Computing Optimal Trajectories of Noise-Driven Systems*

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Optimal Trajectories Occur in...

- The large deviation theory of drift-diffusion processes. (Mathematical probability community, since 1960s.) But large deviation theory predicts only the *leading-order behavior* of mean escape times and related quantities, as the noise strength tends to zero.

- Ray expansions applied to Fokker–Planck or Smoluchowski equations. (Matkowsky, Schuss et al., before 1990; Dykman et al., since 1980s or before; RSM et al., since 1990.) A much more powerful approach: can in principle yield *arbitrarily fine asymptotics*.
  - Recent work: RSM & Stein, PRL 2000, 2001; see also RSM & Stein, SIAM J. Appl. Math. 1997.
  - `http://uranium.math.arizona.edu/∼rsm`

Noise-Perturbed Bistable ODEs

- A Fokker–Planck equation for $\rho = \rho(\mathbf{x}, t)$, and an Itô Langevin equation for $\mathbf{x} \in \mathbf{R}^d$:

$$\begin{aligned} \dot{\rho} &= -\nabla \cdot (\mathbf{b}(\mathbf{x})\rho) + \frac{\epsilon}{2} \frac{\partial^2}{\partial x_i \partial x_j} (D_{ij}(\mathbf{x})\rho), \\ \dot{\mathbf{x}} &= \mathbf{b}(\mathbf{x}) + \epsilon^{1/2} \sigma(\mathbf{x}) \cdot \eta(t). \end{aligned}$$

  Here $\mathbf{D} = (D_{ij}) \equiv \sigma\sigma^t$, and $\eta(t)$ is a vector of independent unit-strength white noises. The factor ϵ is the *applied noise strength*.

- **Suppose the *drift field* $\mathbf{b} = \mathbf{b}(\mathbf{x})$ has two attactors S, S' and a hyperbolic limit set Hy between them.** E.g., S, S' are point attractors and Hy is a saddle; or S, S' are stable limit cycles and Hy is an unstable limit cycle. **As $\epsilon \to 0$, what happens to $\langle \tau_{SS'} \rangle$, the mean time to escape the basin of S, and reach the vicinity of S'?**

Ray Expansions; Stochastic Phenomenology

- If the *quasistationary PDF* $\rho_0 = \rho_0(\mathbf{x})$ is expanded in a *ray expansion*

$$\rho_0(\mathbf{x}) \sim [K_0(\mathbf{x}) + \epsilon K_1(\mathbf{x}) + \cdots] \exp[-W(\mathbf{x})/\epsilon],$$

  and this is substituted into the Fokker–Planck equation, then the balance equations yield ODEs for $K_0, K_1, \ldots$, and W. The rays emanate from S.

- $H(\mathbf{x}, \mathbf{p}) \equiv (1/2)\mathbf{p} \cdot D(\mathbf{x}) \cdot \mathbf{p} + \mathbf{b}(\mathbf{x}) \cdot \mathbf{p}$ arises naturally, as an auxiliary Hamiltonian. The rays are *zero-energy Hamiltonian trajectories*.

- The rays are *optimal trajectories*: the most probable noise-induced fluctuational trajectories extending from S, in the weak-noise limit. The optimal trajectory extending from S to Hy is the MPEP: the *most probable escape path*.

Key Results (Cf. Kramers 1940)

- The function $W = W(\mathbf{x})$ is a sort of Lyapunov function: it is zero at S and increases away from S. Also, it is a *classical action function*: it satisfies the *zero-energy Hamilton–Jacobi equation* $H(\mathbf{x}, \nabla W(\mathbf{x})) = 0$.
  - In simple models (with 'conservative forces', or 'detailed balance'), W can be computed in closed form from the fields $\mathbf{b}$ and $\mathbf{D}$.
  - In general, need to generate the rays emanating from S via Hamilton's equations. Integration will yield $W(\mathbf{x}')$ as $\int_S^{\mathbf{x}'} \mathbf{p} \cdot d\mathbf{x}$.

- Computing the rate of absorption of probability through Hy yields, if S and Hy are *points*,

$$\langle \tau_{SS'} \rangle \sim \frac{2\pi |\det \Lambda^{(Hy)}|}{K_0(Hy)|\lambda_-^{(Hy)}| \det \Lambda^{(S)}} \exp\left[W(Hy)/\epsilon\right]$$

  as $\epsilon \to 0$. Here $\Lambda^{(S)}$, $\Lambda^{(Hy)}$ are the linearizations of $-\mathbf{b}$ at S, Hy; $\lambda_-^{(Hy)}$ is the negative eigenvalue.

Our Numerical Scheme

- The leading pre-exponential function K_0 satisfies:

$$\dot{K}_0 = -\left(\nabla \cdot \mathbf{b}(\mathbf{x}) + \frac{1}{2}\sum_{i,j=1}^{d} D_{ij}(\mathbf{x})\frac{\partial^2 W}{\partial x_i \partial x_j}(\mathbf{x})\right) K_0.$$

  To get $K_0(\mathbf{x}')$, must integrate this from S to $\mathbf{x}'$.

- How to compute the *Hessian matrix* $(W_{,ij}) \equiv (\partial^2 W/\partial x_i \partial x_j)$, along any optimal trajectory?

  $\Rightarrow$ Answer: Manipulation of the H.–J. equation yields a *matrix Riccati equation* for the matrix $(W_{,ij})$, valid along any optimal trajectory.

- A *triangular numerical scheme* now follows:
  - Compute an optimal trajectory $t \mapsto (\mathbf{x}(t), \mathbf{p}(t))$.
  - Simultaneously, integrate the matrix Riccati equation along the optimal trajectory.
  - Also simultaneously, integrate the ODE for K_0 along the optimal trajectory.

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Example: A Periodically Forced Particle

- How does a noise-perturbed, *periodically forced* overdamped particle eventually escape from a potential well $V(x)$? (Application: a mesoscopic particle in a periodically modulated optical trap.)
  - Earlier work: Smelyanskiy, Dykman, & Golding, PRL 1999; Lehmann, Reimann, & Hänggi, PRL 2000.

- To model periodicity, we treat time as just another coordinate! If $\nu = \nu(t)$ is the forcing function, with period τ_F, we use the 2-D Langevin equation

$$\begin{aligned} \dot{x} &= -V'(x) + f\nu(y) + \epsilon^{1/2}\,\eta(t), \\ \dot{y} &= 1. \end{aligned}$$

  Here $0 \leq y < \tau_F$, and y is periodic: $y = \tau_F$ is identified with $y = 0$. The state space with coordinates $\mathbf{X} \equiv (x, y)$ is effectively a cylinder. On this cylinder, the oscillating well bottom is our stable limit cycle S, and the oscillating well top is our unstable limit cycle Hy.

Consequences of Forcing ($f \neq 0$)

- When $f = 0$, the classical action function $W(x, y)$ is equal to $2V(x) + \mathrm{const}$ for all y. But when $f \neq 0$, it must be computed numerically: by integrating along an optimal trajectory from S to (x, y).

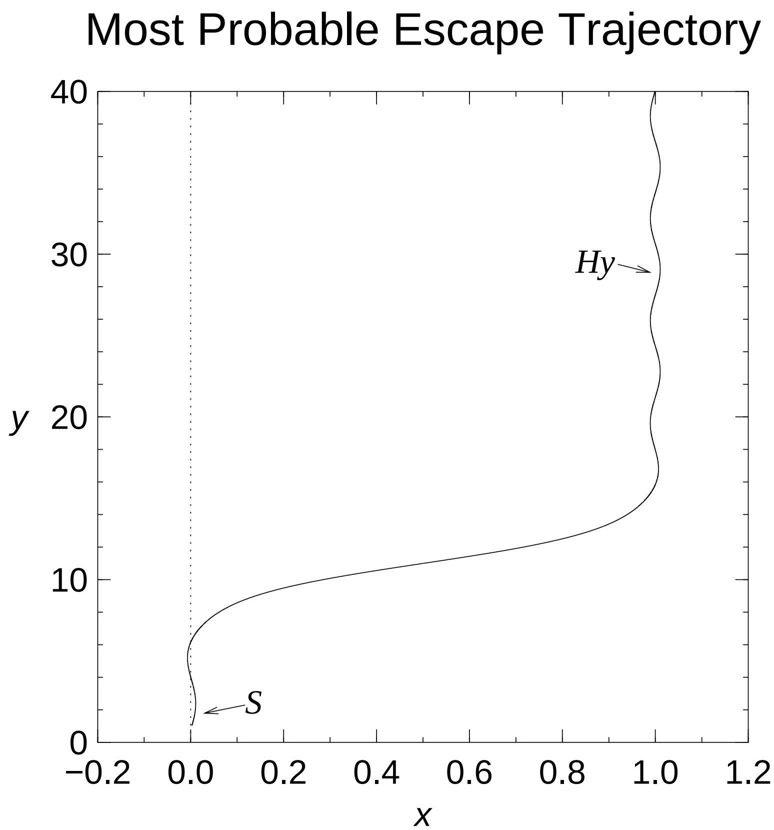
- When $f \neq 0$, there is normally an *infinite discrete set* of optimal trajectories that extend from S to any point $\mathbf{X} \equiv (x, y)$ near Hy.

  $\Rightarrow$ Reason: an optimal trajectory may cycle near Hy an arbitrarily large (integer) number of times before being 'flung back' toward S. Cf. 'multiply illuminated regions' in ray optics.

  $\Rightarrow$ Consequence: the classical action W (and also K_0, etc.) is *infinite-valued*!

$$\rho_0(\mathbf{X}) \sim \sum_{\ell} K_0^{(\ell)}(\mathbf{X}) \exp\left[-W^{(\ell)}(\mathbf{X})/\epsilon\right], \quad \epsilon \to 0,$$

where the infinitely many branches $\{W^{(\ell)}(x, y)\}$ of $W(x, y)$ merge together as $(x, y) \to Hy$.



In this simulation,

- $V(x) = x^2/2 - x^3/3$, so the well bottom is at $x = 0$ and the well top is at $x = 1$.
- The forcing term $f\nu(y)$ equals $0.15 \sin y$.
- S and Hy oscillate around $x = 0$ and $x = 1$.

Computation $\rightarrow$ Theory $\rightarrow$ Experiment

- Theoretical work on the behavior of W and K_0 near Hy shows that at any small inward offset $n = N\epsilon^{1/2}$ from Hy,

  $$\rho_0(n = N\epsilon^{1/2}, y) \sim h_{f,\epsilon}(N, y) \exp(-W(Hy)/\epsilon),$$

  where the quantity $h_{f,\epsilon}(N, y)$, for any N and any fixed 'phase' y in $[0, \tau_F)$, oscillates periodically in $\log \epsilon$ as $\epsilon \to 0$.

  – See RSM & Stein, PRL 2001.

- In consequence, the flux through Hy, at any fixed phase y, should *not* simply fall off exponentially as $\epsilon \to 0$. It too should oscillate, periodically in $\log \epsilon$, as $\epsilon \to 0$.

  Experimental prediction: The phase at which a periodically driven, thermally perturbed, particle is eventually 'sloshed out' of a well should not settle down at any fixed value as $\epsilon \to 0$. The phase distribution should (very!) slowly oscillate.

Noise-Perturbed Bistable PDEs

- How to model a noise-perturbed *spatially extended* system? Use a stochastic PDE, or a Langevin equation with *spatiotemporal* noise.

- Example: a bistable, 1D quartic field theory on the interval $[-L/2, L/2]$.

$$\dot{\phi} = \nabla^2\phi - \phi^3 + \phi + \epsilon^{1/2}\eta(x,t).$$

  Naively, $\phi \equiv \pm 1$ are S, S', and $\phi \equiv 0$ is Hy. How does the noise induce a *droplet* of the S' state to nucleate, and expand to fill the interval?

  – Earlier work: Büttiker & Landauer c. 1980 ($L \to \infty$); also Coleman 1970s; Jona-Lasinio & Faris, mid-1980s.

- Applications of similar noise-perturbed PDEs: thermally activated formation of spatially localized states ('worms') in layers of nematic liquid crystal; thermally activated domain wall formation and motion in micromagnetism.

Our Results on Droplet Nucleation

- Boundary conditions, if $L < \infty$, affect S, S', and Hy, which become *elliptic functions* of x. D, N, P, and anti-P b.c. are all of interest.

- This model has 'detailed balance', and $W(\phi(\cdot))$ can be computed in closed form from $\phi(\cdot)$. No optimal trajectories need to be computed or integrated along! Also, $K(\phi(\cdot)) \equiv 1$.

- To leading order, $\langle \tau_{SS'} \rangle \sim \exp[W(Hy)/\epsilon]$, $\epsilon \to 0$. But computing the *pre-exponential factor* is hard.
  - The *fluctuation determinants* $\det \Lambda^{(S)}$, $\det \Lambda^{(Hy)}$ are determinants of operators on a Hilbert space. (Cf. Coleman & Callan, 1970s.)
  - The lone negative eigenvalue $\lambda_{-}^{(Hy)}$ of $\Lambda^{(Hy)}$ must be computed from a Sturm–Liouville problem involving elliptic functions.

- Key result: $\langle \tau_{SS'} \rangle \sim C\epsilon^{a} \exp[W(Hy)/\epsilon]$, where the prefactor as well as $W(Hy)$ can be computed *explicitly* in terms of elliptic functions, for any L.

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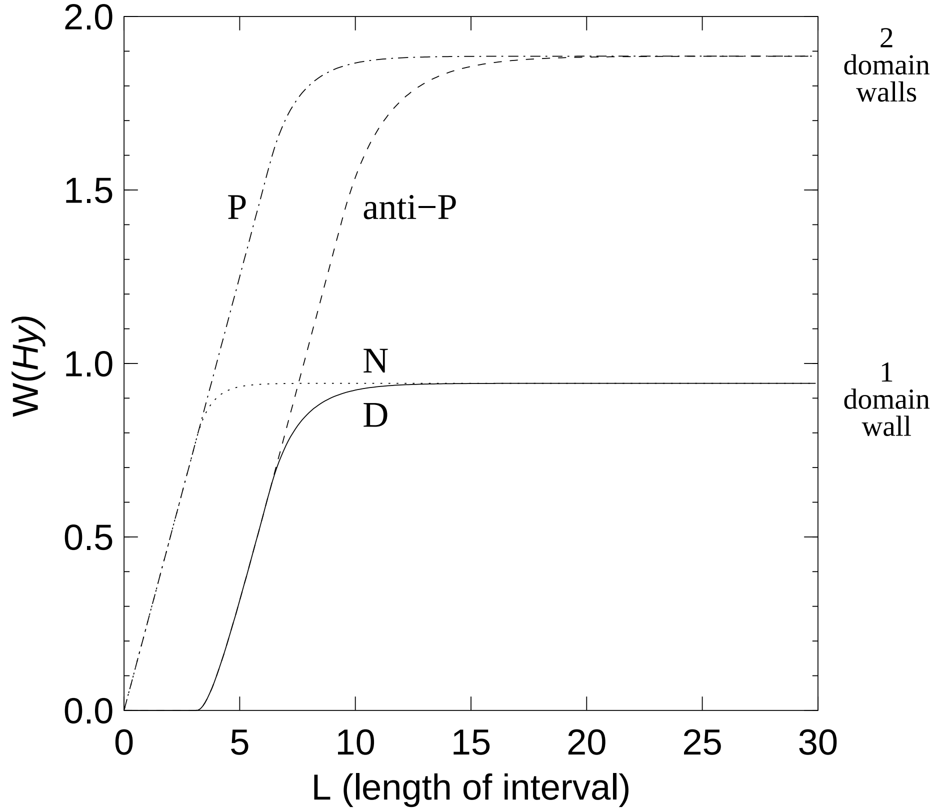
Activation Barrier (for various B.C.s)



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Conclusions

- Optimal trajectories of noise-perturbed systems, including ones with spatial extent, can be computed numerically, and even analytically.

- In the weak-noise limit, the mean time to escape the basin of an attractor S and reach the vicinity of S' will grow exponentially. Both the *exponential growth rate*, i.e., the activation barrier $W(Hy)$, and the *prefactor* can be computed by integrating along the dominant optimal trajectory.
  - This generalizes the Kramers formula for noise-perturbed systems with detailed balance.

- Nontrivial applications in physics include:
  - Thermally activated hopping of a mesoscopic particle between the wells of a periodically modulated optical trap. (No spatial extent.)
  - Thermally activated magnetization reversal in a finite volume. (Nontrivial spatial extent.)