The Most Probable Transition Pathways in Non-Gaussian Stochastic Dynamical Systems

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Our Story

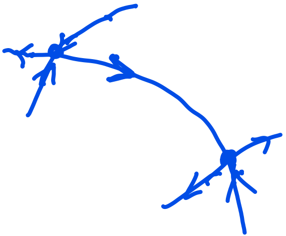
Computing the Most Probable Transition Pathways

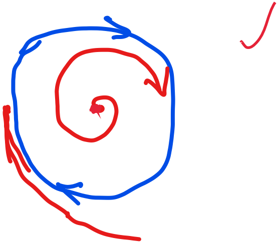
Method 1: An Euler-Lagrange method

Method 2: An Optimal Control method

Our Story: Deterministic ‘counterpart’

Heteroclinic orbits ✓ & Limit cycles ✓





Transition Time = ∞

John Guckenheimer & Philip Holmes:
“Nonlinear Oscillations, Dynamical Systems, and Bifurcations of Vector Fields", 1983

Our Story: Gaussian vs. Non-Gaussian

Gaussian distribution: $X \sim e^{-\frac{1}{2}x^2}$

Maxwellian in stat phys: $e^{-\frac{mx^2}{2kT}}$

Maximum likelihood estimation: $e^{-\frac{1}{2}X_1^2-\frac{1}{2}x_2^2} = e^{-\frac{1}{2}X_1^2} \cdot e^{-\frac{1}{2}x_2^2}$

Kernel method in machine learning: $e^{-\frac{1}{2}x^2}$

$\cdots$

Gaussian distribution:

1. comes from Central Limit Theorem!
2. is the unique fixed point of Fourier transform!

We were/are deeply rooted in Gaussianity!

Our Story:
Gaussianity ≈ Linearity Non-Gaussianity ≈ Nonlinearity

1. Linear operations on Gaussian still output Gaussian!

2. Gaussian particle vs Non-Gaussian particle escape probability from an interval: (0, 1)

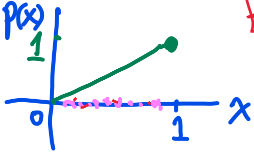
Levy

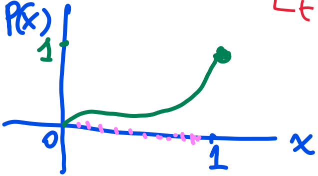
Linear function vs Nonlinear function

L_t

B_t

Brownian

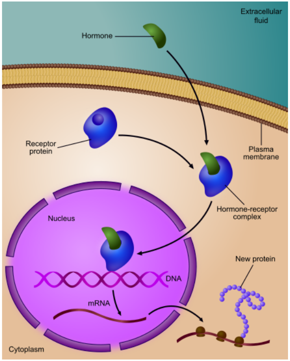




Jinqiao Duan: “An Introduction to Stochstic Dynamics", 2015

Motivation: Transcription in gene expression

Gene expression = Transcription + Translation
Gene (DNA segment) → mRNA → Protein

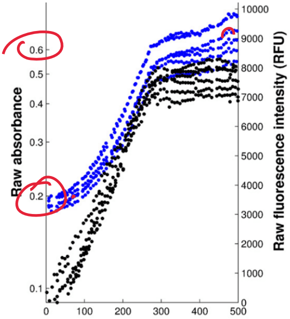


Raser-O'Shea et al.: Science 2010.
Noise in Gene Expression: Origins, Consequences, and Control

Evolution of concentration of a transcription factor

(Protein)

Stefan et al.: PLOS Compu. Biology, 2015



Metastable patterns & Transitions between patterns

Elowitz et al.: Nature 2011. Stochastic differential equation model

Stochastic differential equations: Differential equations with Brownian motion and Lévy motion

Brownian motion B_t:

- Independent increments: $B_{t_2} - B_{t_1}$ and $B_{t_3} - B_{t_2}$ independent
- Stationary increments with $B_t - B_s \sim \mathcal{N}(0, t-s)$
- Continuous sample paths, but nowhere differentiable

I. Karatzas and S. E. Shreve,
Brownian Motion and Stochastic Calculus

Lévy Motion L_t^α

Definition: Lévy motion L_t^α with $0 < \alpha < 2$:
(1) Independent increments
(2) Stationary increments $L_t^\alpha - L_s^\alpha \sim S_\alpha(|t-s|^{\frac{1}{\alpha}}, 0, 0)$
(3) Sample paths are stochastically continuous: $L_t^\alpha \to L_s^\alpha$ in probability as $t \to s$

Note: Sample paths are right continuous with left limit; countable jumps
Jump measure: $\nu_\alpha(dy) = C_\alpha \frac{dy}{|y|^{1+\alpha}}$

Lévy-Khintchine Theorem

A special case $\alpha = 2$: Brownian motion B_t

D. Applebaum,
Lévy Processes and Stochastic Calculus

A large class of Stochastic Differential Equations (SDEs)

Lévy-Itô Decomposition Theorem:

'A stochastic process with independent and stationary increments is the sum of a Brownian motion B_t and a Lévy motion L_t'

White noise:

'Derivative' of a stochastic process with independent and stationary increments

$$dX_t = f(X_t)dt + \sigma\, dB_t + c\, dL_t$$

Back to: Transition phenomena in stochastic dynamical systems

How to examine —

The most probable transition pathway between metastable states

Transition phenomena in stochastic dynamical systems

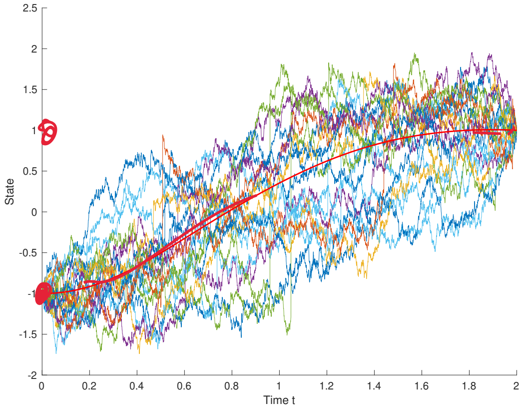
Metastable states:
A metastable state is an unperturbed equilibrium stable state.

The most probable transition pathway:
A ‘reference trajectory’ from one metastable state to another

Small tube around the most probable transition pathway

Probability estimate for solution paths to stay inside this tube

Onsager-Machlup: 1953



Onsager-Machlup action functional

Asymptotic probabilistic estimate for solu paths $X(t)$ lying in a small tube surrounding a 'reference trajectory $z(t)$'

Definition

Consider a tube (of sufficiently small diameter δ) surrounding a reference trajectory $z(t)$. If the probability of the solution paths X_t lying in this tube is estimated by

$$\mathbb{P}(\{\|X - z\| \leq \delta\}) \propto C(\delta) \exp\{-\frac{1}{2}\int_0^T OM(\dot{z}, z)dt\},$$

then integrand $OM(\dot{z}, z)$ is called Onsager-Machulup function.

$\propto$: equivalence for δ small enough.

Minimizer for $\int_0^T OM\, dt$: Most probable transition pathway

The most probable transition pathway
—- Onsager-Machlup action functional (finite noise)

Small tube around the most probable transition path:
Probability estimate for solu paths to stay inside this tube via Onsager-Machlup action functional

1953: SDEs with (Gaussian) Brownian noise;
Onsager-Machlup, Physical Reviews, 1953
Dürr-Bach, Comm. Math. Phys., 1978

$$dX_t = f(X_t)dt + \sigma \, dB_t$$

2019: SDEs with (non-Gaussian) Lévy noise

$$dX_t = f(X_t)dt + \sigma \, dB_t + c \, dL_t$$

Chao & Duan, Nonlinearity, June 2019

Onsager-Machlup action functional: Gaussian noise

$dX_t = f(X_t)dt + \sigma\, dB_t$

Theorem

The Onsager-Machlup function is given, up to an additive constant, by:

$$OM(\dot{z}, z) = \left|\frac{\dot{z} - f(z)}{\sigma}\right|^2 + div\, f(z), \quad (1)$$

where $z(t)$ is a reference trajectory.

$\int_0^T OM(\ )\, dt$

Dürr-Bach, Comm. Math. Phys., 1978

Onsager-Machlup action functional: Non-Gaussian noise $dX_t = f(X_t)dt + \sigma\, dB_t + dL_t$

Theorem

For a class of stochastic systems in the form of with the jump measure satisfying $\int_{|\xi|<1} \xi\nu(d\xi) < \infty$, the Onsager-Machlup function is given, up to an additive constant, by:

$$OM(\dot{z}, z) = |\frac{\dot{z} - f(z)}{\sigma}|^2 + div\, f(z) + 2\frac{\dot{z} - f(z)}{\sigma^2}\int_{|\xi|<1} \xi\nu(d\xi), \quad (2)$$

where $z(t)$ is a reference trajectory.

1. Impact of non-Gaussian Lévy noise: Third term
2. Lévy noise absent: Recover the OM for the Gaussian case

Chao & Duan, Nonlinearity, June 2019.

How to determine the transition time T?

1. Mean exit time

2. Estimate from observation data

3. Theoretical estimation:
$\min_T \min_z \int_0^T OM(\dot{z}(t), z(t))dt$

Huang-Chao-Wei-Duan, Nonlinearity, 2021

Most probable transition pathway: Theoretical results

$$\min \int_0^T OM(\dot{z}(t), z(t))dt$$

Theorem

Assume that the solution z of Euler-Lagrange equation is smooth.

(i) This solution is indeed a local minimizer of OM functional, if $OM(\dot{z}, z)$ is convex in the variable $\dot{z}$.

(ii) This solution is a global minimizer, if $OM(\dot{z}, z)$ is convex in both variables $(\dot{z}, z)$.

Two Methods for computing the most probable transition pathway

Consider the following stochastic differential equation

$$dX(t) = f(X(t))dt + \sigma dB_t, \quad X(0) = x_0 \in \mathbb{R}^d, \tag{3}$$

- $f : \mathbb{R}^d \to \mathbb{R}^d$ is a drift function
- σ: a $d \times k$ diffusion matrix
- B_t: Brownian motion in $\mathbb{R}^k$

Method 1: An Euler-Lagrange method for computing the most probable transition pathway

The most probable path $z(t)$:

$$\min_{z(t)} \int_0^T OM(\dot{z}(t), z(t))dt$$

Corresponding Euler-Lagrange equation:

$$\frac{d}{dt}\frac{\partial OM(\dot{z}, z)}{\partial \dot{z}} = \frac{\partial OM(\dot{z}, z)}{\partial z} \tag{4}$$

That is:

$$\ddot{z}(t) = \frac{\sigma^2}{2} f''(z) + \text{div } f(z)\ f(z) \tag{5}$$

with initial and final conditions: $z(0) = x_0,\ z(T) = x_1$.

Shooting scheme for Euler-Lagrange equation

Shooting scheme for solving initial-final value problem:

- Minimization problem
- So: Machine learning method

X. Chen, J. Duan, J. Hu and D. Li (2023):
Data-driven method to learn the most probable transition pathway and stochastic differential equation. Physica D 443: 133559

Numerical results

Consider a two dimension stochastic gene regulation network

$$
\begin{aligned}
dk &= (a_k + \frac{b_k k^n}{k_0^n + k^n} - \frac{k}{1+k+s})dt + \sigma dB^1(t), \\
ds &= (\frac{b_s}{1+(k/k_1)^p} - \frac{s}{1+k+s})dt + \sigma dB^2(t).
\end{aligned} \tag{6}
$$

- k: concentration of ComK protein
- s: concentration of ComS protein

Sü, Gürol M., et al. (2006)
An excitable gene regulatory circuit induces transient cellular differentiation. Nature 440.7083: 545-550.

J. Hu, X. Chen, and J. Duan (2022)
An Onsager–Machlup approach to the most probable transition pathway for a genetic regulatory network. Chaos, 32.4: 041103.

Numerical results

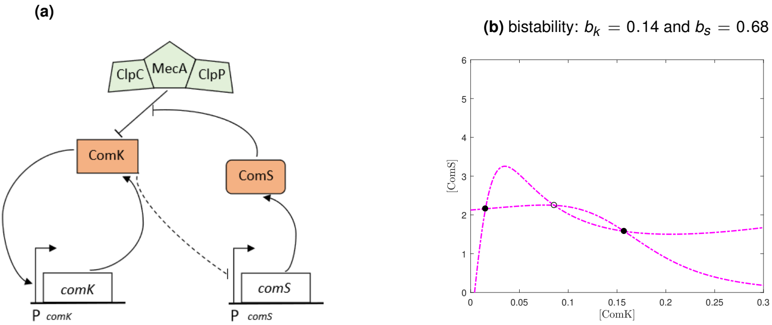


Figure: Gene regulation network. (a) The core competence circuit in B. subtilis (MeKS). (b) Nullclines for this model with parameter $a_k = 0.004$, $k_0 = 0.2$, $k_1 = 0.222$, $n = 2$ and $p = 5$.

Numerical results

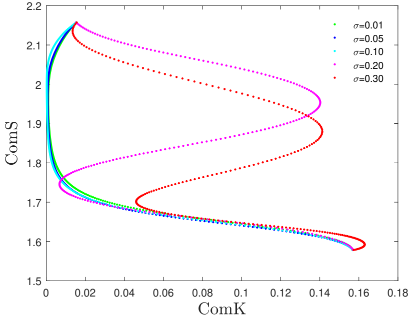


Figure: The most probable transition pathways for bistable dynamics with different noise intensities when noise intensity $\sigma \in (0, 0.3]$ and transition time $T = 5$.

Method 2: An optimal control method for computing the most probable transition pathway

The Onsager-Machlup action functional S^{OM}:

$$S^{OM}(\varphi,\dot{\varphi}) = \frac{1}{2}\int_0^T \{\frac{1}{\sigma^2}|\dot{\varphi} - f(\varphi)|^2 + \text{div } f(\varphi)\}dt. \qquad (7)$$

The minimization of OM action function (1) can be reformulated as the following optimal control problem:

$$\begin{cases} \inf\limits_{\varphi} & \mathcal{J}[\varphi, g] = \int_0^T OM(\varphi(t), g(t))dt + |\varphi(T) - x_1|^2, \\ \text{subject to} & \dot{\varphi}(t) = f(\varphi(t)) + \sigma\, g(t), \\ & \varphi(0) = x_0, \end{cases} \qquad (8)$$

where

$$OM(\varphi(t), g(t)) = \frac{1}{2}(|g(t)|^2 + \text{div } f(\varphi(t))). \qquad (9)$$

W. Wei, T. Gao, X. Chen & J. Duan (2022)
An optimal control method to compute the most likely transition path for stochastic

Machine learning to solve optimal control problem

First step:

- construct neural network NN for g and φ, set them as $g_{NN}(t;\theta)$ and $\varphi_{NN}(t;\theta)$ (θ is the trainable weights and biases)
- g_{NN} and φ_{NN} should satisfy the minimization problem (8)
- g_{NN} and φ_{NN} should satisfy the control term (8)

Second step: construct the loss function as

$$\mathrm{loss} = \tau \mathrm{loss}_{\varphi} + \mathrm{loss}_{g}, \tag{10}$$

where τ is the weight to balance loss_{φ} and loss_{g}, and

$$\mathrm{loss}_{\varphi} = \frac{1}{N_T}\sum_{i=1}^{N_T}(\dot{\varphi}_{NN}(t_i) - f(\varphi_{NN}(t_i)) - \sigma g_{NN}(t))^2 + \tau_1(\varphi_{NN}(0) - x_1)^2,$$

$$\mathrm{loss}_{g} = \frac{1}{2N_T}\sum_{i=1}^{N_T}\left(g_{NN}(t_i)^2 + \nabla f(\varphi_{NN}(t_i))\right)\delta z + \tau_2(\varphi_{NN}(T) - x_2)^2.$$

Last step: use Adam optimizer to train the loss function to get the optimal $g_{NN}(t;\theta^*)$ and $\varphi_{NN}(t;\theta^*)$.

Applications

- **The Rothman carbon cycle model, with random CO_2 injection rate**

  J. Chen, J. Hu, W. Wei and J. Duan (2023)

  A data-driven approach for discovering the most probable transition pathway for a stochastic carbon cycle system. Chaos, 32(11), 113140.

- **A gene regulation model**

  J. Hu, X. Chen, and J. Duan (2022)

  An Onsager–Machlup approach to the most probable transition pathway for a genetic regulatory network. Chaos, 32.4: 041103.

- **A climate model**

  Y. Zheng et al. (2023)

  Early-warning indicator of transition time for noise-induced critical transition of Atlantic Meridional Overturning Circulation.

Conclusion

Computing the most probable transition pathway

Based on the Onsager-Machlup least action theory:

- Euler-Lagrange equation+ neural network method
- Optimal control formulation +neural network method

Thank you!