A least-squares Monte-Carlo approach to rare events simulation

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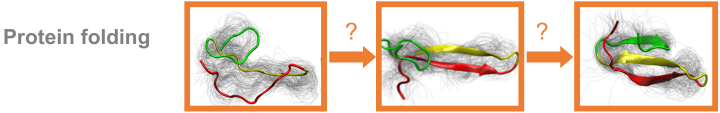
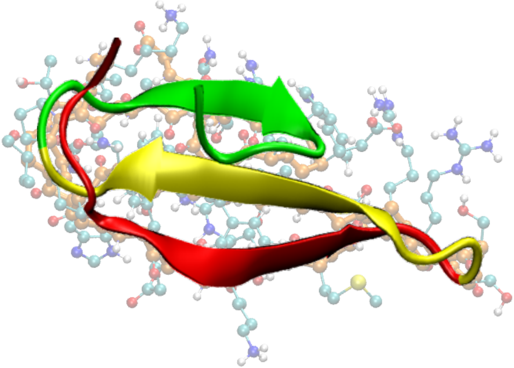
Motivation: conformation dynamics of biomolecules





[Noé et al, PNAS, 2009]

Motivation: conformation dynamics of biomolecules

Given a **Markov process** $(X_t)_{t\geq 0}$, discrete or continuous in time, we want to **estimate probabilities** $p \ll 1$, such as

$$p = P\left(\tau < T\right),$$

with τ the time to reach the target conformation, **free energies**

$$F(\beta) = -\beta^{-1} \log \mathbb{E}\left[e^{-\beta W}\right], \quad \beta > 0\,.$$

or **rates**

$$k = \left(\mathbb{E}[\tau]\right)^{-1}$$

where $\mathbb{E}[\cdot]$ is the expectation with respect to P.

Illustrative example: bistable system

- Overdamped Langevin equation

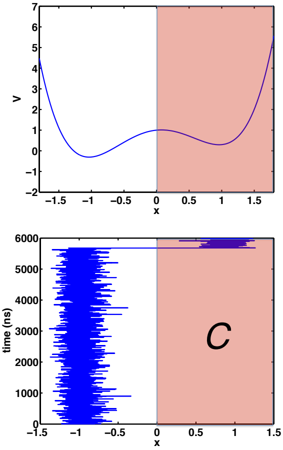
$$dX_t = -\nabla V(X_t)dt + \sqrt{2\epsilon}dB_t \, .$$

- Standard estimator of MGF $\psi = \psi_\epsilon$

$$\hat{\psi}_\epsilon^N = \frac{1}{N}\sum_{i=1}^{N} e^{-\alpha \tau_C^i} \, .$$

- Small noise asymptotics (Kramers)

$$\lim_{\epsilon \to 0} \epsilon \log \mathbb{E}[\tau_C] = \Delta V \, .$$



[Freidlin & Wentzell, 1984], [Berglund, Markov Processes Relat Fields 2013]

Illustrative example, cont'd

- **Relative error** of the MC estimator

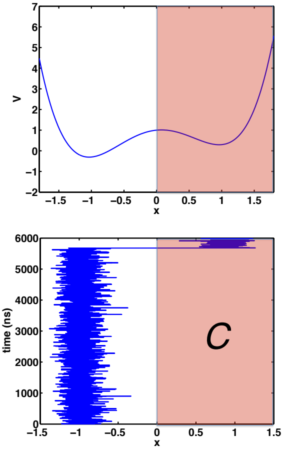
$$\delta_\epsilon = \frac{\sqrt{\mathrm{Var}[\hat{\psi}_N^\epsilon]}}{\mathbb{E}\left[\hat{\psi}_N^\epsilon\right]}$$

- Varadhan's large deviations principle

$$\mathbb{E}\left[(\hat{\psi}_\epsilon^N)^2\right] \gg (\mathbb{E}\left[\hat{\psi}_\epsilon^N\right])^2\,,\ \epsilon \text{ small.}$$

- Unbounded relative error as $\epsilon \to 0$

$$\limsup_{\epsilon\to 0} \delta_\epsilon = \infty$$



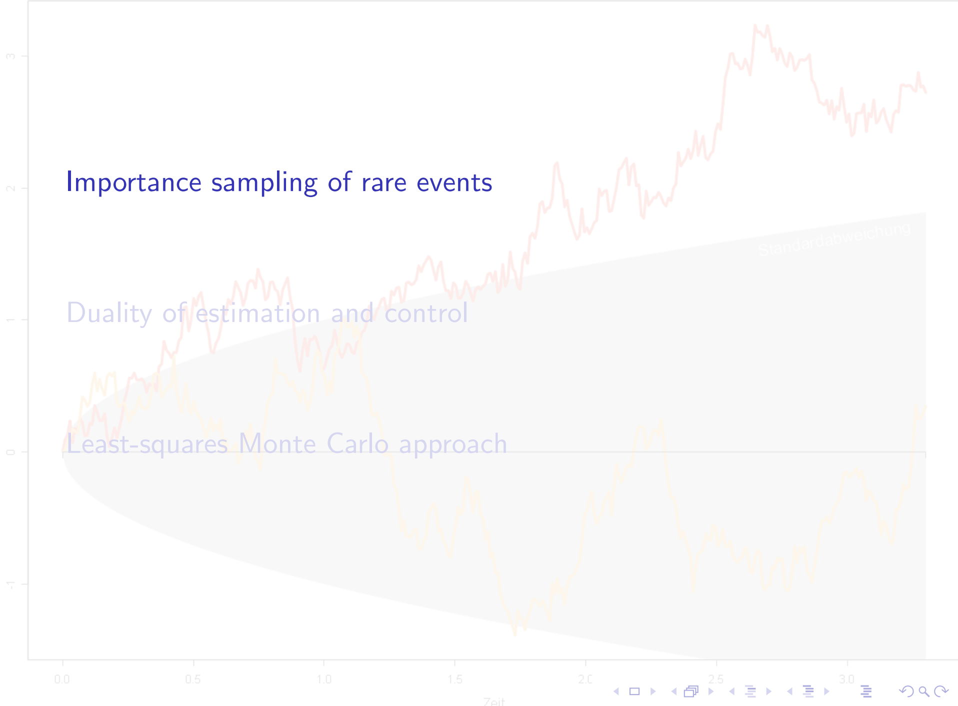
[Dupuis & Ellis, 1997]

Outline

Importance sampling of rare events

Duality of estimation and control

Least-squares Monte Carlo approach


Standardabweichung
Zeit
0.0
0.5
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1.5
2.0
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3.0
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1
2
3

Optimal change of measure: zero variance

Pick another probability measure Q with $\varphi = \frac{dQ}{dP} > 0$, under which the **rare event is no longer rare**, e.g.

$$P(\tau < T) = \mathbb{E}\left[\mathbf{1}_{\{\tau<T\}}\right] = \mathbb{E}_Q\left[\mathbf{1}_{\{\tau<T\}}\varphi^{-1}\right]$$

Zero-variance change of measure is given by

$$\varphi^* = \frac{\mathbf{1}_{\{\tau<T\}}}{\mathbb{E}\left[\mathbf{1}_{\{\tau<T\}}\right]}\,, \text{ i.e. } \quad Q^* = P(\,\cdot\,|\,\tau < T\,)\,,$$

but it depends on the quantity of interest $P(\tau < T)$.

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Idea no. 1

Exponential tilting from large deviations asymptotics

If $\psi_\epsilon \approx \hat{\psi}_\epsilon^N$ satisfies a **large deviations principle**, say,

$$\lim_{\epsilon \to 0} \epsilon \log \mathbb{E}[\hat{\psi}_\epsilon^N] = -\gamma$$

for some $\gamma > 0$. Then asymptotically efficient IS schemes can be based on **exponential family distributions** $Q = Q_\gamma$, such that

$$\lim_{\epsilon \to 0} \epsilon \log \mathbb{E}_Q[(\hat{\psi}_\epsilon^N)^2 \varphi^{-2}] = -2\gamma$$

Log-asymptotic efficiency:

$$\delta_\epsilon = e^{o(1/\epsilon)} \quad \text{as} \quad \epsilon \to 0\,,$$

i.e. the relative error grows subexponentially as $\epsilon \to 0$.

[Siegmund, Ann Stat, 1976], [Glasserman & Kou, AAP, 1997], [Dupuis & Wang, Stochastics, 2004]

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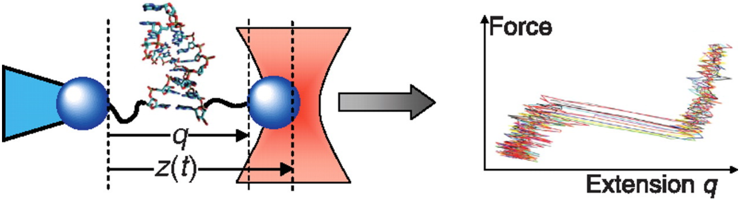
Idea no. 2

Exponential tilting from nonequilibrium forcing



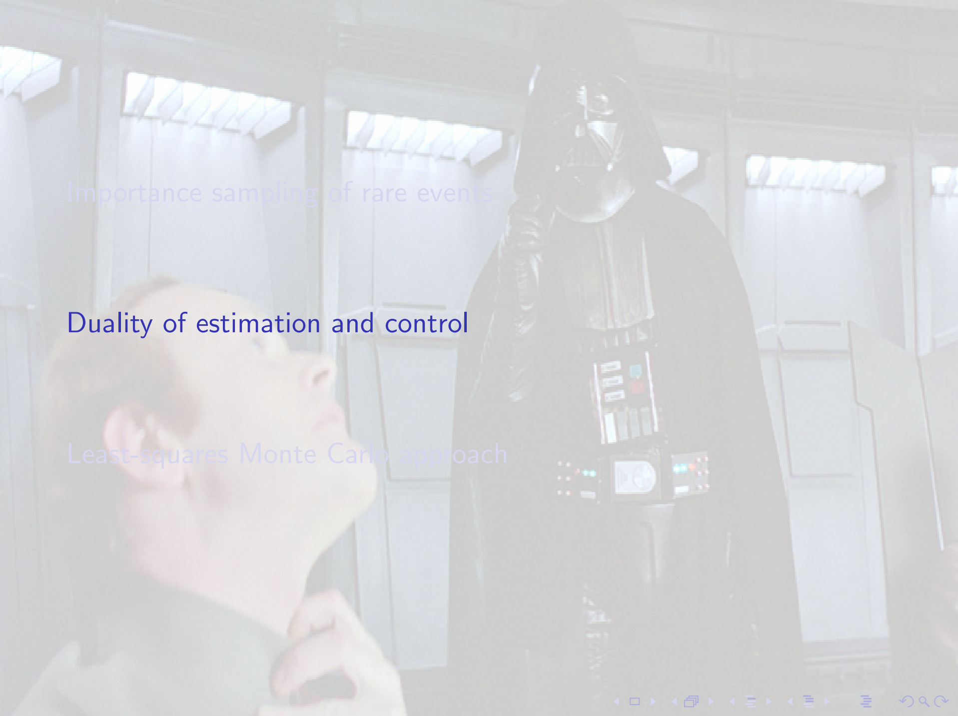
Single molecule pulling experiments, figure courtesy of G. Hummer, MPI Frankfurt

In vitro/in silico **free energy calculation** from forcing:

$$F(\beta) = -\beta^{-1} \log \mathbb{E}\left[e^{-\beta W}\right], \quad \beta > 0\,.$$

Forcing generates a "nonequilibrium" path space measure Q with typically **suboptimal likelihood quotient** $\varphi = dQ/dP$.

[Schlitter, J Mol Graph, 1994], [Hummer & Szabo, PNAS, 2001], Schulten & Park, JCP, 2004], ...



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Variational characterization of free energy

Theorem (Donsker & Varadhan)

For any bounded and measurable function W it holds

$$-\log \mathbb{E}\left[e^{-W}\right] = \min_{Q \ll P} \{\mathbb{E}_Q[W] + KL(Q, P)\}$$

where $KL(Q,P) \geq 0$ is the **relative entropy** between Q and P:

$$KL(Q,P) = \begin{cases} \int \log\left(\frac{dQ}{dP}\right) dQ & \text{if } Q \ll P \\ \infty & \text{otherwise} \end{cases}$$

Sketch of proof: Let $\varphi = dP/dQ$. Then

$$-\log \int e^{-W} dP = -\log \int e^{-W + \log\varphi} dQ \leq \int (W - \log\varphi)\, dQ$$

[Boué & Dupuis, LCDS Report #95-7, 1995], [Dai Pra et al, Math Control Signals Systems, 1996]

Same same, but different. . .

Set-up: uncontrolled ("equilibrium") diffusion process

Let $X = (X_s)_{s \geq 0}$ be a **diffusion process** on $\mathbb{R}^n$,

$$dX_s = b(X_s, s)ds + \sigma(X_s)dB_s \,, \quad X_t = x \,,$$

and

$$W(X) = \int_0^\tau f(X_s, s)\, ds + g(X_\tau) \,,$$

for suitable functions f, g and a **a.s. finite stopping time** $\tau < \infty$.

Aim: Estimate the path functional

$$\psi(x, t) = \mathbb{E}\left[e^{-W(X)}\right]$$

Set-up: controlled ("nonequilibrium") diffusion process

Now given a **controlled diffusion process** $X^u = (X^u_s)_{s \geq 0}$,

$$dX^u_s = (b(X^u_s, s) + \sigma(X^u_s)u_s)ds + \sigma(X^u_s)dB_s\,, \quad X^u_t = x\,,$$

and a probability $Q \ll P$ on $C([0,\infty))$ with **likelihood ratio**

$$\varphi(X^u) = \frac{dQ}{dP}\bigg|_{\mathcal{F}_\tau} = \exp\left(-\int_0^\tau u_s \cdot dB_s - \frac{1}{2}\int_0^\tau |u_s|^2\, ds\right)\,.$$

Now: Estimate the reweigthed path functional

$$\mathbb{E}\big[e^{-W(X)}\big] = \mathbb{E}\big[e^{-W(X^u)}(\varphi(X^u))^{-1}\big]$$

Variational characterization of free energies, cont'd

Theorem (H, 2012/2017)

Technical details aside, let u^* be a minimiser of the cost functional

$$J(u) = \mathbb{E}\left[W(X^u) + \frac{1}{2}\int_t^\tau |u_s|^2\, ds\right]$$

under the **controlled dynamics**

$$dX_s^u = (b(X_s^u, s) + \sigma(X_s^u)u_s)ds + \sigma(X_s^u)dB_s\,, \quad X_t^u = x\,.$$

The **minimiser is unique** with $J(u^*) = -\log\psi(x,t)$. Moreover,

$$\psi(x,t) = e^{-W(X^{u^*})}(\varphi(X^{u^*}))^{-1} \quad \text{(a.s.)}\,.$$

[H & Schütte, JSTAT, 2012], [H et al, Entropy, 2017]

Illustrative example, cont'd

- Exit problem: $f = \alpha$, $g = 0$, $\tau = \tau_C$:

$$J(u^*) = \min_u \mathbb{E}\left[\alpha\tau_C^u + \frac{1}{4\epsilon}\int_0^{\tau_C^u} |u_s|^2\, ds\right]$$

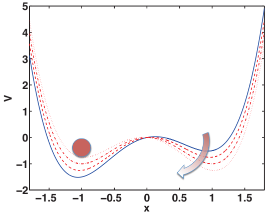
- Recovering **original statistics** by, e.g.,

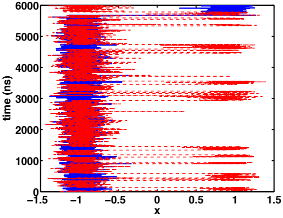
$$\mathbb{E}[\tau_C] = \frac{d}{d\alpha}\bigg|_{\alpha=0} J(u^*)$$

- Optimally tilted potential

$$U^*(x,t) = V(x) - u_t^*\, x$$

with **stationary** feedback $u_t^* = c(X_t^{u^*})$.





Sketch of proof (smooth case w/ classical solution)

By the **Feynman-Kac formula**,

$$\psi(x,t) = \mathbb{E}\left[\exp\left(-\int_0^\tau f(X_t,t)dt - g(X_\tau)\right)\middle| X_t = x\right]$$

solves the linear parabolic BVP on $\Omega \subset [0,\infty) \times \mathbb{R}^n$

$$(\mathcal{A} - f)\psi = f\psi\,, \quad \psi|_{\partial\Omega} = \exp(-g) \qquad \text{with } \mathcal{A} = \frac{\partial}{\partial t} - \mathcal{L}$$

The corresponding **semilinear BVP** for $F = -\log\psi$ reads

$$\mathcal{A}F - \frac{1}{2}|\nabla F|_a^2 + f = 0\,, \quad F|_{\partial\Omega} = g \qquad \text{with } a = \sigma\sigma^T$$

[H et al, JSTAT, 2012]; cf. [Fleming, SIAM J Control, 1978], [Boué & Dupuis, Ann Probab., 1998]

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Sketch of proof, cont'd

The semilinear Hamilton-Jacobi-Bellmann PDE

$$\mathcal{A}F - \frac{1}{2}|\nabla F|_a^2 + f = 0\,, \quad F|_{\partial\Omega} = g \qquad (a = \sigma\sigma^T)$$

is the **dynamic programming equation** for our stochastic control problem; it solution is the value function

$$F(x,t) = \min\{J(u) \colon X_t^u = x\}$$

If $F \in C^{2,1}$ the optimal control has **gradient form**, i.e.

$$u_t^* = -\sigma(X_t^{u^*})^T \nabla F(X_t^{u^*}, t)\,,$$

Generalizations: degenerate diffusions, Markov chains, ...

[Schütte et al, Math Prog, 2012], [Banisch & Hartmann, MCRF, 2016], [H et al, Entropy, 2017]

Sketch of proof, cont'd

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Related work (non-exhaustive)

- **Risk-sensitive control and dynamic games**: [Whittle, Eur J Oper Res, 1994], [James et al, IEEE TAC, 1994], [Dai Pra et al, Math Control Signals Systems, 1996], ...
- **Large deviations and control**: [Fleming, Appl Math Optim, 1977], [Fleming & Sheu, Ann Probab, 1997], [Pavon, Appl Math Optim, 1989], ...
- **Importance sampling of small noise diffusions**: [Dupuis & Wang, Stochastics, 2004], [Dupuis & Wang, Math Oper Res, 2007], [Vanden-Eijnden & Weare, CPAM, 2012], ...
- **Extension to multiscale systems**: [Spiliopoulos et al., SIAM MMS, 2012], [H et al, JCD, 2014], [H et al, Probab Theory Rel F, 2018], [Kebiri et al, Computation, 2018], ...

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From dynamic programming to FBSDE

Let $\Omega \subset [0, T] \times \mathbb{R}^n$ be bounded. The **semilinear HJB equation**

$$\frac{\partial F}{\partial t} + \mathcal{L}F + h(x, F, \sigma^T \nabla F) = 0\,, \; F|_{\partial\Omega} = g$$

for $F \in C^{2,1}$ is equivalent to the **forward-backward SDE**

$$\begin{aligned} dX_s &= b(X_s, s)ds + \sigma(X_s)dB_s\,, \; X_t = x \\ dY_s &= -h(X_s, Y_s, Z_s)ds + Z_s \cdot dB_s\,, \; Y_\tau = g(X_\tau)\,, \end{aligned}$$

where $t \leq s \leq \tau \leq T$ and

$$Y_s = F(X_s, s)\,, \quad Z_s = \sigma(X_s)^T \nabla F(X_s, s).$$

Formal derivation: Itô's Lemma

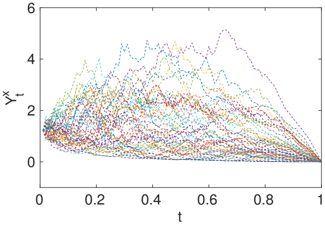
[Pardoux & Peng, LNCIS 176, 1992], [Kobylanski, Ann Probab, 2000]

Some remarks

- The **solution is a triplet** (X, Y, Z) where the pair $(Y_s, Z_s)_s$ is adapted to the filtration generated by $(X_s)_s$.
- Hence $Y_t = F(x, t)$ is a **deterministic** function of the initial data (x, t), and $-Z_t$ is the **optimal control** u^* at time t.
- The backward SDE is **not a time-reversed SDE**; e.g. for $h \equiv 0$ and $Y_T = X_T$, the pair $(Y_s, Z_s) \equiv (X_T, 0)$ satisfies

$$dY_s = Z_s \cdot dB_s \,,$$

but it is **not adapted**.



- **A fix:** L^2 projection onto the filtration generated by $(X_s)_s$.

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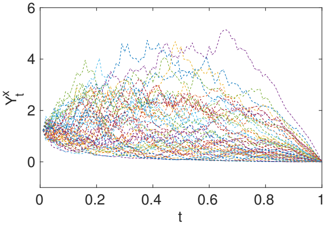

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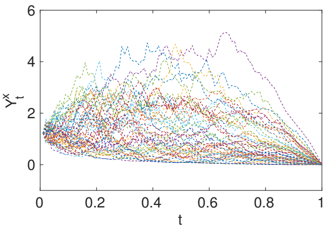

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Numerical discretisation of FBSDE

The **FBSDE is decoupled** and an explicit scheme can be based on

$$\hat{X}_{n+1} = \hat{X}_n + \Delta t\, b(\hat{X}_n, t_n) + \sqrt{\Delta t}\, \sigma(\hat{X}_n)\xi_{n+1}$$
$$\hat{Y}_{n+1} = \hat{Y}_n - \Delta t\, h(\hat{X}_n, \hat{Y}_n, \hat{Z}_n) + \sqrt{\Delta t}\, \hat{Z}_n \cdot \xi_{n+1}$$

Since $\hat{Y}_n$ **is adapted** we have $\hat{Y}_n = \mathbb{E}\big[\hat{Y}_n | \mathcal{F}_n\big]$ and thus

$$\begin{aligned}\hat{Y}_n &= \mathbb{E}\big[\hat{Y}_{n+1} + \Delta t\, h(\hat{X}_n, \hat{Y}_n, \hat{Z}_n) | \mathcal{F}_n\big] \\ &\approx \mathbb{E}\big[\hat{Y}_{n+1} + \Delta t\, h(\hat{X}_n, \hat{Y}_{n+1}, \hat{Z}_{n+1}) | \mathcal{F}_n\big]\end{aligned}$$

where $\mathcal{F}_n = \sigma(\hat{X}_0, \ldots, \hat{X}_n)$ using that $\hat{Z}_n$ is independent of ξ_{n+1}.

[Gobet et al, AAP, 2005], [Bender & Steiner, Num Meth F, 2012], [Kebiri et al, Proc IHP, 2018]

Numerical discretisation of FBSDE, cont'd

The conditional expectation

$$\hat{Y}_n := \mathbb{E}\big[\hat{Y}_{n+1} + \Delta t\, h(\hat{X}_n, \hat{Y}_{n+1}, \hat{Z}_{n+1}) | \mathcal{F}_n\big]$$

can be computed by **least-squares**:

$$\mathbb{E}\big[S|\mathcal{F}_n\big] = \operatorname*{argmin}_{Y \in L^2,\, \mathcal{F}_n\text{-measurable}} \mathbb{E}[|Y - S|^2]\,.$$

Specifically,

$$\hat{Y}_n \approx \operatorname*{argmin}_{Y = Y_K(\hat{X}_n)} \frac{1}{M} \sum_{m=1}^{M} \Big| Y - \hat{Y}_{n+1}^{(m)} - \Delta t\, h\big(\hat{X}_n^{(m)}, \hat{Y}_{n+1}^{(m)}, \hat{Z}_{n+1}^{(m)}\big)\Big|^2,$$

where $Y_K(x) = \alpha_1 \phi_1(x) + \ldots + \alpha_K \phi_K(x)$.

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Numerical discretisation of FBSDE, cont'd

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More remarks

- The scheme is **strongly convergent** of order $1/2$ in $\Delta t \to 0$ as $M, K \to \infty$.
- A (fictitious) **zero-variance change of measure** is given by

$$\left.\frac{dQ}{dP}\right|_{\mathcal{F}_\tau} = \exp\left(\int_0^\tau Z_s \cdot dB_s^u + \frac{1}{2}\int_0^\tau |Z_s|^2\, ds\right),$$

  for $\tau \leq T$ and the discretisation bias can be further reduced by using **importance sampling**.
- **Generalisations include** unbounded & random τ, singular terminal condition, least-squares w/ change of drift.
- **Alternative algorithms:** stochastic gradient descent, cross-entropy minimisation, approximate policy iteration.

[Turkedjiev, PhD thesis, 2013], [Kruse & Popier, SPA, 2016], [Kebiri & H, Preprint, 2018]

Numerical illustration

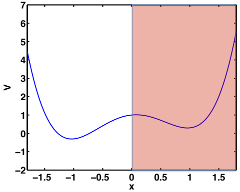
Example I: hitting probabilities

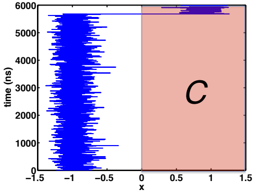
Probability of **hitting the set** $C \subset \mathbb{R}$ before time T:

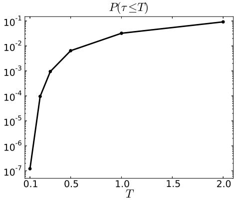
$$-\log \mathbb{P}(\tau \leq T) = \min_u \mathbb{E}\left[\frac{1}{4}\int_0^{\tau \wedge T} |u_t|^2 \, dt - \log \mathbf{1}_{\partial C}(X^u_{\tau \wedge T})\right],$$

with τ denoting the first hitting time of C under the dynamics

$$dX^u_t = (u_t - \nabla V(X^u_t))\, dt + \sqrt{2\epsilon}\, dB_t$$







[Zhang et al, SISC, 2014], [Richter, MSc thesis, 2016], [H et al, Nonlinearity, 2016]

Example I, cont'd

Probability of **hitting** $C \subset \mathbb{R}$ before time T, starting from $x = -1$:

$$-\log \mathbb{P}(\tau \leq T) = \min_u \mathbb{E}\left[\frac{1}{4}\int_0^{\tau \wedge T} |u_t|^2\, dt - \log \mathbf{1}_{\partial C}(X^u_{\tau \wedge T})\right],$$

(BSDE with singular terminal condition and random stopping time)

Simulation parameters	$F^{\epsilon}_{ref}(0,x)$	$\bar{F}^{\epsilon}(0,x)$	Var
$K = 8,\ M = 300,\ T = 5,\ \Delta t = 10^{-3},\ \epsilon = 1$	0.3949	0.3748	10^{-3}
$K = 5,\ M = 300,\ T = 1,\ \Delta t = 10^{-3},\ \epsilon = 1$	1.7450	1.6446	0.0248
$K = 5,\ M = 400,\ T = 1,\ \Delta t = 10^{-4},\ \epsilon = 0.6$	4.3030	4.5779	10^{-3}
$K = 6,\ M = 450,\ T = 1,\ \Delta t = 10^{-4},\ \epsilon = 0.5$	4.5793	4.6044	$5 \cdot 10^{-4}$

with K the number of Gaussians and M the number of realisations of the forward SDE.

[Ankirchner et al, SICON, 2014], [Kruse & Popier, SPA, 2016], [Kebiri et al, Proc IHP, 2018]

Example II: High-dimensional PDE

First exit time of a **Brownian motion** from an n-sphere of radius r:

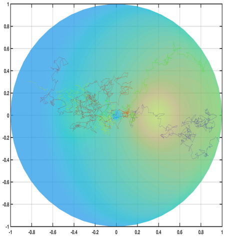
$$\tau = \inf\{t > 0 \colon x + B_t \notin S_r^n\}$$

Cumulant generating function of first exit time satisfies

$$-\log \mathbb{E}_x[\exp(-\alpha\tau)] = \min_u \mathbb{E}_x \left[\alpha\tau^u + \frac{1}{2}\int_0^{\tau^u} |u_t|\, dt\right]$$

- BSDE on random time horizon with homogeneous terminal condition
- mean first exit time $\mathbb{E}_x[\tau] = \frac{r^2 - |x|^2}{n}$
- Least-squares MC w/ $K = 3, M \sim 10^2$

	$n = 3$	$n = 10$	$n = 100$	$n = 1000$
exact	1.00	1.00	1.00	1.00
CMC	0.98	0.99	1.08	1.04
LSMC	0.99	1.01	0.96	0.98



[Kebiri & H, Preprint, 2018]

Conclusions, outlook and open problems

- Adaptive importance sampling scheme based on **dual variational formulation**; resulting control problem features short trajectories with **minimum variance estimators**.
- **Variational problem** boils down to an uncoupled FBSDE with only one additional spatial dimension.
- **Error analysis** for unbounded stopping time & singular terminal condition is open, **least-squares algorithm** requires some fine-tuning (ansatz functions, change of drift, ...).
- Clever choice of ansatz functions should involve **dimension reduction**—preliminary results for slow-fast systems

$$\sup\{|\hat{Y}_t^\delta - Y_t| : 0 \le t \le T\} \le C_{M,K,\Delta t}\sqrt{\delta} \quad \delta = \frac{\tau_{\text{fast}}}{\tau_{\text{slow}}}$$

as $\Delta t = \mathcal{O}(\delta) \to 0$ and $M, K \to \infty$ (analogously for $\hat{Z}_t$).

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Thank you for your attention!

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