Simulation of Mean First Passage Time on embedded two-dimensional domains

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Introduction
Several physical and biological problems have been formulated and studied as mean first passage time (MFPT) problems. Some of these include the time it takes for a predator to locate its prey, the arrival of diffusing surface-bound molecules at a localized signaling region on cell membrane, among others.

Mean first-passage time (MFPT) is defined as the average timescale for a predator to locate its prey, the arrival of diffusing surface-bound molecules to a localized signaling region on cell membrane, among others.

Numerics

We then solve the MFPT problem on the entire rectangular grid.

MFPT on a domain with moving trap

We first discretize the problem using the closest point method and multigrid solvers for elliptic equations on surfaces.

Mathematical Model

The MFPT of a Brownian particle starting from point \(x \in \Omega\) to be absorbed by a stationary trap \(\Omega_0\) satisfies

\[
\frac{\partial u}{\partial t} = -1, \quad x \in \Omega, \quad \Omega_0
\]

\[
\partial_\nu u = 0, \quad x \in \partial \Omega, \quad u = 0, \quad x \in \partial \Omega_0.
\]

MFPT on a domain with moving trap

After a change of variables to reverse time, the MFPT \(u(x, t)\) for a Brownian particle starting from \(x \in \Omega\) satisfies the boundary value problem

\[
\frac{\partial u}{\partial t} = 1, \quad x \in \Omega, \quad \Omega_0(t)
\]

\[
\partial_\nu u = 0, \quad x \in \partial \Omega, \quad u = 0, \quad u \in \partial \Omega_0(t);
\]

\[
u(x, 0) = u(x, 2\pi/\omega).
\]

Average/expected MFPT

The escape time of the particle from all possible starting positions in the domain is given by the average/expected MFPT.

Results: Domain with stationary traps

MFPT in a disk with traps arranged on a ring

Consider \(m\) stationary absorbing traps of radius \(r\) that are equally-spaced on a ring of radius \(r\) concentric within a unit disk. Using strong localized perturbation theory, we derive a transcendental equation for the optimal radius of the ring \(r_0\) that minimizes the average MFPT from problem (1):

\[
\frac{C_m}{2\pi} \left(1 - \frac{r_0^2}{r^2}\right) = m - \frac{1}{2} - \frac{r_0^2}{2r^2}.
\]

We implement the absorbing boundary condition

\[
\frac{\partial u}{\partial n} = 0, \quad x \in \partial \Omega,
\]

Using the closest point method, we numerically compute the MFPT for a Brownian particle to be captured by an absorbing trap in various 2D domains.

Optimizing the fundamental Neumann eigenvalue for the Laplacian in a domain containing an absorbing trap (for example, a punctured disk) using the closest point method.

Numerics

We then solve the MFPT problem on the entire rectangular grid.

Grid points in the domain give physically solutions to the problem, while those outside are used to implement boundary conditions.

We implement the absorbing boundary condition \(u = 0\) on the trap and the reflecting boundary condition \(\nabla u \cdot \nu = 0\) on the boundary of the disk using the method of images by extending the solution in various ways, using the closest point function.

Finite difference algorithm

To solve the MFPT problem on a general 2D domain containing an absorbing trap (for example, a punctured disk) using the closest point method:

We first discretize the problem using a \(\{0, 1\}\) finite difference discretization on a rectangular region.

Embed our domain of interest into the rectangular grid and represent the domain using a closest point function.

Optimizing the fundamental Neumann eigenvalue for the Laplacian in a domain containing an absorbing trap (for example, a punctured disk) using the closest point method.

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Optimal location and MFPT for two stationary traps in an elliptical domain

Consider a unit disk with two absorbing traps on its horizontal axis, that is continuously deformed into an absorbing region, while its area is conserved. Upon solving (1) on a slightly perturbed unit disk, we obtain a two-term asymptotic expansion for the optimal locations of the traps and the optimal average MFPT in terms of the semi-minor axis \(a\) as

\[
x_{\text{trapes}}(b) = 0.4536 + \frac{1}{b} - 1 \cdot 3.5959, \quad \pi x_{\text{trapes}}(b) = 0.5120 - \frac{1}{b} - 0.2149.
\]

Below is a comparison of the asymptotics (4) and the numerical results obtained from closest point method.

Results: Domain with moving periodic trap

Optimizing the radius of rotation of a periodic moving trap in a disk

The boundary value problem (2) is solved as an initial value problem, using the MFPT for a stationary trap as initial condition. The simulation is run for several periods, until a stopping criterion is satisfied:

\[
u(x, t) - u(x, k + 1) | < \text{tol}
\]

where \(T = 2\pi/\omega\) is the period of oscillation of the disk.

For the case of a single rotating trap in a unit disk, the traps prefers to stay at the centre of the domain when the angular frequency is small. A bifurcation occurs at \(\omega_0 \approx 3.131\) (analysis predicted \(\omega = 3.026\) [3], after which the trap moves closer to the boundary of the disk as the angular frequency increases.

MFPT on irregular and general curved surfaces with stationary traps

References

