Learning to reflect – On data driven approaches to stochastic optimal control

Algorithms & Computationally Intensive Inference seminars – University of Warwick

Lukas Trottner
based on joint works with Sören Christensen, Asbjørn Holk Thomsen and Claudia Strauch

29 November 2024

University of Birmingham Kiel University Aarhus University Heidelberg University

Framework for data-driven stochastic optimal control

- consider a d-dimensional ergodic diffusion

$$\mathrm{d}X_t = b(X_t)\,\mathrm{d}t + \sigma(X_t)\,\mathrm{d}W_t,$$

- we assume that the drift b is unknown
- which challenges arise from this uncertainty when we want to optimally control the process and how can they be solved in a data-driven way?
- concrete control problems considered in the literature:
  1. impulse controls in 1D (Christensen, Strauch (*AOAP*, 2023); Christensen, Dexheimer, Strauch (2023+))
  2. reflection controls (singular) (Christensen, Strauch, T. (*Bernoulli*, 2024); Christensen, Holk Thomsen, T. (*JUQ*, 2024))

Framework for data-driven stochastic optimal control

- consider a d-dimensional ergodic diffusion

$$\mathrm{d}X_t = b(X_t)\,\mathrm{d}t + \sigma(X_t)\,\mathrm{d}W_t,$$

- we assume that the drift b is unknown
- which challenges arise from this uncertainty when we want to optimally control the process and how can they be solved in a data-driven way?
- concrete control problems considered in the literature:
  1. impulse controls in 1D (Christensen, Strauch (*AOAP*, 2023); Christensen, Dexheimer, Strauch (2023+))
  2. reflection controls (singular) (Christensen, Strauch, T. (*Bernoulli*, 2024); Christensen, Holk Thomsen, T. (*JUQ*, 2024))

Challenge

Exploration vs. exploitation

Reflection control problem

- consider a d-dimensional Langevin diffusion

$$\mathrm{d}X_t = -\nabla V(X_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t;$$

  if ergodic: stationary density $\pi \propto \exp(-V(\cdot))$
- we play the following game:
  1. the aim is to keep the process close to a target state, say 0, at minimal long run costs
  2. normally reflect the process in a domain D that we are free to choose:

$$\mathrm{d}X_t^D = -\nabla V(X_t^D)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t + n(X_t^D)\,\mathrm{d}L_t^D, \quad \text{where } L_t^D = \lim_{\varepsilon\downarrow 0} \frac{1}{\varepsilon}\int_0^s \mathbf{1}_{(\partial D)_\varepsilon}(X_s^D)\,\mathrm{d}s$$

  3. costs:

$$J_T(D) = \underbrace{\int_0^T c(X_t^D)\,\mathrm{d}t}_{c \text{ increasing in } |x|} + \underbrace{\kappa L_T^D}_{\text{reflection costs}}$$

Reflection control problem

- consider a d-dimensional Langevin diffusion

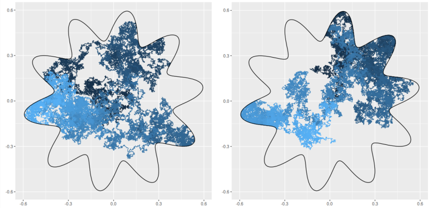
$$\mathrm{d}X_t = -\nabla V(X_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t;$$

  if ergodic: stationary density $\pi \propto \exp(-V(\cdot))$
- we play the following game:
  1. the aim is to keep the process close to a target state, say 0, at minimal long run costs
  2. normally reflect the process in a domain D that we are free to choose:

$$\mathrm{d}X_t^D = -\nabla V(X_t^D)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t + n(X_t^D)\,\mathrm{d}L_t^D, \quad \text{where } L_t^D = \lim_{\varepsilon \downarrow 0} \frac{1}{\varepsilon} \int_0^s \mathbf{1}_{(\partial D)_\varepsilon}(X_s^D)\,\mathrm{d}s$$

  3. costs:

$$J_T(D) = \underbrace{\int_0^T c(X_t^D)\,\mathrm{d}t}_{c \text{ increasing in } |x|} + \underbrace{\kappa L_T^D}_{\text{reflection costs}}$$



Reflection control problem

- consider a d-dimensional Langevin diffusion

$$\mathrm{d}X_t = -\nabla V(X_t)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t;$$

  if ergodic: stationary density $\pi \propto \exp(-V(\cdot))$
- we play the following game:
  1. the aim is to keep the process close to a target state, say 0, at minimal long run costs
  2. normally reflect the process in a domain D that we are free to choose:

$$\mathrm{d}X_t^D = -\nabla V(X_t^D)\,\mathrm{d}t + \sqrt{2}\,\mathrm{d}W_t + n(X_t^D)\,\mathrm{d}L_t^D, \quad \text{where } L_t^D = \lim_{\varepsilon\downarrow 0}\frac{1}{\varepsilon}\int_0^s \mathbf{1}_{(\partial D)_\varepsilon}(X_s^D)\,\mathrm{d}s$$

  3. costs:

$$J_T(D) = \underbrace{\int_0^T c(X_t^D)\,\mathrm{d}t}_{c \text{ increasing in } |x|} + \underbrace{\kappa L_T^D}_{\text{reflection costs}}$$

- Ergodic optimal control: for an admissible domain class Θ determine

$$D^* \in \operatorname*{arg\,min}_{D\in\Theta} \underbrace{\lim_{T\to\infty}\frac{1}{T}\mathbb{E}[J_T(D)]}_{=:J(D)} \quad (\rightsquigarrow \text{shape optimisation problem})$$

- Data-driven optimal control: If V is unknown, determine an estimator $\widehat{D}$ of D^* based on observations of the (controlled) process

Ergodic costs

- let $\mathbf{D}$ be a class of C^2-domains such that for any $D \in \mathbf{D}$ we have $\inf_{x,y\in\overline{D}} p_1^D(x,y) > 0$ for bicontinuous transtion densities p_t^D
- for any $D \in \mathbf{D}$, X^D is ergodic with invariant density

$$\pi_D(x) = \frac{\exp(-V(x))}{\int_D \exp(-V(x))} \; (= \pi(x)/\pi(D) \text{ if free diffusion is ergodic})$$

Theorem

For any $D \in \mathbf{D}$, it holds that

$$J(D) = \int_D c(x)\pi_D(x)\,\mathrm{d}x + \kappa \int_{\partial D} \pi_D(x)\,\mathcal{H}_{d-1}(\mathrm{d}x).$$

and

$$\mathbb{E}^x\Big[\Big|\frac{1}{T}\Big(\int_0^T c(X_t^D)\,\mathrm{d}t + \kappa L_T^D\Big) - J(D)\Big|\Big] \lesssim_D \frac{1}{\sqrt{T}}, \quad x \in D.$$

If $\mathrm{e}^{-V} \in L^1(\mathbb{R}^d)$, then in particular

$$J(D) = J(D,\pi) = \frac{1}{\int_D \pi(y)\,\mathrm{d}y}\Big(\int_D c(y)\pi(y)\,\mathrm{d}y + \kappa \int_{\partial D} \pi(y)\,\mathcal{H}^{d-1}(\mathrm{d}y)\Big).$$

Invariant density estimation

Multivariate kernel density estimator:

$$\hat{\pi}_{\boldsymbol{h},T}(x) := \frac{1}{\prod_{i=1}^d h_i} \int_0^T \mathbb{K}((x - X_t)/\boldsymbol{h})\,\mathrm{d}t, \quad \mathbb{K}(x) := \prod_{i=1}^d K(x_i), \quad x/\boldsymbol{h} := (x_i/h_i)_{i=1,\dots,d}.$$

Results from Strauch (*AOS*, 2018) show that if X satisfies both a Poincaré inequality and a Nash inequality, then under anisotropic $\boldsymbol{\beta}$-Hölder smoothness assumptions on π and sufficient order of K, there exists an adaptive bandwith choice $\hat{\boldsymbol{h}}_T$ such that

$$\mathbb{E}^\pi\Big[\|\hat{\pi}_{\hat{\boldsymbol{h}}_T,T} - \pi\|_\infty^p\Big]^{1/p} \lesssim \Psi_{d,\boldsymbol{\beta}}(T) := \begin{cases} \sqrt{\log T/T}, & d = 1, \\ \frac{\log T}{\sqrt{T}}, & d = 2, \\ \left(\frac{\log T}{T}\right)^{\frac{\overline{\beta}}{2\overline{\beta}+d-2}}, & d \geq 3, \end{cases} \quad \text{where } \overline{\boldsymbol{\beta}} = \Big(\frac{1}{d}\sum_{i=1}^d \frac{1}{\beta_i}\Big)^{-1}.$$

Learning the optimal reflection boundary

Proposition

Let $\hat{\pi}_T^* := \hat{\pi}_{\hat{\boldsymbol{h}}_T,T} \vee \underline{\pi}$, where $\pi \geq \underline{\pi}$ on $B(0,\overline{\lambda})$. Let Θ be a family of domains s.t. $B(0,\underline{\lambda}) \subset D \subset B(0,\overline{\lambda})$ and $\mathcal{H}^{d-1}(\partial D) \leq \Lambda$ for any $D \in \Theta$. For

$$\widehat{D}_T \in \operatorname*{arg\,min}_{D\in\Theta} J(D, \hat{\pi}_T^*),$$

it holds for a warm start μ that

$$\mathbb{E}^{\mu}\Big[J(\widehat{D}_T, \pi) - \min_{D\in\Theta} J(D,\pi)\Big] \lesssim \Psi_{d,\boldsymbol{\beta}}(T).$$

Learning the optimal reflection boundary

Proposition

Let $\hat{\pi}_T^* := \hat{\pi}_{\hat{\boldsymbol{h}}_T,T} \vee \underline{\pi}$, where $\pi \geq \underline{\pi}$ on $B(0,\overline{\lambda})$. Let Θ be a family of domains s.t. $B(0,\underline{\lambda}) \subset D \subset B(0,\overline{\lambda})$ and $\mathcal{H}^{d-1}(\partial D) \leq \Lambda$ for any $D \in \Theta$. For

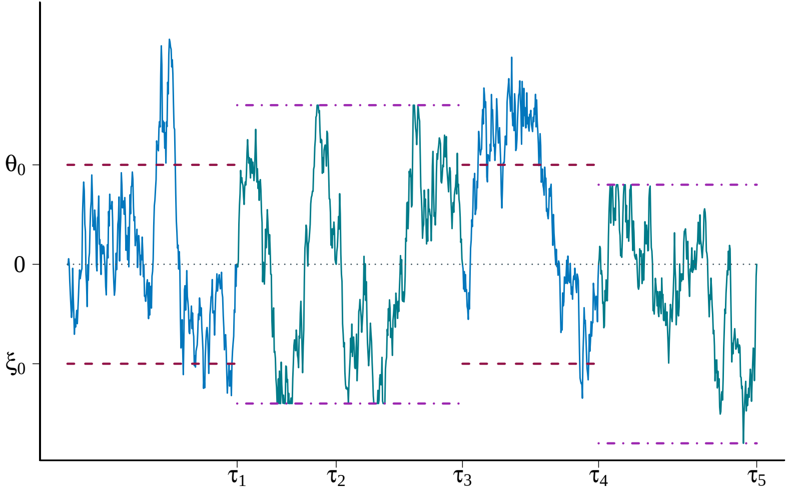
$$\widehat{D}_T \in \operatorname*{arg\,min}_{D \in \Theta} J(D, \hat{\pi}_T^*),$$

it holds for a warm start μ that

$$\mathbb{E}^\mu\Big[J(\widehat{D}_T, \pi) - \min_{D \in \Theta} J(D, \pi)\Big] \lesssim \Psi_{d,\boldsymbol{\beta}}(T).$$

- ⇝ this gives a bound on the simple regret only
- ⇝ how can we use this to determine strategies that overcome exploration vs. exploitation tradeoff with sublinear regret rate?

Episodic domain learning in 1D



Regret bound for episodic domain learning

Theorem (Christensen, Strauch, T. (2024)[1]; Christensen, Holk, T. (2024)[2])

There exists a purely data-driven episodic domain learning strategy $\widehat{Z}$ such that the expected regret per time unit satisfies

$$\frac{1}{T}\mathbb{E}\Big[\int_0^T c(X_t^{\widehat{Z}})\,\mathrm{d}t + \kappa L_T^{\widehat{Z}}\Big] - J(D^*) \lesssim \begin{cases} \frac{\sqrt{\log T}}{T^{1/3}}, & d = 1, \\ \Big(\frac{(\log T)^2}{T}\Big)^{\frac{1}{3}}, & d = 2, \\ \Big(\frac{\log T}{T}\Big)^{\frac{\overline{\beta}}{3\overline{\beta}+d-2}}, & d \geq 3. \end{cases}$$

[1]Strauch, Christensen and Trottner (2024). Learning to reflect: A unifying approach to data-driven control strategies. *Bernoulli*
[2]Christensen, Holk Thomsen and Trottner (forthcoming). Data-driven rules for multidimensional reflection problems. *SIAM/ASA J. Uncert. Quantif.*

Regret bound for episodic domain learning

Theorem

There exists a purely data-driven episodic domain learning strategy $\widehat{Z}$ such that the expected regret per time unit satisfies

$$\frac{1}{T}\mathbb{E}\Big[\int_0^T c(X_t^{\widehat{Z}})\,\mathrm{d}t + \kappa L_T^{\widehat{Z}}\Big] - J(D^*) \lesssim \begin{cases} \frac{\sqrt{\log T}}{T^{1/3}}, & d = 1, \\ \Big(\frac{(\log T)^2}{T}\Big)^{\frac{1}{3}}, & d = 2, \\ \Big(\frac{\log T}{T}\Big)^{\frac{\overline{\beta}}{3\overline{\beta}+d-2}}, & d \geq 3. \end{cases}$$

- 1D case: for S_T the (random) exploration time and N_T the number of exploration intervals until time T, choose a strategy such that for some $m, M > 0$,

$$\mathbb{P}(T^{-2/3}S_T \leq M) \lesssim T^{-1/3} \quad \text{and} \quad \limsup_{T\to\infty} T^{-2/3}\mathbb{E}[N_T] \leq M$$

- if $(c_n)_{n\in\mathbb{N}}$ is a binary sequence with $c_n = 0$ if n-th period is exploration, this is satified provided that for some $a > 0$

$$n^{2/3} \leq |\{i \leq n \,:\, c_i = 0\}| \leq n^{2/3} + a.$$

Regret bound for episodic domain learning

Theorem

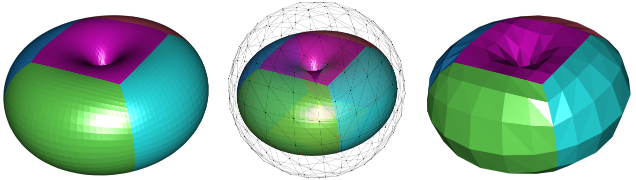
There exists a purely data-driven episodic domain learning strategy $\widehat{Z}$ such that the expected regret per time unit satisfies

$$\frac{1}{T}\mathbb{E}\Big[\int_0^T c(X_t^{\widehat{Z}})\,\mathrm{d}t + \kappa L_T^{\widehat{Z}}\Big] - J(D^*) \lesssim \begin{cases} \frac{\sqrt{\log T}}{T^{1/3}}, & d = 1, \\ \Big(\frac{(\log T)^2}{T}\Big)^{\frac{1}{3}}, & d = 2, \\ \Big(\frac{\log T}{T}\Big)^{\frac{\overline{\beta}}{3\overline{\beta}+d-2}}, & d \geq 3. \end{cases}$$

- multivariate case: X does not hit points for $d \geq 2$ $\rightsquigarrow$ construction of stochastic exploration/exploitation intervals as in the one-dimensional case not feasible
- instead: alternate between exploration/exploitation intervals with deterministic lengths $a_i \asymp 2^i$ and exploitation lengths $b_i \asymp a_i/\Psi_{d,\beta}(a_i)$ (+ asymptotically negligible stochastic fluctuation for exploitation lengths to make sure that the process is inside of proposed reflection domain)
- for technical reasons estimated reflection domain in i-th exploitation interval calculated only from data in i-th exploration interval

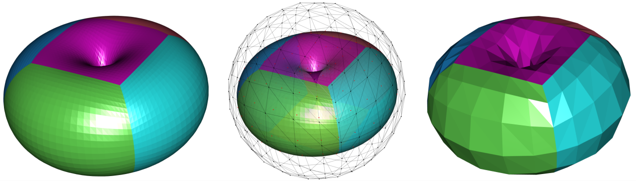
Numerical shape optimisation

- as target domains Θ only allow strongly star-shaped sets at 0 (appropriate when continuous costs c are minimised close to the origin) $\rightsquigarrow$ $\partial D = \{r(q)q \,:\, q \in S^{d-1}\}$ for some radial function $r:\, S^{d-1} \to (0,\infty)$
- for N points $\{q_i\}_{i=1}^N \subset S^{d-1}$ consider the polytope $\widetilde{D}$ with vertices $\{p_i\}_{i=1}^N = \{r(q_i)q_i\}_{i=1}^N$ $\rightsquigarrow$ $\widetilde{D}$ can be split into N simplices $\{S_I\}_{I\in\mathcal{J}}$ with facets $\{F_I\}_{I\in\mathcal{J}}$ opposite the origin



Numerical shape optimisation

- as target domains Θ only allow strongly star-shaped sets at 0 (appropriate when continuous costs c are minimised close to the origin) $\rightsquigarrow \partial D = \{r(q)q \,:\, q \in S^{d-1}\}$ for some radial function $r : S^{d-1} \to (0, \infty)$
- for N points $\{q_i\}_{i=1}^N \subset S^{d-1}$ consider the polytope $\widetilde{D}$ with vertices $\{p_i\}_{i=1}^N = \{r(q_i)q_i\}_{i=1}^N \rightsquigarrow \widetilde{D}$ can be split into N simplices $\{S_l\}_{l\in\mathcal{J}}$ with facets $\{F_l\}_{l\in\mathcal{J}}$ opposite the origin

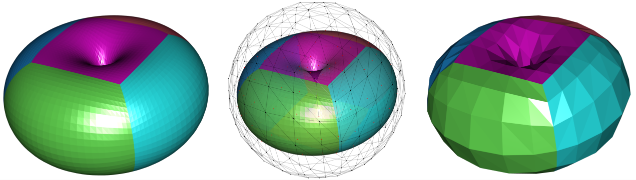


- for $\boldsymbol{r} = \{r_i\}_{i=1}^N = \{r(q_i)\}_{i=1}^N$ we have

$$J(D) \approx J(\widetilde{D}) \equiv J(\boldsymbol{r}) = \frac{1}{\sum_{l\in\mathcal{J}} \int_{S_l} e^{-V(x)}\,dx} \sum_{l\in\mathcal{J}} \left(\int_{S_l} c(x) e^{-V(x)}\,dx + \kappa \int_{F_l} e^{-V(x)}\,\mathcal{H}^{d-1}(dx) \right)$$

Numerical shape optimisation

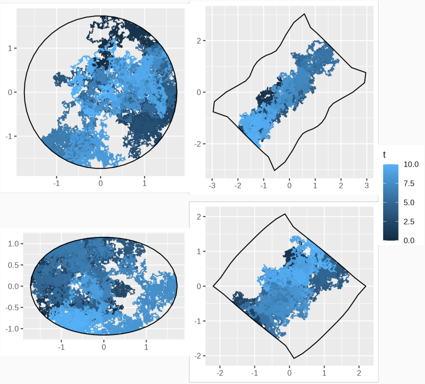
- as target domains Θ only allow strongly star-shaped sets at 0 (appropriate when continuous costs c are minimised close to the origin) $\rightsquigarrow \partial D = \{r(q)q \,:\, q \in S^{d-1}\}$ for some radial function $r : S^{d-1} \to (0,\infty)$
- for N points $\{q_i\}_{i=1}^N \subset S^{d-1}$ consider the polytope $\widetilde{D}$ with vertices $\{p_i\}_{i=1}^N = \{r(q_i)q_i\}_{i=1}^N \rightsquigarrow \widetilde{D}$ can be split into N simplices $\{S_I\}_{I\in\mathcal{J}}$ with facets $\{F_I\}_{I\in\mathcal{J}}$ opposite the origin



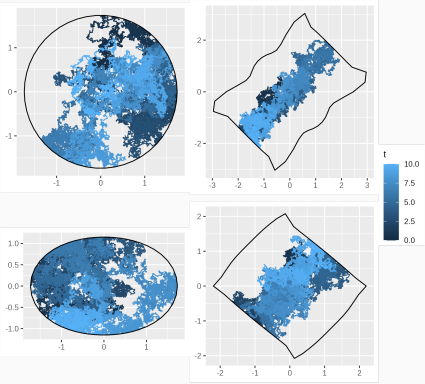
- for $\boldsymbol{r} = \{r_i\}_{i=1}^N = \{r(q_i)\}_{i=1}^N$ we have

$$J(D) \approx J(\widetilde{D}) \equiv J(\boldsymbol{r}) = \frac{1}{\sum_{I\in\mathcal{J}} \int_{S_I} \mathrm{e}^{-V(x)}\,\mathrm{d}x} \sum_{I\in\mathcal{J}} \left(\int_{S_I} c(x)\mathrm{e}^{-V(x)}\,\mathrm{d}x + \kappa \int_{F_I} \mathrm{e}^{-V(x)}\,\mathcal{H}^{d-1}(\mathrm{d}x) \right)$$

- we derive explicit expressions for $\nabla J(\boldsymbol{r})$ to employ a gradient descent algorithm for shape optimisation

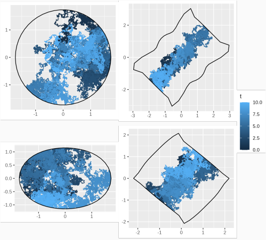


Simulated optimal shapes and corresponding path realisations of reflected processes. Top left: Brownian motion with norm cost. Top right: Ornstein–Uhlenbeck process with norm cost. Bottom left: Brownian motion with skewed cost. Bottom right: Ornstein–Uhlenbeck process with skewed cost.



	Brownian motion	Ornstein–Uhlenbeck
norm cost function	2.22 (2.31)	1.18 (1.15)
skewed cost function	2.83 (2.91)	1.66 (1.74)

Table 1: Average realized costs vs. expected average long term costs (in brackets)



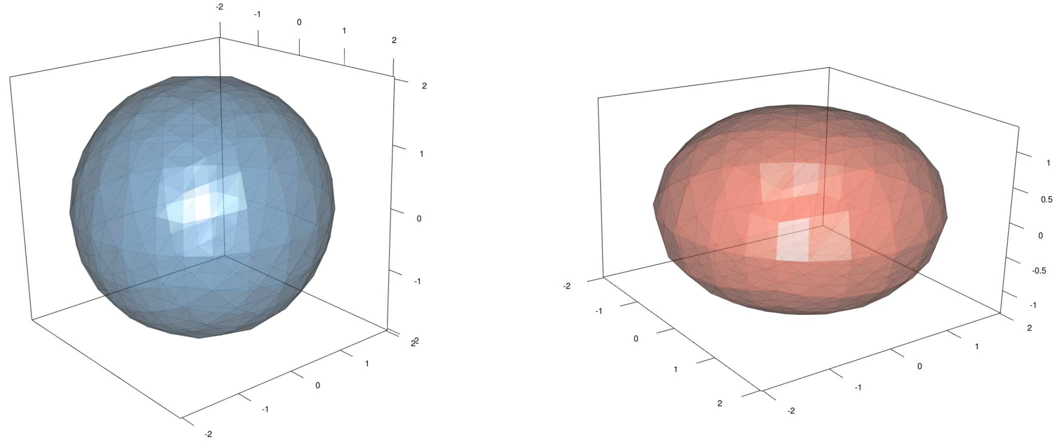
- Simulation of reflected diffusion (Słomiński, *SPA* 1994): simulate proposal

$$X^{\text{prop}}_{(n+1)\Delta} = X_{n\Delta} - \nabla V(X_{n\Delta})\Delta + \sqrt{2\Delta}\xi_{n+1}, \quad (\xi_i)_i \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, I_d),$$

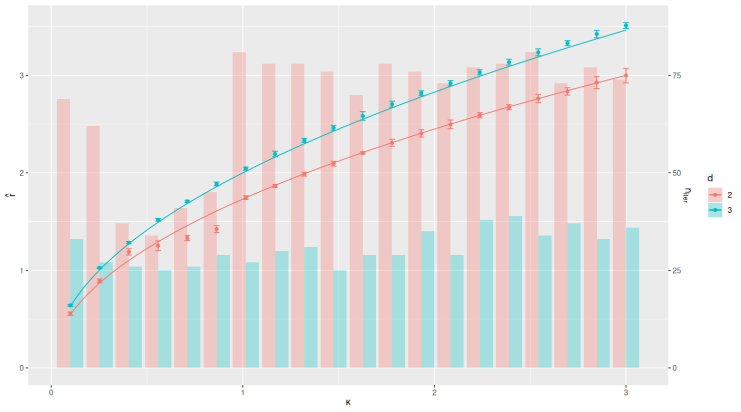
  then set

$$X_{(n+1)\Delta} = \text{Proj}_D(X^{\text{prop}}_{(n+1)\Delta}), \quad L_{(n+1)\Delta} = L_{n\Delta} + |X^{\text{prop}}_{(n+1)\Delta} - X_{(n+1)\Delta}|$$

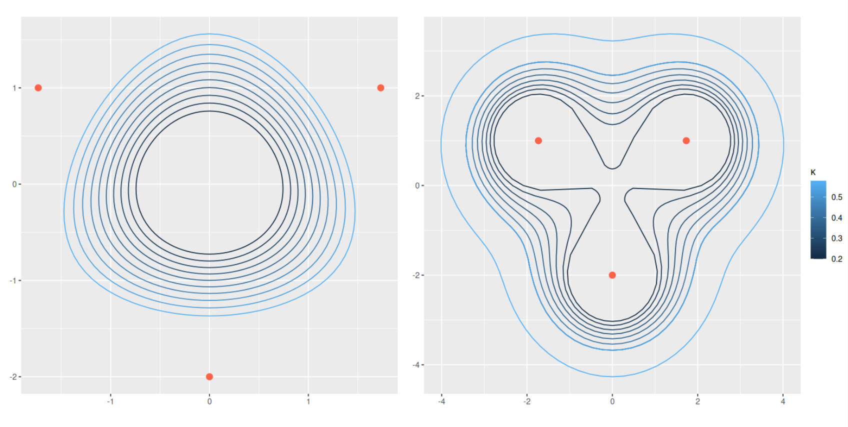
- this works well for polyhedral domains D in low dimensions because projection can be simulated efficiently
- Fishman et al. (*NeurIPS*, 2023) demonstrate weak convergence of Metropolis approximation and Rejection approximation of reflected Brownian motion
- this is motivated by denoising reflected diffusion models (Lou and Ermon, *ICML* 2023), see also Holk, Strauch and T. (2024+) for a first statistical analysis



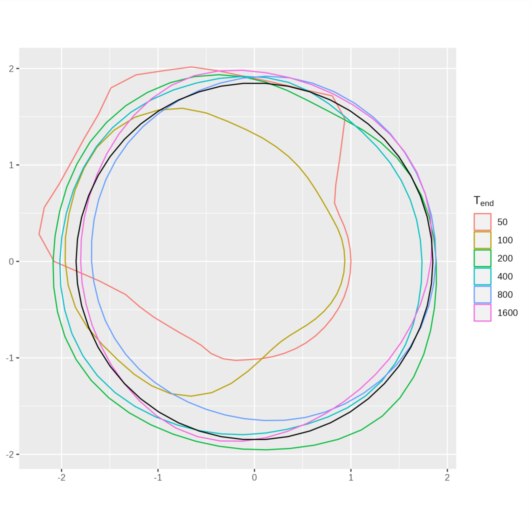
Optimised shapes for Brownian motion with reflection cost $\kappa = 1$ and cost function $c = |\cdot|$ (left) and $c(x, y, z) = \sqrt{x^2 + 5y^2 + z^2}$ (right).



For each value of κ, we use the BFGS algorithm (using the built-in R implementation optim) to find an approximate optimal shape. To not bias the results towards a ball, we initialize the algorithm with $r_i = 1 + \frac{1}{2}U_i$, where $U_i \sim \mathrm{Unif}[-1, 1]$ for $i = 1, \dots, N$ ($N \approx 200$). Once the approximate optimal values $\hat{r}_1, \hat{r}_2, \dots, \hat{r}_N$ are found, we plot the mean of these along with error bars with height of their standard deviation. For reference we draw a curve of the theoretical optimal radius $r^* = \sqrt{(d+1)\kappa}$. Finally, we also add a bar-plot illustrating the number of iterations of the BFGS algorithm were needed to compute the shapes.



For each κ, we plot the optimized reflection boundaries, where π is a mixture of three Gaussians with means at the points marked in red. Left: Norm cost function, $c = |\cdot|$. Right: Cost function $c(x) = \min\{|x - \mu_1|, |x - \mu_2|, |x - \mu_3|\}$.



Estimates of the optimal shape (black) using kernel estimates after increasing periods of exploration. Notably, after only $T = 150$, the estimated optimal shape has an associated cost only 0.61% higher than the true optimum.

References

S. Christensen, N. Dexheimer, and C. Strauch. **Data-driven optimal stopping: A pure exploration analysis.** 2023. arXiv: 2312.05880 [math.ST].

S. Christensen and C. Strauch. **"Nonparametric learning for impulse control problems—Exploration vs. exploitation".** In: *Ann. Appl. Prob.* 33.2 (2023), pp. 1569 –1587.

S. Christensen, C. Strauch, and L. Trottner. **"Learning to reflect: a unifying approach for data-driven stochastic control strategies".** In: *Bernoulli* 30.3 (2024), pp. 2074–2101.

S. Christensen, A. H. Thomsen, and L. Trottner. **"Data-driven rules for multidimensional reflection problems".** In: *SIAM/ASA J. Uncertain. Quantif.* 12.4 (2024), pp. 1240–1272.

N. Fishman et al. **"Metropolis Sampling for Constrained Diffusion Models".** In: *Advances in Neural Information Processing Systems*. Vol. 36. 2023, pp. 62296–62331.

A. Holk, C. Strauch, and L. Trottner. **Statistical guarantees for denoising reflected diffusion models.** 2024. arXiv: 2411.01563 [math.ST].

L. Słomiński. **"On approximation of solutions of multidimensional SDEs with reflecting boundary conditions".** In: *Stochastic Process. Appl.* 50.2 (1994), pp. 197–219.

C. Strauch. **"Adaptive invariant density estimation for ergodic diffusions over anisotropic classes".** In: *Ann. Statist.* 46.6B (2018), pp. 3451–3480.

References

S. Christensen, N. Dexheimer, and C. Strauch. **Data-driven optimal stopping: A pure exploration analysis.** 2023. arXiv: 2312.05880 [math.ST].

S. Christensen and C. Strauch. **"Nonparametric learning for impulse control problems—Exploration vs. exploitation".** In: *Ann. Appl. Prob.* 33.2 (2023), pp. 1569 –1587.

S. Christensen, C. Strauch, and L. Trottner. **"Learning to reflect: a unifying approach for data-driven stochastic control strategies".** In: *Bernoulli* 30.3 (2024), pp. 2074–2101.

S. Christensen, A. H. Thomsen, and L. Trottner. **"Data-driven rules for multidimensional reflection problems".** In: *SIAM/ASA J. Uncertain. Quantif.* 12.4 (2024), pp. 1240–1272.

N. Fishman et al. **"Metropolis Sampling for Constrained Diffusion Models".** In: *Advances in Neural Information Processing Systems*. Vol. 36. 2023, pp. 62296–62331.

A. Holk, C. Strauch, and L. Trottner. **Statistical guarantees for denoising reflected diffusion models.** 2024. arXiv: 2411.01563 [math.ST].

L. Słomiński. **"On approximation of solutions of multidimensional SDEs with reflecting boundary conditions".** In: *Stochastic Process. Appl.* 50.2 (1994), pp. 197–219.

C. Strauch. **"Adaptive invariant density estimation for ergodic diffusions over anisotropic classes".** In: *Ann. Statist.* 46.6B (2018), pp. 3451–3480.

Thank you for your attention!