Nonequilibrium Markov processes conditioned on large deviations

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Large Deviation Theory in Principle and Practice
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Work with

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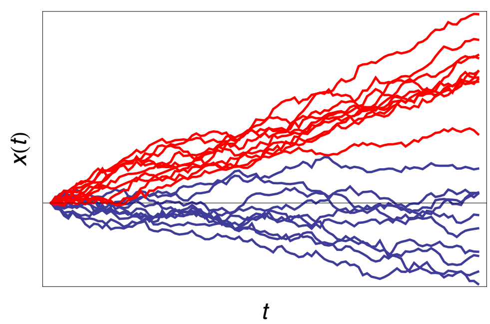
Problem

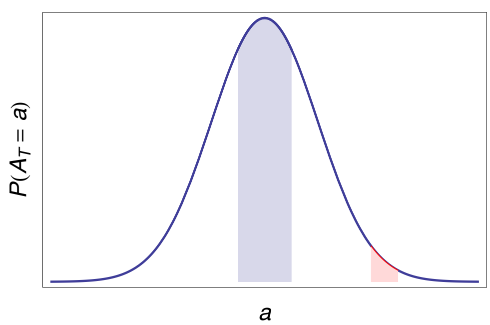
Physical

- Stochastic process: X_t
- Observable: $A_T[x]$
- Look at trajectories leading to $A_T = a$
- Find effective process describing these trajectories



Mathematical

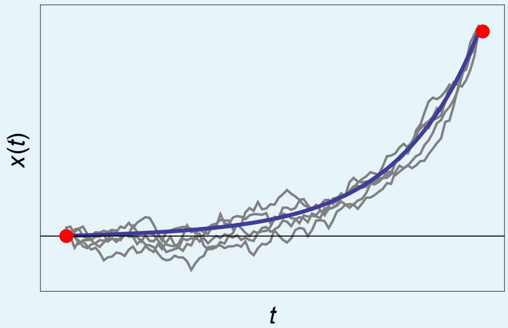
- Markov process: $\{X_t\}_{t=0}^{T}$
- Conditioned process: $X_t | A_T = a$
- Is it a Markov process?
- Construct its generator



Path integral formulation

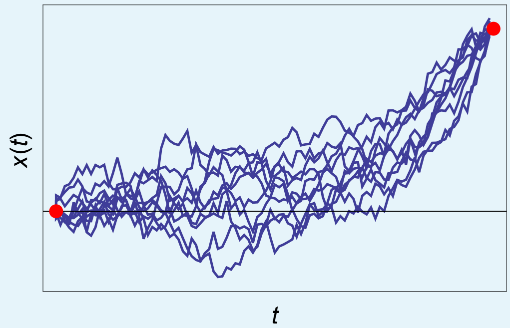
$$P(A_T = a) = \int_{A_T[x]=a} \mathcal{D}[x]\ e^{-I[x]/\epsilon}$$

Low noise



- Fluctuation from single path
- Reactive path or instanton
- WKB approx of path integral

Not low noise



- Fluctuation from many paths
- No reactive path
- Whole fluctuation process

Process

- Markov process: X_t
  - One or many particles
  - Equilibrium or nonequilibrium
  - Includes external forces, reservoirs
- Master (Fokker-Planck) equation:

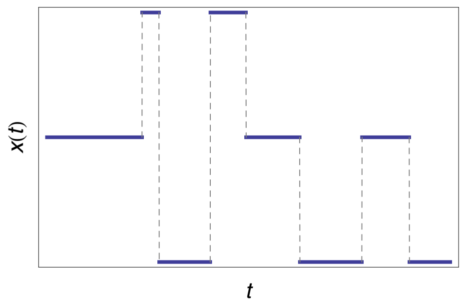
$$\partial_t p(x,t) = L^\dagger p(x,t)$$

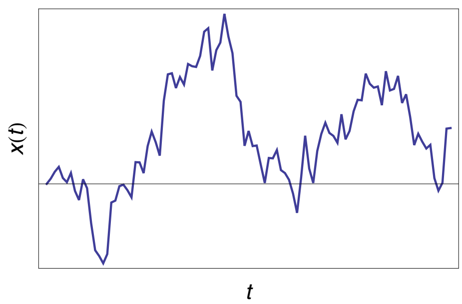
- Generator:

$$\partial_t E_x[f(X_t)] = E_x[Lf(X_t)]$$

- Path measure:

$$P[x] = P(\{x_t\}_{t=0}^T)$$





Examples of Markov processes

Pure jump process

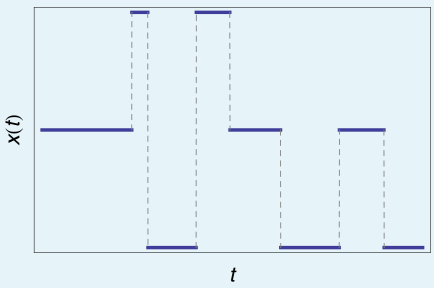
- Transition rates:

$$W(x,y) = P(x \to y \text{ in } dt)/dt$$

- Escape rates:

$$\lambda(x) = \sum_y W(x,y) = (W1)(x)$$

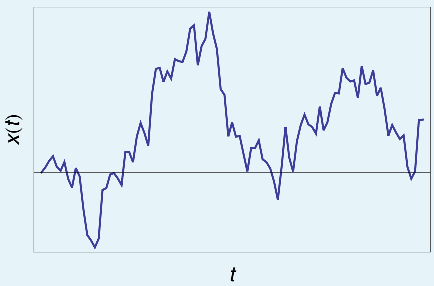
- Generator: $L = \underbrace{W}_{\text{off-diag}} - \underbrace{\lambda}_{\text{diag}}$



Pure diffusion

- SDE: $dX_t = F(X_t)dt + \sigma dW_t$
- Generator:

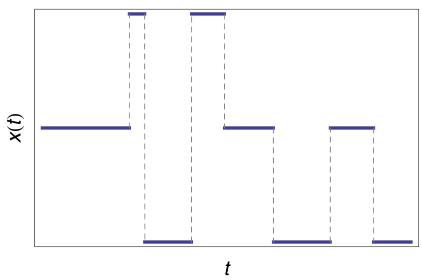
$$L = F \cdot \nabla + \frac{D}{2}\nabla^2, \qquad D = \sigma\sigma^T$$



Conditioning observable

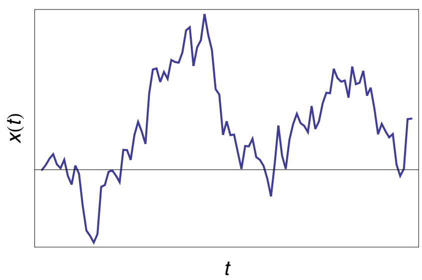
- Random variable: $A_T[x]$
- Jump processes:

$$A_T = \frac{1}{T}\int_0^T f(X_t)\, dt + \frac{1}{T}\sum_{\Delta X_t \neq 0} g(X_{t^-}, X_{t^+})$$



- Diffusions:

$$A_T = \frac{1}{T}\int_0^T f(X_t)\, dt + \frac{1}{T}\int_0^T g(X_t) \circ dX_t$$



Examples

- Occupation time $X_t \in \Delta$
- Mean number jumps (activity), current
- Work, heat, entropy production,...

Rare event conditioning

Large deviation principle

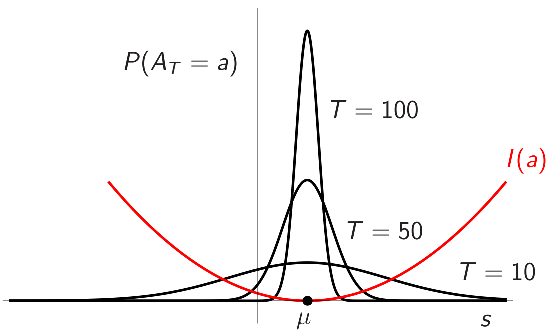
$$P(A_T = a) \approx e^{-TI(a)}$$

- Meaning of $\approx$:

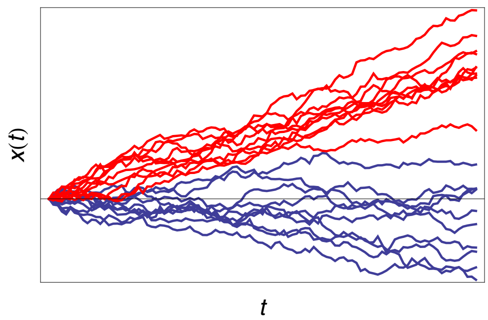
$$\lim_{T\to\infty} -\frac{1}{T} \ln P(A_T = a) = I(a), \qquad P(A_T = a) = e^{-TI(a)+o(T)}$$

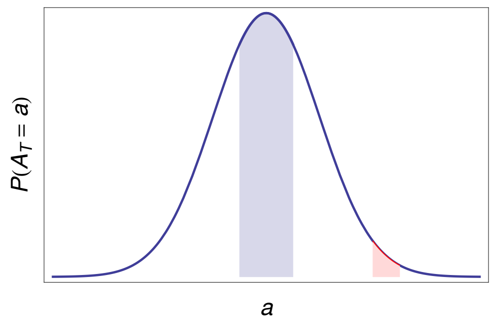
- Rate function: $I(a)$

- Exponentially rare fluctuations
- Applies to many systems and observables
- Zero of I = Law of Large Numbers
- Small fluct. = Central Limit Thm



Conditioned process





- Conditioned process: $X_t | A_T = a$
- Path distribution:

$$P^a[x] = P[x|A_T = a] = \frac{P[x, A_T = a]}{P(A_T = a)} = P[x]\,\frac{\delta(A_T[x] - a)}{P(A_T = a)}$$

- Path microcanonical ensemble

- Not necessarily Markov for $T < \infty$
- Becomes equivalent to Markov process as $T \to \infty$
- Driven process $\hat{X}_t$

Spectral elements

Scaled cumulant function

$$\Lambda_k = \lim_{T\to\infty} \frac{1}{T} \ln E[e^{TkA_T}]$$

- $k \in \mathbb{R}$

Gärtner-Ellis Theorem

Λ_k differentiable, then

1. LDP for A_T
2. $I(a) = \sup_k \{ka - \Lambda_k\}$

Perron-Frobenius

$$\mathcal{L}_k r_k = \Lambda_k r_k$$

- Tilted (twisted) operator: $\mathcal{L}_k$
- Dominant eigenvalue: Λ_k
- Dominant eigenfunction: r_k

Jump processes

$$\mathcal{L}_k = We^{kg} - \lambda + kf$$

Diffusions

$$\mathcal{L}_k = F \cdot (\nabla + kg) + \frac{D}{2}(\nabla + kg)^2 + kf$$

Driven process $\hat{X}_t$

Generator

$$L_k = r_k^{-1}\mathcal{L}_k r_k - r_k^{-1}(\mathcal{L}_k r_k)$$

- Generalization of Doob's transform (1957)
- Action:

$$(L_k h)(x) = \frac{1}{r_k(x)}(\mathcal{L}_k r_k h)(x) - \Lambda_k h(x)$$

- Markov operator: $(L_k 1) = 0$
- Path distribution:

$$\underbrace{P_k^{\text{driven}}[x]}_{\text{new}} = r_k^{-1}(X_0)\, e^{T(kA_T - \Lambda_k)}\, r_k(X_T)\ \underbrace{P[x]}_{\text{original}}$$

Main result

$$\begin{array}{cccl} X_t \| A_T = a & \overset{T\to\infty}{\cong} & \hat{X}_t & k(a) = I'(a) \\ P^a[x] & \approx & P^{\text{driven}}_{k(a)}[x] & \text{almost all paths} \\ B_T \to b^* & \Rightarrow & B_T \to b^* & \text{in probability} \\ A_T = a & & A_T \to a & \end{array}$$

- Same typical states
- Different fluctuations in general
- Similar to ensemble equivalence (microcanonical/canonical)
- Similar to asymptotic equipartition (information theory)
- $I(a)$ must be convex

Analogy with equilibrium ensembles

Equilibrium systems

Microcanonical	Canonical
$P^u(\omega) = P(\omega \| H = u)$	$P_\beta(\omega) = \dfrac{e^{-\beta H(\omega)}}{Z(\beta)}$

- Same typical states in thermo limit $N \to \infty$
- Different fluctuations

Nonequilibrium systems

$$\underbrace{X_t \,|\, A_T = a}_{\substack{\text{conditioned}\\ \text{microcanonical}}} \quad \overset{T\to\infty}{\cong} \quad \underbrace{\hat{X}_t}_{\substack{\text{driven}\\ \text{canonical}}}$$

- Same typical states in ergodic limit $T \to \infty$
- Different fluctuations

Driven process: Explicit form

Jump process

- Original process: $W(x,y)$
- Driven process:

$$W_k(x,y) = r_k^{-1}(x)\, W(x,y)\, e^{kg(x,y)}\, r_k(y), \qquad k = I'(a)$$

- [Evans PRL 2004, Jack and Sollich PTPS 2010]

Diffusion

- Reference SDE:

$$dX_t = F(X_t)dt + \sigma dW_t$$

- Driven SDE:

$$dY_t = F_k(Y_t)dt + \sigma dW_t$$

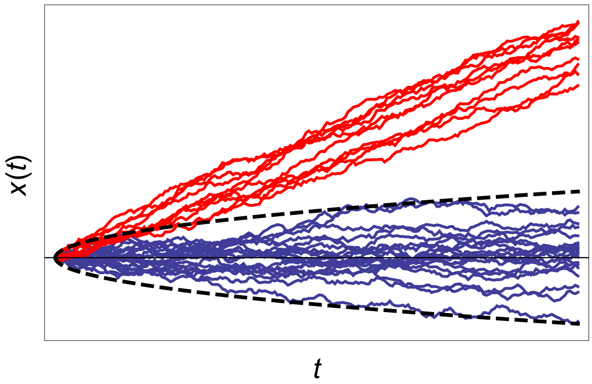
- Modified drift:

$$F_k(y) = F(y) + D(kg + \nabla \ln r_k), \qquad k = I'(a)$$

Application: Brownian motion

- Process: W_t
- Typical trajectories: $w_t \sim \sqrt{t}$
- Atypical trajectories:

$$A_T = \frac{W_T}{T} = \frac{1}{T}\int_0^T dW_t$$



Effective process

$$W_t | A_T = a \quad \overset{T\to\infty}{\cong} \quad \hat{X}_t = W_t + \underbrace{at}_{\text{added drift}}$$

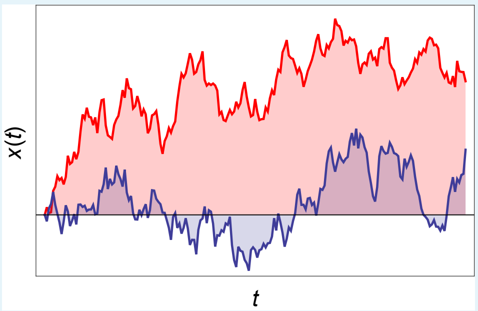
Langevin equation

$$dX_t = -\gamma X_t dt + \sigma dW_t$$

Area

$$A_T = \frac{1}{T}\int_0^T X_t dt$$

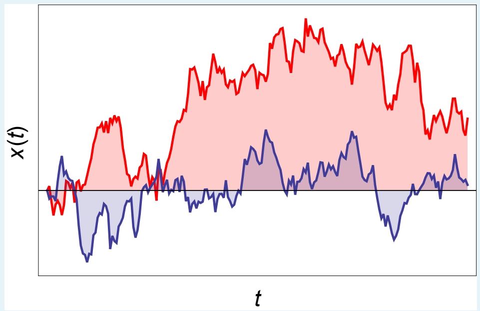
- $F_a(x) = -\gamma x + \gamma a$
- Modified drift



Empirical variance

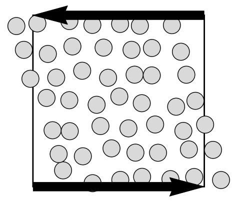
$$A_T = \frac{1}{T}\int_0^T X_t^2 dt$$

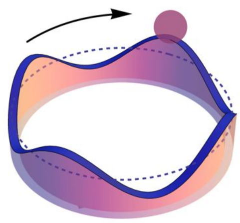
- $F_a = -\sigma^2 x/(2a)$
- Modified friction

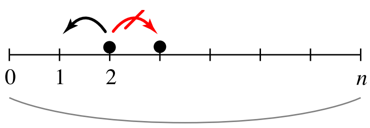


Applications

- Sheared fluids
  - [Mike Evans 2004]
- Interacting particle systems
  - ASEP, ZRP, Spin-Glauber, rotators, etc.
  - [Talk of Rob Jack]
- Diffusions
  - Current or occupation conditioning
- Chemical reactions
- Open quantum systems
  - [Talk of Juan Garrahan]
- Random walks on graphs







- Effective (nonequilibrium) process for fluctuations
- Conditioning induces non-local forces/long-range interactions
- Nonequilibrium = conditioning equilibrium?

Conclusion

$$\underbrace{X_t \,|\, A_T = a}_{\substack{\text{conditioned} \\ \text{microcanonical}}} \quad \stackrel{T\to\infty}{\cong} \quad \underbrace{\hat{X}_t}_{\substack{\text{driven} \\ \text{canonical}}}$$

- Effective process for fluctuations
- Process (ensemble) equivalence

Other links and applications

- Variational principles for large deviations [Varadhan, Eyink,...]
- Nonequilibrium maximum entropy [Filyukov, Evans,...]
- Stochastic optimal control [Fleming,...]
- Quasi-stationary distributions

Ongoing work

- Nonequilibrium systems
- Numerical large deviations

Large deviations in principle and practice

What we have in principle

- General theory of steady states and fluctuations
- Legendre structure underlying large deviation functions
- Different limits: system size, time, noise [source of general results]
- Same language for equilibrium and nonequilibrium

Problems in practice

- Large deviation functions are hard to obtain
- Nonequilibrium is difficult [system dependent, non-hermitian]
- True also for equilibrium [eg free energy of real systems]

To develop

- Approximation methods for large deviations
- Numerical methods
- Response theory

References

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Phys. Rev. Lett. **111**, 120601, 2013

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Variational and optimal control representations of conditioned and driven processes
To appear in JSTAT. arxiv:1506.05291

`www.physics.sun.ac.za/~htouchette`

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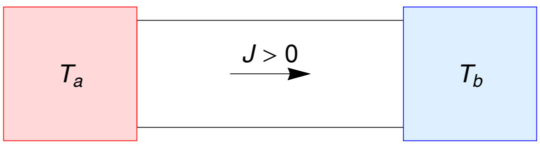
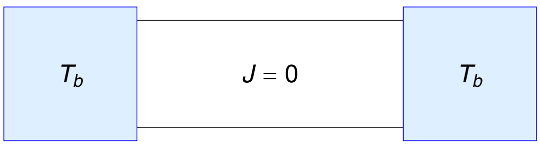
Nonequilibrium systems

Nonequilibrium	Equilibrium





- Microscopic dynamics:

$$W^{\text{noneq}}(x \to y)?$$

- Many models possible

- Microscopic dynamics known
- Detailed balance:

$$\frac{W^{\text{eq}}(x \to y)}{W^{\text{eq}}(y \to x)} = e^{\beta \Delta E}$$

Evans's hypothesis [PRL 2004; JPA 2005]

$$W^{\text{noneq}}(x \to y) = W^{\text{eq}}(x \to y|J)$$

- Nonequilibrium = conditioning of equilibrium

Markov conditioning

- State conditioning [Doob 1957]

$$X_t \mid X_T \in \mathcal{A} \qquad \text{target point or set}$$

- Schrödinger bridge [Schrödinger 1931]

$$X_t \mid p(x,T) = q(x) \qquad \text{target distribution}$$

- Quasi-stationary distributions

$$\underbrace{X_t}_{\text{absorbing}} \mid \text{not reaching absorbing state} \equiv \underbrace{\hat{X}_t}_{\text{non-absorbing}}$$

Here

- $X_t|A_T$ with A_T defined on $[0,T]$
- Requires generalization of Doob's transform
- Asymptotic equivalence

Other applications

Conditional limit theorems

- Sequence of RVs: $X_1, X_2, \ldots, X_n, \quad X_i \sim P(x)$
- Sample mean: $S_n = \frac{1}{n}\sum_{i=1}^{n} f(X_i)$
- Conditional marginal:

$$\lim_{n\to\infty} P(X_i = x|S_n = s) = \frac{e^{kf(x)}}{E[e^{kf(X)}]} P(x)$$

Control representations of PDEs

$$\begin{array}{cccc} \text{PDE} & \overset{I=-\ln\phi}{\longrightarrow} & \text{Hamilton-Jacobi equation} & \text{(Hopf-Cole)} \\ \phi(x,t) & & \downarrow & \\ \partial_t\phi = L\phi & & \text{Dynamic programming} & \\ & & \downarrow & \\ & & \text{Optimal stochastic control} & = \ \text{Doob transform} \end{array}$$

- [Fleming, Sheu, Whittle, Dupuis-Ellis – 80s and 90s]