP from an LDP (here from I to V).

- **Propagator LDP:**
$$P(x,t|x_0,0) \asymp e^{-V(x,t|x_0,0)/\varepsilon} \tag{73}$$

- **Quasi-potential:**
$$V(x,t|x_0,0) = \inf_{x(t):x(0)=x_0,x(t)=x} I[x] \tag{74}$$

    - Also called the pseudo or **quasi-potential** or simply the rate function.
    - Non-negativity: $V(x,t|x_0,0) \geq 0$

- **Instanton:**
$$\begin{aligned} x^*(t) &= \arg \inf_{x(t):x(0)=x_0,x(t)=x} I[x] \\ V(x,t|x_0,0) &= I[x^*] \end{aligned} \tag{75}$$

    - Also called the **minimum action** or **most probable path**.
    - Most likely path among all (exponentially) unlikely fluctuation paths from x_0 to x.
    - Determines the propagator in the low-noise limit.
    - There may be more than one instanton (more than one solution of the variational problem defining the quasi-potential).

- **Euler-Lagrange (EL) equation:** $x^*(t)$ is an optimizer of $I[x]$ so that
$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0, \qquad x(0) = x_0, \quad x(t) = x \tag{76}$$

    - Action density or Lagrangian:
$$L(x,\dot{x}) = \frac{1}{2\sigma^2}(\dot{x} - F(x))^2 \tag{77}$$

    - Explicit EL equation:
$$\ddot{x} - F(x)F'(x) = 0, \qquad x(0) = x_0, \quad x(t) = x. \tag{78}$$

    This is a second-order ODE with two boundary conditions.

- **Hamilton's equations:** To any Lagrangian dynamics can be associated an equivalent Hamiltonian dynamics.

    - Hamiltonian:
$$H(x,p) = p \cdot \dot{x}_p - L(\dot{x}_p, x), \qquad p = \frac{\partial L}{\partial \dot{x}_p} \tag{79}$$

    - Conjugate momentum:
$$p = \frac{\partial L}{\partial \dot{x}} = \dot{x} - F \tag{80}$$

    - Explicit Hamiltonian:
$$H(x,p) = \frac{p^2}{2} + pF(x) \tag{81}$$

- ◦ Hamilton's equations:

$$\dot{x} = \frac{\partial H}{\partial p} = p + F(x)$$
$$\dot{p} = -\frac{\partial H}{\partial x} = -pF'(x) \tag{82}$$

  - $*$ Two first-order ODEs.
  - $*$ Energy is conserved: $\dot{H} = 0$

- ◦ Quasi-potential:

$$V(x, t|x_0, 0) = I[x^*] = \int_0^t L(x^*, \dot{x}^*)dt = \int_{x_0}^x p^* dx^*, \tag{83}$$

  where p^* is the instanton momentum.

- **Remark:** The Lagrangian and Hamiltonian equations are only auxiliary dynamics for finding the instanton; the real dynamics is the SDE.

- *Hamilton-Jacobi equation:

$$\frac{\partial V}{\partial t} + H\left(x, \frac{\partial V}{\partial x}\right) = 0, \tag{84}$$

  where $V = V(x, t|x_0, 0)$.

- *Bellman's optimality principle:

$$V(x, t|x_0, 0) = \inf_{x'}\{V(x, t|x', s) + V(x', s|x_0, 0)\} \tag{85}$$

  for any intermediate times $s \in [0, t]$.

- **Example:** The Lagrangian of the Langevin equation (33) with $\sigma = 1$ is

$$L = \frac{1}{2}(\dot{x} + \gamma x)^2 \tag{86}$$

  and leads to the EL equation

$$\ddot{x} - \gamma^2 x = 0. \tag{87}$$

  The Hamiltonian is

$$H = \frac{p^2}{2} - \gamma p x \tag{88}$$

  and leads instead to

$$\dot{x} = p - \gamma x, \qquad \dot{p} = \gamma p x. \tag{89}$$

2.4. Stationary large deviations

- **Remark:** Assume that the ODE $\dot{x} = F(x)$ has a unique attractor located, without loss of generality, at $x = 0$. We can always translate the attractor at 0 if need be. The case of many attractors will not be treated in the lectures; see further reading.

- **Stationary LDP:**

$$P(x) \asymp e^{-V(x)/\varepsilon} \tag{90}$$

- **Quasi-potential:**
$$V(x) = \inf_{x(t):x(-\infty)=0,x(0)=x} I[x] \tag{91}$$
- **Instanton:**
$$x^*(t) = \arg \inf_{x(t):x(-\infty)=0,x(0)=x} I[x] \tag{92}$$
- **Remarks:**
  - The terminal conditions $x(-\infty) = 0$ and $x(0) = x$ arise because we want the stationary distribution in the long-time limit. Thus, we should choose $x(0)$ on the attractor (here assumed to be $x = 0$) and $x(\infty) = x$. By time-translation invariance of the Lagrangian (or action), this is equivalent to $x(-\infty) = 0$ and $x(0) = x$.
  - *In the infinite time limit, it does not matter whether you start at the attractor or not: from any initial condition, the system will go to the attractor in finite time with zero action. Consequently, the initial condition $x(-\infty) = 0$ above can be changed to $x(-\infty) =$ anywhere.
  - *It can be proved more generally that
$$V(x) = \inf_{t>0} \inf_{x(0)=0,x(t)=x} I[x]. \tag{93}$$
    Thus, a priori, the stationary quasi-potential is found by minimizing over all paths going from the attractor to the point x of interest after a time t. However, in many cases (all cases known to me) the minimization selects only those paths that achieve this in infinite time.
- Euler-Lagrange equation: Same as (76) but with terminal conditions $x(-\infty) = 0$, $x(0) = x$.
- Hamilton's equations: Same as (82) but with correct terminal conditions.
- Hamilton-Jacobi equation:
$$H(x, V'(x)) = 0. \tag{94}$$
  Explicitly:
$$FV' + \frac{\sigma^2}{2} V'^2 = 0. \tag{95}$$
- General properties of the quasi-potential:
  - $V(x) \geq 0$ with equality iff $x = 0$ (more generally, for x on the attractor).
  - $V(x)$ is continuous but not necessarily differentiable; see Exercise 9 of Sec. 3.4.
- General properties of the instanton $x^*(t)$:
  - $H(x^*, p^*) = 0$ but $p^* \neq 0$.
  - Line integral:
$$V(x) = \int_0^x p^* \cdot dx^*. \tag{96}$$
    Note that time is absent from this representation.
  - Interpretation: The system naturally stays at the attractor; it needs noise to be pushed away from it. The quasi-potential is the optimal "push" cost needed to reach x; the instanton is the optimal path to get there.

2.5. *Escape problem

- Kramers escape:
  - Thermal system at inverse temperature β.
  - Reaction coordinate or macrostate: x
  - Free energy: $F(x)$
  - Canonical distribution:
$$P_\beta(x) = \frac{e^{-\beta F(x)}}{Z(\beta)} \tag{97}$$
  - What is the probability of escape from a metastable state to a stable state as $\beta \to \infty$ ($T \to 0$)? See Fig. 2 left.
- General escape problem (Fig. 2 right):
  - Domain around an attractor: D
  - Boundary ∂D
  - Escape time: $\tau_\varepsilon = \inf\{t : X_t \in \partial D\}$
- Large deviation estimate:
$$\lim_{\varepsilon \to 0} P\left(e^{(V^*-\delta)/\varepsilon} < \tau_\varepsilon < e^{(V^*+\delta)/\varepsilon}\right) = 1 \tag{98}$$
  for any $\delta > 0$.
  - Interpretation: $\tau_\varepsilon \asymp e^{V^*/\varepsilon}$ with probability 1 as $\varepsilon \to 0$.
  - Escape quasi-potential:
$$V^* = \inf_{x \in \partial D} \inf_{t>0} V(x, t|x_0, 0) \tag{99}$$
  - Escape instanton: Instanton reaching the boundary ∂D.
- **Example:** For Kramers's problem, $V^* = \Delta F$, the potential height. (Arrhenius law).

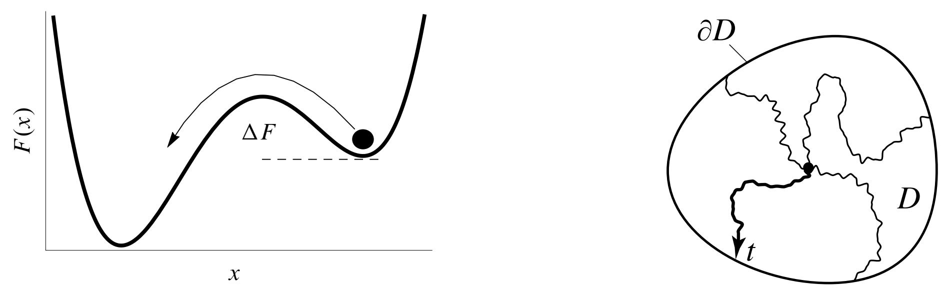


Figure 2: Left: Kramers's escape problem. Right: General escape problem.

2.6. Exercises

1. (Laplace principle) Prove the Laplace principle for general sums, as in (66), and for general integrals, in as in (68). Do you need any conditions on these for approximations to be valid?

2. (Action) Re-do the calculation of Sec. 2.1 leading to the expression of the path distribution $P[x]$ and action $I[x]$. Do the calculation using first the Itō convention and then the Stratonovich convention. Are there any differences between the two conventions?

3. (Hamilton equations) Show that the Hamiltonian H is conserved under Hamilton's equations (82). Then show that that $H(x^*, p^*) = 0$ for the stationary instanton. Can you find another path with zero energy? What differentiates this path from the instanton?

4. (Langevin equation) Find the instanton for the quasi-potential $V(x, t|x_0, 0)$ of the Langevin equation. Repeat for the stationary quasi-potential $V(x)$. Verify in both cases that the quasi-potentials satisfy their corresponding Hamilton-Jacobi equations. Finally, compare the instantons with the decay paths obtained by solving the corresponding noiseless ODE with the terminal conditions reversed. Do you see any relation between the natural paths and the instantons?

5. (Quadratic well) Consider the vector SDE in $\mathbb{R}^2$ with $\mathbf{F} = -\nabla U$ and

$$U(x, y) = \frac{x^2 + y^2}{2}. \tag{100}$$

Show that the natural decay path of this system satisfies the ODE $\dot{r} = -r$. Then find the equation of the stationary instanton as well as the associated quasi-potential $V(x, y)$ or $V(r, \theta)$. Do you see any relation between the decay path and instanton? Can you write the action $I[\mathbf{x}]$ in a simple form in polar coordinates?

6. (Vector SDEs) Derive the action $I[\mathbf{x}]$ for a set of n coupled SDEs or, equivalently, for an SDE taking values in $\mathbb{R}^d$. Do you need any conditions on the diffusion matrix to derive the action?

7. (Linear stream) Find the stationary quasi-potential $V(x, y)$ for the 2D system

$$\dot{\mathbf{x}} = B\mathbf{x} + \boldsymbol{\xi} \tag{101}$$

with

$$B = \begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}, \tag{102}$$

$\mathbf{x} = (x \;\; y)^T$, and $\boldsymbol{\xi} = (\xi_x \;\; \xi_y)^T$ a vector of independent Gaussian white noises. Note that this a normal system in the sense of Exercise 2 of Sec. 1.3. Is this SDE gradient? Source: [FW84, Sec. 4.4, p. 123].

8. (Noisy Van der Pol oscillator) Find the quasi-potential $V(x, v)$ of the noisy Van der Pol oscillator (57). [Hint: Use polar coordinates.]

9. ***(WKB approximations)** Consider the following ansatz for the propagator:

$$P(x, t|x_0, 0) = e^{-a/\varepsilon + b + c\varepsilon + d\varepsilon^2 + \cdots}. \tag{103}$$

(a) Use this ansatz in the Fokker-Planck equation (39) to derive the Hamilton-Jacobi equation (84).

(b) Repeat for the stationary distribution to arrive at the Hamilton-Jacobi equation (95).

10. *(**Bellman's principle**) Write Bellman's optimality principle (85) for $s = t - \Delta t$ and derive from the resulting expression the Hamilton-Jacobi equation (84). Source: [DZ98, Ex. 5.7.36, p. 237].

11. *(**Numerical instantons**) Solve numerically the Euler-Lagrange equation for the Langevin equation to obtain $V(x, t|x_0, 0)$ and $V(x)$. Repeat for Hamilton's equations. Is there any way these equations can be used to avoid numerical instabilities?

2.7. Further reading

- Laplace principle and Laplace integrals: Chap. 6 of [BO78].
- First work on fluctuation paths (Onsager and Machlup): [OM53].
- Low-noise large deviations: Sec. 6.1 of [Tou09], [Gra89], Chap. 4 of [FW84] (for the mathematically minded), [LMD98].
- Other large deviation limits and large deviation theory: [Ell95], [DZ98], [Tou09].
- Escape problem: [Kra40], [HTB90], [Mel91], [Gar85].
- Applications: [LMD98].
- Numerical methods for finding instantons: [ERVE02], [Cam12].
- Bellman's optimality principle and dynamic programming: [Bel54], Wikipage, [FS06].

3. Reversible versus non-reversible systems

3.1. Gradient systems

- SDE:

$$dX_t = -\nabla U(X_t)dt + \sqrt{\varepsilon}\,\sigma\, dW_t, \qquad X_t \in \mathbb{R}^d \tag{104}$$

  - Potential: $U(x)$
  - Diffusion matrix: $D = \sigma\sigma^T$.
  - Assumptions:
    1. $U(x)$ has a unique attractor at $x = 0$ corresponding to a unique minimum of $U(x)$.
    2. D is constant and proportional to the identity matrix.
    3. $U(x)$ is such that the stationary distribution exists and is unique (ergodic systems).

- **Stationary LDP:**

$$P(x) \asymp e^{-V(x)/\varepsilon} \tag{105}$$

- **Quasi-potential:** $V(x) = 2U(x)$

Proof 1 (Direct minimization). Assume $D = \mathbb{1}$ without loss of generality. Then for any path $\{x_t\}_{t=0}^T$ we have

$$\begin{aligned} I[x] &= \frac{1}{2}\int_0^T |\dot{x} + \nabla U|^2 dt \\ &= \frac{1}{2}\int_0^T |\dot{x} - \nabla U|^2 dt + 2\int_0^T \dot{x}\cdot\nabla U\, dt \\ &= \frac{1}{2}\int_0^T |\dot{x} - \nabla U|^2 dt + 2\int_0^T \nabla U \cdot dx \\ &\geq 2[U(x_T) - U(x_0)]. \end{aligned} \tag{106}$$

Thus $I[x] \geq 2U(x)$ if $x_0 = 0$ and ends at $x_T = x$. The minimum is achieved for $\dot{x} = \nabla U$ which links these two points in infinite time. □

- Remark: For finite time $I[x] > 2U(x)$, which means that $V(x, t|0, 0) > V(x)$.

Proof 2 (Hamilton's equations). The instanton is such that $H = 0$ and $p \neq 0$. This implies $p = 2\nabla U$ from (81), so that, from (96),

$$V(x) = \int_0^x p^* \cdot dx^* = 2\int_0^x \nabla U \cdot dx = 2U(x). \tag{107}$$

□

- **Natural dynamics or decay path:**

$$\dot{x}_{\text{decay}} = -\nabla U(x_{\text{decay}}), \qquad x_{\text{decay}}(0) = x \tag{108}$$

  - Pure, dissipative hill-descent dynamics.
  - First-order ODE.

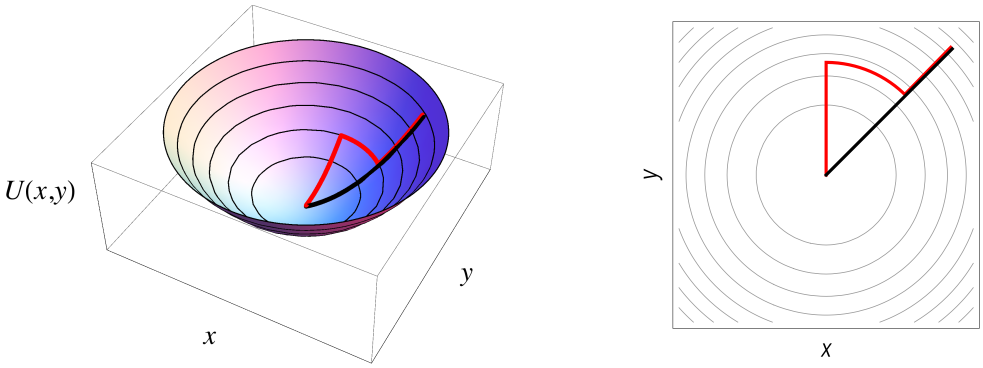


Figure 3: Two instantons for the quadratic well. Black: Smooth instanton solving the Euler-Lagrange equation. Red: Continuous, piecewise smooth instanton.

- **Instanton or adjoint dynamics:**

$$\dot{x}^* = \nabla U(x^*), \qquad x^*(0) = 0 \tag{109}$$

  - Follows from the first Hamilton's equations.
  - Pure hill climber: the dissipation of the hill descent is reversed.
  - First-order ODE (compare with the EL equation which is second-order).
  - **Time-reversal of decay path:**

$$x^*(t) = x_{\text{decay}}(-t), \quad t \in (-\infty, 0] \tag{110}$$

  - Reversible system: satisfies detailed balance.
  - Related to the Kolmogorov loop law: see Exercise 10.
  - Adjoint force:

$$\dot{x} = F_A(x), \qquad F_A = -F. \tag{111}$$

- **Remark:** SDEs on $\mathbb{R}$ are gradient: forces $F(x)$ on $\mathbb{R}$ can always be written as the derivative of a potential, $F(x) = -U'(x)$. Periodic SDEs on the circle are not always gradient; see Exercise 9.

- **Example:** Langevin equation: see Exercise 4 of Sec. 2.6.

- **Example:** Quadratic well in $\mathbb{R}^2$: see Exercise 5 of Sec. 2.6. We have seen in that exercise that the instanton satisfies the ODE $\dot{r} = r$. However, this is not the only instanton minimizing the action in the infinite-time limit: Fig. 3 shows another one, which is continuous but not C^1. The smooth instanton is the one given by the adjoint dynamics.

3.2. Transversal systems

- SDE:

$$dX_t = -\nabla U(x)dt + R(x)dt + \sqrt{\varepsilon}\,\sigma\, dW_t \tag{112}$$

  - Force: $F(x) = -\nabla U(x) + R(x)$
  - Transversal condition: $\nabla U(x) \cdot R = 0$

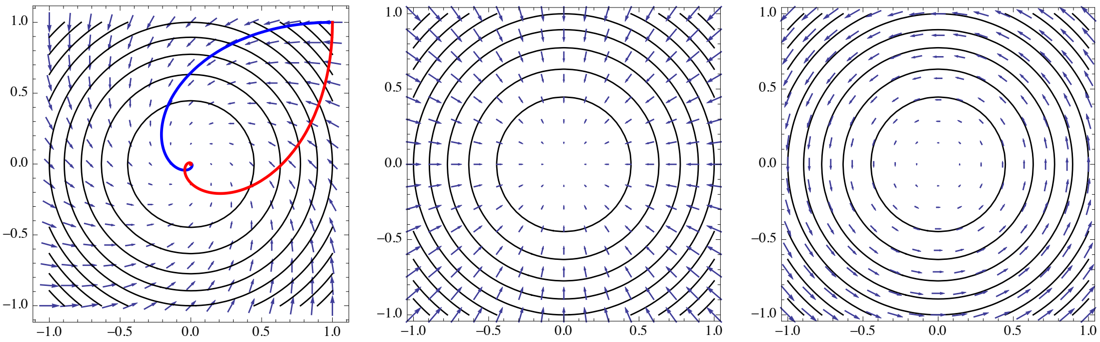


Figure 4: Linear transversal system. Left: Natural decay path (blue) and instanton (red) superimposed on the vector plot of total force. Middle: Vector plot of the dissipative force. Right: Vector plot of the stream force. The black lines in the plots are equi-potentials of the quasi-potential $V(x, y)$.

  - G force is orthogonal to the gradient descent force $-\nabla U$.

- **Stationary LDP:**

$$P(x) \asymp e^{-V(x)/\varepsilon} \tag{113}$$

- **Quasi-potential:** $V(x) = 2U(x)$

  - Same result as gradient case, yet the force is different. R plays no role in the quasi-potential.
  - Proof: Follow the direct minimization of the gradient case, but include now the R component. Then use the transversality condition to arrive at the same bound. See Exercise 4.

- Natural dynamics:

$$\dot{x} = -\nabla U(x) + R(x) \tag{114}$$

- **Instanton or adjoint dynamics:**

$$\dot{x} = \nabla U(x) + R(x) \tag{115}$$

  - Reverse the dissipation; keep the sign of R.
  - Adjoint force:

$$\dot{x} = F_A(x), \qquad F_A = F + D\nabla V. \tag{116}$$

  - Non-reversible system: the instanton dynamics is not the time-reverse of the decay path.
  - Related to the Kolmogorov loop law: see Exercise 10.
  - Proof: Substitute this dynamics in $I[x]$, use the transversality condition, and verify that the bound (106) is attained.

- **Example:** The linear stream of Exercise 7, Sec. 2.6, is transversal. Its dissipative and stream forces are shown in Fig. 4. The fact that the instanton is not the time reversal of the decay path is also shown there.

3.3. General systems

- SDE:

$$dX_t = F(X_t)dt + \sqrt{\varepsilon}\,\sigma\, dW_t, \qquad X_t \in \mathbb{R}^d \tag{117}$$

  - Force F is not necessarily gradient or transversal.
  - Still assume unique fixed point at $x = 0$.
  - Still assume D constant and proportional to the identity matrix. (Can be relaxed.)

- **Stationary LDP:** $P(x) \asymp e^{-V(x)/\varepsilon}$

- **Quasi-potential:**

$$V(x) = \inf_{x(t):x(-\infty)=0, x(0)=x} I[x] \tag{118}$$

- Fokker-Planck current:

$$J = FP - \frac{D}{2}\nabla P \tag{119}$$

- **Stream function:**

$$R = \lim_{\varepsilon\to 0} \frac{J}{P} = F + \frac{D}{2}\nabla V \tag{120}$$

- **Force decomposition:**

$$F = K + R \tag{121}$$

  - Dissipative force:

$$K = -\frac{D}{2}\nabla V \tag{122}$$

  - Stream force: R
  - Tranversality: $K \cdot R = 0$
  - **Interpretation:** The force F can be decomposed into a dissipative (purely gradient) force K, which completely determines V, and a stream force, orthogonal to K, which does not play any role in V. The orthogonality holds only if D is constant and proportional to the identity matrix. For more general systems, we have $\nabla V \cdot R = 0$ instead of $K \cdot R = 0$.

- Natural dynamics:

$$\dot{x} = F(x) = K(x) + R(x) \tag{123}$$

- **Instanton or adjoint dynamics:**

$$\dot{x} = -K(x) + R(x) \tag{124}$$

  - Reverse the sign of dissipation; keep the sign of the (rotation) stream.
  - Adjoint force:

$$\dot{x} = F_A(x), \qquad F_A = F + D\nabla V. \tag{125}$$

  - Cannot be defined a priori: we need $V(x)$ (and the instanton) to obtain K and R.
  - Non-reversible system: the instanton dynamics is not the time-reverse of the decay path. Equivalent to $R \neq 0$.
  - Related to the Kolmogorov loop law: see Exercise 10.
  - Proof: see Exercise 4.

- Remark: A gradient and non-gradient systems can have the same quasi-potential; they will differ in that $R = 0$ for the former while $R \neq 0$ for the latter.

3.4. Exercises

1. (Noisy Van der Pol oscillator) Consider again the noisy Van der Pol oscillator (Exercise 8, Sec. 2.6). Find the stream force of this system. Then find a different SDE having the same quasi-potential as this system, but with a null stream force, $K = 0$.

2. (Three well system) Consider the gradient SDE with potential

$$U(x, y) = 3e^{-x^2-(y-1/3)^2} - 3e^{-x^2-(y-5/3)^2} - 5e^{-(x-1)^2-y^2} - 5e^{-(x+1)^2-y^2} + \frac{x^4 + (y-1/3)^2}{5}. \quad (126)$$

Find all the critical points of this potential, including the two minima at $(\pm 1, 0)$ and the shallow minimum at $(0, 1.5)$. Determine whether the instanton connecting the two deep minima goes via the shallow minimum or via the saddle-point between them. Source: [MSVE06].

3. (Time reversibility) Show for a gradient system that the instanton is the time reversal of the natural decay path.

4. (Transversal systems) Prove that $V = 2U$ for transversal systems using the WKB approximation of Exercise 9 of Sec. 2.6 or the Hamilton-Jacobi equation. Then adapt your proof to cover the general systems described in Sec. 3.3.

5. (General diffusion) Re-derive all the results of this section for a general invertible diffusion matrix D. That is, do not assume, as done before, that D is constant or proportional to the identity matrix. What happens to the whole formalism if D is not invertible?

6. (State-dependent diffusion) Show that an SDE with gradient force $F = -\nabla U$ is not reversible in general if it has a state-dependent diffusion matrix $D(x)$. What can we say in general about the quasi-potential of such a system?

7. (Maier-Stein system [MS93]) Consider the 2D SDE

$$\begin{aligned} \dot{x} &= x - x^3 - \alpha x y^2 + \xi_x \\ \dot{y} &= -y - x^2 y + \xi_y, \end{aligned} \quad (127)$$

where ξ_x and ξ_y are two independent Gaussian white noises.

(a) Find and classify the fixed points (stable, unstable, saddles) of the noiseless system.

(b) Show that this system is gradient iff $\alpha = 1$. For this case, find the force potential U and the quasi-potential V. Analyze these functions in view of the fixed points found in (a).

8. (Maier-Stein-Graham system [Gra95]) Consider the following simplification of the system above:

$$\begin{aligned} \dot{x} &= x - x^3 + \xi_x \\ \dot{y} &= y - y^3 - 2x^2 y + \xi_y, \end{aligned} \quad (128)$$

in which the x motion is decoupled from the y motion.

(a) Find and classify the fixed points (stable, unstable, saddles) of the noiseless system.

(b) Is this system gradient?

(c) Find the quasi-potential $V(x, y)$ of the system, as well as the dissipative function $K(x, y)$ and stream function $R(x, y)$. The analyze these functions.

(d) Analyze the dynamics of the instantons for points inside and outside the strip $y^2 = 1$.

9. *(**Diffusion on the circle**) Consider the following diffusion on the circle (or ring):

$$d\theta_t = [\gamma - U'(\theta_t)]dt + dW_t, \qquad \theta_t \in [0, 2\pi), \tag{129}$$

where $U(\theta) = U_0 \cos\theta$, U_0 and γ are real numbers, and W_t is a normal BM. Simulate this SDE to understand the role of γ and U. Is this system gradient? Derive its stationary quasi-potential $V(\theta)$. Show that $V = 2U$ iff $\gamma = 0$. Source: [Gra95].

10. *(**Kolmogorov loop law**) Consider a path $\{x_t\}_{t=0}^T$ of a Markov system and the time-reversal $\{x^R\}_{t=0}^T$ of this path defined by

$$x^R(t) = x(T - t). \tag{130}$$

The Kolmogorov loop law or Kolmogorov criterion asserts that this system is reversible (in the sense of detailed balance) iff $P[x] = P[x^R]$ for all loop paths, that is, all paths ending at their starting point. Use this result to show that, for reversible systems, the instanton is the time reverse of the decay path. Then prove that, for non-reversible systems, the instanton cannot be the time reverse of the decay path.

11. *(**Potential function**) Consider a 'loop' sequence of states $x_1, x_2, \ldots, x_n$ that finishes with the starting state, $x_n = x_1$, and a certain function $g(x, y)$ of two variables. Prove that, if

$$\mathcal{G}(x_1, \ldots, x_n) := \sum_{i=1}^{n-1} g(x_i, x_{i+1}) = 0 \tag{131}$$

for all loop sequences, then there exists a 'potential' function $G(x)$ such that $g(x, y) = G(x) - G(y)$, and

$$\mathcal{G}(x_1, \ldots, x_n) = G(x_n) - G(x_1) \tag{132}$$

for non-loop sequences. Can you think of a differential analog of this result? What is the relation with the previous exercise? Is the cost of climbing a mountain potential-like?

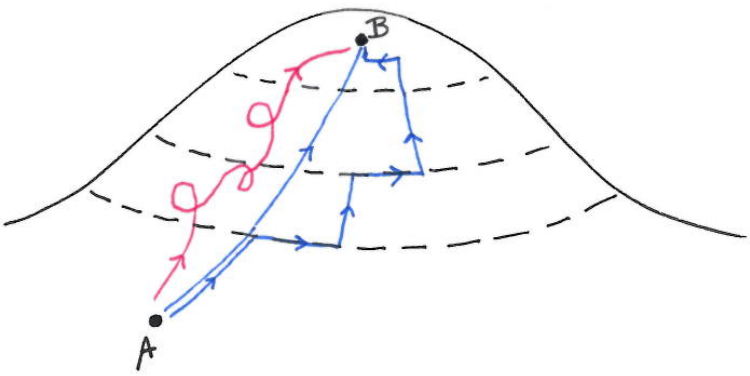
3.5. Further reading

- Instanton and adjoint dynamics: [Gra95].
- Other examples: [Gra89], [Cam12].
- Applications: [LMD98], [LM97].
- Time-reversibility: [OM53], [LMD98], [LM97].
- Kolmogorov loop law: See Wikipage.
- Many attractors: Sec. 7.14 of [Gra89], [Gra95].
- Quasi-potential of general 2D non-reversible systems: [Cam12].
- *Large deviation for stochastic PDEs: [FJL82], [BSG+07].

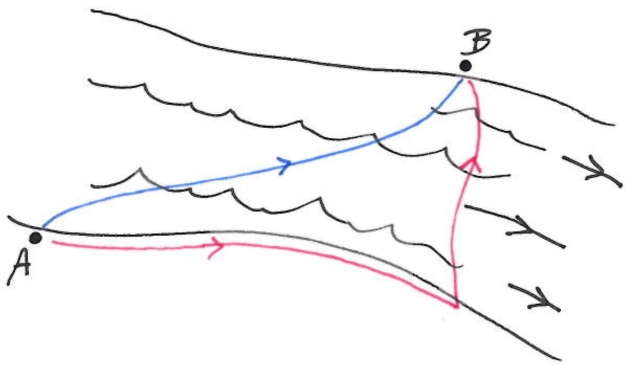
Epilogue: Mountains and rivers

System	Dynamics	Stream	Detailed balance?	Type
Reversible	Pure gradient, $D \propto \mathbb{1}$	$R = 0$	Yes	Mountain
Non-reversible	Non pure gradient or $D \not\propto \mathbb{1}$	$R \neq 0$	No	River or sinkhole

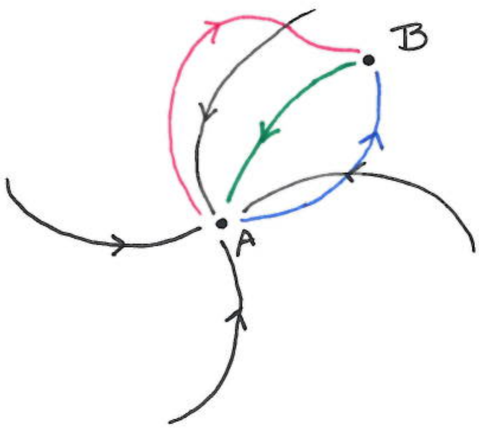
- **Mountains:**



- **Rivers:**



- **Sink holes:**



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