Path integrals for classical Markov processes

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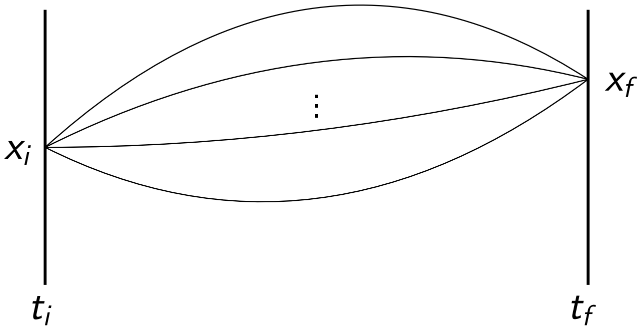
- Slides: `www.maths.qmul.ac.uk/~ht/talks.html`

Quantum path integral



- Propagator:

$$K({\color{red}x_f}, {\color{red}t_f} | {\color{blue}x_i}, {\color{blue}t_i}) = \langle {\color{red}x_f}, {\color{red}t_f} | {\color{blue}x_i}, {\color{blue}t_i} \rangle$$

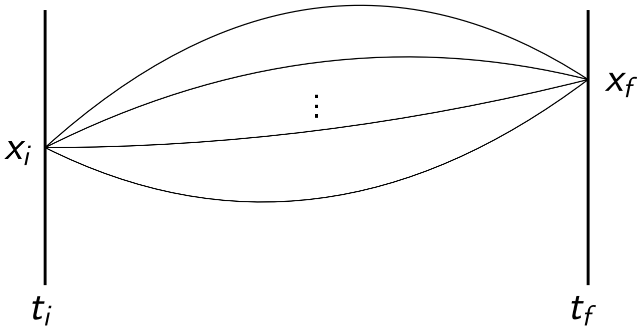
- Propagation:

$$\psi({\color{red}x_f}, {\color{red}t_f}) = \int K({\color{red}x_f}, {\color{red}t_f} | {\color{blue}x_i}, {\color{blue}t_i})\, \psi({\color{blue}x_i}, {\color{blue}t_i})\, d{\color{blue}x_i}$$

- Path integral:

$$K({\color{red}x_f}, {\color{red}t_f} | {\color{blue}x_i}, {\color{blue}t_i}) = \int_{x({\color{blue}t_i})}^{x({\color{red}t_f})} \mathcal{D}[x]\, e^{iS[x]/\hbar} = \sum_{\text{all paths}} e^{iS[\text{path}]/\hbar}$$

Classical path integral



- Propagator:

$$P(x_f, t_f | x_i, t_i) = \text{Prob}\{x(t_i) \to x(t_f)\}$$

- Propagation (Kolmogorov-Chapmann equation):

$$P(x_f, t_f) = \int P(x_f, t_f | x_i, t_i)\, P(x_i, t_i)\, dx_i$$

- Path integral:

$$P(x_f, t_f | x_i, t_i) = \int_{x(t_i)}^{x(t_f)} \mathcal{D}[x]\, e^{-S[x]/\epsilon} = \sum_{\text{all paths}} e^{-S[\text{path}]/\epsilon}$$

Comparison

Quantum path integral

- K quantum amplitude
- Interference possible
- Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = H\psi(x,t)$$

- H hermitian
- $\hbar \to 0$: semi-classical limit

Classical path integral

- P classical probability
- No interference
- Fokker-Planck equation:

$$\frac{\partial}{\partial t}P(x,t) = LP(x,t)$$

- L non-hermitian in general
- $\epsilon \to 0$: low-noise limit

Type of stochastic processes

- Continuous time Markov processes
- Stochastic differential equations

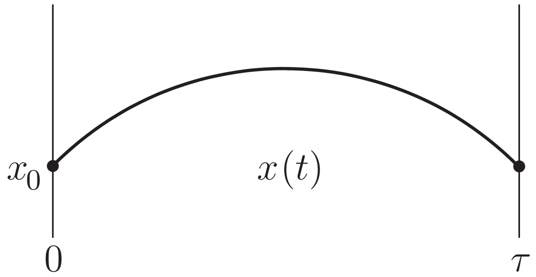
Stochastic differential equations

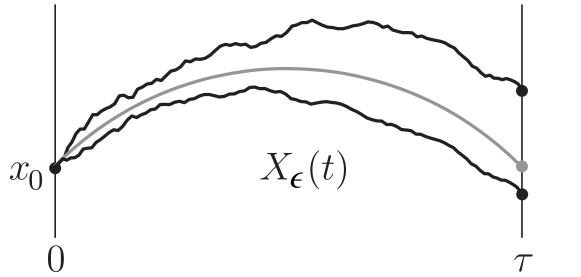
- Deterministic dynamics (ODE):

$$\dot{x}(t) = F(x)$$

- Perturbed dynamics (SDE):

$$\dot{X}_\epsilon(t) = F(X_\epsilon) + \underbrace{\sqrt{\epsilon}\,\xi(t)}_{\text{noise}}$$



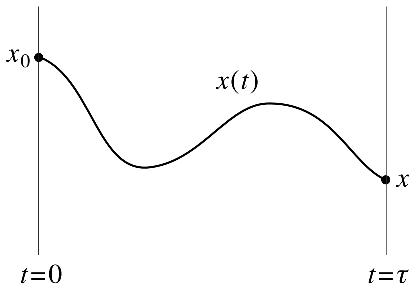


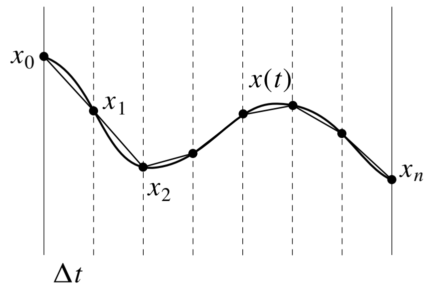
$$x_{t+\Delta t} = x_t + F(x_t)\Delta t \qquad X_{t+\Delta t} = X_t + F(X_t)\Delta t + \sqrt{\epsilon}\,\Delta W_t$$

- Gaussian white noise:

$$\Delta W_t \sim \mathcal{N}(0, \Delta t)$$

Path integral





- Time discretization:

$$\begin{aligned} P[x] &= \lim_{n\to\infty} P(x_1, x_2, \ldots, x_n | x_0) \\ &= \lim_{n\to\infty} P(x_n|x_{n-1}) \cdots P(x_2|x_1) P(x_1|x_0) \end{aligned}$$

- Infinitesimal propagator:

$$P(x', t+\Delta t | x, t) = \frac{1}{\sqrt{2\pi\epsilon\Delta t}} \exp\left(-\frac{\Delta t}{2\epsilon} \left[\frac{x'-x}{\Delta t} - F(x) \right]^2 \right)$$

- Path distribution:

$$P[x] = c\, e^{-S[x]/\epsilon}, \qquad S[x] = \int_0^\tau L(\dot{x}, x)\, dt, \qquad L = \frac{1}{2}[\dot{x} - F(x)]^2$$

Dominant path approximation

- Low-noise approximation:

$$P(x_f, t_f | x_i, t_i) = \int \mathcal{D}[x]\, e^{-S[x]/\epsilon}$$
$$\approx e^{-\min S[x]/\epsilon} \qquad \epsilon \to 0$$
$$= e^{-S[x^*]/\epsilon}$$

- Final result:

$$P(x_f, t_f | x_i, t_i) \approx e^{-V(x_f, t_f | x_i, t_i)/\epsilon}$$
$$V(x_f, t_f | x_i, t_i) = \min_{x(t): x(t_i)=x_i, x(t_f)=x_f} S[x]$$

- Dominant path:

$$x^*(t) : \min S[x] \quad \Rightarrow \quad \delta S = 0$$

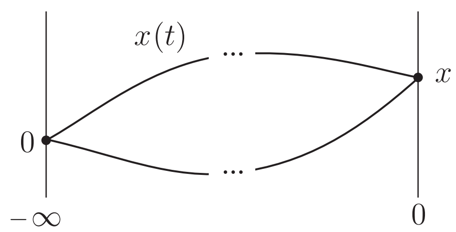
- Euler-Lagrange equation:

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{x}} - \frac{\partial L}{\partial x} = 0, \qquad x(t_i) = x_i, x(t_f) = x_f$$

Applications

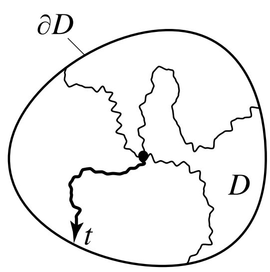
- Stationary distribution:

$$P(x) \approx e^{-V(x)/\epsilon}$$
$$V(x) = \min_{x(t): x(-\infty)=0, x(0)=x} S[x]$$



- Exit time:

$$\tau_\epsilon \approx e^{V^*/\epsilon} \quad \text{in probability}$$
$$V^* = \min_{x \in \partial D} \min_{t \geq 0} V(x, t | x_0, 0)$$



- Exit path = dominant path = instanton
- Exit location = $x(\tau_\epsilon)$
- Semiclassical or WKB approximation

Example: Ornstein-Uhlenbeck process

- SDE:

$$\dot{x}(t) = -\gamma x(t) + \sqrt{\epsilon}\,\xi(t)$$

- Stationary distribution:

$$P(x) \approx e^{-V(x)/\epsilon}, \qquad V(x) = \min_{x(t):x(0)=x_0, x(\infty)=x} S[x]$$

- Euler-Lagrange equation:

$$\ddot{x} - \gamma^2 x = 0, \qquad x(-\infty) = 0,\ x(0) = x$$

- Instanton solution:

$$x^*(t) = xe^{\gamma t}, \qquad (\dot{x}^* = \gamma x^*)$$

- Solution:

$$V(x) = S[x^*] = \gamma x^2$$

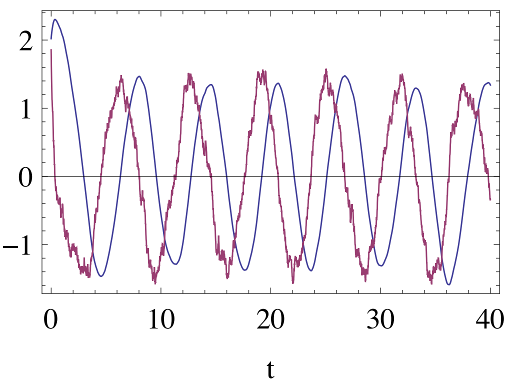
  - $P(x)$ Gaussian
  - Instanton = time reverse of deterministic dynamics ($\epsilon = 0$)

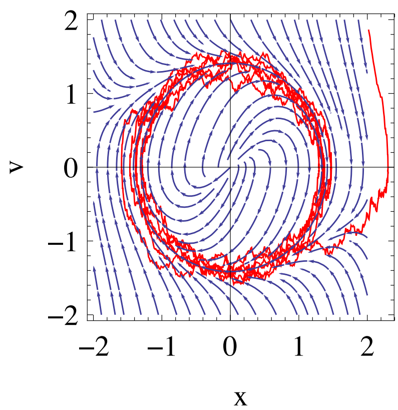
Example: Noisy van der Pol oscillator

- SDE:

$$\begin{aligned} \dot{x} &= v \\ \dot{v} &= -x + v(\alpha - x^2 - v^2) + \sqrt{\epsilon}\,\xi(t) \end{aligned}$$

- Bifurcation:
  - Stable fixed point: $\alpha < 0$
  - Stable limit cycle: $\alpha > 0$



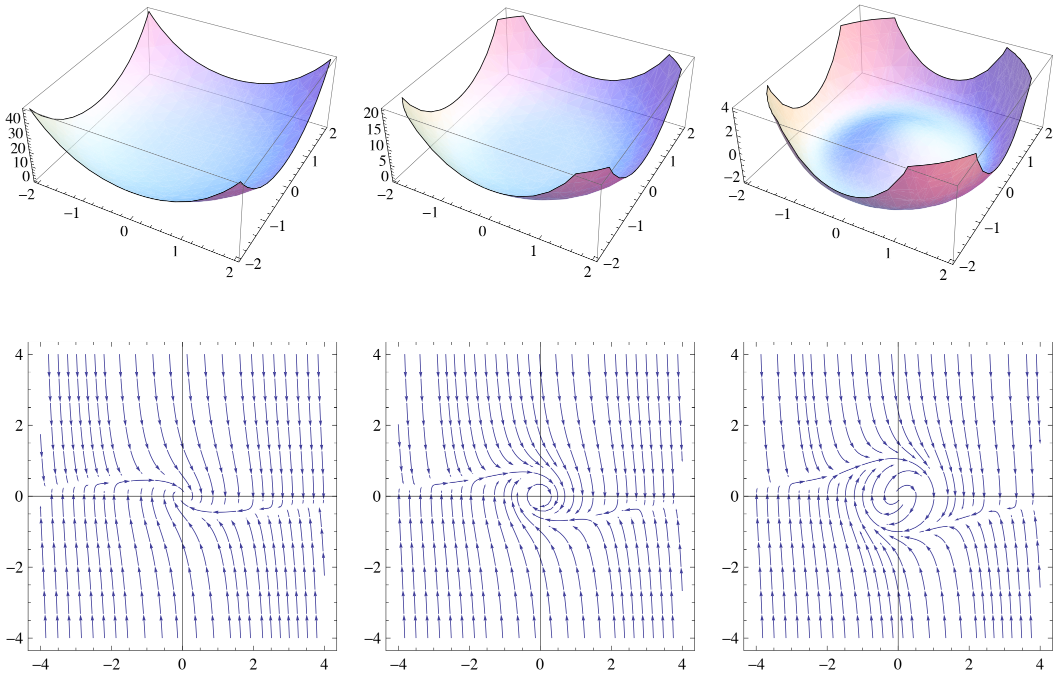


- Stationary distribution: $P(r, \theta) \approx e^{-W(r)/\epsilon}$
- $W(r)$ given by Hamilton-Jacobi equation

Noisy van der Pol oscillator (cont'd)

- Solution:

$$W(r) = -\alpha r^2 + \frac{r^4}{2}$$



Gradient vs non-gradient

Gradient system

$$\dot{x} = F(x) + \sqrt{\epsilon}\,\xi(t), \qquad F(x) = -\nabla U(x)$$

- $V(x) = 2U(x)$
- Instanton = time-reversed deterministic dynamics
- Instanton equation: $\dot{x}^* = \nabla U(x^*)$

Non-gradient system

- $F \neq -\nabla U$
- Instanton $\neq$ time-reversed deterministic dynamics
- Instanton dynamics: $\dot{x}^* = F(x) + \nabla V(x)$

- Equilibrium vs nonequilibrium systems
- Detailed balance vs non-detailed balance

Example: Linear, non-gradient system

$$\dot{x} = Bx + \sqrt{\epsilon}\,\xi, \qquad B = \begin{pmatrix} -1 & -1 \\ 1 & -1 \end{pmatrix}$$

- Non-gradient: $\dot{x} \neq -\nabla U$
- Stationary distribution:

$$P(x) \approx e^{-V(x,y)/\epsilon}$$

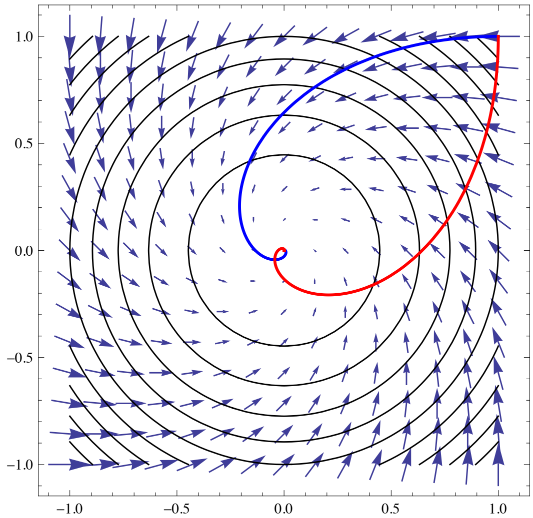
- Quasi-potential:

$$V(x,y) = x^2 + y^2$$

- Instanton:

$$\dot{x} = (-B_s + B_a)x = B^* x$$

$$B^* = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = -B^T$$



Summary

$$P(x_f, t_f | x_i, t_i) = \int_{x(t_i)}^{x(t_f)} \mathcal{D}[x]\, P[x], \qquad P[x] = e^{-S[x]/\epsilon}$$

- Action:

$$S[x] = \int_{t_i}^{t_f} [\dot{x}_t - F(x_t)]^T A(x_t) [\dot{x}_t - F(x_t)]\, dt$$

- Dominant path approximation:

$$V(x_f, t_f | x_i, t_i) = \min_{x(t): x(t_i) = x_i, x(t_f) = x_f} S[x]$$

- Calculate all sorts of transition, escape probabilities
- Similar to semiclassical or WKB approximation
- Nonlinear equations difficult to solve in general
- Other noises: colored, Poisson, etc.

Applications

Physics

- Brownian motion
- Diffusion, transport
- Irreversible processes
- Noisy systems
- Biophysics

Engineering

- Control, reliability
- Signal analysis, filtering
- Queueing

- Statistics, sampling
- Finance

Further reading

H. Kleinert
Path Integrals in Quantum Mechanics, Statistics, Polymer Physics, and Financial Markets
World Scientific, 2005 [Chaps. 2, 4 and 20]

M. I. Freidlin, A. D. Wentzell
Random Perturbations of Dynamical Systems
Springer, New York, 1984, Chap. 4 [for the braves!]

R. Graham
Macroscopic potentials, bifurcations and noise in dissipative systems
F. Moss, P. V. E. McClintock (eds), Noise in Nonlinear Dynamical Systems, Cambridge University Press, 1989 [ask me a copy]

H. Touchette
The large deviation approach to statistical mechanics
Physics Reports 478, 1-69, 2009 [Sec. 6.1]

Reading on stochastic processes

- N. G. van Kampen
  Stochastic Processes in Physics and Chemistry
  North-Holland, 1992
- B. Øksendal
  Stochastic Differential Equations
  Springer, 2000 [recommended]
- K. Jacobs
  Stochastic processes for Physicists: Understanding Noisy Systems
  Cambridge, 2010 [recommended]
- D. J. Higham
  An algorithmic introduction to numerical simulation of stochastic differential equations
  SIAM Review 43, 525-546, 2001

Exercises

1. Re-do the calculation of page 6 to obtain the path distribution and the corresponding action.
2. Derive the expression of the propagator's quasi-potential $V(x_f, t_f; x_i, t_i)$ for the Ornstein-Ulhenbeck process using the dominant path approximation. [Hint: Follow the stationary solution on page 9.] Check that the propagator verifies the time-dependent Fokker-Planck equation exactly.
3. Derive the stationary quasi-potential $W(r)$ for the noisy van der Pol oscillator (page 10). Can you write down another dynamical system having the same quasi-potential?
4. Show for a gradient system that the instanton is the time-reverse of the deterministic path.
5. Derive the general result for the stationary quasi-potential shown on page 12.
6. What is the expression of the classical action $S[x]$ using the Stratonovitch calculus convention? Is there any choice of calculus convention in quantum mechanics?