Large deviation simulations: Equilibrium vs nonequilibrium systems

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Problems

Large deviation problem

$$P(A_n \in B) \approx e^{-nI}$$

Dual problem

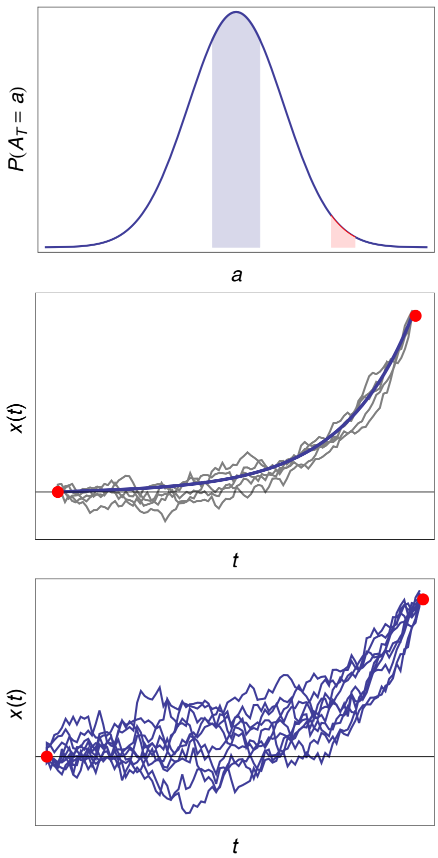
$$E[e^{kA_n}] \approx e^{n\lambda(k)}$$

- Generating function
- Spectral problem (Kac)

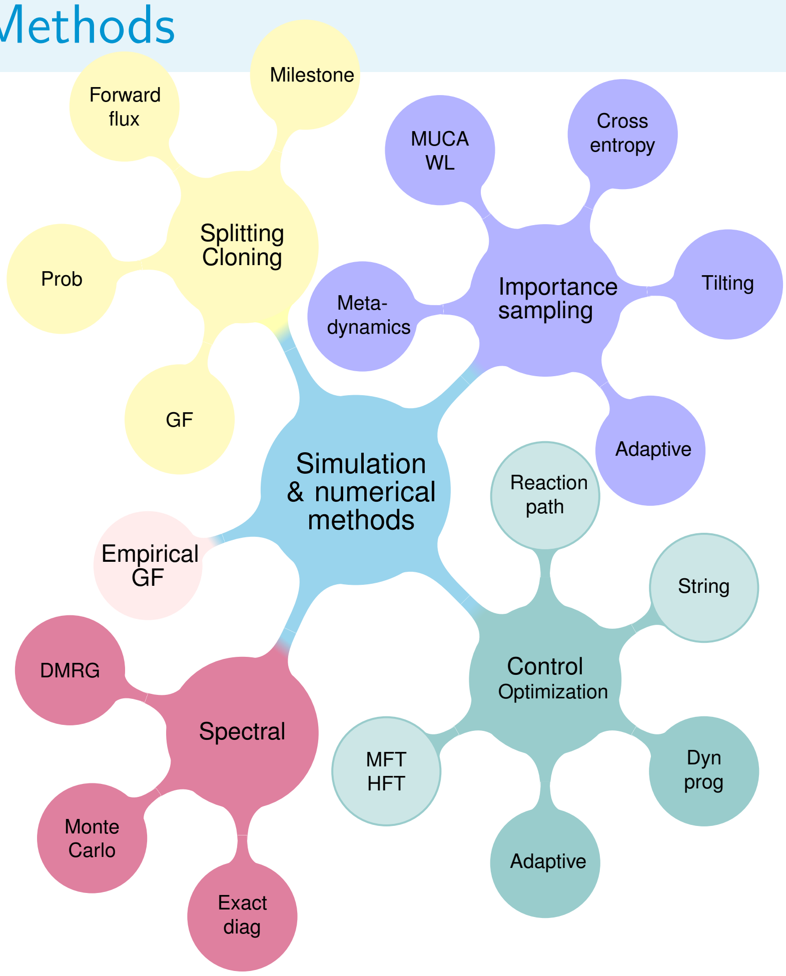
Prediction problem

How is the fluctuation created?

- Reaction or optimal path
- Fluctuation process
- Conditioning



Methods



Questions

- Equilibrium or nonequilibrium method?
- Equilibrium vs nonequilibrium fluctuations
- Nonequilibrium more difficult?

Methods covered

- Spectral
- Optimization
- Importance sampling

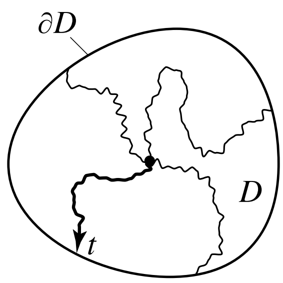
Low-noise large deviations

- Process:

$$dX_t^\varepsilon = F(X_t^\varepsilon)dt + \sqrt{\varepsilon}\, dW_t, \qquad X_0 \in O$$

- Transition rare event:

$$P(X_\tau^\varepsilon \in B | X_0 \in O) \approx e^{-V/\varepsilon}, \qquad \varepsilon \to 0$$



Freidlin-Wentzell-Graham

$$V = \inf_{x\in B} \underbrace{V(x)}_{\text{quasi-potential}} = \inf_{x\in B} \inf_{x_0\in O, x_t = x} \underbrace{\frac{1}{2}\int_0^t (\dot{x}_s - F(x_s))^2 ds}_{\text{FW action, Lagrangian } J[x]}$$

- Deterministic control problem
- Optimal path $\{x_t^*\}$
- $V(x)$ solves Hamilton-Jacobi-Bellman equation (1st order)

Low-noise large deviations (cont'd)

Fluctuation created by optimal path

Conditioning

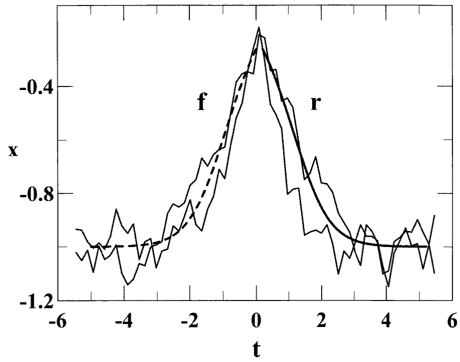
- $P[x] \approx e^{-J[x]/\varepsilon}$ max
- $P[x|\text{escape event}]$ concentrates on optimal path

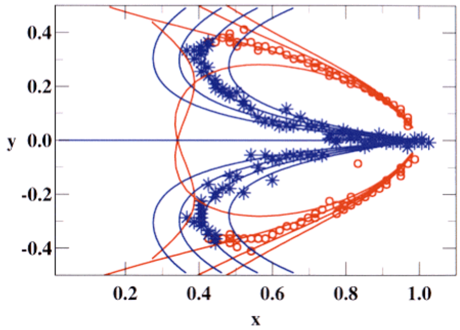
Equilibrium

- Optimal path = relaxation path^R
- $V(x) = J[x^R_{\text{relax}}]$

Nonequilibrium

- Optimal path $\neq$ relaxation path^R
- Current loops
- Transversal decomposition [Graham 80's]





[Luchinsky et al 1997]

Applications

SDEs

$$dX_t = F(X_t)dt + \sqrt{\varepsilon}\,\text{noise}$$

- Escape, transition paths, escape time
  [Onsager-Machlup 1953] [Freidlin-Wentzell 70s] [Graham 80-90s] ...
- Experiments [Luchinsky and McClintock 90s]
- Metastability [Olivieri-Vares 2005]

SPDEs

$$d\rho(x,t) = F[\rho]dt + \sqrt{\varepsilon}\,\text{noise}$$

- Heat equation [Faris, Jona-Lasinio 1982]
- Ginzburg equation [Graham 1990s]
- Reaction-diffusion [Vanden-Eijnden 2000s]
- 2D fluid equations [Laurie-Bouchet 2014]
- MFT/HFT [Bertini et al 2000s]

Long-time large deviations

- Process:

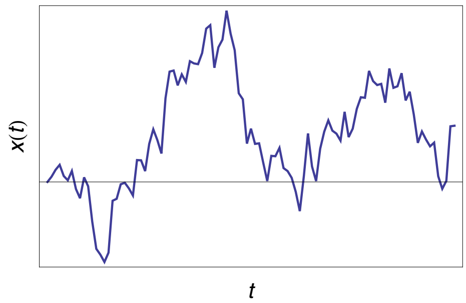
$$dX_t = F(X_t)dt + \sigma dW_t$$

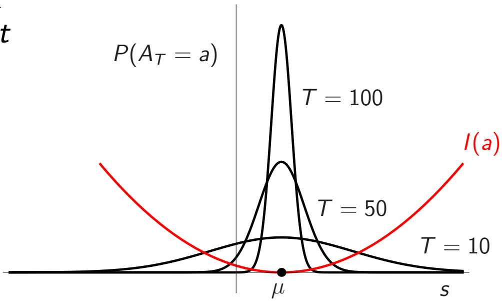
- Observable:

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

- Large deviation principle (LDP):

$$P(A_T = a) \approx e^{-TI(a)}, \quad T\to\infty$$





Examples

- Occupation time, empirical density
- Current, mean speed, activity
- Work, heat, entropy production (stochastic thermo)

Dual problem

Scaled cumulant function

$$\lambda(k) = \lim_{T\to\infty}\frac{1}{T}\ln E[e^{TkA_T}]$$

Gärtner-Ellis Theorem

$\lambda(k)$ differentiable, then

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

Feynman-Kac-Perron-Frobenius

$$\mathcal{L}_k r_k = \lambda(k) r_k$$

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

Jump processes

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

Diffusions

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

Spectral problem

Equilibrium

- X_t reversible, g gradient, f arbitrary
- $\mathcal{L}_k$ non-Hermitian but conjugated to Hermitian:

$$\mathcal{H}_k = \rho^{1/2}\mathcal{L}_k\rho^{-1/2}, \qquad \psi_k^2 = r_k l_k$$

- Real spectrum (quantum problem)

Nonequilibrium

- X_t nonreversible OR g non-gradient, f arbitrary
- $\mathcal{L}_k$ non-Hermitian, not conjugated to Hermitian
- Complex spectrum
- Full spectral problem:

$$\begin{aligned} \mathcal{L}_k r_k &= \lambda(k) r_k \\ \mathcal{L}_k^\dagger l_k &= \lambda(k) l_k \end{aligned} \qquad r_k(x) l_k(x) \stackrel{|x|\to\infty}{\longrightarrow} 0$$

Algorithms

Markov chains

- Non-symmetric positive matrices
- Direct diagonalization
- Power method
- DMRG [Gorissen-Vanderzande 2011]

Diffusions

- Equilibrium: (Quantum) spectral methods
- Nonequilibrium: Fourier decomposition, basis functions

Cloning/splitting

- Particle/trajectory simulation
- Yields SCGF
- No eigenvector

Other approach: Optimization and control

$$A_T = \tilde{A}(\rho_T, J_T) = \int f(x)\underbrace{\rho_T(x)}_{\text{dist.}}dx + \int g(x)\underbrace{J_T(x)}_{\text{current}}dx$$

Drift optimization

$$I(a) = \inf_{u:E_u[A_T]=a} \frac{1}{2\sigma^2}\int (u(x)-F(x))^2 \rho^u_{\text{inv}}(x)\,dx$$

- Requires stationary distribution ρ^u_{inv}

Stochastic optimal control

$$I(a) = \lim_{T\to\infty} \inf_{u:A^u_T\to a} \frac{1}{2\sigma^2 T}\int_0^T (u(X^u_t)-F(X^u_t))^2 dt$$

- Controlled process: X^u_t
- Constrained control (dual for SCGF is unconstrained)
- Solves Hamilton-Jacobi-Bellman equation (2nd order)

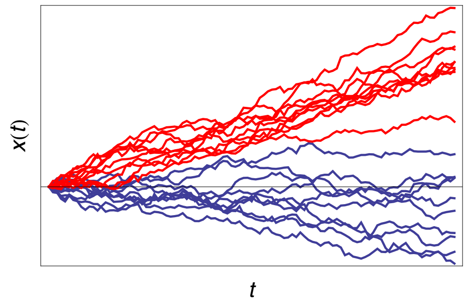
Fluctuation process

Optimal control process

$$d\hat{X}_t = F_k(\hat{X}_t)dt + \sigma dW_t$$

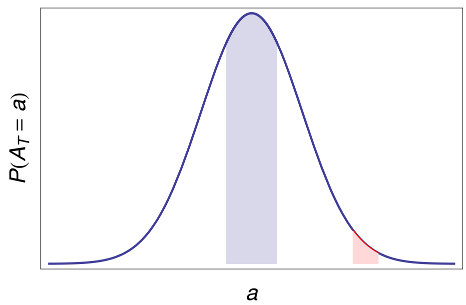
- Optimal drift:

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



Conditioning

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



- Effective process creating the fluctuation
- Process generalization of optimal path

[Chetrite HT, PRL 2013, AHP 2015, JSTAT 2015]

Equilibrium vs nonequilibrium

$$A_T = \tilde{A}(\rho_T, J_T) = \int f(x) \underbrace{\rho_T(x)}_{\text{dist.}} dx + \int g(x) \underbrace{J_T(x)}_{\text{current}} dx$$

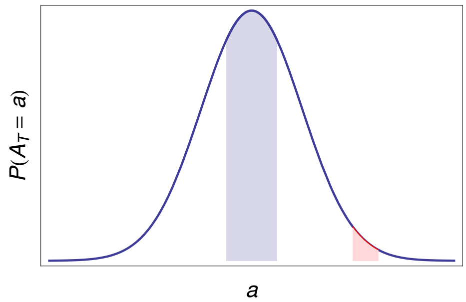
X_t	g	$\hat{X}_t$
Reversible	0	Reversible Same spectrum Rayleigh-Ritz variational principle
	Gradient	Reversible Rayleigh-Ritz variational principle
	Non-gradient	Non-reversible
Non-reversible	0	Non-reversible Donsker-Varadhan principle
	Other	Non-reversible

- Process closest to X_t that creates fluctuation
- Distance: $\|u - F\|_{\rho^u_{\text{inv}}}$ or $\frac{1}{T} S(P_{\hat{X}} \| P_X)$

Simulations: Importance sampling

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

$$\text{sample size } = L \sim e^T$$



Importance sampling

- Change process: $X_t \to \hat{X}_t$
- Make $A_T = a$ typical
- Change of measure:

$$P(A_T = a) = E_X[\mathbb{1}_a(A_T)] = E_{\hat{X}}\left[\frac{dP_X}{dP_{\hat{X}}} \mathbb{1}_a(A_T)\right]$$

- Estimator:

$$\hat{P}_L(a) = \frac{1}{L} \sum_{j=1}^{L} \mathbb{1}_a(A_T^{(j)}) R$$

Efficiency

Zero-variance process

- Conditioned process: $X_t | A_T = a$
- Estimator variance:

$$\mathrm{var}_{\hat{X}}(\hat{P}_L) = \frac{E_{\hat{X}}[R^2 \mathbb{1}_a(A_T)] - p^2}{L} = 0$$

Effective process

- Not zero variance
- Asymptotic optimality:

$$\lim_{T\to\infty} -\frac{1}{T} \ln E_{\hat{X}}[R^2 \mathbb{1}_a(A_T)] = 2I(a)$$

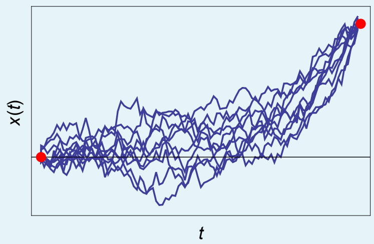
- Variance goes to 0 with largest rate
- Exponential tilting:

$$P_{\text{driven}}[x] \approx P_k[x] = \frac{e^{TkA_T[x]} P[x]}{E[e^{TkA_T}]}$$

Connections

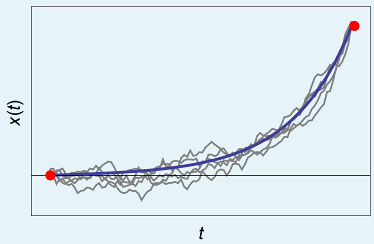
$\sigma > 0$

- Stochastic optimal control
- Quadratic cost function (log RND)
- Nonlinear HJB equation (2nd order)
- Similar to cross-entropy minimization



$\sigma \to 0$

- Deterministic optimal control
- Quadratic cost function (log RND)
- Nonlinear HJB (1st order, viscosity)



Optimal controller		Value function		
Dyn programming	$\longleftrightarrow$	HJB equations	$\longleftrightarrow$	Exponential tilting
$\hat{X}_t$		LD functions		

Conclusions

LD ≡ control/optimization ≡ spectral
Type of fluctuations determines class of control designs

Equilibrium fluctuations

Reversible control
Hermitian spectral problem

Nonequilibrium fluctuations

Non-reversible control
Non-hermitian spectral problem

Future work

- Adapt methods from quantum mechanics
- Methods for non-hermitian operators
- HJB-based methods
- Adaptive control methods
- Error bars
- Benchmarking

References

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More pointers at
www.physics.sun.ac.za/~htouchette/ldt