Mathematical Analysis of the Narrow Escape Problem

Ulm Applied Analysis Seminar

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References:

- T. Lelièvre, M. Rachid, and G. Stoltz. 2024
  A spectral approach to the narrow escape problem in the disk

- Preprints in preparation on extensions: general domains, general dimension, more precise asymptotics

Outline

The narrow escape problem

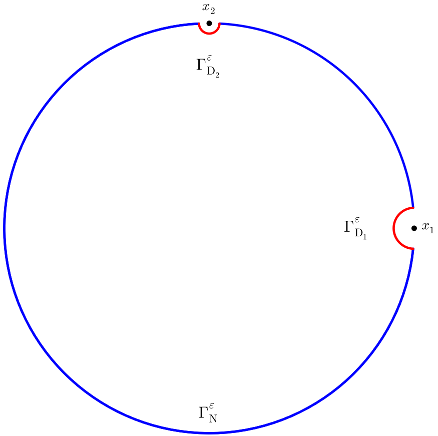
- Domain Ω_ε with small doors:

$$\Omega_\varepsilon = \Omega \setminus \bigcup_{n=1}^{N} \overline{B}\left(x_n, r_n^\varepsilon\right)$$

- Brownian particle:

$$\mathrm{d}X_t = \sqrt{2}\,\mathrm{d}W_t$$

- Reflecting boundary $\Gamma_{\mathrm{N}}^\varepsilon$
- N exit doors $\Gamma_{\mathrm{D}_1}^\varepsilon, \ldots \Gamma_{\mathrm{D}_N}^\varepsilon$



Let $\tau := \inf\{t \geqslant 0, X_t \in \Gamma_{\mathrm{D}}^\varepsilon\}$ where

$$\Gamma_{\mathrm{D}}^\varepsilon = \bigcup_{n=1}^{N} \Gamma_{\mathrm{D}_n}^\varepsilon$$

Objective: Characterize first exist event (τ, X_τ) in the limit $\varepsilon \to 0$

The narrow escape problem: motivation and references

Motivations from biology and chemistry:

- Escape of ions through small openings in cell membranes
- Early stages of viral infection
- Escape of diffusing molecules to active sites

Vast existing literature, but few rigorous results:

- D. Holcman and Z. Schuss. J. Stat. Phys., 2004
- O. Bénichou and R. Voituriez. Phys. Rev. Letters, 2008
- H. Ammari, K. Kalimeris, H. Kang, and H. Lee. J. Math. Pures Appl. (9), 2012
- D. Holcman and Z. Schuss. SIAM Rev., 2014
- X. Chen and A. Friedman. SIAM J. Math. Anal., 2011

Focus in the literature on the mean escape time starting from a point: $\mathbf{E}_x[\tau]$

Recalls on the exponential distribution

The exponential distribution $\mathrm{Exp}(\lambda)$ is the probability measure with density

$$f_\lambda(x) = \begin{cases} \lambda\,\mathrm{e}^{-\lambda x} & \text{if } x \geqslant 0 \\ 0 & \text{if } x < 0 \end{cases}$$

Key properties of the exponential distribution

Suppose that $Z_1 \sim \mathrm{Exp}(\lambda_1)$ and $Z_2 \sim \mathrm{Exp}(\lambda_2)$ are independent. Then

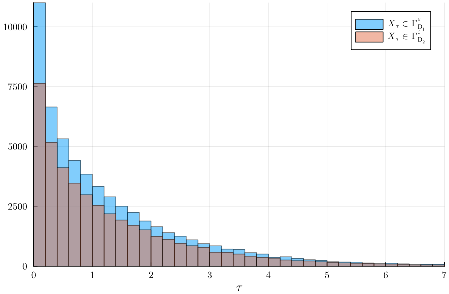
- Let $M := \min\{Z_1, Z_2\}$. Then $M \sim \mathrm{Exp}(\lambda_1 + \lambda_2)$.
- Let

  $$I = \begin{cases} 1 & \text{if } Z_1 \leqslant Z_2 \\ 2 & \text{if } Z_1 > Z_2 \end{cases}$$

  Then $\mathbf{P}[I = i] = \frac{\lambda_i}{\lambda_1+\lambda_2}$ for $i \in \{1, 2\}$
- The random variables I and M are independent

We simulate $M = 10^5$ Brownian paths started from $X_0 \sim \mathcal{U}(\Omega_\varepsilon)$ until escape

- Size of exit doors $r_1^\varepsilon = 0.1$, $r_2^\varepsilon = 0.05$
- We record $\left(\tau, \mathrm{index}(X_\tau)\right)$ for each exit event



Observations:

- Escape time τ appears to follow an exponential distribution
- The index of the exit door appears to be independent of τ

Preliminary numerical experiments (2/3)

Link with a partial differential equation

Let $T_\varepsilon := \Omega_\varepsilon \to \mathbf{R}$ be defined as $T_\varepsilon(x) := \mathbf{E}_x[\tau]$. Then T_ε satisfies

$$\begin{cases} -\Delta T_\varepsilon = 1 & \text{on } \Omega_\varepsilon \\ \partial_n T_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ T_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{D}}^\varepsilon \end{cases}$$

Sketch of proof. Assuming a smooth solution T_ε exists, we have by Itô's formula

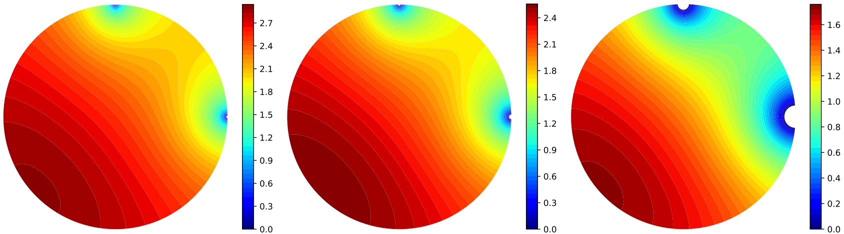
$$\mathrm{d}T_\varepsilon(X_t) = \Delta T_\varepsilon(X_t)\,\mathrm{d}t + \sqrt{2}\nabla T_\varepsilon(X_t)\cdot \mathrm{d}W_t$$

Writing this equation in integral form and taking the expectation, we obtain

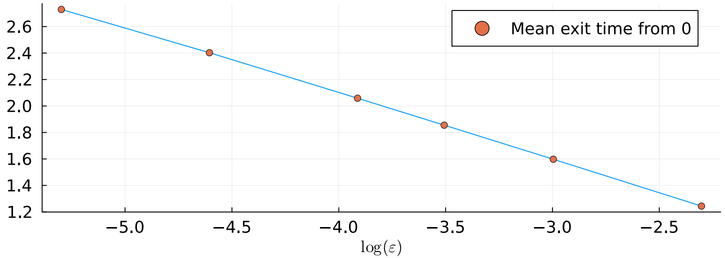
$$\mathbf{E}\Big[T_\varepsilon(X_\tau) - T_\varepsilon(X_0)\Big] = -\mathbf{E}[\tau] \qquad \to \qquad T_\varepsilon(x) = \mathbf{E}[\tau]$$

Preliminary numerical experiments (3/3)

Finite element simulation for mean exit time starting from x (here $r_1^\varepsilon = 2r_2^\varepsilon = \varepsilon$)



(a) $\varepsilon = 0.01$ (b) $\varepsilon = 0.02$ (c) $\varepsilon = 0.1$



Outline

The narrow escape problem

The quasi-stationary distribution approach

Mathematical results

Numerical illustration

The quasi-stationary distribution

- **Goal:** Rewrite the narrow escape problem as a spectral problem
- **Motivation:** For $\varepsilon \ll 1$, particle reaches local equilibrium before leaving

Definition: quasi-stationary distribution[1,2]

The QSD ν_ε is the probability measure with support Ω_ε such that

$$\forall t \geqslant 0, \qquad X_0 \sim \nu_\varepsilon \quad \Rightarrow \quad \mathcal{L}aw(X_t \,|\, \tau > t) = \nu_\varepsilon$$

Property (Yaglom limit): For any $X_0 \in \Omega_\varepsilon$ and measurable A

$$\lim_{t \to \infty} \mathbf{P}\left[X_t \in A \,|\, \tau > t\right] = \nu_\varepsilon(A)$$

[1] S. Méléard and D. Villemonais. Probab. Surv., 2012.
[2] T. Lelièvre and G. Stoltz. Acta Numer., 2016, Section 6.3.1.

Illustration of the Yaglom limit

Fokker-Planck equation:

$$\begin{cases} \partial_t \rho_\varepsilon = \Delta \rho_\varepsilon & \text{on } \Omega_\varepsilon \\ \partial_n \rho_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ \rho_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{D}}^\varepsilon \end{cases}$$

gives evolution of $\mathcal{L}aw(X_t \,|\, \tau > t)$

On the right, $X_0 \sim \mathcal{N}(0, 0.04)$

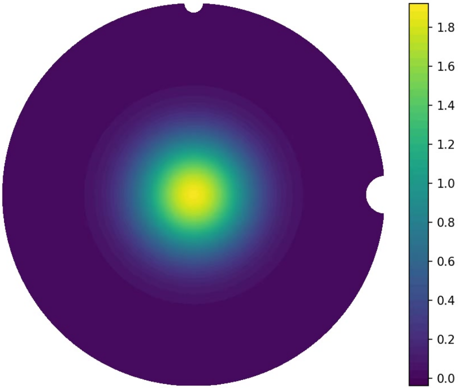


Figure: Evolution of $\mathcal{L}aw(X_t \,|\, \tau > t)$

Fundamental properties of the QSD

Assume that $X_0 \sim \nu_\varepsilon$. Then

- The exit time τ is exponentially distributed $\sim \mathrm{Exp}(\lambda_\varepsilon)$

$$\begin{aligned}\mathbf{P}_{\nu_\varepsilon}[\tau \geqslant s+t] &= \mathbf{P}_{\nu_\varepsilon}[\tau \geqslant s+t \,|\, \tau \geqslant s]\, \mathbf{P}_{\nu_\varepsilon}[\tau \geqslant s] \\ &= \mathbf{P}_{\nu_\varepsilon}[\tau \geqslant t]\, \mathbf{P}_{\nu_\varepsilon}[\tau \geqslant s].\end{aligned}$$

- The exit point X_τ is independent of the exit time τ

$$\begin{aligned}\mathbf{P}_{\nu_\varepsilon}[X_\tau \in A, \tau \geqslant t] &= \mathbf{P}_{\nu_\varepsilon}[X_\tau \in A \,|\, \tau \geqslant t]\, \mathbf{P}_{\nu_\varepsilon}[\tau \geqslant t] \\ &= \mathbf{P}_{\nu_\varepsilon}[X_\tau \in A]\, \mathbf{P}_{\nu_\varepsilon}[\tau \geqslant t]\end{aligned}$$

Goal. Study λ_ε and $\mathbf{P}_{\nu_\varepsilon}[X_\tau \in \Gamma^\varepsilon_{\mathrm{D}_i}]$ for $i \in \{1, \dots, N\}$ in the limit $\varepsilon \to 0$

Explicit formulas for mean exit time and exit point

Spectral characterization of the QSD

Consider the first eigenpair $(u_\varepsilon, \lambda_\varepsilon)$ of the eigenvalue problem

$$\begin{cases} -\Delta u_\varepsilon = \lambda_\varepsilon u_\varepsilon & \text{on } \Omega_\varepsilon \\ \partial_n u_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ u_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{D}}^\varepsilon \end{cases}$$

Then the QSD is given by

$$\nu_\varepsilon = \frac{u_\varepsilon(x)\,\mathrm{d}x}{\int_{\Omega_\varepsilon} u_\varepsilon}$$

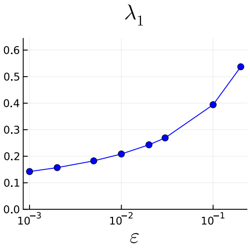
(It can be shown that u_ε has a sign and $\lambda_\varepsilon > 0$)

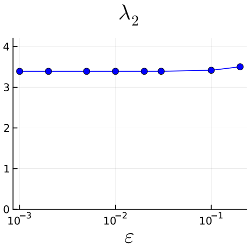
- The mean exit time satisfies $\mathbf{E}_{\nu_\varepsilon}[\tau] = \frac{1}{\lambda_\varepsilon}$
- The distribution of the exit point satisfies

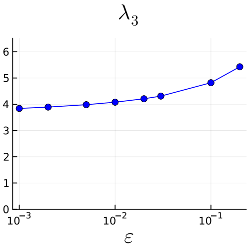
$$\mathbf{P}_{\nu_\varepsilon}[X_\tau \in \Gamma_{\mathrm{D_i}}^\varepsilon] = -\frac{\int_{\Gamma_{\mathrm{D}_i}^\varepsilon} \partial_n u_\varepsilon \,\mathrm{d}\sigma}{\int_{\Gamma_{\mathrm{D}}} \partial_n u_\varepsilon \,\mathrm{d}\sigma}$$

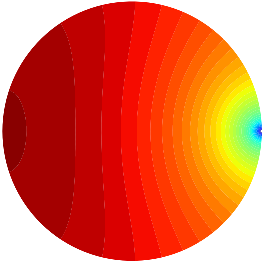
$\to$ The QSD distribution gives information on exit time and exit point

Numerical illustration of the eigenfunctions

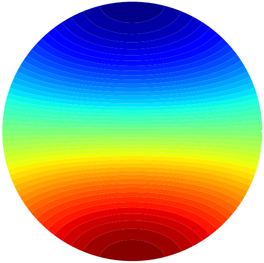




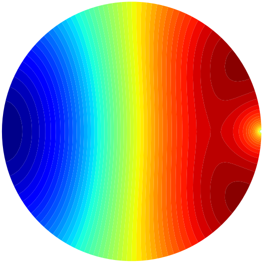




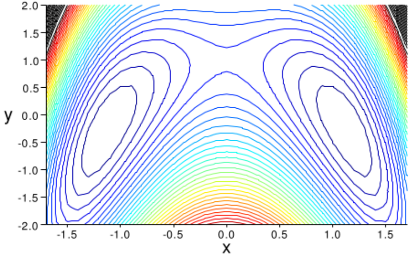
(a) First eigenfunction



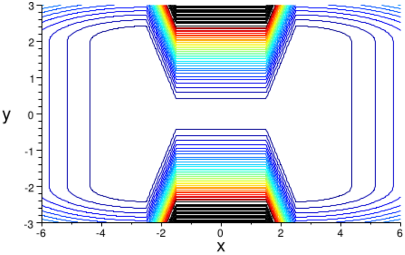
(b) Second eigenfunction



(c) Third eigenfunction



(a) Energetic barrier (well studied)



(b) Entropic barrier (no full understanding)

Overdamped Langevin dynamics in external potential V:

$$\mathrm{d}X_t = -\nabla V(X_t)\,\mathrm{d}t + \sqrt{2\beta^{-1}}\,\mathrm{d}W_t.$$

- For metastability of energetic origin, the QSD is useful to study exit events from the basin of attraction of a local minimum. Arrhenius approximation when $\beta \gg 1$:

$$\lambda_i \propto \mathrm{e}^{-\beta\left(V_{\mathrm{saddle}} - V_{\mathrm{min(i)}}\right)}$$

- Understanding the exit events enables to construct discrete state-space approximation

Why we work in domain $\Omega_\varepsilon = \Omega \setminus \bigcup \overline{B}(x_i, r_i)$

The QSD ν_ε is related to the first eigenpair of

$$\begin{cases} -\Delta u_\varepsilon = \lambda_\varepsilon u_\varepsilon & \text{in } \Omega_\varepsilon \\ \partial_n u_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ u_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{D}_i}^\varepsilon \end{cases}$$

The solution u_ε enjoys better regularity[1] if there is an angle between $\Gamma_{\mathrm{N}}^\varepsilon$ and $\Gamma_{\mathrm{D}}^\varepsilon$

- If angle between $\Gamma_{\mathrm{N}}^\varepsilon$ and $\Gamma_{\mathrm{D}_i}^\varepsilon$ is $= \pi$: $\partial_n \nu_\varepsilon \notin L^2(\partial\Omega)$
- If angle between $\Gamma_{\mathrm{N}}^\varepsilon$ and $\Gamma_{\mathrm{D}_i}^\varepsilon$ is $< \pi$: $\partial_n \nu_\varepsilon \in L^2(\partial\Omega)$

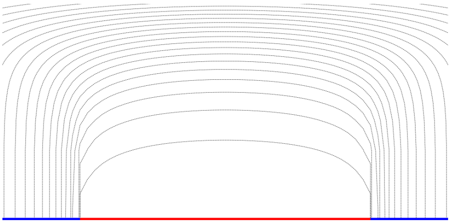


Figure: Contour lines of ν_ε for flat boundary.

[1] T. Jakab, I. Mitrea, and M. Mitrea. Indiana Univ. Math. J., 2009.

Outline

Goal: approximate the first eigenpair $(\lambda_\varepsilon, u_\varepsilon)$ of

$$\begin{cases} -\Delta u_\varepsilon = \lambda_\varepsilon u_\varepsilon & \text{on } \Omega_\varepsilon \\ \partial_n u_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ u_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{D}}^\varepsilon \end{cases}$$

When $\varepsilon \to 0$, it holds $|\Gamma_{\mathrm{D}}^\varepsilon| \to 0$ so we expect $\lambda_\varepsilon \to 0$ and $u_\varepsilon \to \mathrm{cst}$. This motivates looking for a solution of the form $u_\varepsilon = 1 + v_\varepsilon$, with

$$\begin{cases} -\Delta v_\varepsilon = \lambda_\varepsilon + \lambda_\varepsilon v_\varepsilon & \text{on } \Omega_\varepsilon \\ \partial_n v_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ v_\varepsilon = -1 & \text{on } \Gamma_{\mathrm{D}}^\varepsilon \end{cases}$$

Taking formally the limit $\varepsilon \to 0$, we find that $v_\varepsilon/\lambda_\varepsilon$ should converge to a function w satisfying

$$\begin{cases} -\Delta w = 1 & \text{on } \Omega \\ \partial_n w = 0 & \text{on } \partial\Omega \setminus \{x_1\} \end{cases}$$

Construction of the function w for 1 exit door (1/2)

Let $\Lambda\colon \mathbf{R}^d \to \mathbf{R}$ denote the fundamental solution of the Laplacian :

$$\Lambda(x) \propto \begin{cases} -\log(x) & \text{if } d = 2 \\ \frac{1}{|x|^{d-2}} & \text{if } d \geqslant 3 \end{cases}$$

Lemma (Construction of a quasimode)

If $\partial\Omega$ is smooth, there exists a smooth function of the form $w(x) = -\frac{\Lambda(x-x_1)}{\alpha_{\Omega,d}} + R(x)$ defined on Ω such that

$$\begin{cases} -\Delta w = 1 & \text{on } \Omega \\ \partial_n w = 0 & \text{on } \partial\Omega \setminus \{x_1\} \end{cases}$$

and the smooth remainder term $R\colon \Omega \to \mathbf{R}$ satisfies

$$R(x) = \begin{cases} \mathcal{O}(1) & \text{if } d = 2 \\ \mathcal{O}\big(-\log|x-x_1|\big) & \text{if } d = 3 \\ \mathcal{O}\big(|x-x_1|^{-(d-3)}\big) & \text{if } d \geqslant 4 \end{cases}$$

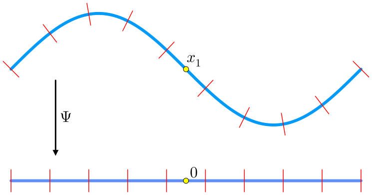
The factor $\alpha_{\Omega,d}$ is given by, denoting by w_d the surface of the unit sphere in $\mathbf{R}^d$:

$$\alpha_{\Omega,d} = \frac{w_d}{2|\Omega|} \times \begin{cases} 1 & \text{if } d = 2 \\ d-2 & \text{if } d \geqslant 3 \end{cases}$$

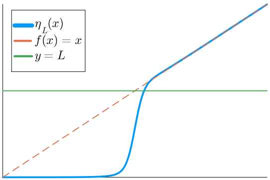
Sketch of proof. Consider the change of variables

$$\Psi\colon \Omega \cap B(x_1, \delta) \to \mathbb{R}^+ \times \mathbb{R}^{d-1}$$

that locally flattens the boundary $\partial\Omega$ and satisfies $\Psi(x_1) = 0$



(a) Local change of coordinates



(b) Smooth cutoff function

We use the ansatz $w(x) = -\frac{\eta_L \circ \Lambda \circ \Psi(x)}{\alpha_{\Omega,d}} + S(x)$ with $w(x) = S(x)$ if $x \notin B(x_1, \delta)$

- In the first term $\eta_L \circ \Lambda \circ \Psi(x)$ equals $\Lambda(x - x_1)$ to leading order, in a neighborhood of x_1
- By substitution we look for S satisfying

$$\begin{cases} -\Delta S = 1 - \alpha_{\Omega,d}^{-1}\Delta(\eta_L \circ \Lambda \circ \Psi) & \text{on } \Omega \\ \partial_n S = 0 & \text{on } \partial\Omega \end{cases}$$

$\rightsquigarrow$ This problem admits a unique mean-zero weak solution if RHS is mean-zero[1]

[1] J. Aramaki. Commun. Math. Anal., 2018.

For convenience, let $\widetilde{\Lambda} = \eta_L \circ \Lambda \circ \Psi$. Two steps are required to conclude the proof:

- **To determine** $\alpha_{\Omega,d}$
  - we first prove that $\Delta\widetilde{\Lambda} \in L^1(\Omega)$
  - then use Green's theorem:

$$\begin{aligned}\int_\Omega \Delta\tilde{\Lambda} &= \lim_{\lambda\to 0}\int_{\Omega\setminus B(x_1,\lambda)} \Delta\tilde{\Lambda}\,\mathrm{d}\Omega \\ &= \lim_{\lambda\to 0}\int_{\partial\Omega\setminus B(x_1,\lambda)} \partial_n\tilde{\Lambda}\,\mathrm{d}\sigma + \lim_{\lambda\to 0}\int_{\partial B(x_1,\lambda)\cap\Omega} \partial_n\tilde{\Lambda}\,\mathrm{d}\sigma \\ &= 0 + \frac{(d-2)w_d}{2}\end{aligned}$$

- **To prove that S is a subsingular term**, we use an integral representation of the solution (layer potential techniques[1]). To leading order around x_1, it holds that

$$S(x) = -\int_\Omega \Lambda(x-y)\,\Delta S(y)\,\mathrm{d}y$$

[1] H. Ammari, H. Kang, and H. Lee. American Mathematical Soc., 2009.

Recall that

- It should hold that $u_\varepsilon \approx 1 + \lambda_\varepsilon w$ for $\varepsilon \ll 1$
- The Dirichlet boundary condition requires that $u_\varepsilon = 0$ on $\Gamma_{\mathrm{D}}^\varepsilon$.
- Close to x_1, the function $w(x)$ equals $-\frac{\Lambda(x-x_1)}{\alpha_{\Omega,d}}$ to leading order.

This motivates the approximation

$$\widehat{\lambda}_\varepsilon = \frac{\alpha_{\Omega,d}}{\Lambda(r_1^\varepsilon)} = \alpha_{\Omega,d} \times \begin{cases} \dfrac{-1}{\log(r_1^\varepsilon)} & \text{if } d = 2 \\ (r_1^\varepsilon)^{d-2} & \text{if } d \geqslant 3 \end{cases}$$

The pair $(\widehat{\lambda}_\varepsilon, \widehat{u}_\varepsilon)$, with $\widehat{u}_\varepsilon := 1 + \widehat{\lambda}_\varepsilon w$, satisfies the initial problem with small residuals

$$\begin{cases} -\Delta \widehat{u}_\varepsilon = \widehat{\lambda}_\varepsilon \widehat{u}_\varepsilon - \widehat{\lambda}_\varepsilon^2 w & \text{on } \Omega_\varepsilon \\ \partial_n u_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ u_\varepsilon = \widehat{\lambda}_\varepsilon R & \text{on } \Gamma_{\mathrm{D}}^\varepsilon \end{cases}$$

Towards a rigorous error estimate for $\widehat{\lambda}_\varepsilon$ for 1 exit door

We take for granted[1] that $u_\varepsilon, \widehat{u}_\varepsilon$ (normalized to be probability densities) satisfy

- $\langle u_\varepsilon, u_\varepsilon \rangle = |\Omega|^{-\frac{1}{2}} + \mathcal{O}(\widehat{\lambda}_\varepsilon)$
- $\langle \widehat{u}_\varepsilon, u_\varepsilon \rangle = |\Omega|^{-\frac{1}{2}} + \mathcal{O}(\widehat{\lambda}_\varepsilon)$

By Green's identity, we have

$$\begin{aligned}\lambda_\varepsilon \langle \widehat{u}_\varepsilon, u_\varepsilon \rangle &= -\langle \widehat{u}_\varepsilon, \Delta u_\varepsilon \rangle \\ &= -\langle \Delta \widehat{u}_\varepsilon, u_\varepsilon \rangle + \langle \partial_n \widehat{u}_\varepsilon, u_\varepsilon \rangle_{\Gamma^\varepsilon} - \langle \widehat{u}_\varepsilon, \partial_n u_\varepsilon \rangle_{\Gamma^\varepsilon} \\ &= \widehat{\lambda}_\varepsilon \langle \widehat{u}_\varepsilon, u_\varepsilon \rangle - \widehat{\lambda}_\varepsilon^2 \langle w, u_\varepsilon \rangle + 0 - \widehat{\lambda}_\varepsilon \langle R, \partial_n u_\varepsilon \rangle_{\Gamma^\varepsilon_{\mathrm{D}}}\end{aligned}$$

Therefore we deduce that

$$\left| \lambda_\varepsilon - \widehat{\lambda}_\varepsilon \right| \langle \widehat{u}_\varepsilon, u_\varepsilon \rangle \leqslant \mathcal{O}(\widehat{\lambda}_\varepsilon^2) + \widehat{\lambda}_\varepsilon \|R\|_{L^\infty(\Gamma^\varepsilon_{\mathrm{D}})} \|\partial_n u_\varepsilon\|_{L^1(\Gamma^\varepsilon_{\mathrm{D}})}$$

The function $\partial_n u_\varepsilon$ is (up to renormalization) a probability density, so it has a sign and

$$\|\partial_n u_\varepsilon\|_{L^1(\Gamma^\varepsilon_{\mathrm{D}})} = \left| \langle \partial_n u_\varepsilon, 1 \rangle_{L^2(\Gamma^\varepsilon_{\mathrm{D}})} \right| = \left| \langle \Delta u_\varepsilon, 1 \rangle \right| = \lambda_\varepsilon \left| \langle u_\varepsilon, 1 \rangle \right|$$

[1] T. Lelièvre, M. Rachid, and G. Stoltz. 2024.

General result with N doors

We define

$$K_\varepsilon^i := \begin{cases} -\dfrac{1}{\log(r_i^\varepsilon)} & \text{if } d = 2 \\ (r_i^\varepsilon)^{d-2} & \text{if } d \geqslant 3 \end{cases} \qquad \overline{K}_\varepsilon := K_1 + \cdots + K_N$$

Theorem (Eigenvalue)

The mean exit time when $X_0 \sim \nu_\varepsilon$ is given by $\mathbf{E}_{\nu_\varepsilon}[\tau] = \frac{1}{\lambda_\varepsilon}$, where

$$\lambda_\varepsilon = \alpha_{\Omega,d}\overline{K}_\varepsilon + \begin{cases} \mathcal{O}\left(\overline{K}_\varepsilon^2\right) & \text{for } d = 2 \\ \mathcal{O}\left(\overline{K}_\varepsilon^2 \log\left(\overline{K}_\varepsilon\right)\right) & \text{for } d = 3 \\ \mathcal{O}\left(\overline{K}_\varepsilon^{\frac{d-1}{d-2}}\right) & \text{for } d \geqslant 4 \end{cases}$$

Elements of proof. Construct w_i as previously for each door and define

$$\widehat{u}_\varepsilon = 1 + \sum_{i=1}^{N} \widehat{\lambda}_i^\varepsilon w_i$$

Fix $\widehat{\lambda}_i^\varepsilon$ by requiring that $\widehat{u}_\varepsilon = 0$ on $\Gamma_{\mathrm{D}_i}^\varepsilon$ and noting that $\widehat{u}_\varepsilon \approx 1 + \widehat{\lambda}_i^\varepsilon w_i$ on $\Gamma_{\mathrm{D}_i}^\varepsilon$

Theorem (Exit door distribution)

Assume that $\partial\Omega$ is smooth. Then for $i \in \{1, \dots, N\}$, it holds that

$$\mathbf{P}_{\nu_\varepsilon}\left[X_\tau \in \Gamma^\varepsilon_{\mathrm{D}_i}\right] = \frac{K^i_\varepsilon}{\overline{K}_\varepsilon} + \begin{cases} \mathcal{O}\left(\overline{K}_\varepsilon\right) & \text{for } d = 2 \\ \mathcal{O}\left(\overline{K}_\varepsilon \log\left(\overline{K}_\varepsilon\right)\right) & \text{for } d = 3 \\ \mathcal{O}\left(\overline{K}_\varepsilon^{\frac{1}{d-2}}\right) & \text{for } d > 3 \end{cases}$$

Idea of proof

- Let ν^k_ε denote the QSD with only door i, with corresponding eigenvalue λ^i_ε
- For small ε, it holds that $\nu_\varepsilon \approx \nu^i_\varepsilon$ in total variation
- By the properties of the QSD, it holds for all $t > 0$ that

$$\mathbf{P}_{\nu_\varepsilon}\left[X_\tau \in \Gamma^\varepsilon_{\mathrm{D}_i}\right] = \frac{\mathbf{P}_{\nu_\varepsilon}\left[X_{t\wedge\tau} \in \Gamma^\varepsilon_{\mathrm{D}_i}\right]}{\mathbf{P}_{\nu_\varepsilon}\left[X_{t\wedge\tau} \in \Gamma^\varepsilon_{\mathrm{D}}\right]} \approx \frac{\mathbf{P}_{\nu^i_\varepsilon}\left[X_{t\wedge\tau} \in \Gamma^\varepsilon_{\mathrm{D}_i}\right]}{\mathbf{P}_{\nu_\varepsilon}\left[X_{t\wedge\tau} \in \Gamma^\varepsilon_{\mathrm{D}}\right]}$$

$$\leqslant \frac{1 - \mathrm{e}^{-\lambda^i_\varepsilon t}}{1 - \mathrm{e}^{-\lambda_\varepsilon t}} \xrightarrow[\varepsilon\to 0]{} \frac{K^i_\varepsilon}{\overline{K}_\varepsilon}$$

Distribution of the exit door: idea of an analytic proof

Let $\nu_\varepsilon^{!k}$ denote the QSD without door k, with density $u_\varepsilon^{!k}$ and eigenvalue $\lambda_\varepsilon^{!k}$. Then

$$
\begin{aligned}
-\langle \partial_n u_\varepsilon, 1 \rangle_{\Gamma^\varepsilon_{\mathrm{D}_k}} &\approx -\frac{1}{|\Omega|} \langle \partial_n u_\varepsilon, u_\varepsilon^{!k} \rangle_{\Gamma^\varepsilon_{\mathrm{D}_k}} \\
&= -\frac{1}{|\Omega|} \left(\left\langle \Delta u_\varepsilon, u_\varepsilon^{!k} \right\rangle_{\Omega_\varepsilon} - \left\langle u_\varepsilon, \Delta u_\varepsilon^{!k} \right\rangle_{\Omega_\varepsilon} \right) \\
&= -\frac{1}{|\Omega|} \left(\left\langle \Delta u_\varepsilon, u_\varepsilon^{!k} \right\rangle_{\Omega_\varepsilon} - \left\langle u_\varepsilon, \Delta u_\varepsilon^{!k} \right\rangle_{\Omega_\varepsilon} \right) \\
&= \frac{1}{|\Omega|} \left(\lambda_\varepsilon - \lambda_\varepsilon^{!k} \right) \left\langle u_\varepsilon, u_\varepsilon^{!k} \right\rangle_{\Omega_\varepsilon} \approx \frac{\alpha_{\Omega,d} K_\varepsilon^k}{|\Omega|^2}
\end{aligned}
$$

Outline

Sampling the QSD: Fleming–Viot particle system

- **Initialization**: Sample M independent particles $X_0^1, \dots, X_0^M \sim \mu$
- **Evolution**: Each particle evolves independently according to the dynamics

$$\mathrm{d}X_t^i = \sqrt{2}\,\mathrm{d}W_t^i \quad + \quad \text{Reflecting boundary condition}$$

- **Resampling**: When a particle i reaches an absorbing state
  - Pick particle j among remaining particles, uniformly at random
  - Move particle i to position of particle j instantly
- **Output**: For $M, t \gg 1$, the empirical measure approximates the QSD[1,2]

$$\frac{1}{M}\sum_{i=1}^{M} \delta_{X_t^i} \xrightarrow[M\to\infty]{\text{weak}} \mathbf{P}_\mu[X_t \in \cdot \,|\, \tau > t]$$

[1] D. Villemonais. ESAIM Probab. Stat., 2014.
[2] L. Journel and P. Monmarché. Ann. Appl. Probab., 2025.

Monte Carlo simulation of the narrow escape problem

Given $X_0^1, \dots, X_0^M$ output of Fleming–Viot, repeat the following steps:

1. Propose move by Euler–Maruyama discretization:

$$\widehat{X}_{n+1} = X_n + \sqrt{2\Delta t}\,\xi_n, \qquad \xi_n \sim \mathcal{N}(0, \mathrm{I}_d)$$

2. If $\widehat{X}_{n+1} \in B(x_i, r_i^\varepsilon)$, register exit event for door $i \in \{1, \dots, N\}$. **Done**
3. Else if $\widehat{X}_{n+1} \notin \Omega$, reject move (reflecting boundary)
4. Else, set $X_{n+1} = \widehat{X}_{n+1}$

This approach is computationally expensive

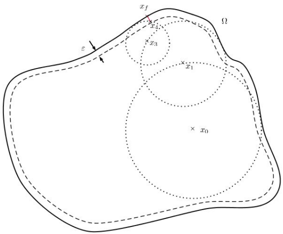
- Time step should be small compared to $(r_i^\varepsilon)^2$ for $i \in \{1, \dots, N\}$
- Mean exit time increases as $\varepsilon \to 0$

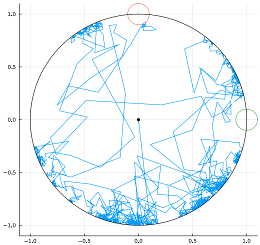
Example: in dimension 3 with $r_i^\varepsilon \propto \varepsilon$, the mean exit time scales as $\frac{1}{\varepsilon}$

$\rightsquigarrow$ Simulation cost of M exit events scales as $M\varepsilon^{-3}$

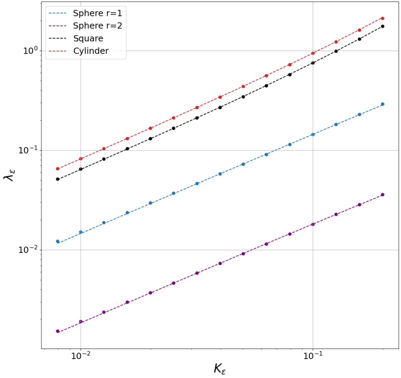
When far from the boundary, instead of Euler–Maruyama we use walk-on-spheres

- Compute radius $r_n = \text{dist}(X_n, \partial\Omega_\varepsilon)$.
- Sample the exit point X_{n+1} from $B(X_n, r_n)$, uniformly on $\partial B(X_n, r_n)$
- Sample exit time $\Delta t_n \sim \mathcal{T}_{r_n}$, with $\mathcal{T}_{r_n}$ the law of first exit time from the ball
- Update time: $t_{n+1} = t_n + \Delta t_n$





Measure of the exit time through the Finite Element Method (FEM)



Recall that $\mathbf{E}_{\nu_\varepsilon}[\tau] = \lambda_\varepsilon^{-1} \approx \widehat{\lambda}_\varepsilon^{-1}$ with

$$\widehat{\lambda}_\varepsilon = \alpha_{\Omega,d}\overline{K}_\varepsilon, \quad \alpha_{\Omega,d} := \frac{\max\{1, d-2\}w_d}{2|\Omega|}$$

We fit $\alpha_{\Omega,3}$ based on data simple shapes:

Shape Ω	$\alpha_{\Omega,3}$	$\alpha_{\Omega,3}$ (simu)
Sphere radius 1	1.500	1.46
Sphere radius 2	0.187	0.18
Cube	6.282	6.28
Cylinder	8.000	8.06

Summary and perspectives

We presented new results on the asymptotic scaling of exit time and position

- We considered general domains and general dimension
- We used a spectral approach based on the quasi-stationary distribution

Perspectives:

- Obtain more precise asymptotics in ε
- Treat the case of "flat" boundaries
- Consider (kinetic) Langevin dynamics
- Study asymptotic scaling of exit event starting from a deterministic point

Exit time

Function $T_\varepsilon(x) := \mathbf{E}_x[\tau]$ satisfies

$$\begin{cases} -\Delta T_\varepsilon = 1 & \text{on } \Omega_\varepsilon \\ \partial_n T_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ T_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{D}}^\varepsilon \end{cases}$$

Exit probability

Function $P_\varepsilon(x) := \mathbf{P}_x[X_\tau \in \Gamma_{\mathrm{D}_i}^\varepsilon]$ satisfies

$$\begin{cases} -\Delta P_\varepsilon = 0 & \text{on } \Omega_\varepsilon \\ \partial_n P_\varepsilon = 0 & \text{on } \Gamma_{\mathrm{N}}^\varepsilon \\ P_\varepsilon = \delta_{ij} & \text{on } \Gamma_{\mathrm{D}_j}^\varepsilon \end{cases}$$

Thank you for your attention!

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