Transition Phenomena in Stochastic Dynamical Systems

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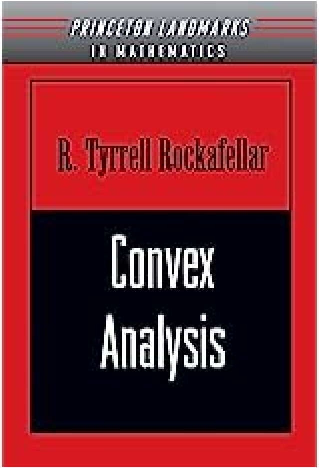
Once upon a time.......
My undergraduate thesis was in computational optimization

Advised by Professor Fei Pusheng (trained in Hamburg University, Germany) at Wuhan University, China.



Optimization was NOT a popular subject .....
Most students were studying finite element method, operator-splitting method, and numerical ODEs (stiff ODEs, A-stability, Runge-Kutta scheme).....

My path drifts to dynamical systems, especially stochastic dynamical systems.

Now, Convex Analysis and Computational Optimization are at the heart of the current AI revolution......

My presentations at Dalat:
The most probable transition pathway in Transition Dynamics is an optimization problem!

So my path reconnects to my old path in Dalat.....

...... We all will live happily ever after Dalat conference!

Lecture 1: Introduction to Stochastic Dynamics

What Are Stochastic Dynamical Systems?

Lecture 1:
Introduction to Stochastic Dynamical Systems

Recall:
Deterministic Dynamical Systems

$$\dot{x} = f(x)$$

Examples:
Newton's sceond law
Hodgkin-Huxley system
Michaelis–Menten kinetics
SIR Model for Spread of Disease

What to Do with Dynamical Systems?

Recall: Solving Algebraic Equations —
New ideas and new math branches —
Complex numbers, algebraic geometry, Fermat's last theorem, Newton's method, optimization....

Structures and properties of “solutions"!

Solving Differential Equations —
New ideas and new math branches —
Qualitative theory, geometric methods, topological indexes, invariant sets and chaos, time-discretization/Poincare map

Structures and properties of “trajectories"!
"Dynamical Systems": Prediction

What are Stochastic Dynamical Systems?

Stochastic Differential Equations:

$$\dot{x} = f(x, \text{noise})$$

Examples:

Dynamical systems under noisy fuctuations!

Stochastic Dynamical Systems: Pre-History

• Statistical mechanics (Maxwell, Boltzmann, density, distribution, ergodicity)

• Math theory of Brownian motion
Einstein 1905
Smoluchowski 1906
Wiener 1920s
Lévy 1930s

• Langevin Equation 1908

• Fokker-Planck equation 1914 & 1917

• Kolmogrov equations for stochastic processes, 1930s

Stochastic Dynamical Systems: History

1940-60s: Stochastic calculus
Itô, Doeblin, Gikhman-Skorohod
1970s: Stochastic differential equations (SDEs)
Ikeda-Watanabe, L. Arnold, Friedman

1976: Klaus Hasselmann (Nobel in Physics 2021)
Climate system: Stochastic slow-fast dynamics

1980s: Stochastic flows, cocycles
Elworthy, Baxendale, Bismut, Ikeda, Kunita, Xue-Mei Li,...

1980s—: Non-equilibrium statistic mechanics
1980s: Nelson stochastic mechanics
Recent advances: Jean-Claude Zambrini & Qiao Huang 2022
1985–: Oksendal - Stochastic Differential Equations

1990s: Dynamical systems approaches for SDEs
L. Arnold and Bremen School

Statistical features of noisy fluctuations:

Stochastic Differential Equations:

$$\dot{x} = f(x, \text{noise})$$

Noise: A special stochastic process
Heavy tail or light tail probability densities

Non-Gaussian distribution or Gaussian distribution

Question:

What does a stochastic diffential equation look like?

How to take noise into account in math modeling?

How to describe noise?

• Math theory of Brownian motion
Einstein 1905
Smoluchowski 1906
Wiener 1923
Lévy 1937

Noisy process $\xi_t(\omega)$:
Independent increments & stationary increments

(Note: We deal with increments everyday in math and science!)

What could be a probability distribution for the "random increments"?

Central Limit Theorem: Independent measurements and then “averaging"

$X_1, X_2, \cdots, X_n$ are independent, identically distributed (iid) random variables (i.e., ‘measurements’)

Central Limit Theorem

A stable random variable X comes from “averaging the measurements": $\lim_{n\to\infty} \frac{X_1+\cdots+X_n-b_n}{a_n} = X$ in distribution for some constants a_n, b_n ($a_n \neq 0$)

Notation: $X \sim S_\alpha, \quad 0 < \alpha \leq 2$

$\alpha-$stable random variable

α: Non-Gaussianity index

A special case: $\alpha = 2$

Well-known normal random variable emerges when $\alpha = 2$
$\mathbb{E}X_i = \mu, \ \ \mathrm{Var}(X_i) = \sigma^2$

Central limit theorem: A normal random variable comes from "averaging the measurements"
$\lim_{n\to\infty} \frac{X_1+\cdots+X_n-n\mu}{\sigma\sqrt{n}} = X \ \sim \mathcal{N}(0,1)$ in distribution Namely,
$\lim_{n\to\infty} \mathbb{P}(\frac{X_1+\cdots+X_n-n\mu}{\sigma\sqrt{n}} \leq x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} e^{-x^2/2} dx$

Gaussian vs. Non-Gaussian random variables

Gaussian: Normal random variable $X \sim \mathcal{N}(0,1)$
Probability density function $f(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$

$$\mathbb{P}(X \leq x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \, dx$$

Non-Gaussian: $\alpha-$stable random variable $X \sim S_\alpha, \ 0 < \alpha < 2$
Probability density function $f_\alpha(x)$

$$\mathbb{P}(X \leq x) = \int_{-\infty}^{x} f_\alpha(x) \, dx$$

Prob density function for a Gaussian random variable

$X \sim \mathcal{N}(0,1)$

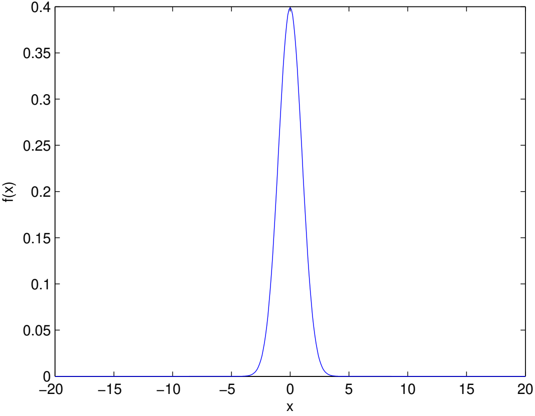


Figure: "Bell shape": Exponential decay, light tail

Prob density function for a non-Gaussian, $\alpha-$stable random variable

$X \sim S_\alpha$

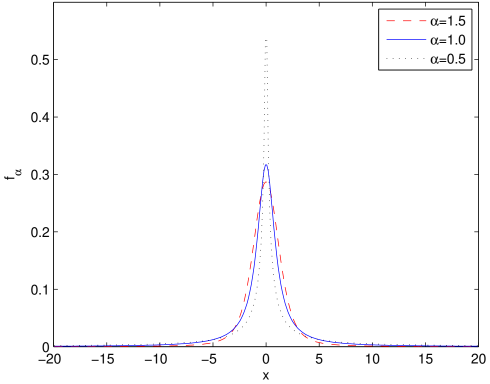


Figure: Polynomial decay, heavy tail

Lévy Motion L_t^α

Definition: Lévy motion L_t^α with $0 < \alpha < 2$:
(1) $L_0^\alpha = 0, \; a.s.$
(2) Stationary increments $L_t^\alpha - L_s^\alpha \sim S_\alpha(|t-s|^{\frac{1}{\alpha}}, 0, 0)$
(3) L_t^α has independent increments

Note: Paths are stochastically continuous (i.e., right continuous with left limit; countable jumps): $L_t^\alpha \to L_s^\alpha$ in probability as $t \to s$
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**
J. Duan: **An Intro to Stochastic Dynamics**

A special case: 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
J.-F. Le Gall:
Brownian Motion, Martingales, 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

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

'General' form of stochastic governing laws

Recall:

General form of Newton's second law:
$\ddot{x} = F(x)$

General form of dynamical systems/governing laws:
$\dot{x} = f(x)$

Goals of Random Dynamical Systems

Subjects: Structures and Properties of “trajectories or orbits"

Methods: Geometric, analytical, probabilistic or computational

Phenomena:
Transition, transport, diffusion, critical dynamics, control, peculiar

Applications:
Microscopic mechanisms
Unresolved scales
Random algorithms (stochastic gradient descent)
Open quantum dynamics
Stochastic biodynamics
Climate dynamics
Stochastic Dynamics+Data Science

Stochastic Dynamical Systems: Some current activities

- SDEs and SPDEs with Lévy Noise
- Gaussian vs Non-Gaussian Noise
- Local vs Non-local Generators/Partial Diff Eqns
- Markov vs Non-Markov Approaches
- Hamiltonian vs Dissipative Dynamics
- Interactions with:
  Non-equilibrium statistical mechanics
  Open quantum dynamics
  Geophysical systems
  Biophysical dynamics
- Interface with:
  Data science

Stochastic Dynamical Systems: Some current activities

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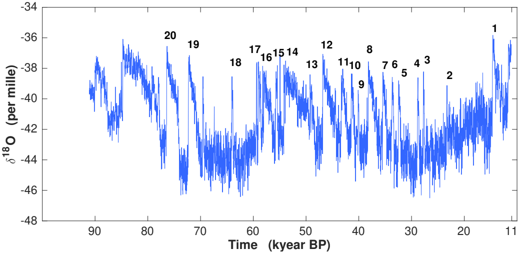
Lecture 2:
Transition Phenomena

What Are Transition Phenomena ?

Motivation: Climate transitions in Greenland Ice-Core data

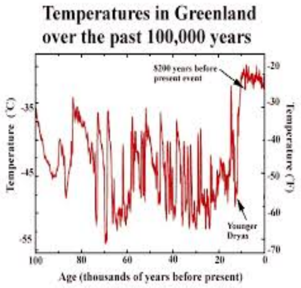
Dansgaard-Oeschger events: Abrupt shifts in temperature

$\delta^{18}O$ record between 10000 and 90,000 years before present.



Measured temperature for the past 100000 years

Niels Bohr Institute: Ditlevsen 1999



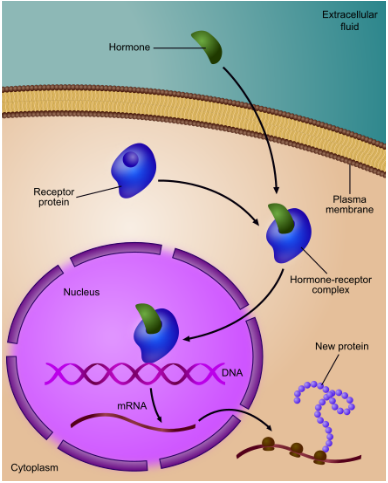
Metastable patterns & Transitions between patterns

Stochastic differential equation model:

$\dot{x}(t) =$ vector field $+$ Lévy noise

Motivation: Transcription in gene expression

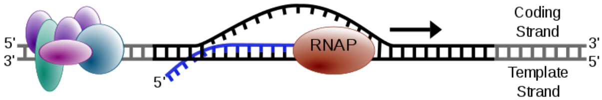
Gene expression = Transcription + Translation
Gene (DNA segment) $\rightarrow$ mRNA $\rightarrow$ Protein



Transcription

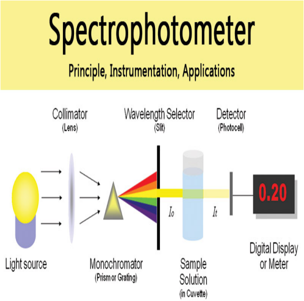
Transcription: Gene $\to$ mRNA

Transcription factor:
A protein activating or repressing transcription



Measurement data: Concentration of a transcription factor

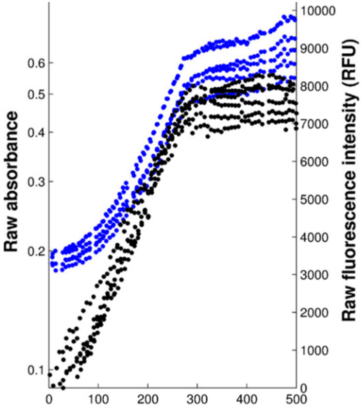
Transcription factor ('**a protein**'):
High concentration means active transcription
So its concentration evolution matters



Absorbance or Fluorescence intensity:
Correspond to concentration of a transcription factor

Data: Evolution of concentration of a transcription factor

Stefan et al.: PLOS Compu. Biology, 2015



Metastable patterns & Transitions between patterns

Noisy gene expression: From experts in domain science

- Raser-O'Shea: Science, 2010
  Noise in Gene Expression: Origins, Consequences, and Control
  Sources of Randomness: fluctuating biochemical reactions, variation in cell division, random mutation

- Elowitz: Nature 2011, Science 2007
  Stochastic differential equations for evolution of concentration of transcription factors
  Differential equation model: $\dot{x}(t) = \cdots$

What are transition phenomena?

State transitions from one 'regime' to another regime:

- **Climate change:** Temperature shifts between metastable states
- **Transitions in gene regulation:** Transcription is a transition —- from low concentration to high concentration in proteins
- **Many others—**
  Contaminant transport to reach a specific region
  Tumor cell density decreases zero (cancer-free)
  Abrupt changes in physics and chemistry

No transition between stable equilibrium states in deterministic dynamical systems

A dynamical system:

$$\frac{dx}{dt} = f(x)$$

Dynamical patterns: Stable or unstable equilibrium points, ...

J. Guckenheimer and P. J. Holmes
Nonlinear Oscillations, Dynamical Systems, and Bifurcations of Vector Fields., 1983.

Transition in stochastic dynamical systems?

Mechanism: **Interaction between nonlinearity & uncertainty**

$$\frac{dX_t}{dt} = f(X_t) + \text{Noise}$$

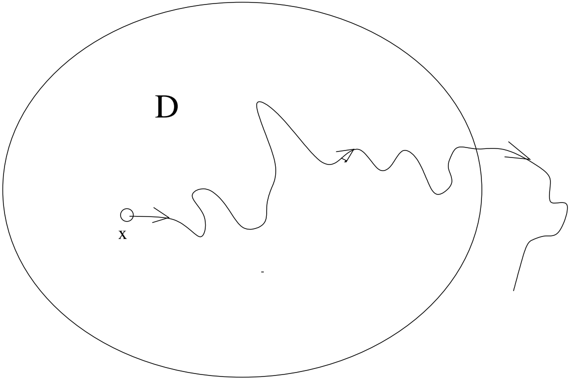
Metastable stable states: Stable equilibrium states of $\dot{x} = f(x)$

Trajectories may '**connect**' metastable states.

Mean exit time of solution orbit from a domain

$$dX_t = f(X_{t-})dt + \sigma(X_{t-})dB_t + dL_t, \quad X_0 = x,$$

where B_t is a Brownian motion, L_t is a Lévy motion with generating triplet $(0, 0, \nu)$.
Mean exit time from a domain D:



First exit time τ_x of a solution path (i.e., a ‘particle’) starting at x from a bounded domain D as

$$\tau_x(\omega) \triangleq \inf\{t \geq 0, X_t(\omega, x) \notin D\}.$$

The mean exit time is then denoted by

$$u(x) = \mathbb{E}^x \tau_x(\omega),$$

for $x \in D$.

Theorem

Mean exit time $u(x)$, for a solution path starting at $x \in D$, satisfies the following nonlocal partial differential equation

$$Au = -1, \quad u|_{D^c} = 0, \tag{1}$$

where A is the generator

$$Au = f \cdot \nabla u + \frac{1}{2} Tr[\sigma\sigma^T H(u)] \tag{2}$$

$$+ \int_{\mathbb{R}^n \setminus \{0\}} [u(x+y) - u(x) - I_{\{\|y\|<1\}}\, y \cdot \nabla u(x)]\, \nu(dy), \tag{3}$$

and D^c is the complement of the bounded domain D in $\mathbb{R}^n$.

Escape probability

Likelihood for a system transition from one regime to another

- **Contaminant transport:** likelihood for contaminant to reach a specific region
- **Climate:** likelihood for temperature to be within a range
- **Tumor cell density:** likelihood for tumor density to decrease (becoming cancer-free)

How to quantify escape probability?

Question:

Can we use the nonlocal operator or related PDE to investigate stochastic dynamics?

$$dX_t = f(X_t)dt + dL_t^{\alpha}$$

• **Examine** quantities that carry dynamical information:

Escape probability

Likelihood of transition between different dynamical regimes!

Escape probability from a domain D

Consider a SDE

$$dX_t = f(X_t)dt + dL_t^{\alpha}, \quad X_0 = x \in D$$

Escape probability $p(x)$:
Likelihood that a “particle **x**" first escapes D and lands in U

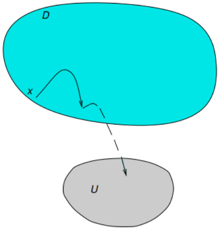


Figure: Domain D, with a target domain U in D^c

A surprising connection between escape probability and harmonic functions!

What is a harmonic function?

Recall: What is a harmonic function?

It is a solution of the Laplace equation:

$$\Delta h(x) = 0$$

But Δ is the generator of Brownian motion B_t

So we say:
$h(x)$ is a harmonic function with respect to Brownian motion

An analogy:

Harmonic function with respect to Lévy motion L_t^{α}:

$$(-\Delta)^{\frac{\alpha}{2}} h(x) = 0$$

where $(-\Delta)^{\frac{\alpha}{2}}$ is the generator of L_t^{α}

Note: Feedback of Probability Theory to Analysis!

A further analogy:

Consider a stochastic system

$$dX_t = f(X_t)dt + dL_t^{\alpha}$$

Generator for solution process X_t:

$$A_{\alpha}h(x) = f^T(x)\nabla h(x) - K_{\alpha}\,(-\Delta)^{\frac{\alpha}{2}}h(x)$$

Harmonic function with respect to X_t: $A_{\alpha}h(x) = 0$

Nonlocal deterministic partial differential equation

What is the connection between escape probability & harmonic functions?

Escape probability from a domain D

Escape probability $p(x)$:
Likelihood that a "particle **x**" first escapes D and lands in U

Exit time: $\tau_{D^c}(x)$ is the first time for X_t to escape D

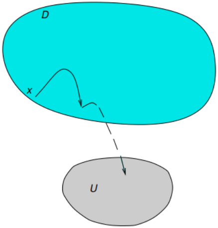


Figure: Domain D, with a target domain U in D^c

Connection: Escape probability & harmonic function

$$dX_t = f(X_t)dt + dL_t^\alpha, \quad X_0 = x \in D$$

For

$$\varphi(x) = \begin{cases} 1, & x \in U, \\ 0, & x \in D^c \setminus U, \end{cases}$$

$$\begin{aligned} \mathbb{E}[\varphi(X_{\tau_{D^c}(x)})] &= \int_{\{\omega: X_{\tau_{D^c}} \in U\}} \varphi(X_{\tau_{D^c}}) d\mathbb{P}(\omega) \\ &\quad + \int_{\{\omega: X_{\tau_{D^c}} \in D^c \setminus U\}} \varphi(X_{\tau_{D^c}}) d\mathbb{P}(\omega) \\ &= \mathbb{P}\{\omega : X_{\tau_{D^c}} \in U\} \\ &= p(x) \end{aligned}$$

But, left hand side is a harmonic function with respect to X_t
Liao 1989

Escape probability from a domain D

$$dX_t = f(X_t)dt + dL_t^\alpha, \quad X_0 = x \in D$$

Escape probability $p(x)$: Likelihood that a ”particle **x**" first escapes D and lands in U

Theorem

Escape probability p is solution of Balayage-Dirichlet problem

$$\begin{cases} A_\alpha p = 0, \\ p|_U = 1, \\ p|_{D^c \setminus U} = 0, \end{cases} \tag{4}$$

where A_α is the generator for X_t.

Qiao, Kan & Duan, 2013

Einstein theory for Brownian motion

Einstein: 1905
Macroscopic theory for particles following Brownian motion (liquid is motionless)

$$\frac{dX_t}{dt} = 0 \; + \; \frac{dB_t}{dt}, \quad X_0 = \xi$$

$X_t = \xi + B_t \sim \mathcal{N}(\xi, t)$ Probability density: $p(x,t) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{(x-\xi)^2}{2t}}$

$$p_t = \frac{1}{2} p_{xx} \; (= \frac{1}{2} \Delta p)$$

Fokker-Planck eqn

Fokker, 1914; Planck, 1917

L. C. Evans: *Introduction to Stochastic Differential Equations* 2014

Fokker-Planck equation

For a system described by a scalar stochastic differential equation with Brownian motion (a Gaussian process),

$$dX_t = b(X_t)dt + dB_t, \quad X_0 = \xi$$

$b(x)$: Vector field (or drift term)
$p(x,t)$: Probability density function for the solution X_t
Fokker-Planck equation contains the usual Laplacian operator Δ,

$$p_t = \frac{1}{2}\Delta p - (b(x)p)_x.$$

Fokker-Planck eqn = Laplace + Liouville

Nonlocal Laplace operator ?

Nonlocal operators & nonlocal partial differential equations

Main Ideas:

(i) Solution process of a stochastic system is a Markov process

(ii) Markov process $\rightarrow$ Semigroups

(iii) Generator A for solution process:

Nonlocal operators!
Pseudo-partial differential operators
Partial differential equations

Generator of a Markov stochastic process X_t: $X_0 = x$

Semigroup: For observable φ

$$P_t\varphi(x) \triangleq \mathbb{E}\varphi(X_t)$$
$$P_{t+s} = P_t P_s$$

Generator: Derivative of semigroup P_t at time 0

$$A\varphi(x) \triangleq \frac{d}{dt}|_{t=0} P_t\varphi(x)$$

Generator A carries info about stochastic process X_t

Fokker-Planck equation for probability density evolution:
$\partial_t p(x,t) = A^* p(x,t)$

Adjoint operator in L^2: A^*

Example: Generator of B_t

Generator for Brownian motion $X_t = x + B_t$ is Laplacian: $\frac{1}{2}\Delta$

$$\mathbb{E}f(X_t) = \frac{1}{\sqrt{2\pi t}} \int f(y)\, e^{-\frac{(y-x)^2}{2t}} dy$$

$$\begin{aligned} \frac{\mathbb{E}f(X_t) - f(x)}{t} &= \frac{1}{\sqrt{2\pi}} \int \frac{z\sqrt{t} f'(x) + \frac{1}{2} z^2 t f''(x + \theta z\sqrt{t})}{t}\, e^{-\frac{z^2}{2}} dz \\ &= \frac{1}{2}\frac{1}{\sqrt{2\pi}} \int z^2 f''(x + \theta z\sqrt{t})\, e^{-\frac{z^2}{2}} dz. \end{aligned}$$

$$Af(x) = \frac{d}{dt}|_{t=0}\mathbb{E}f(X_t) = \frac{1}{2} f''(x)$$

$$A = \frac{1}{2}\Delta$$

Example: Generator of L_t^α

Generator for $\alpha-$stable Lévy motion is:
Nonlocal operator

$$A_\alpha \varphi = \int_{\mathbb{R}^1 \setminus \{0\}} [\varphi(x+y) - \varphi(x)] \, \nu_\alpha(dy)$$

$\nu_\alpha(dy) = C_\alpha \frac{dy}{|y|^{d+\alpha}}$: Jump measure for L_t^α
C_α, K_α: Constants depending on α

Applebaum 2009

Fourier analysis for generator of L_t^α

$$
\begin{aligned}
A_\alpha \varphi &= \int_{\mathbb{R}^1\setminus\{0\}} [\varphi(x+y) - \varphi(x)]\, \nu_\alpha(dy) \\
\mathbb{F}(A_\alpha u(x)) &= \mathbb{F} \int_{\mathbb{R}^1\setminus\{0\}} [\varphi(x+y) - \varphi(x)]\, \nu_\alpha(dy) \\
&= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}^1} e^{-ikx} \int_{\mathbb{R}^1\setminus\{0\}} [\varphi(x+y) - \varphi(x)]\, \nu_\alpha(dy)\, dx \\
&= c_\alpha \int_y \frac{1}{|y|^{1+\alpha}} dy \cdot \frac{1}{\sqrt{2\pi}} \int_x e^{-ikx} [\varphi(x+y) - \varphi(x)] dx \\
&= c_\alpha \int_y \frac{1}{|y|^{1+\alpha}} [e^{iky} - 1] dy \cdot \mathbb{F}(u) = -\gamma_\alpha |k|^\alpha \mathbb{F}(u)
\end{aligned}
$$

Recall: $\mathbb{F}(-\Delta u(x)) = \|k\|^2 \mathbb{F}(u)(k)$
Hence: Generator $A_\alpha \sim -(-\Delta)^{\frac{\alpha}{2}}$

Eigenvalues for generator of L_t^α

$$A_\alpha \varphi = \int_{\mathbb{R}^1 \setminus \{0\}} [\varphi(x+y) - \varphi(x)]\, \nu_\alpha(dy) \sim -(-\Delta)^{\frac{\alpha}{2}}$$

Nonlocal Laplace operator:
Looking like an integral operator!
But behaving like a differential operator!

Eigenvalues on $D = (-\pi, \pi)$: $0 < \alpha < 2$

$$\lambda_n = \left(\frac{n}{2} - \frac{(2-\alpha)}{8}\right)^\alpha + o(\frac{1}{n}).$$

$$0 < \lambda_1 < \lambda_2 \leq \cdots \leq \lambda_n \leq \cdots, \text{ for } n = 1, 2, \cdots.$$

Eigenfunctions φ_n form a complete orthonormal basis in $L^2(D)$.

The larger the α value, the stronger the dissipation!

Generator for solution process X_t

Stochastic Differential Equation (SDE):

$$dX_t = f(X_t)dt + dL_t^{\alpha}$$

Generator for solution process X_t:

$$A_\alpha h(x) \triangleq f^T(x)\nabla h(x) - K_\alpha \, (-\Delta)^{\frac{\alpha}{2}} h(x)$$

Fokker-Planck operator
$=$ Liouville operator $+$ Nonlocal Laplace operator

Nonlocal Fokker-Planck equation

For a system described by a scalar stochastic differential equation with $\alpha-$stable Lévy motion L_t^α (a non-Gaussian process), $\alpha \in (0,2)$

$$dX_t = b(X_t)dt + dL_t^\alpha, \quad X_0 = \xi$$

$p(x,t)$: probability density function for the solution X_t
Nonlocal Fokker-Planck equation contains the nonlocal Laplacian operator A_α,

$$p_t = \frac{1}{2}A_\alpha p - (b(x)p)_x$$

$$A_\alpha f(x) \triangleq -(-\Delta)^{\alpha/2} f(x) = c_\alpha \int_{\mathbb{R}^1\setminus\{0\}} \frac{f(x+y)-f(x)}{|y|^{1+\alpha}} dy, \ \ 0<\alpha<2,$$

When the vector field $b(\cdot)$ depends on the distribution of X_t:
The divergence term $(bp)_x$ becomes nonlinear!

Lecture 3:
Variational Methods for the Most Probable Transition Pathways

The Most Probable Transition Pathways via Onsager-Machlup Least Action Principle

Euler-Lagrange equations

Transition phenomena in stochastic dynamical systems

A "rare" but dynamically important shift event between two metastable states

Definition:
A metastable state is an unperturbed equilibrium stable state.

Most probable transition pathway —

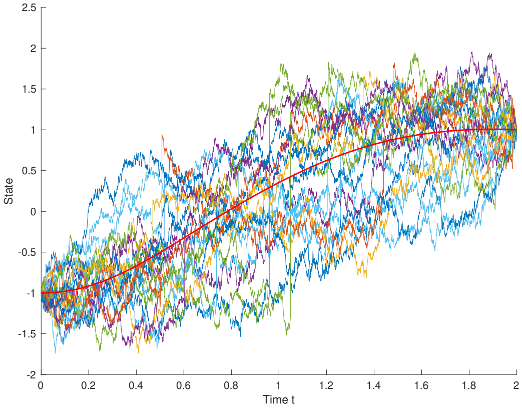
A 'reference trajectory' from one metastable state to another

Small tube around the most probable transition pathway

Idea —

Probability estimate for solution paths to stay inside a 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.

$\propto$: denotes the equivalence relation for δ small enough.
Max $\mathbb{P}(\{\|X - z\| \leq \delta\})$ or Min $\int_0^T OM\, dt$: Most probable transition pathway

How to get the most probable transition pathway?

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

Minimizer $z_m(t)$: Most probable transition pathway

$z_m(0) = x_0, \quad z_m(T) = x_1$

Two metastable states: x_0, x_1

Most probable transition pathways: Need to derive Onsager-Machlup action functional

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

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

2019: SDEs with (non-Gaussian) Lévy noise

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

Chao & Duan, Nonlinearity, June 2019

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$\propto$: denotes the equivalence relation for δ small enough Min $\int_0^T OM\, dt$: Most probable transition pathway $z_m(t)$

Derivation of Onsager-Machlup action functional
One dimensional case

Consider the following scalar stochastic differential equation, for $t \in [0, T]$

$$dX_t = f(X_t)dt + c\, dB_t + dL_t,$$
$$X_0 = x_0.$$

Onsager-Machlup action functional

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:

$$OM(\dot{z}, z) = (\frac{\dot{z} - f(z)}{c})^2 + f'(z) + 2\frac{\dot{z} - f(z)}{c^2} \int_{|\xi|<1} \xi\nu(d\xi), \quad (5)$$

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

Contribution of Lévy noise: Third term
When jump measure is absent: Recover the OM function 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

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

Huang-Chao-Wei-Duan– Estimating the Most Probable Transition Time for Stochastic Dynamical Systems. Nonlinearity, 2021, vol. 34, 4543

Most probable path $z_m(t)$ via Euler-Lagrange equation

The most probable path $z_m(t)$:
Minimizer for Onsager-Machlup functional $\int_0^T OM(\dot{z}(t), z(t))dt$:
Corresponding Euler-Lagrange equation:

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

That is:

$$\ddot{z}_m(t) = \frac{c^2}{2} f''(z_m) + f'(z_m)f(z_m) - f'(z_m)\int_{|\xi|<1} \xi \; \nu(d\xi)$$

with initial and final conditions: $z_m(0) = x_0, z_m(T) = x_1$.
Shooting method

Most probable transition pathway: Theoretical results

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 $(\dot{z}, z)$.

Derivation of Onsager-Machlup action functional High dimensional case

Consider the following stochastic differential equation system, for $t \in [0, T]$

$$dX(t) = f(X(t))dt + BdW(t) + dL(t), t \in [0, 1],$$

with initial data $X(0) = x_0 \in \mathbb{R}^d$, where B is a nondegenerate $d \times d$ matrix.

Derivation of Onsager-Machlup action functional High dimensional case

Assumption on the vector field:
Let F be a mapping from $\mathbb{R}^d$ to $\mathbb{R}^d$. For each $x \in \mathbb{R}^d$, assume that $DF(x)$ is a symmetric matrix from $\mathbb{R}^d$ to $\mathbb{R}^d$. Then, there exists a smooth function $V : \mathbb{R}^d \to \mathbb{R}$, such that for all $x \in \mathbb{R}^d$, DV(x)=F(x).

Explanation:
The dual space of $\mathbb{R}^d$ is itself. Also, the tangent bundle and cotangent bundle are both $\mathbb{R}^{2d}$. So for each $x \in \mathbb{R}^d$, $F(x)$ can be regard as a 1-form. Then it is a closed 1-form due to the symmetry of $DF(x)$. Thus by the Poincaré lemma, it is an exact form, i.e. there exists a smooth function $V : \mathbb{R}^d \to \mathbb{R}$, such that for all $x \in \mathbb{R}^d$, $DV(x) = F(x)$. $\square$

Derivation of Onsager-Machlup action functional
High dimensional case

Theorem

Assume that the diffusion matrix B is nondegenarate such that $B^{-1}f$ is C_b^2 in x, φ^h , and the Lévy jump measure ν satisfies that $\int_{|x|<1} |x|\nu(dx) < \infty$. Let $g(x) = (B^{-1})^*(B^{-1}f(x))$. If the gradient $\nabla_x g(x)$ is symmetric, then the Onsager-Machlup action functional is $\int_0^1 L(\varphi^h, \dot{\varphi}^h)ds$, with Lagrangian

$$L(\varphi^h, \dot{\varphi}^h) = \frac{1}{2}|B^{-1}[f(\varphi^h(t)) - \dot{\varphi}^h(t) - \eta]|^2 + \frac{1}{2}Tr[\nabla_x f(\varphi^h(s))], \tag{6}$$

with $\eta = \int_{|\xi|<1} \xi\nu(d\xi)$.

Jianyu Chen and Jianyu Hu:
Transition pathways for a class of high dimensional stochastic dynamical systems with Lévy noise. *Chaos*, 2021.

Remarks

1. We see that, the quadratic term is the main term, while the divergence term comes from the Itô correction of Brownian motion. Moreover, only small jumps contribute to the Onsager-Machlup action functional and the effect is similar to adding the mean value of small jumps to the drift.

2. We require the symmetry of the gradient $\nabla_x g(x)$. We apply the Poincaré lemma which requires the symmetry condition to obtain the original function.

Open problems in deriving Onsager-Machlup action functionals

For SDEs with non-Gaussian noise:

1. Remove the gradient structure for the vector fields
2. Include multiplicative noise

Example: A stochastic genetic regulatory system

Genetic regulatory system (Smolen et al. Amer. J. Physiol. 1998):

$$\dot{X}_t = \frac{k_f X_t^2}{X_t^2 + K_d} - k_d X_t + R_{bas}, \qquad X_0 = x_0,$$

X_t: Concentration of a transcription factor activator ('**protein**')

Vector field ('drift'): $f(x) = \frac{k_f X_t^2}{X_t^2 + K_d} - k_d X_t + R_{bas}$.

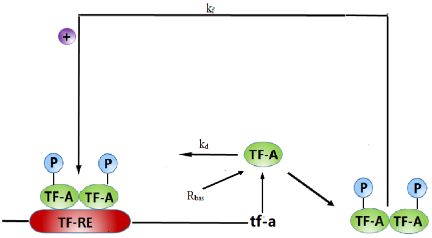


Figure: Genetic regulatory model

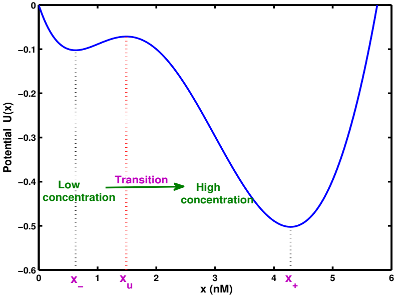


Figure: The bistable potential U for the TF-A monomer concentration model. $k_f = 6\ \mathrm{min}^{-1},\ K_d = 10,\ k_d = 1\ \mathrm{min}^{-1}$, and $R_{bas} = 0.4\ \mathrm{min}^{-1}$.

The potential function $U(x)$ is given by $f(x) = -U'(x)$.
Two stable states: $x_- \approx 0.62685\ \mathrm{nM}, \qquad x_+ \approx 4.28343\ \mathrm{nM}$;
The unstable state (a saddle point): $x_u \approx 1.48971\ \mathrm{nM}$.

The stochastic genetic regulation system:

$$\dot{X}_t = \frac{k_f X_t^2}{X_t^2 + K_d} - k_d X_t + (R_{bas} + \epsilon \dot{B}_t), \qquad X_0 = x_0,$$

Noise intensity: ϵ Standard Gaussian noise: B_t

Noise sources on basal synthesis rate R_{bas}:

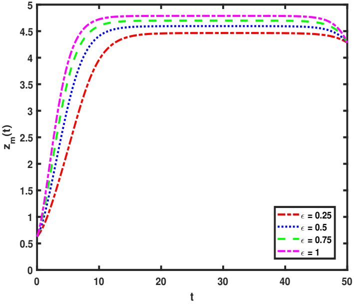
- External noisy environment;
- Inherent uncertainty: such as the biochemical reactions, the concentrations of other proteins, and gene mutations.

Raj & Oudenaarden: Ann. Rev. Biophys. 2009.

The most probable pathways: Brownian noise
Noise intensity: $\epsilon = 0.25,\ 0.5,\ 0.75,\ 1$

Euler-Lagrange eqn:

$$\ddot{z}_m(t) = \frac{\epsilon^2}{2} f''(z_m) + f'(z_m) f(z_m), \quad t \in (0, T),$$
$$z_m(0) = x_- \approx 0.62685\ , \quad z_m(T) = x_+ \approx 4.28343.$$



Cheng, Wang, Duan & Li, Physica A, 2019

The most probable pathways: Computing

Low dimensions: Shooting method

High dimensions:
Yang Li, Jinqiao Duan and Xianbin Liu:
A Machine Learning Framework for Computing the Most Probable Paths of Stochastic Dynamical Systems
Phys. Review E. 2021.

Jianyu Chen and Jianyu Hu:
Transition pathways for a class of high dimensional stochastic dynamical systems with Lévy noise
Chaos. 2021.

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

An optimal control method to compute the most likely transition

Conclusion

Introducing Stochastic Dynamical Systems

Examining Transition Phenomena via Onsager-Machlup Action Functionals

Analyzing the Most Probable Transition Pathways