Stochastic optimal control and transition paths on manifold and graph

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Outline

Stochastic optimal control formulation for transition path theory

- Optimal control for Markov process on continuous states:
  - Running cost via Girsanov Thm for Brownian motion
  - Committor function $\to$ optimal control

- Drift-diffusion on manifold:
  - Voronoi tessellation on point cloud,
  - Upwind scheme $\to$ reversible Markov chain, convergence with refined graph
  - Optimality of the controlled random walk?

- Optimal control for general Markov chain:
  - Control applies to the transition rate Q,
  - Running cost in finite time horizon (Girsanov Thm for jump process),
  - SOC in infinite time horizon (optimal change of measure in Càdlàg path space),
  - Discrete committor function $\to$ optimal control

Transition path problem for diffusion processes

- Take $\Omega = C([0, +\infty); \mathbb{R}^d)$ and $(\Omega, \mathscr{F}_t, \mathscr{F}_\infty, P)$.
- Goal:

$$\mathrm{d}X_t = -\nabla U(X_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}B$$

  Transition path connecting from local attractor A to local attractor B (fix noise level).
  Rare event: efficient computations? manifold suggested by point clouds?

- Define a controlled process

$$\mathrm{d}\tilde{X}_t = (-\nabla U(\tilde{X}_t) + v(\tilde{X}_t))\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}B$$

  Optimality? solvable?

Stochastic optimal control: infinite time horizon

Reinterpret the transition path theory using stochastic optimal control (SOC) in the infinite time horizon

$$\gamma(x) := \inf_{v} \mathbb{E}_P \left[\int_0^{\tau} \frac{1}{2} |v(\tilde{X}_s)|^2 \, \mathrm{d}s + f(\tilde{X}_\tau) \right]$$

$$\text{s.t.} \quad \text{under } P, \; \mathrm{d}\tilde{X}_t = (\vec{b}(\tilde{X}_t) + v(\tilde{X}_t)) \, \mathrm{d}t + \sqrt{2\varepsilon} \, \mathrm{d}B, \quad \tilde{X}_0 = x \in \overline{A \cup B}^c,$$

$$\tau = \inf\{t \geq 0; \tilde{X}_t \in \overline{A \cup B}\}.$$

Boundary cost functional $f(\tilde{X}_\tau)$ is

$$f(x) = \begin{cases} +\infty, & \text{in } \bar{A}; \\ 0, & \text{in } \bar{B}. \end{cases}$$

If in finite time horizon $[0, T]$, it can be directly solved by HJE

Reformulated as optimal change of measures

- Original: s.t. under P, $\mathrm{d}\tilde{X}_t = (\vec{b}(\tilde{X}_t) + v(\tilde{X}_t))\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}B$
- Define process
$$Z_t = \exp\Big(\int_0^t \frac{v(\tilde{X}_s)}{\sqrt{2\varepsilon}} dB_s - \frac{1}{4\varepsilon}\int_0^t v(\tilde{X}_s)^2 ds\Big), \quad t \geq 0.$$
Under P, Z_t is positive, martingale, mean 1.
Define $P^v(A) := \int_{\Omega\cap A} Z_t dP$ for all $A \in \mathscr{F}_t$ or symbolically $\frac{dP^v}{dP}\big|_{\mathscr{F}_t} = Z_t$.
- New: under P^v, $\mathrm{d}\tilde{X} = \vec{b}(\tilde{X}_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}B$

- Convert the running cost [Girsanov Thm for Brownian motion],
$$\mathbb{E}_P^x\left(\int_0^t \frac{1}{2}|v(\tilde{X}_s)|^2\,\mathrm{d}s\right) = -2\varepsilon\mathbb{E}_P^x\Big(\log\frac{dP^v}{dP}\Big|_{\mathscr{F}_t}\Big)$$
- Value function becomes
$$\gamma(x) = \min_{v\in\mathscr{A},P^v} \mathbb{E}_P^x\left[f(\tilde{X}_\tau) - 2\varepsilon\log\frac{dP^v}{dP}\Big|_{\mathscr{F}_\tau}\right],$$
s.t. under P^v, $\mathrm{d}\tilde{X} = \vec{b}(\tilde{X}_t)\,\mathrm{d}t + \sqrt{2\varepsilon}\,\mathrm{d}B.$

Novikov condition and regularization

- Admissible velocity given by the Novikov condition $\mathscr{A} := \{v : \ \mathbb{E}_P\left(e^{\frac{1}{4\varepsilon}\int_0^\tau |v(\tilde{X}_s)|^2\,\mathrm{d}s}\right) < \infty\}$
- Regularization by δ-cutoff

$$f_\delta(x) = \begin{cases} -\log\delta & \text{for } x \in A; \\ 0 & \text{for } x \in B. \end{cases}$$

- Using elliptic estimates to justify $\delta \to 0$

Solvable optimal control by committor function

- Committor function h (probability of hitting B before A),

$$Qh = 0 \qquad \text{with BCs } h|_A = 0,\ h|_B = 1; \quad \text{generator } Q = \varepsilon\Delta + b\cdot\nabla$$

- Probability representation of h via

$$h(x) = \mathbb{E}_P^x(e^{-f(X_\tau)}), \qquad \forall x \in (A\cup B)^c.$$

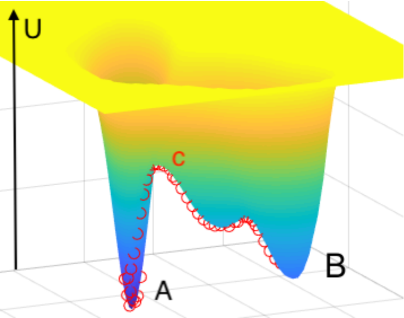
- Optimal control is given by $v^* = -\nabla\gamma = 2\varepsilon\nabla\ln h$
- $\gamma(x)$ satisfies static HJE $H(p,x) = \frac{1}{2}|p|^2 - b\cdot p$,

$$H(\nabla\gamma(x),x) = \varepsilon\Delta\gamma, \ \text{in } (\overline{A\cup B})^c, \qquad \gamma = f \ \text{on } \overline{A\cup B}$$

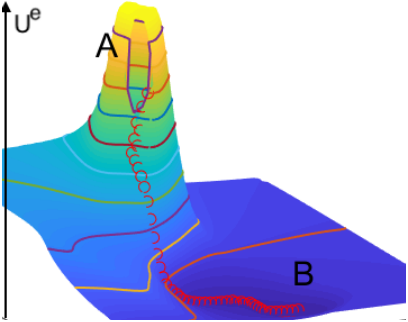
- In reversible case $\to$ effective potential $U^e = U - 2\varepsilon\ln h$, effective equilibrium $\pi^e = h^2\pi$

[Bolhuis, Chandler, Dellago, Geissler, '02][Weinan E, Vanden-Eijnden, '06]

Simulation for transition path: rare event $\to$ a.s.



$\Longrightarrow$



Part II: Drift-diffusion on manifold

- Voronoi tessellation on point cloud,
- Upwind scheme $\rightarrow$ reversible Markov chain (convergence with refined graph)
- Optimality of the controlled random walk?

Reversible Fokker-Planck on manifold, finite volume scheme

- Voronoi tessellation:
  Collected point $\{x_i\}_{i=1}^N \subset \mathscr{M}$, well distributed;
  $\mathscr{M}$ is d-dimensional closed manifold embedded into $\mathbb{R}^\ell$
  Cell $C_i = \{x : d(x, x_i) \leq d(x, x_j), j \neq i\}$;
  Interface Γ_{ij} between cell C_i and C_j (perpendicular bisector);
  Nearest neighbor index set $\mathscr{N}_i$ not include itself.
- Reversible case, equilibrium $\pi \propto e^{-U/\varepsilon}$, $\tilde{t} = \varepsilon t$, drop tilde

$$\partial_{\tilde{t}} \rho = \frac{1}{\varepsilon} \partial_t \rho = \Delta \rho + \nabla \cdot (\rho \nabla U) = \nabla \cdot \left(\pi \nabla \left(\frac{\rho}{\pi} \right) \right).$$

- Finite volume method: (piecewise constant approximation) ρ_i at C_i,

$$\frac{\mathrm{d}}{\mathrm{d}t} \rho_i |C_i| \approx \frac{\mathrm{d}}{\mathrm{d}t} \int_{C_i} \rho \mathscr{H}^d(C_i) \approx \sum_{j \in \mathscr{N}_i} \int_{\Gamma_{ij}} \pi \mathbf{n} \cdot \nabla \left(\frac{\rho}{\pi} \right) \mathscr{H}^{d-1}(\Gamma_{ij})$$

- Finite volume scheme

$$\frac{\mathrm{d}}{\mathrm{d}t} \rho_i |C_i| = \sum_{j \in \mathscr{N}_i} |\Gamma_{ij}| \frac{\pi_i + \pi_j}{2} \frac{1}{|x_i - x_j|} \left(\frac{\rho_j}{\pi_j} - \frac{\rho_i}{\pi_i} \right) =: \sum_{j=1}^N Q_{ji} \rho_j |C_j|$$

In graph calculus notation

- Graph gradient

$$\nabla_{ij} u := \frac{u_j - u_i}{|x_i - x_j|},$$

- Graph divergence for flux $F = (F_{ij})$, $F_{ij} = -F_{ji}$

$$\text{div}_i F := \frac{1}{|C_i|} \sum_{j \in \mathcal{N}_i} |\Gamma_{ij}| F_{ij}$$

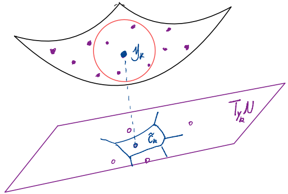
- Thus the scheme recast as

$$\frac{\mathrm{d}}{\mathrm{d}t} \rho_i = \text{div}_i \left(\frac{\pi_i + \pi_j}{2} \nabla_{ij} \frac{\rho}{\pi} \right)$$

- Compare with continuous eq

$$\partial_t \rho = \nabla \cdot \left(\pi \nabla \left(\frac{\rho}{\pi} \right) \right).$$

Tangent plane approximation → Voronoi cells



Input: Set bandwidth r and threshold s

- Approximation of tangent plane $T_{x_k}\mathscr{M}$:
  Span $\{\beta_{n,r,1},\cdots,\beta_{n,r,d}\}$, the first d orthonormal eigenvectors of covariance matrix

$$\mathscr{C}_{n,r}(x_k)=\frac{1}{n}\sum_{i=1}^{\bar{N}_k}(x_{k,i}-x_k)(x_{k,i}-x_k)^\top\in\mathbb{R}^{\ell\times\ell},\quad x_{k,i}\text{ in large ball } B^{\mathbb{R}^\ell}_{\sqrt{r}}(x_k).$$

- Projection map: $\iota_k(u):\mathbb{R}^\ell\to\mathbb{R}^d$; $\iota_k(u)=(u^\top\beta_{n,r,1},\cdots,u^\top\beta_{n,r,d})$.
  Project points in the small ball $B^{\mathbb{R}^\ell}_{r}(x_k)$ via $\tilde{\iota}_k(x)=\iota_k(x-x_k)$.

- Voronoi tessellation in $\mathbb{R}^d$.

- Compute approximated volumes $|\tilde{C}_k|$ and approximated areas $|\tilde{\Gamma}_{k\ell}|=\max\{\mathscr{H}^{d-1}(\tilde{C}_{k,0}\cap\tilde{C}_{k,\ell}),s\}$.

Error estimate for the finite volume scheme

- Geodesic approximated by Euclidean distance:

$$\|x' - x\|_{\mathbb{R}^\ell} = d(x,x')(1 + O(d^2(x,x'))).$$

- Approximation of the volume of a Voronoi cell $|C_k|$

$$|\tilde{C}_k| = |C_k| + O(r^{d+1})$$

- Approximation of the area of a Voronoi face $|\Gamma_{k\ell}|$

$$|\tilde{\Gamma}_{k\ell}| = |\Gamma_{k\ell}| + O(r^d).$$

Theorem (YG., Liu, Wu, ACHA 23')

Let $e_i(t) := \rho(x_i,t) - \rho_i(t)$. *With probability greater than* $1 - \frac{1}{N^2}$,

$$\max_{t\in[0,T]} \sum_i e_i(t)^2 \frac{|C_i|}{\pi_i} \le \Big(\sum_i e_i(0)^2 \frac{|C_i|}{\pi_i} + cr\Big) e^{2T}$$

$r \sim$ *diameter of Voronoi cell*

Random walk approximation: master equation $\frac{\mathrm{d}}{\mathrm{d}t}p = Q^* p$

Q-matrix $\Longrightarrow$ jump rate λ_i and transition probability P_{ji} (from j to i, stochastic matrix):

$$\lambda_i := \sum_{j\neq i} Q_{ij} = \sum_{j\in\mathcal{N}_i} \frac{\pi_i+\pi_j}{2\pi_i|C_i|}\frac{|\Gamma_{ij}|}{|y_i-y_j|}, \quad i=1,2,\cdots,n;$$

$$P_{ji} := \frac{1}{\lambda_j} Q_{ji} = \frac{\pi_i+\pi_j}{2\lambda_j\pi_j|C_j|}\frac{|\Gamma_{ij}|}{|y_i-y_j|}, \quad j\in\mathcal{N}_i; \quad P_{ji}=0, \quad j\notin\mathcal{N}_i.$$

Recast as a master equation of a Markov process:

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\rho_i|C_i| = \sum_{j\in\mathcal{N}_i} \lambda_j P_{ji}\rho_j|C_j| - \lambda_i\rho_i|C_i|, \quad \text{distribution } p_i=\rho_i|C_i|,}$$

It satisfies $\sum_j P_{ij}=1$ and the detailed balance property

$$P_{ji}\lambda_j\pi_j|C_j| = P_{ij}\lambda_i\pi_i|C_i|.$$

Construct controlled random walk on graph, reversible case

Recall optimal control, effective potential and equilibrium:

$$v^* = 2\varepsilon \nabla \ln h, \quad U^e = U - 2\varepsilon \ln h, \quad \pi^e = e^{-\frac{U^e}{\varepsilon}} = h^2 \pi$$

- Discrete committor function

$$\sum_{j=1}^{N} Q_{ij} h_j = 0, \; i \neq i_a \text{ or } i_b, \quad h_{i_a} = \delta, h_{i_b} = 1$$

- Equilibrium (inherit from continuous form): $\pi_i^e := h_i^2 \pi_i$
- Master equation of controlled Markov process

$$\frac{\mathrm{d}}{\mathrm{d}t} \rho_i |C_i| = \sum_{j \in \mathcal{N}_i} |\Gamma_{ij}| \frac{h_i h_j (\pi_i + \pi_j)}{2} \frac{1}{|x_i - x_j|} \left(\frac{\rho_j}{h_j^2 \pi_j} - \frac{\rho_i}{h_i^2 \pi_i} \right), \quad i = 1, \cdots, N.$$

- Controlled Q-matrix (Doob's h-transformation), for $i \neq j$

$$Q_{ij}^h = \frac{h_j}{h_i} \frac{(\pi_i + \pi_j)}{2\pi_i |C_i|} \frac{|\Gamma_{ij}|}{|x_i - x_j|} = \frac{h_j}{h_i} Q_{ij}, \quad Q_{ii}^h = -\sum_{j \neq i} Q_{ij}^h.$$

Part III: Optimal control for general Markov chain

- Control applies to the transition rate Q,
- Running cost in finite time horizon (Girsanov Thm for jump process),
- SOC in infinite time horizon (optimal change of measure in Càdlàg path space),
- Discrete committor function $\to$ optimal control

Optimality for finite time OC, Doob transformation

- Given a generator Q_{ij}, introduce control velocity

$$\vec{v}_t(i) = (v_t(i,j))_{j=1:N} \geq 0, \text{ and } \tilde{Q}_t(i,j) = Q_{ij} v_t(i,j), j \neq i.$$

- Running cost for finite time horizon $\tilde{L}(i,\vec{v}_t) = \sum_{j\neq i} Q_{ij} \text{Ent}(v_t(i,j))$, $\text{Ent}(r) = r\log r - r + 1$

$$\gamma(p_0) = \min_{\vec{v},\vec{p}} \left\{ \sum_i f(i) p_T(i) + \int_0^T \sum_i \tilde{L}(i,\vec{v}_t) p_t(i)\,\mathrm{d}t \right\},$$

$$\text{s.t. } \frac{\mathrm{d}}{\mathrm{d}t} p_i = \sum_{j=1}^N (v_t(j,i) Q_{ji} p_t(j) - v_t(i,j) Q_{ij} p_t(i)), \quad p_{t=0}(i) = p_0(i).$$

- The optimal control is given by the Doob type h-transformation

$$v_t(i,j) = \frac{h_t(j)}{h_t(i)},\ Q_t^h(i,j) := \frac{h_t(j)}{h_t(i)} Q(i,j),\ i,j \in \Gamma,\ j \neq i, \quad Q_{ii}^h := -\sum_{j\neq i, j\in\Gamma} Q_{ij}^h = -\lambda_i^h.$$

h solves linear backward eq. $\frac{\mathrm{d}}{\mathrm{d}t} h_t(i) + \sum_j Q_{ij} h_t(j) = 0,\ h_T(i) = e^{-f(i)}$.
γ solves HJE $\frac{\mathrm{d}}{\mathrm{d}t}\phi_t(i) + H(i,\vec{\phi}) = 0, \quad H(i,\vec{\phi}) := \sum_j Q_{ij}(e^{\phi(j)-\phi(i)} - 1)$.

SOC in infinite time, running cost via Girsanov transformation

- Girsanov Thm for pure jump (time-homogeneous case)

$$Z_t := e^{\int_0^t [\lambda^h(X_s^h) - \lambda(X_s^h)]\,\mathrm{d}s - \log \frac{h(X_t^h)}{h(X_0^h)}}, \quad t \geq 0$$

is positive, P-martingale, and of mean 1. Thus define P^h via $\frac{\mathrm{d}P^h}{\mathrm{d}P}\Big|_{\mathscr{F}_t} = Z_t$

$$(X^h, P, Q^h) \longrightarrow (X^h, P^h, Q)$$

The time marginal representation for finite time horizon (consistent with entropy)

$$\mathbb{E}^P(\log \frac{\mathrm{d}P^h}{\mathrm{d}P}\Big|_{\mathscr{F}_t}) = -\int_0^t \sum_i p_s^h(i) \sum_j Q_{ij} \mathrm{Ent}(\frac{h_s(j)}{h_s(i)})\,\mathrm{d}s.$$

- Stochastic optimal control formulation in the infinite time horizon

$$\gamma(x) = \min_{h, h_i > 0} \mathbb{E}_P\{f(X_\tau^h) + \log \frac{\mathrm{d}P}{\mathrm{d}P^h}\Big|_{\mathscr{F}_\tau}\}$$

s.t. X^h is the controlled process with generator Q^h under P, $X^h(0) = x \notin A \cup B$.

Optimality given by committor function and Doob transformation

Theorem

Transition path problem for Markov chain is formulated as

$$\gamma(i) = \min_{\vec{h}, h_i > 0} \mathbb{E}^P \left\{ f(X^h(\tau)) - \int_0^\tau (\lambda^h(X_s^h) - \lambda(X_s^h))\, \mathrm{d}s + [\log h(X_\tau^h) - \log h(X_0^h)] \right\},$$

s.t. $(X_t^h)_{t\geq 0}$ *is a Markov chain with generator* Q^h *under* P, $X_0^h = i \in (A \cup B)^c$.

The optimal control is given by discrete committor function, for $i \in (A \cup B)^c$,

$$\gamma(i) = -\log h^*(i) = -\log \mathbb{E}_P^i(e^{-f(X_\tau)}), \qquad \sum_j Q_{ij} h_j^* = 0, \quad h^*|_A = \delta,\ h^*|_B = 1.$$

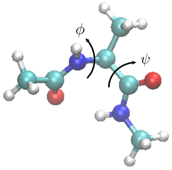
Optimal controlled jump rate doesn't change $\lambda_i^{h^*} := -Q_{i,i}^{h^*} = -Q_{i,i} = \lambda_i,\ i \notin A \cup B$

Remark: Optimal change of measure formulation (importance sampling, need parameterized $\tilde{P}$)

$$\gamma(x) = \min_{\tilde{P} \ll P} \mathbb{E}^P \left\{ f(\tilde{X}_\tau) - \log \frac{\mathrm{d}\tilde{P}}{\mathrm{d}P}\Big|_{\mathscr{F}_\tau} \right\},$$

s.t. $(\tilde{X})_{t\geq 0}$ is a Markov chain with generator Q under $\tilde{P}$, $x \notin A \cup B$.

Alanine dipeptide and two backbone dihedral angles



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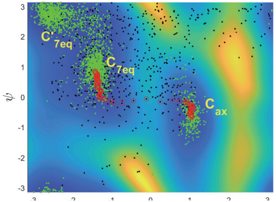

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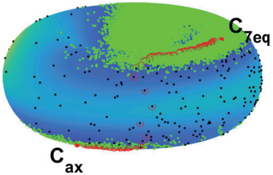

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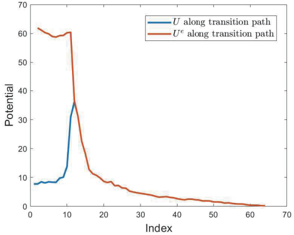

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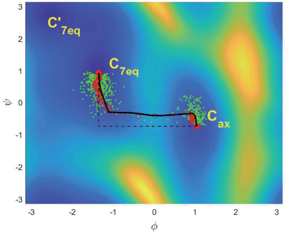

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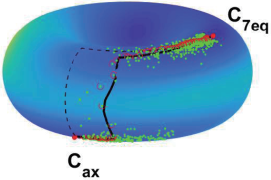

Conclusion

- Transition path theory via stochastic optimal control in infinite time horizon
- Finding optimal control $=$ optimal change of measure (parameterized) in path space
- Girsanov Thm: Running cost is the cost of changing measures:
  relative entropy on path space: quadratic for diffusion; entropy for Markov chain
- Optimal solution is given by continuous/discrete committor function (linear problem)
- Helps design optimally controlled random walk (rare event $\rightarrow$ almost surely)

Thank you!