Nonequilibrium Markov processes conditioned on large deviations

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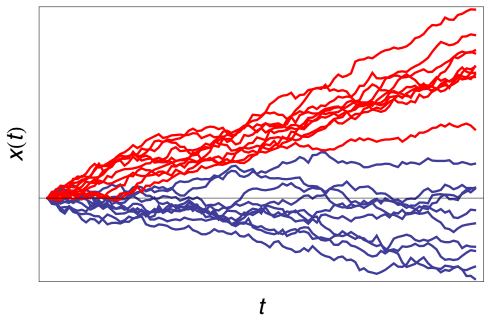
Problem

- Markov process: $\{X_t\}_{t=0}^T$
- Observable (rv): A_T
- Conditioned process: $X_t | A_T = a$

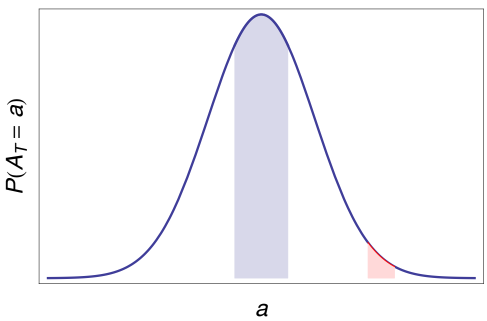


Questions

1. Conditional process Markov?
2. Generator?
3. Relation with X_t?

Connections

- Markov conditioning (Doob)
- Nonequilibrium systems
- Rare event simulations
- Quasi-stationary distributions
- Stochastic control (Fleming)



Markov conditioning

Doob conditioning (1957)

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

- Brownian bridge: $W_t|W_1 = 0$

Schrödinger bridge (1931)

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

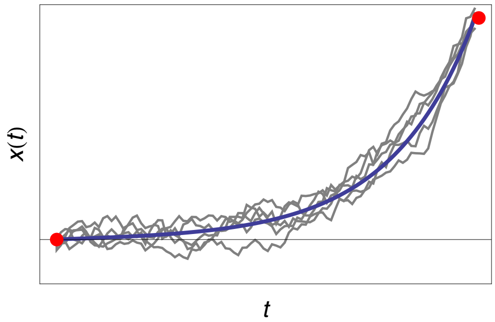
- Classical (Markov) representation of QM
- Nelson's mechanics

Here

- $X_t|\mathcal{A}_T$ with $\mathcal{A}_T$ defined on $[0, T]$
- Requires generalization of Doob's transform
- Asymptotic equivalence

Comparison with optimal paths

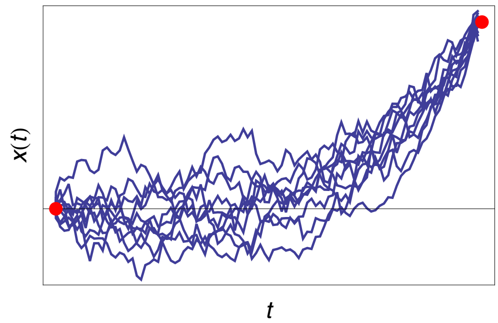
Low noise limit



- Concentration in path space
- Prob dominated by single path
- Dominant path, most probable path, instanton

Fluctuation path

Arbitrary noise



- No concentration
- Prob coming from many paths
- No dominating path

Fluctuating dynamics

Process

- Markov process: $X_t \in \mathcal{E}$
- State space: $\mathcal{E}$
- Time interval (horizon): $t \in [0, T]$
- Generator:

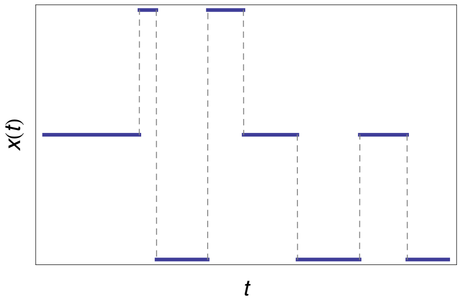
$$\partial_t E_x[f(X_t)] = E_x[Lf(X_t)]$$

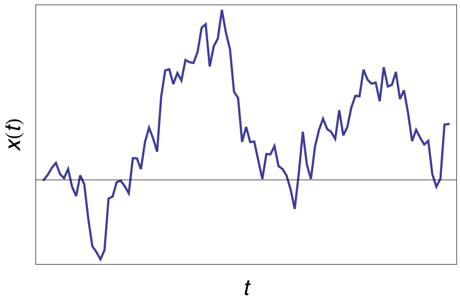
- Master (Fokker-Planck) equation:

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

- Path measure:

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





Examples of Markov processes

Pure jump process

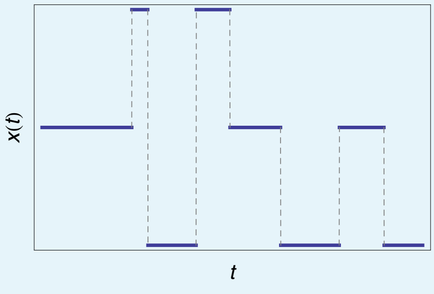
- Transition rates:

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

- Escape rates:

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

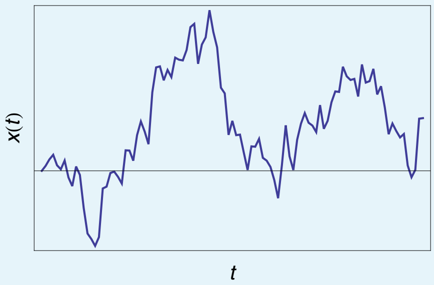
- Generator: $L = \underbrace{W}_{\text{off-diag}} - \underbrace{\lambda}_{\text{diag}}$



Pure diffusion

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

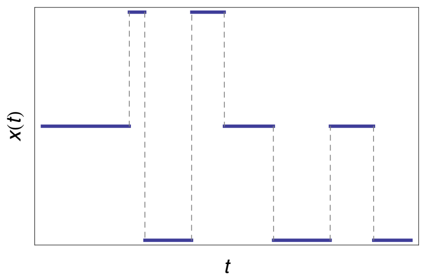
$$L = F \cdot \nabla + \frac{D}{2}\nabla^2, \qquad D = \sigma\sigma^T$$



Conditioning observable

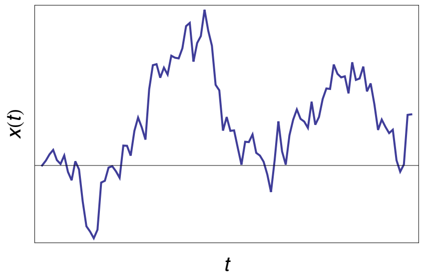
- Observable: $A_T[x]$
- Jump processes:

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



- 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

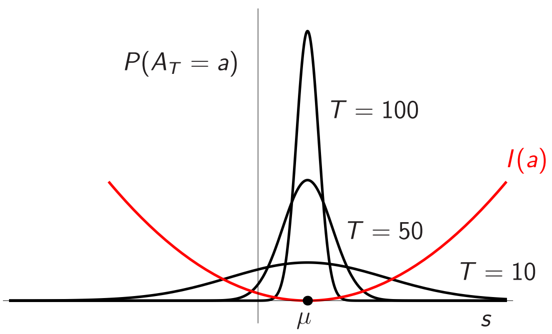
$$P(A_T = a) \asymp e^{-TI(a)}$$

- Meaning of $\asymp$:

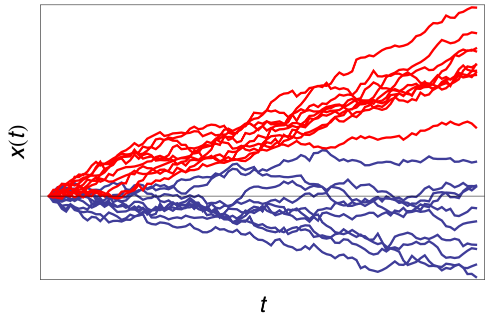
$$\lim_{T\to\infty} -\frac{1}{T}\ln P(A_T = a) = I(a), \qquad P(A_T = a) = e^{-TI(a)+o(T)}$$

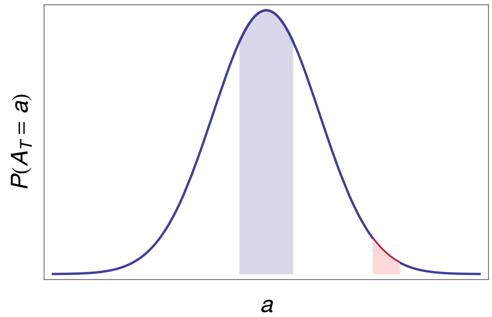
- Rate function: $I(a)$

- Zero of I = Law of Large Numbers
- Concentration point(s): $I(a^*) = 0$
- Small fluctuations = Central Limit Theorem



Conditioned process





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

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

- Path microcanonical ensemble

- Not Markov for $T < \infty$
- Becomes equivalent to Markov process as $T \to \infty$
- Non-conditioned process realizing conditioning

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. $I(a) = \sup_k \{ka - \Lambda_k\}$

Feynman-Kac-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

Definition

- Process Y_t
- Generator:

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

- Generalized Doob transform
- Positive, Markov operator: $(L_k 1) = 0$
- Path measure:

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

- Radon-Nikodym derivative

Main result

Hypotheses

- A_T satisfies LDP
- Rate function $I(a)$ convex
- Other properties of spectral elements (gap, regular r_k)

Result

$X_t \| A_T = a$	$\overset{T\to\infty}{\cong}$	Y_t	$k(a) = I'(a)$
$P^a[x]$	$\asymp$	$P_{k(a)}^{\text{driven}}[x]$	almost everywhere
$B_T \to b^*$	$\Rightarrow$	$B_T \to b^*$	in probability
$A_T = a$		$A_T \to a$	

- Same typical states
- Different fluctuations (LDPs) in general

Idea of the proof

Microcanonical	Canonical	Driven
$X_t \| A_T = a$		Y_t
	$P_k^{\text{cano}}[x] = \dfrac{e^{kTA_T[x]}}{E[e^{kTA_T}]} P[x]$	
$P^a[x] = P[x \| A_T = a]$		$P_k^{\text{driven}}[x]$

Driven $\longrightarrow$ canonical

- $P_k^{\text{driven}}[x] \asymp P_k^{\text{cano}}[x]$
- Same large deviations

Microcanonical $\longrightarrow$ canonical

- $P^a[x] \asymp P_k^{\text{cano}}[x]$ if $I(a)$ convex
- Same typical states
- General result about conditioning vs tilting

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: Langevin equation

$$dX_t = -\gamma X_t dt + \sigma dW_t \qquad \longrightarrow \qquad X_t | A_T = a$$

Area under path

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

- $f(x) = x$, $g = 0$
- Rate function: $I(a) = \frac{\gamma^2 a^2}{2\sigma^2}$
- Eigenfunction: $r_k(x) = e^{kx/\gamma}$
- Modified drift:

$$F_{k(a)}(x) = -\gamma x + \frac{a}{\gamma}$$

- $k(a) = I'(a)$

Empirical variance

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

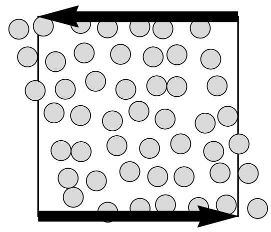
- $f(x) = x^2$, $g = 0$
- Modified drift:

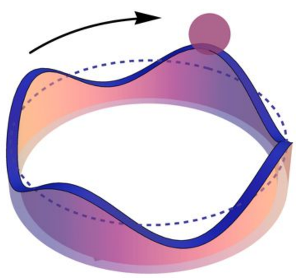
$$F_{k(a)} = -\frac{\sigma^2}{2a} x$$

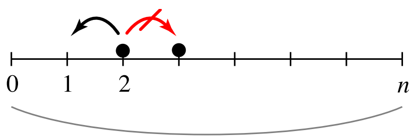
- Modified friction

Other applications

- Sheared fluids
  - R.M.L. Evans PRL 2004; JPA 2005
  - Baule & Evans PRL 2008; PRE 2008
- Diffusion on circle
  - Conditioning on current
  - Chetrite & HT PRL 2013
  - Nemoto & Sasa PRE 2011, PRL 2014
- Interacting particles on lattices
  - Conditioning on current
  - TASEP: Schütz *et al.* JSTAT 2010; JSP 2011
  - Zero-range: Harris *et al.* 2013
  - Glauber-Ising: Jack & Sollich PTPS 2010
  - East model: Jack & Sollich JPA 2014
  - Rotators: Knezevic & Evans PRE 2014



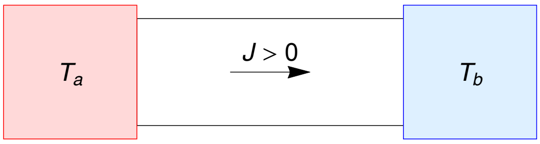


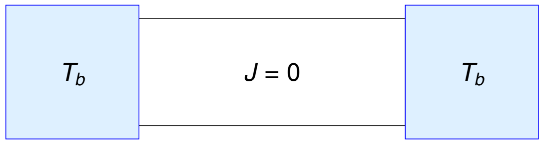


Conditioning typically induces long-range interaction

Nonequilibrium systems

Nonequilibrium	Equilibrium





- Microscopic dynamics:

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

- Many models possible

- Microscopic dynamics known
- Detailed balance:

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

Mike Evans's hypothesis

PRL 2004; JPA 2005

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

- Nonequilibrium = conditioning of equilibrium
- True? Approximation?

Other connections

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

PDE $\overset{I = -\ln \phi}{\longrightarrow}$ Hamilton-Jacobi equation (Hopf-Cole)

$\phi(x, t)$ $\downarrow$

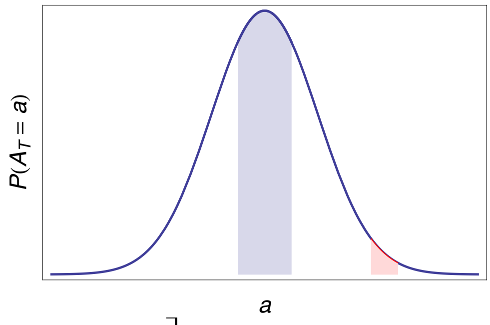
$\partial_t \phi = L\phi$ Dynamic programming

$\downarrow$

Optimal stochastic control = Doob transform

- Fleming, Sheu, Dupuis 1980's, 1990's

Large deviation simulations



- $A_T = a$ exponentially rare
- Direct sampling: sample size $\sim e^T$
- Importance sampling (reweighting)
  - Change process
  - Make $A_T = a$ typical

$$P(A_T = a) = E_X[\delta(A_T - a)] = E_Y\left[\frac{dP_X}{dP_Y}\,\delta(A_T - a)\right]$$

Driven process Y_t

- Makes $A_T = a$ typical
- Good (optimal) change of process
- Problem: Y_t based on r_k, Λ_k and $I(a)$

Learning algorithm [Borkar 2008]

1. Direct sampling + feedback $\rightarrow$ iterative estimation of r_k
2. Control leading to driven process

Conclusions

$$\underbrace{X_t \,|\, A_T = a}_{\text{conditioned}} \overset{T\to\infty}{\cong} \underbrace{Y_t}_{\text{driven}}$$

- Effective Markov dynamics for rare events
- Explicit interpretation of asymptotic equivalence
- Similar to equivalence of equilibrium ensembles
- Generalization of Markov conditioning and bridges
- Links: QSD, stochastic control, conditional limit theorems

Future work

- Large deviation simulations
- Consequences for nonequilibrium systems

References

- R. Chetrite, H. Touchette
  Nonequilibrium microcanonical and canonical ensembles and their equivalence
  Phys. Rev. Lett. **111**, 120601, 2013

- R. Chetrite, H. Touchette
  Nonequilibrium Markov processes conditioned on large deviations
  arxiv:1405.5157

- H. Touchette
  General equivalence and nonequivalence of ensembles: Thermodynamic, macrostate, and measure levels
  arxiv:1403.6608

- H. Touchette
  The large deviation approach to statistical mechanics
  Phys. Rep. **478**, 1-69, 2009

- `www.maths.qmul.ac.uk/~ht`