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.

  – http://uranium.math.arizona.edu/~rsm
Noise-Perturbed Bistable ODEs

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

$$
\dot{\rho} = -\nabla \cdot (b(x) \rho) + \frac{\epsilon}{2} \frac{\partial^2}{\partial x_i \partial x_j} (D_{ij}(x) \rho),
$$

$$
\dot{x} = b(x) + \epsilon^{1/2} \sigma(x) \cdot \eta(t).
$$

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

- Suppose the drift field $b = b(x)$ has two attractors $S, S'$ 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 $\langle T_{SS'} \rangle$, the mean time to escape the basin of $S$, and reach the vicinity of $S'$?
Ray Expansions;  
Stochastic Phenomenology

• If the quasistationary PDF \( \rho_0 = \rho_0(x) \) is expanded in a ray expansion

\[
\rho_0(x) \sim [K_0(x) + \epsilon K_1(x) + \cdots] \exp \left[ -W(x)/\epsilon \right],
\]

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 \( S \).

• \( H(x, p) \equiv (1/2)p \cdot D(x) \cdot p + b(x) \cdot p \) 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 \( H_y \) is the MPEP: the most probable escape path.
Key Results (Cf. Kramers 1940)

- The function \( W = W(x) \) is a sort of Lyapunov function: it is zero at \( S \) and increases away from \( S \). Also, it is a \textit{classical action function}: it satisfies the \textit{zero-energy Hamilton–Jacobi equation} \( H(x, \nabla W(x)) = 0 \).

  - In simple models (with ‘conservative forces’, or ‘detailed balance’), \( W \) can be computed in closed form from the fields \( b \) and \( D \).
  - In general, need to generate the rays emanating from \( S \) via Hamilton’s equations. Integration will yield \( W(x') \) as \( \int_{S}^{x'} p \cdot dx \).

- Computing the rate of absorption of probability through \( H_y \) yields, if \( S \) and \( H_y \) are \textit{points},

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

as \( \epsilon \to 0 \). Here \( \Lambda^{(S)}, \Lambda^{(H_y)} \) are the linearizations of \( -b \) at \( S, H_y \); \( \lambda_{-}^{(H_y)} \) is the negative eigenvalue.
Our Numerical Scheme

- The leading pre-exponential function $K_0$ satisfies:

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

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

- 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 $t \mapsto (x(t), p(t))$.
  - Simultaneously, integrate the matrix Riccati equation along the optimal trajectory.
  - Also simultaneously, integrate the ODE for $K_0$ along the optimal trajectory.
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.)


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

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

Here $0 \leq y < \tau_F$, and $y$ is periodic: $y = \tau_F$ is identified with $y = 0$. The state space with coordinates $X \equiv (x, y)$ 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 \(2V(x) + \text{const}\) 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 \(X \equiv (x, y)\) 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!

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

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

- \( V(x) = \frac{x^2}{2} - \frac{x^3}{3} \), 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 \( H_y \) oscillate around \( x = 0 \) and \( x = 1 \).
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 $\epsilon \to 0$.


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

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

Activation Barrier (for various B.C.s)

- P
- anti-P
- N
- D

W(Hy) vs. L (length of interval)

1 domain wall
2 domain walls
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 $W(H_y)$, 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.)