Rare Events in Stochastic Systems

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March 1, 2007



Outline

SIS Model (Epidemiology)

- The Setup
- Mean Extinction Time
- Large System Size Asymptotics of MET
- Near-Continuum (Fokker-Planck) Approximation

Large Deviations for Markov Jump Processes

- One-Step MJP
- Large System Size Regime
- Large and Moderate Deviations
- Hamilton-Jacobi Equation

Schlögl Model (Chemical Kinetics)

- The Setup
- Deterministic Description
- Mean Switching Times and Asymptotics
- Solving the Hamilton-Jacobi Equation



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One-step Markov Jump Process

- n = number of infected people,
- N = total number of people (kept constant),
- Λ = infection rate.

$$n \to n+1 \qquad \text{with rate} \quad \lambda_n = \Lambda n\left(1-\frac{n}{N}\right),$$

$$n \to n-1 \qquad \text{with rate} \quad \mu_n = n.$$

Mean Extinction Time τ_n is the Mean First Passage Time from the state n to the state 0.

Backward Equation

$$-1 = \lambda_n \tau_{n+1} - (\lambda_n + \mu_n)\tau_n + \mu_n \tau_{n-1}$$

with boundary condition $\tau_0 = 0$.

The Exact Solution

$$\tau_n = \sum_{m=1}^{n} \left[\frac{1}{\mu_m} + \prod_{i=1}^{m-1} \frac{\mu_i}{\lambda_i} \sum_{j=m+1}^{\infty} \frac{1}{\mu_j} \prod_{k=1}^{j-1} \frac{\lambda_k}{\mu_k} \right]$$



$N \gg 1, n = \mathcal{O}(N)$

Assumptions

- $\lambda_n = N\bar{\lambda}(n/N)$ and $\mu_n = N\bar{\mu}(n/N)$, with $\bar{\lambda}(x)$ and $\bar{\mu}(x)$ smooth functions.
- The "effective potential" $\Phi(x) = -\int_0^x \log \frac{\bar{\lambda}(\xi)}{\bar{\mu}(\xi)} d\xi$.

Three Cases

- $\Lambda < 1$, Subthreshold: $\tau_n \sim \log N$,
- $\Lambda = 1$, Threshold: $\tau_n \sim \sqrt{N}$,
- $\Lambda > 1$, Superthreshold: $\tau_n \sim e^{N\Phi(n_e/N)}$, with a unique interior equilibrium $n_e = N\left(1 - \frac{1}{\Lambda}\right)$.



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Near-Continuum Approximation of Discrete Backward Equation

$$-1 = (\bar{\lambda}(x) - \bar{\mu}(x))T'(x) + \frac{1}{2N}(\bar{\lambda}(x) + \bar{\mu}(x))T''(x)$$

Stochastic Differential Equation

$$dX = (\bar{\lambda}(X) - \bar{\mu}(X))dt + \frac{1}{\sqrt{N}}\sqrt{\bar{\lambda}(X) + \bar{\mu}(X)}dW$$

The MET Solution

$$T(x) = 2N \int_0^x \int_y^\infty \frac{e^{-N(V(z)-V(y))}}{\bar{\lambda}(z) + \bar{\mu}(z)}\, dz\, dy$$

$N \gg 1$ Asymptotics for the Superthreshold Case

$$T(x) \sim e^{NV(x_e)},$$

with different "effective potential" $V(x) = -2\int_0^x \frac{\bar{\lambda}(\xi)-\bar{\mu}(\xi)}{\bar{\lambda}(\xi)+\bar{\mu}(\xi)}\, d\xi$.



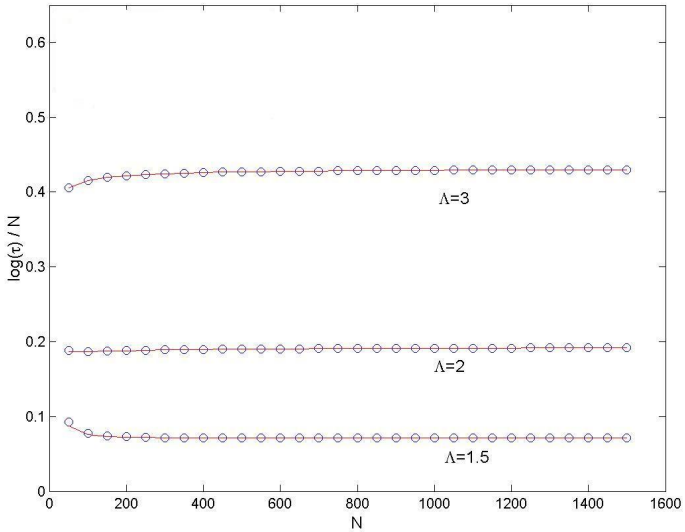
Exponential Extinction Times

$$\log(\text{Extinction Time}) = N \times \text{Potential}(x_e)$$

Exact Potential

Two Potentials

- $\Phi(x) = -\int_0^x \log \frac{\bar{\lambda}(\xi)}{\bar{\mu}(\xi)} d\xi$
- $V(x) = -2\int_0^x \frac{\bar{\lambda}(\xi)-\bar{\mu}(\xi)}{\bar{\lambda}(\xi)+\bar{\mu}(\xi)} d\xi$



Fokker-Planck approximation is not good enough for exponentially large observables.

Exponential Extinction Times

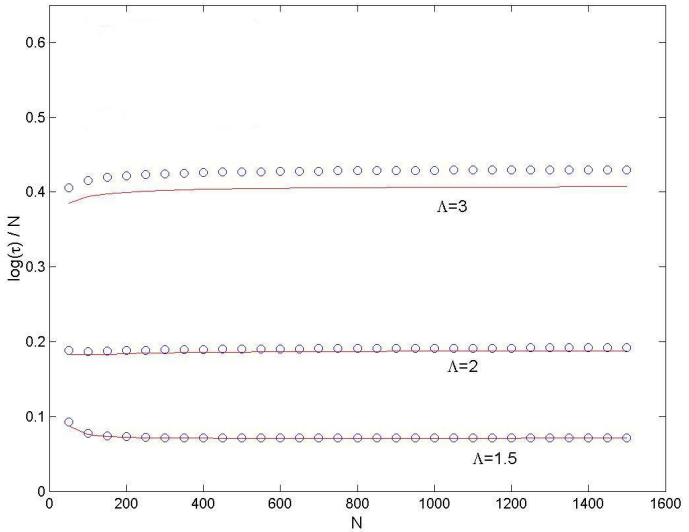
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Fokker-Planck Potential

Two Potentials

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One-step Markov Jump Process $X(t)$

$$\begin{aligned} U_n \qquad & n \to n+1, \\ D_n \qquad & n \to n-1. \end{aligned}$$

Master Equation

$$\frac{dP_n(t)}{dt} = U_{n-1}P_{n-1}(t) + D_{n+1}P_{n+1}(t) - (U_n + D_n)P_n(t)$$

for the probabilities $P_n(t) = \mathbb{P}\{X(t) = n\}$.



- Rescale the jump sizes and the rates,
- Rates $u(x) := \epsilon U_n$ and $d(x) := \epsilon D_n$,
- *Intensive variable* $x = n/N = \epsilon n$.

Rescaled Master Equation

$$\frac{\partial P_\epsilon(x,t)}{\partial t} = \epsilon^{-1}\{u(x-\epsilon)P_\epsilon(x-\epsilon,t) - u(x)P_\epsilon(x,t)\}+$$
$$+\epsilon^{-1}\{d(x+\epsilon)P_\epsilon(x+\epsilon,t) - d(x)P_\epsilon(x,t)\},$$

for the probabilities $P_\epsilon(x,t) = \mathbb{P}\{X(t) = x/\epsilon\}$.

Expansion up to the order $\mathcal{O}(\epsilon^0)$

- Liouville Equation: $\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[(u(x) - d(x))P(x,t)\right]$,
- Leads to the ODE: $\dot{x} = u(x) - d(x)$.



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for the probabilities $P_\epsilon(x,t) = \mathbb{P}\{X(t) = x/\epsilon\}$.

Expansion up to the order $\mathcal{O}(\epsilon^1)$

- Fokker-Planck Equation: $\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[(u(x)-d(x))P(x,t)\right] + \frac{\epsilon}{2}\frac{\partial^2}{\partial x^2}\left[(u(x)+d(x))P(x,t)\right]$,
- Leads to the SDE: $dx = (u(x)-d(x))\,dt + \sqrt{\epsilon(u(x)+d(x))}\,dW$.



Rare event (large deviation) ansatz $P(x,t) = e^{-\Phi(x,t,\epsilon)/\epsilon}$ (same ϵ!).

Rescaled Master Equation

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$$-\epsilon^{-1} e^{-\Phi(x,t)/\epsilon} \frac{\partial \Phi(x,t)}{\partial t} = \epsilon^{-1} u(x) \left[e^{-\Phi(x-\epsilon,t)/\epsilon} - e^{-\Phi(x,t)/\epsilon} \right] +$$

$$+\epsilon^{-1} d(x) \left[e^{-\Phi(x+\epsilon,t)/\epsilon} - e^{-\Phi(x,t)/\epsilon} \right]$$



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Hamilton-Jacobi Equation

$$\Phi_t + u(x)(e^{\Phi_x} - 1) + d(x)(e^{-\Phi_x} - 1) = 0$$



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Fokker-Planck Equation

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}\left[(u(x) - d(x))P(x,t)\right] + \frac{\epsilon}{2}\frac{\partial^2}{\partial x^2}\left[(u(x) + d(x))P(x,t)\right]$$

The *wrong* Hamilton-Jacobi Equation

$$\Phi_t + (u(x) - d(x))\Phi_x + \frac{u(x) + d(x)}{2}(\Phi_x)^2 = 0$$



[Not so] Rare event (moderate deviation) ansatz $P(x,t) = e^{-\Phi(x,t)/\delta}$ with $\delta = \epsilon^{\alpha}$ for $0 < \alpha < 1$.

Now both Master and Fokker-Planck Equations lead to the same

Hamilton-Jacobi Equation

$$\Phi_t + (u(x) - d(x))\Phi_x + \frac{\epsilon}{\delta}\frac{u(x)+d(x)}{2}(\Phi_x)^2 + o\left(\frac{\epsilon}{\delta}\right) = 0$$



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Take-Home Message

Fokker-Planck approximation is valid only for up to moderate deviations $e^{-\Phi(x,t)/\delta}$, NOT for large deviations $e^{-\Phi(x,t)/\epsilon}$!



Hamilton-Jacobi form

$$\Phi_t + u(x)(e^{\Phi_x} - 1) + d(x)(e^{-\Phi_x} - 1) = \Phi_t + H(x, \Phi_x) = 0$$

- Read off the Hamiltonian

$$H(x, p) = u(x)(e^{p} - 1) + d(x)(e^{-p} - 1),$$

- Set up the Hamiltonian System

$$\begin{cases} \frac{dx}{dt} = u(x)e^{p} - d(x)e^{-p} \\ \frac{dp}{dt} = -u'(x)(e^{p} - 1) - d'(x)(e^{-p} - 1), \end{cases}$$

- Along the Hamiltonian paths,

$$\frac{d\Phi}{dt} = \Phi_t + \Phi_x \frac{dx}{dt} = -H(x, p) + p\frac{dx}{dt}.$$



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$$2R + A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 3R$$

$$R \underset{k_4}{\overset{k_3}{\rightleftharpoons}} B$$

- Introduced by Schlögl in 1972, as a catalysis model.
- Keep the concentrations N_A and N_B constant.
- Interested in the dynamics of $X(t) := N_R(t)$.
- The simplest description: deterministic, rate equation.



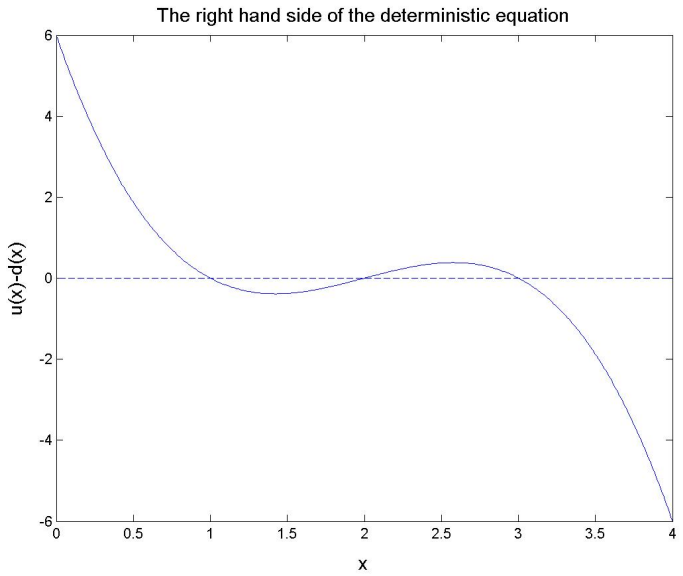
Proportion to the system size

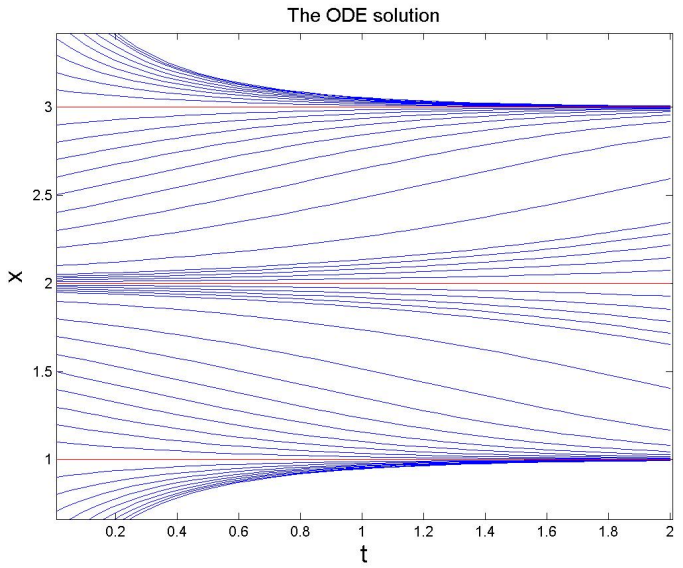
$$x(t) = \frac{X(t)}{N}$$

Governing ODE

$$\frac{dx}{dt} = k_1 x^2 + k_4 - k_2 x^3 - k_3 x = u(x) - d(x)$$

- Simple to analyze.
  Stable-Unstable-Stable.





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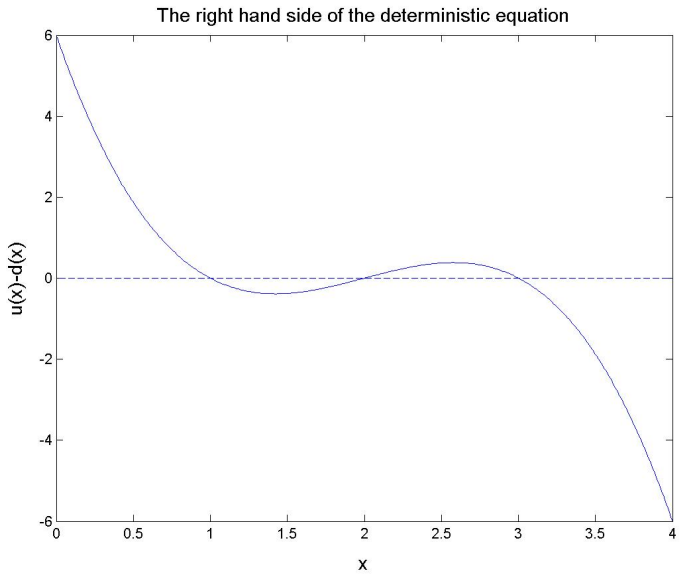
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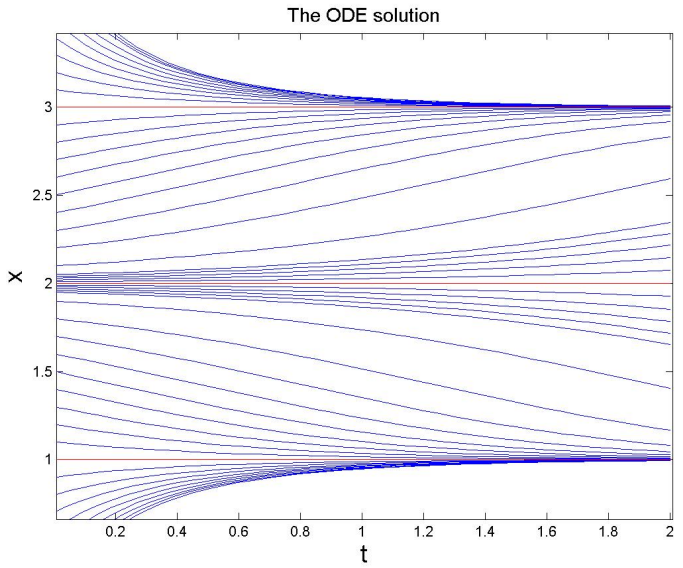
$$\frac{dx}{dt} = k_1 x^2 + k_4 - k_2 x^3 - k_3 x = u(x) - d(x)$$

- Simple to analyze.
  Stable-Unstable-Stable.

BUT

- Works only for large and well stirred systems.
- Does not detect intrinsic fluctuations.
- Switches between stable equilibriums are not allowed.
- Which of the two stable states is more stable?





Discrete Model

$$2R + A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 3R$$

$$R \underset{k_4}{\overset{k_3}{\rightleftharpoons}} B$$

$$(N_R =)\ n \to n+1 \qquad \text{with rate} \quad U_n = k_1 \frac{n(n-1)}{N} + k_4 N,$$

$$(N_R =)\ n \to n-1 \qquad \text{with rate} \quad D_n = k_2 \frac{n(n-1)(n-2)}{N^2} + k_3 n.$$

- To determine which deterministically stable state is "more stable", we need to compare the mean switching times between them, $\tau_{n_2 \to n_1}$ and $\tau_{n_1 \to n_2}$.
- We have the exact solution

$$\tau_{n \to n_1} = \sum_{m=n_1+1}^{n} \left[\frac{1}{D_m} + \prod_{i=1}^{m-1} \frac{D_i}{U_i} \sum_{j=m+1}^{\infty} \frac{1}{D_j} \prod_{k=1}^{j-1} \frac{U_k}{D_k}, \right]$$

for $n > n_1$.

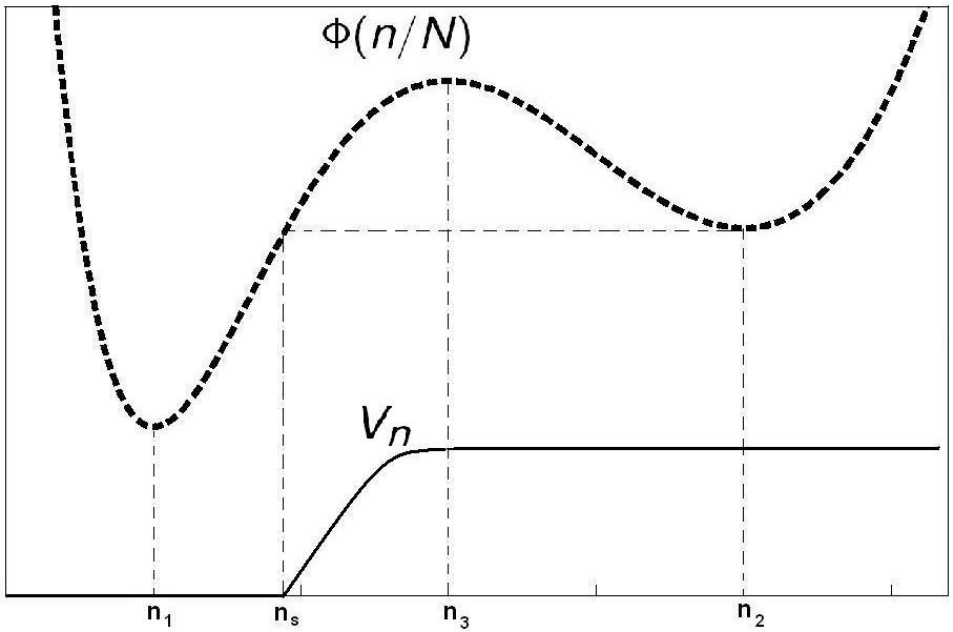


The leading order of the exponent $V_n = \frac{1}{N} \log \tau_{n \to n_1}$

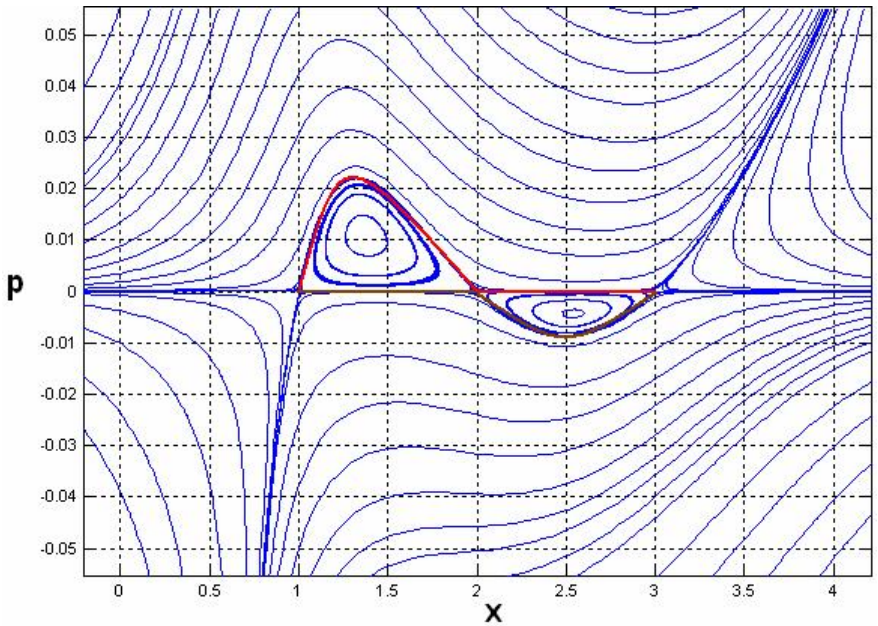
$$V_n \sim \begin{cases} 0 & \text{for} \quad n \in [n_1, n_s] \\ \Phi(n/N) - \Phi(n_2/N) & \text{for} \quad n \in [n_s, n_3] \\ \Phi(n_3/N) - \Phi(n_2/N) & \text{for} \quad n \in [n_3, \infty) \end{cases}$$

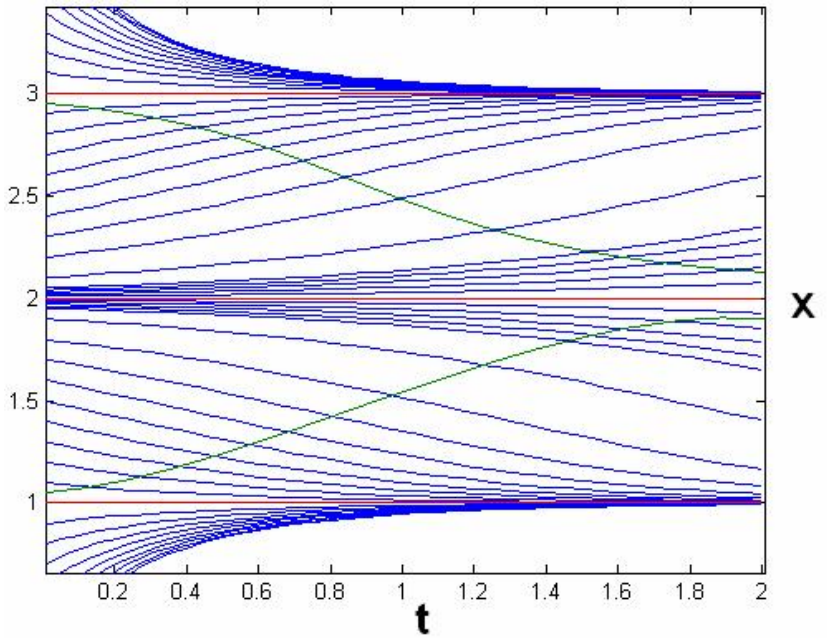
$$\Phi(n/N) = -\int_0^{n/N} \log \frac{u(x)}{d(x)}\, dx,$$

$$\Phi(n_s/N) = \Phi(n_2/N).$$



- Backward Equation $-1 = \mathcal{L}T$ for mean switching times leads to Homogeneous H-J Equation $H(x, \Phi_x) = 0$ for the exponent function.
- For One-Step MJP: $H(x,p) = u(x)(e^p - 1) + d(x)(e^{-p} - 1) = 0$. $p = 0$ (deterministic path) or $p = \log(d(x)/u(x))$.
- $\Phi(x) = \int p(x)dx$ = Area in the phase plane.





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Conclusions

- Fokker-Planck (diffusion) approximation is not good enough for exponentially - in system size - rare events,
- The paths that contribute the most to the Mean First Passage Time are NOT always the most likely ones.



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Future Work

- Finding unambiguous way to get the exponent bypassing the exact solution.
- Shortest/First Passage Time paths in multidimensional systems (no exact solutions available).



Acknowledgements

- Charles Doering, Mathematics, University of Michigan,
- Leonard Sander, Physics, University of Michigan,
- Eric Vanden-Eijnden, Courant Institute, NYU.

- Geophysical Fluid Dynamics Program, Woods Hole Oceanographic Institution,
- Department of Mathematics and Michigan Center for Theoretical Physics, University of Michigan.

Thank You!

