Traps, Holes, and Spots: Analysis and Modeling of Localization Behavior for Some Partial Differential Equations

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Outline of the Talk

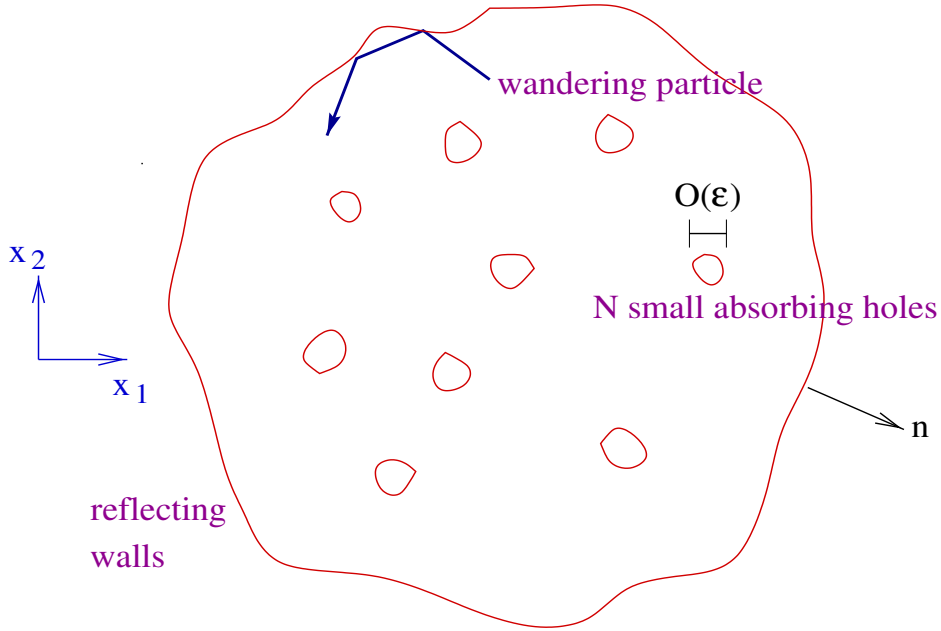
1. An Eigenvalue Optimization Problem in a Planar Domain
   - Asymptotic expansions, the Neumann Green's function, and Optimal Trap locations (Kolokolnikov, Titcombe, MJW).
   - Boundary Traps and a Narrow Escape Problem (Kolokolnikov, Pillay, MJW)
   - Analogous problems in a spherical domain (Cheviakov, Kolokolnikov, MJW)
2. Diffusion of Receptor Proteins on a Cylindrical Membrane
   - The reaction rate with one trap (Falcke, Straube, MJW)
   - Steady-state diffusion with many traps (Bressloff, Earnshaw, MJW)
3. Spot Solutions to Reaction-Diffusion Models
   - The stability of spots for the GM model (Kolokolnikov, MJW)
   - Self-Replication of spots for the Gray-Scott model (Chen, MJW). A self-destruction–self-replication "attractor"?
   - Self-Replication of spots for the Schnakenburg model on a growing domain (Kolokolnikov, MJW, Wei)

Eigenvalue Problem with Interior Traps

$$\Delta u + \lambda u = 0\,, \quad x \in \Omega\backslash\Omega_p\,; \qquad \int_{\Omega\backslash\Omega_p} u^2\,dx = 1\,,$$

$$\partial_n u = 0 \quad x \in \partial\Omega\,, \quad u = 0\,, \quad x \in \partial\Omega_p\,.$$

- Here $\Omega_p = \cup_{i=1}^{N}\Omega_{\varepsilon_i}$ are N interior non-overlapping holes or traps, each of 'radius' $O(\varepsilon) \ll 1$. The holes are assumed to be identical up to a translation and rotation.
- Also $\Omega_{\varepsilon_i} \to x_i$ as $\varepsilon \to 0$, for $i = 1, \ldots, N$. The centers x_i are arbitrary.



The Eigenvalue Optimization Problem

Goal: Let $\lambda_0 > 0$ be the fundamental eigenvalue. For $\varepsilon \to 0$ (small hole radius) find the hole locations x_i, for $i = 1, \ldots, N$, that maximize λ_0. In other words, chose the trap locations to minimize the lifetime of a wandering particle in the domain, i.e. where are the best places to fish?

Specific Questions:

- For $N = 1$ (one hole), is there a unique x_0 that maximizes λ_0? Can one find domains Ω where there are several values of x_0 that locally maximize λ_0?
- For the unit ball $\Omega = |x| \leq 1$, determine ring-type configurations of holes $x_1, ..., x_N$ that maximize λ_0.

Reference: T. Kolokolnikov, M. Titcombe, MJW, Optimizing the Fundamental Neumann Eigenvalue for the Laplacian in a Domain with Small Traps, EJAM Vol. 16, No. 2, (2005), pp. 161-200.

Previous Studies I

For the Neumann problem, with N circular holes each of radius $\varepsilon \ll 1$, Ozawa (Duke J. 1981) proved that

$$\lambda_0 \sim \frac{2\pi N \nu}{|\Omega|} + O(\nu^2), \quad \nu \equiv \frac{-1}{\log \varepsilon} \ll 1\,.$$

Since this is independent of x_i, $i = 1, \ldots, N$, we need the neglected $O(\nu^2)$ term to optimize λ_0. For the Dirichlet problem, Ozawa (1981) proved

$$\lambda_0 \sim \lambda_{0d} + 2\pi \sum_i^N \left[u_0(x_i)\right]^2 \nu + O(\nu^2)\,.$$

To optimize λ_0, put the hole at a local maxima of u_0 (Harrell, (SIMA 2001)). For the Neumann or Dirichlet case, MJW, Henshaw, Keller (SIAP, 1993) showed

$$\lambda_0 \sim \lambda_*(\nu; x_1, ..x_N) + O(\varepsilon/\nu)\,,$$

where λ_* (which "sums" all the log terms) satisfies a PDE that must be solved numerically. Highly accurate results for λ_0, but no analytical insight on how to optimize λ_0 wrt hole locations.

Eigenvalue Asymptotics I

A singular perturbation analysis shows that all of the logarithmic terms are contained in the solution to

$$\Delta u^* + \lambda^* u^* = 0\,, \quad x \in \Omega \backslash \{x_1, \ldots, x_N\}\,,$$

$$\int_\Omega (u^*)^2 dx = 1\,; \qquad \partial_n u^* = 0\,, \quad x \in \partial\Omega\,,$$

$$u^* \sim A_j\, \nu_j\, \log|x - x_j| + A_j\,, \quad x \to x_j\,, \;\; j = 1, \ldots, N\,.$$

Here $\nu_j \equiv -1/\log(\varepsilon d_j)$, where d_j is the logarithmic capacitance of the j^{th} hole defined by

$$\Delta_y v = 0\,, \quad y \notin \Omega_j \equiv \varepsilon^{-1}\Omega_{\varepsilon_j}\,,$$

$$v = 0\,, \quad y \in \partial\Omega_j\,,$$

$$v \sim \log|y| - \log d_j + o(1)\,, \quad |y| \to \infty\,.$$

The highlighted term together with the normalization condition provides $N+1$ constraints for the $N+1$ unknowns λ^* and A_j, for $j = 1, \ldots, N$.

Eigenvalue Asymptotics II

Define the G-function $G(x, x_0, \lambda^*)$ for the Helmholtz operator as

$$\Delta G + \lambda^* G = -\delta(x - x_0)\,, \quad x \in \Omega\,; \quad \partial_n G = 0\,, \quad x \in \partial\Omega\,,$$

$$G(x;, x_0, \lambda^*) = -\frac{1}{2\pi} \log|x - x_0| + R(x; x_0, \lambda^*)\,.$$

Here R is its "regular part". Then, $u^* = -2\pi \sum_{k=1}^{N} A_k \nu_k G(x; x_k, \lambda^*)$. Satisfying the point constraint at each x_j gives the homogeneous system

$$A_j \left(1 + 2\pi\nu_j R(x_j; x_j, \lambda^*)\right) + 2\pi \sum_{\substack{k=1 \\ k\neq j}}^{N} A_k \nu_k G(x_j; x_k, \lambda^*) = 0\,, \quad j = 1, \ldots, N\,.$$

Consider the first eigenvalue for which $\lambda^* \to 0$ as $\varepsilon \to 0$. Set the determinant to zero and then use for $\lambda^* \ll 1$ that

$$G(x; x_0, \lambda^*) \sim -\frac{1}{|\Omega|\lambda^*} + G_m(x; x_0)\,, \quad R(x; x_0, \lambda^*) \sim -\frac{1}{|\Omega|\lambda^*} + R_m(x; x_0)\,,$$

where G_m and R_m are the Neumann G-function and its regular part.

Eigenvalue Expansion: A Two-Term Result

Principal Result: For N small circular holes centered at $x_1, \ldots, x_N$ with logarithmic capacitances $d_1, \ldots, d_N$, then

$$\lambda_0(\varepsilon) \sim \lambda^* \,, \quad \lambda^* = \frac{2\pi}{|\Omega|} \sum_{j=1}^{N} \nu_j - \frac{4\pi^2}{|\Omega|} \sum_{j=1}^{N} \sum_{k=1}^{N} \nu_j \nu_k \left(\mathcal{G}\right)_{jk} + O(\nu^3) \,.$$

Here $\nu_j \equiv= -1/\log(\varepsilon d_j)$ and $\left(\mathcal{G}\right)_{jk}$ are the entries of a certain Neumann Green's function matrix $\mathcal{G}$.

For N-circular holes each of radius ε (for which $d_j = 1$), then with $\nu = -1/\log(\varepsilon)$,

$$\lambda_0(\varepsilon) \sim \lambda^* \,, \quad \lambda^* = \frac{2\pi N \nu}{|\Omega|} - \frac{4\pi^2 \nu^2}{|\Omega|} p(x_1, \ldots, x_N) + O(\nu^3) \,,$$

where

$$p(x_1, \ldots, x_N) \equiv \sum_{j=1}^{N} \sum_{k=1}^{N} \left(\mathcal{G}\right)_{jk} \,.$$

Therefore, for N circular holes and $\nu \ll 1$, λ_0 has a local maximum at a local minimum point of the "Energy-like" function $p(x_1, \ldots, x_N)$.

The Neumann Green's Function

The Neumann Green's function $G_m(x;x_0)$, with regular part $R_m(x;x_0)$, satisfies:

$$\Delta G_m = \frac{1}{|\Omega|} - \delta(x-x_0)\,, \quad x \in \Omega\,,$$

$$\partial_n G_m = 0\,, \quad x \in \partial\Omega\,; \qquad \int_\Omega G_m\, dx = 0\,,$$

$$G_m(x,x_0) = -\frac{1}{2\pi}\log|x-x_0| + R_m(x,x_0)\,;$$

The Green's matrix $\mathcal{G}$ is determined in terms of the hole-interaction term $G_m(x_i;x_j) \equiv G_{mij}$, and the self-interaction $R_m(x_i;x_i) \equiv R_{mii}$ by

$$\mathcal{G} \equiv \begin{pmatrix} R_{m11} & G_{m12} & \cdots & \cdots & G_{m1N} \\ G_{m21} & R_{m22} & G_{m23} & \cdots & \cdots \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ G_{mN1} & \cdots & \cdots & G_{mNN-1} & R_{mNN} \end{pmatrix}.$$

One Hole: Uniqueness of Maximizer?

Corollary: For the case of one circular hole of radius ε, centered at x_1, then

$$\lambda_0(\varepsilon) \sim \frac{2\pi\nu}{|\Omega|} - \frac{4\pi^2\nu^2}{|\Omega|} R_m(x_1; x_1) + O(\nu^3)\,, \quad \nu \equiv -1/\log\varepsilon\,.$$

Thus λ_0 is maximized for a hole location that minimizes $R_m(x_1; x_1)$.

Is there a unique point x_1 in Ω that minimizes $R_m(x_1; x_1)$, and consequently maximizes λ_0?

- Require properties of $R_m(x; x_1)$ and $\nabla R_{m0} \equiv \nabla R_m(x : x_1)|_{x=x_1}$ (complex analysis).
- In a symmetric dumbbell-shape domain x_1 is unique. However, multiple roots of $\nabla R_m = 0$ can occur in non-symmetric dumbbell-shape domains (proof by complex analysis).

Multiple Holes in the Unit Disk

Let Ω be the unit circle, so that $|\Omega| = \pi$. Then, G_m and R_m are

$$G_m(x;\xi) = -\frac{1}{2\pi}\log|x-\xi| + R_m(x;\xi)$$

$$R_m(x;\xi) = -\frac{1}{2\pi}\log\left|x|\xi| - \frac{\xi}{|\xi|}\right| + \frac{(|x|^2+|\xi|^2)}{2} - \frac{3}{4}\,.$$

For the unit disk, the problem of minimizing $p(x_1,\ldots,x_N)$ is equivalent to the problem of minimizing the function $\mathcal{F}(x_1,\ldots,x_N)$ defined by

$$\mathcal{F}(x_1,\ldots,x_N) = -\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N}\log|x_j-x_k| - \sum_{j=1}^{N}\sum_{k=1}^{N}\log|1-x_j\bar{x}_k| + N\sum_{j=1}^{N}|x_j|^2\,,$$

for $|x_j| < 1$ and $x_j \neq x_k$ when $j \neq k$.

We consider the restricted optimization problem where $\mathcal{F}$ is optimized over certain ring-type configurations of holes. We then compare the results with those computed with optimization software from MATLAB.

A Related Concentration Problem: Unit Disk

Our eigenvalue optimization problem is equivalent to minimizing

$$\mathcal{F}(x_1,\ldots,x_N) = -\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N}\log|x_j-x_k| - \sum_{j=1}^{N}\sum_{k=1}^{N}\log|1-x_j\bar{x}_k| + N\sum_{j=1}^{N}|x_j|^2\,,$$

for $|x_j|<1$, and $x_j\neq x_k$ when $j\neq k$.

In contrast, by taking a certain limit of a variational formulation of the GL model of superconductivity in the unit disk, Lefter, Radulescu (1996) and Sandier, Soret (2000) showed that equilibrium vortices at $x_1,\ldots,x_N$ inside the unit disk $|x_j|<1$ with a common winding number are located at a minimum point of the renormalized energy $\mathcal{W}$ defined by

$$\mathcal{W}(x_1,\ldots,x_N) = -\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N}\log|x_j-x_k| - \sum_{j=1}^{N}\sum_{k=1}^{N}\log|1-x_j\bar{x}_k|\,.$$

This problem differs from that of the eigenvalue problem only by the confinement potential $N\sum_{j=1}^{N}|x_j|^2$.

One-Ring Configurations: Unit Disk

Two Patterns: I (one ring), II (ring with a center hole). Specifically,

$$x_j = re^{2\pi ij/N}\,, \quad j = 1, \ldots, N\,, \quad \text{(P I)}\,,$$

$$x_j = re^{2\pi ij/(N-1)}\,, \quad j = 1, \ldots, N-1\,,\ x_N = 0\,, \quad \text{(P II)}\,.$$

More generally, we can construct m ring patterns with m rings of radii $r_1, \ldots, r_m$, with $r_j < r_{j+1}$, inside the unit disk. Assume that there are J_k holes on the ring of radius r_k. On the k^{th} ring, for $k = 1, \ldots, m$, the centres of the holes are assumed to satisfy

$$\xi_j^{(k)} = r_k e^{2\pi ij/J_k} e^{i\phi_k}\,, \quad j = 1, \ldots, J_k\,.$$

Here ϕ_k is a phase angle with $\phi_1 = 0$.

For each pattern we can calculate $p(x_1, \ldots, x_N)$ explicitly and then optimize over the ring radii.

Pattern I

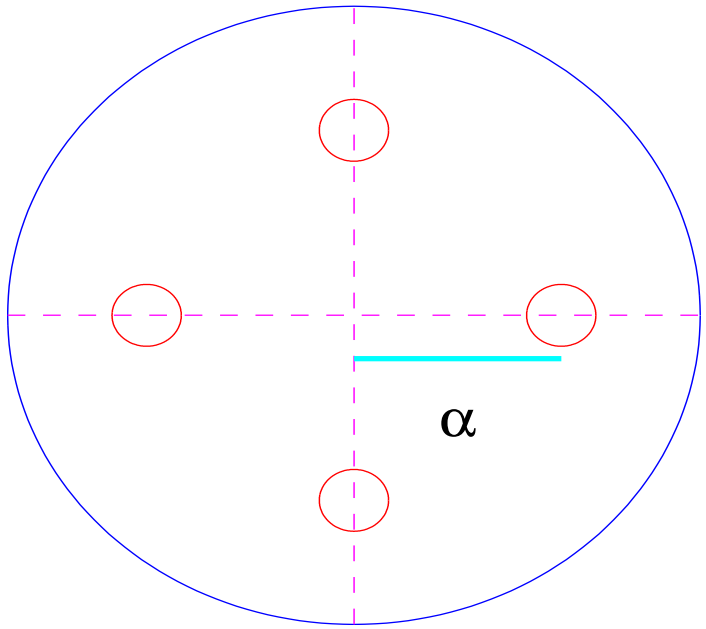
Principal Result: (Pattern I): Let $N > 1$, then $p = p_*/(2\pi)$ satisfies

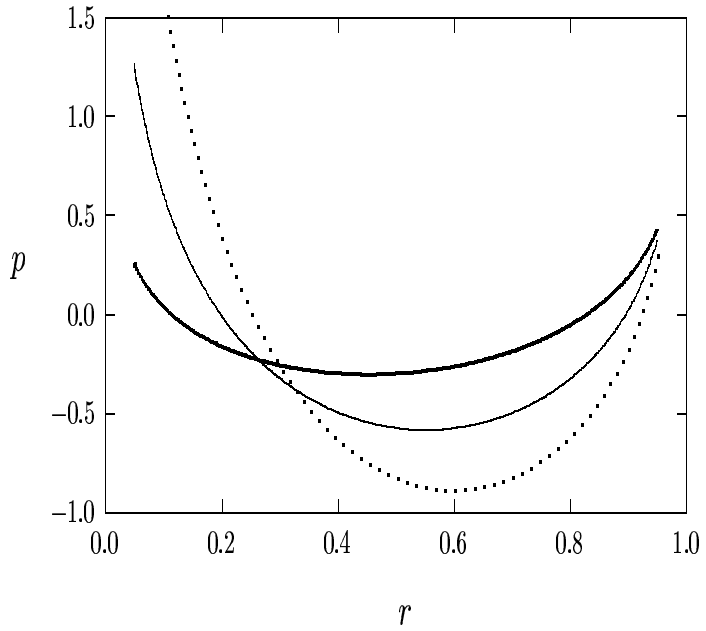
$$p_* = -N \log(N r^{N-1}) - N \log\left(1 - r^{2N}\right) + r^2 N^2 - \frac{3N^2}{4} .$$

Hence $p(r)$ has a unique minimum at $r = r_c$, where

$$\frac{r^{2N}}{1 - r^{2N}} = \frac{N-1}{2N} - r^2 .$$

Left: 4 holes on a ring. Right: p versus r for $N = 2, 3, 4$ holes on a ring.





Pattern II

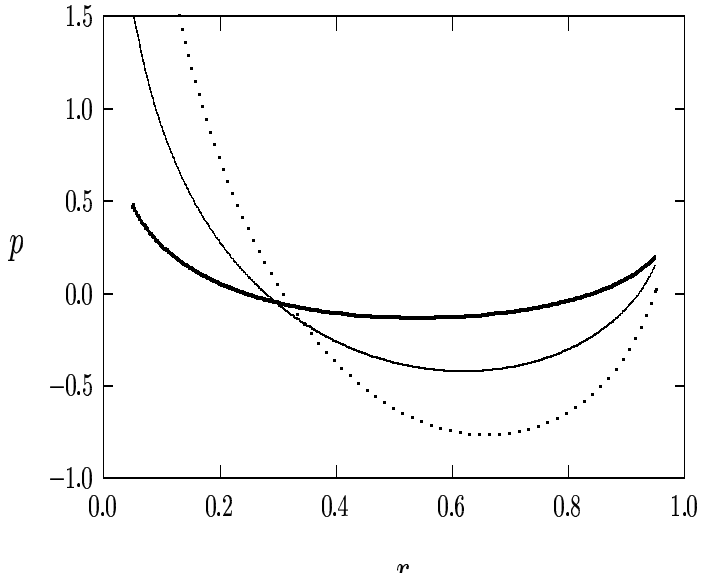
Principal Result: (Pattern II): Let $N > 1$, then $p = p_*(r)/(2\pi)$ satisfies

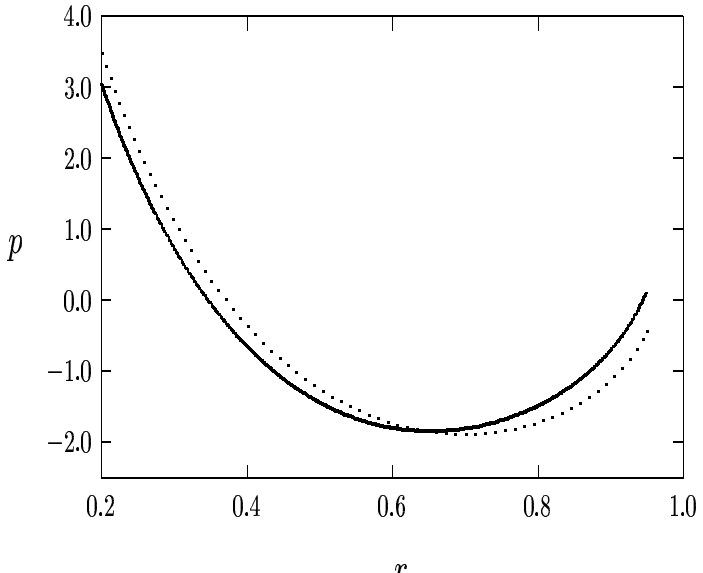
$$p_* = -(N-1)\log\left[(N-1)r^N\right] + r^2 N(N-1) - \frac{3N^2}{4}$$
$$-(N-1)\log\left(1 - r^{2(N-1)}\right) .$$

Hence $p(r)$ has a unique minimum at $r = r_c$, where

$$\frac{r^{2N-2}}{1-r^{2N-2}} = \frac{N}{N-1}\left(\frac{1}{2} - r^2\right) .$$

Left: $N = 2, 3, 4$ holes on a ring and a center hole. Right: 7 holes on a ring (heavy solid) and 6 holes on a ring with an extra center hole (dotted).



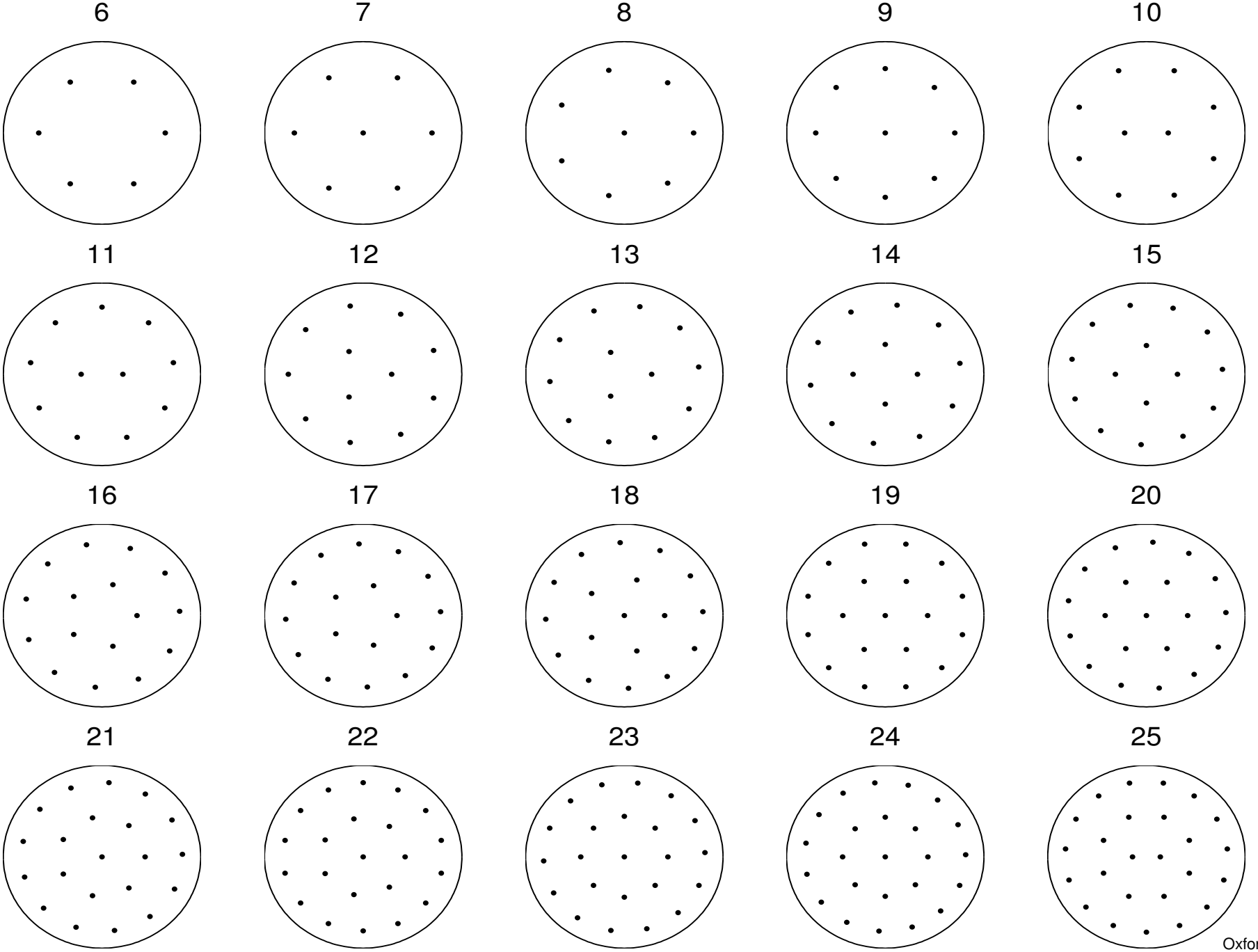


Restricted Optimization: m-ring Patterns

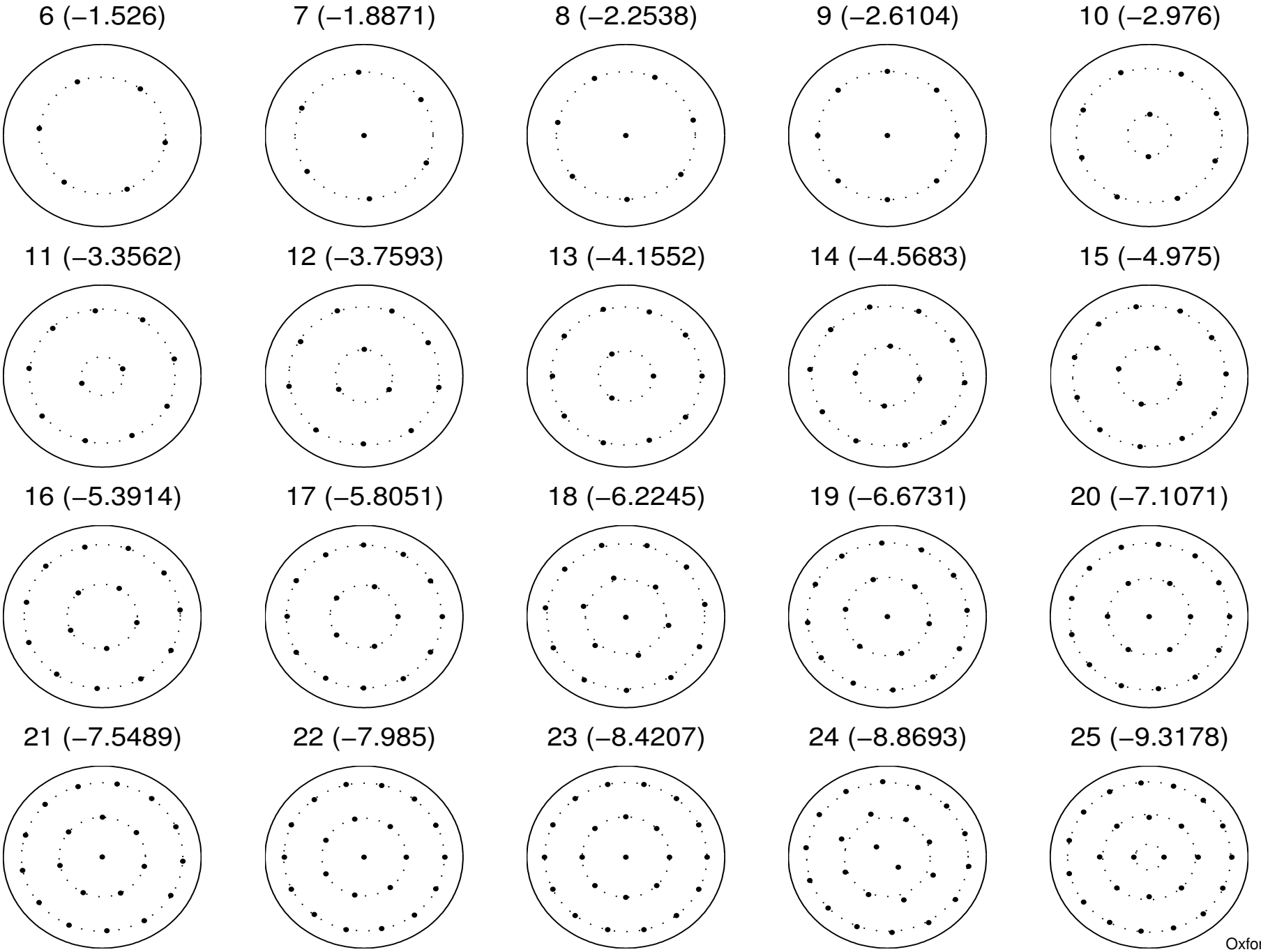
N	optimal pattern	$p_{\min}$	optimum r_j	second best pattern	p
6	(6)	-1.5260	0.642	[1](5)	-1.5134
7	[1](6)	-1.8871	0.698	(7)	-1.8398
8	[1](7)	-2.2538	0.702	(2,6)	-2.1732
9	[1](8)	-2.6104	0.705	(2,7)	-2.5754
10	(2,8)	-2.9686	0.222, 0.737	[1](9)	-2.9549
11	(2,9)	-3.3498	0.212, 0.736	(3,8)	-3.3449
12	(3,9)	-3.7546	0.288, 0.760	(2,10)	-3.7175
13	(3,10)	-4.1511	0.277, 0.758	(4,9)	-4.1457
14	(4,10)	-4.5660	0.327, 0.776	(3,11)	-4.5336
15	(4,11)	-4.9728	0.316, 0.773	(5,10)	-4.9636
16	(5,11)	-5.3903	0.354, 0.788	(4,12)	-5.3652
17	(5,12)	-5.8040	0.343, 0.785	[1](5,11)	-5.7921
18	[1](5,12)	-6.2242	0.408, 0.797	(6,12)	-6.2195
19	[1](6,12)	-6.6713	0.429, 0.809	[1](5,13)	-6.6422
20	[1](6,13)	-7.1052	0.418, 0.805	[1](7,12)	-7.0983
21	[1](7,13)	-7.5480	0.436, 0.815	[1](6,14)	-7.5257
22	[1](7,14)	-7.9844	0.426, 0.811	[1](6,15)	-7.9313
23	[1](8,14)	-8.4204	0.442, 0.819	[1](7,15)	-8.4058
24	[1](8,15)	-8.8566	0.433, 0.816	(2,8,14)	-8.8561
25	(2,8,15)	-9.3056	0.141, 0.469, 0.824	(3,8,14)	-9.3020

Table 1: Numerical results for the optimum configuration within the class of two and three-ring patterns with or without a centre hole. The first three columns indicate the optimum configuration, the minimum value of p, and the optimum ring radii. The last two columns correspond to the second best pattern. The notation $[1](5, 12)$ indicates a two-ring pattern with a centre hole, which has 5 and 12 holes on the inner and outer rings, respectively.

Restricted Optimization: m-ring Patterns II

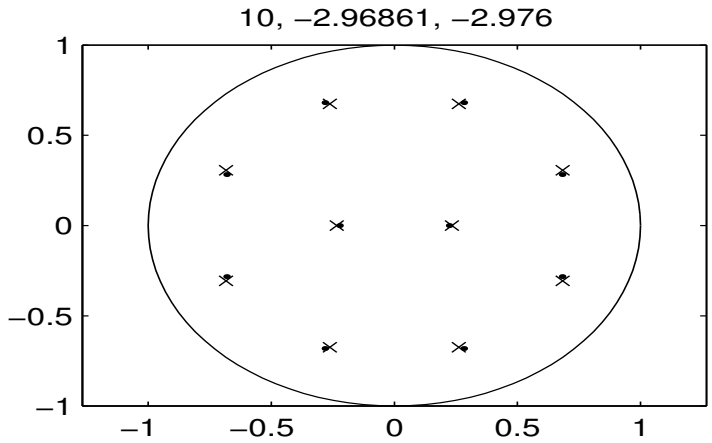


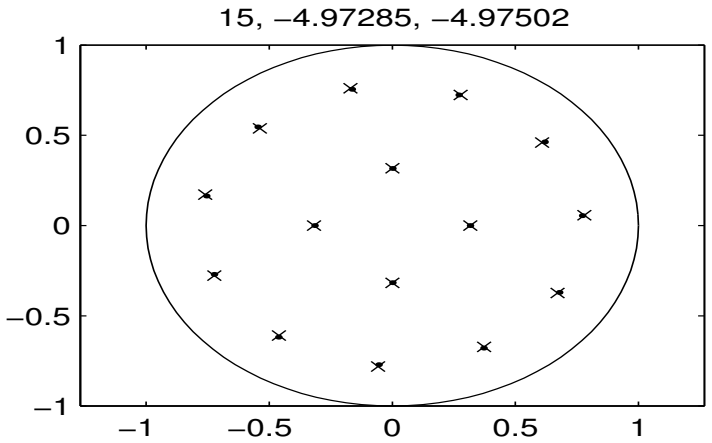
Full Optimization: m-ring Patterns II

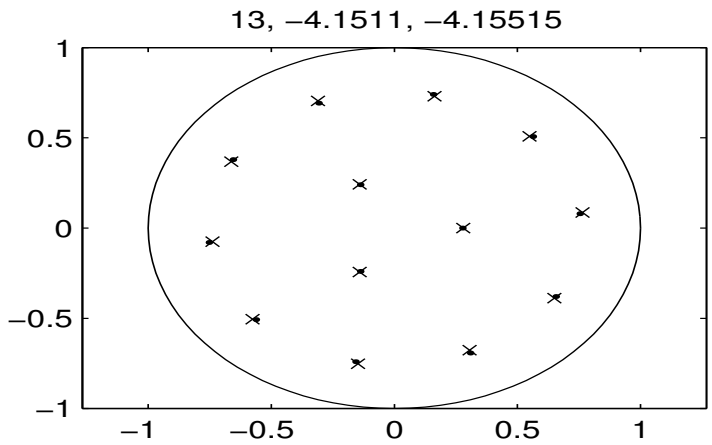


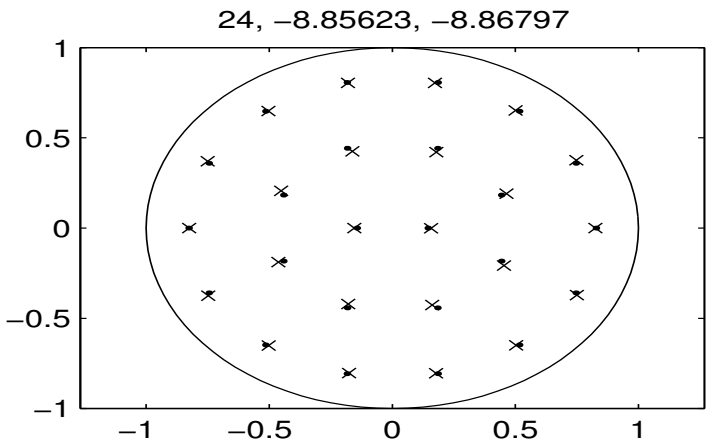
Comparison: Restricted and Full Optimization

Optimization with respect to radii (dots) is compared with a MATLAB optimization with respect to $2N$ variables









Open: Is a Hexagonal Lattice the optimal arrangement for $N \gg 1$?

Open: Optimal Configurations in Other Domains such as a Square?

Eigenvalue Problem with Boundary Traps: I

Consider the 2-D problem with boundary traps

$$\Delta u + \lambda u = 0\,, \quad x \in \Omega\,; \qquad \int_\Omega u^2\,dx = 1\,,$$

$$\partial_n u = 0 \quad x \in \partial\Omega_r\,, \quad u = 0\,, \quad x \in \partial\Omega_a = \cup_{j=1}^N \partial\Omega_{\varepsilon_j}\,.$$

Assume that $\partial\Omega_{\varepsilon_j} \to x_j$ as $\varepsilon \to 0$ and $|\partial\Omega_{\varepsilon_j}| = 2\varepsilon$ for $j = 1, \ldots, N$. Then, with $\nu \equiv -1/\log[\varepsilon/2]$, the first eigenvalue λ_1 satisfies

$$\lambda_1 \sim \frac{\pi N \nu}{|\Omega|} - \frac{\pi^2\nu^2}{|\Omega|}\sum_{j=1}^N\sum_{k=1}^N (\mathcal{G})_{jk} + O(\nu^3)\,,$$

where $(\mathcal{G})_{jk} \equiv G_m(x_j; x_k)$ for $j \neq k$ and $(\mathcal{G})_{jj} \equiv R_m(x_j; x_j)$ where $G_m(x; x_0)$ and $R_m(x; x_0)$ are now the "surface" Neumann G-function:

$$\Delta G_m = \frac{1}{|\Omega|}\,, \quad x \in \Omega\,; \qquad \int_\Omega G_m(x; x_0)\,dx = 0\,,$$

$$\partial_n G_m = 0\,, \;\; x \in \partial\Omega_r \backslash \{x_0\}\,; \quad G_m(x, x_0) = -\frac{1}{\pi}\log|x - x_0| + R_m(x, x_0)\,.$$

Eigenvalue Problem with Boundary Traps: II

Some consequences and open issues:

- For one patch, λ_1 and the associated "outer" eigenfunction u_1 are

$$\lambda_1 \sim \frac{\pi\nu}{|\Omega|} - \frac{\pi^2\nu^2}{|\Omega|} R_m(x_1, x_1) + \cdots ,$$

$$u_1 \sim |\Omega|^{-1/2} - \frac{\pi\nu}{|\Omega|^{1/2}} G_m(x; x_1) + O(\nu^2) .$$

  Open: Is the point that minimizes R_m, and consequently maximizes λ_1, related to extrema of the boundary curvature?

- For N patches on the boundary of the unit disk, for which R_m is independent of x_j, the optimal arrangement is to choose x_j with $|x_j| = 1$ for $j = 1, \ldots, N$ such that $\mathcal{F}(x_1, \ldots, x_N)$ is minimized, where

$$\mathcal{F}(x_1, \ldots, x_N) = -\sum_{j=1}^{N} \sum_{\substack{k=1 \\ k \neq j}}^{N} \log |x_j - x_k| .$$

  Clearly, we must choose the roots of unity. Open: what about the optimal arrangement for a general boundary?

Narrow Escape: A Boundary Trap in 2-D

Consider Brownian motion with diffusivity D in a 2-D domain Ω with a boundary that is insulated except for a small absorbing patch $\partial\Omega_a$ with $|\partial\Omega_a| = 2\varepsilon$. Assume that $\partial\Omega_a \to x_1$ as $\varepsilon \to 0$ and that the initial point for the Brownian motion is $X(0) = x \in \Omega$.

Let $v(x)$ be the mean first passage time (MFPT)

$$v(x) = E\left[\tau | X(0) = x\right] .$$

It is well-known that $v(x)$ satisfies

$$\Delta v = -\frac{1}{D} , \quad x \in \Omega ,$$
$$\partial_n v = 0 \quad x \in \partial\Omega_r ; \quad v = 0 , \quad x \in \partial\Omega_a .$$

Goal: Calculate $v(x)$ as $\varepsilon \to 0$.

History: The paper [SSH]: "Narrow Escape Part II: The Circular Disk", A. Singer, Z. Schuss, D. Holcman, J. Stat. Phys. Vol. 122, (2006), pp. 465-489. Very complicated analysis based on dual integral equations, special functions etc.... (also Narrow Escape Part I: (the Sphere) J. Stat. Phys. (2006) 26 pages, Narrow Escape Part III: Non-Smooth Domains etc...).

Narrow Escape: A Boundary Trap in 2-D

Alternative More General Derivation: Expand v in terms of the eigenfunctions u_i for $i \geq 1$. Then,

$$v = \frac{1}{D\lambda_1}\left(\int_\Omega u_1\,dx\right)u_1 + \sum_{i=2}^{\infty}\frac{1}{D\lambda_i}\left(\int_\Omega u_i\,dx\right)u_i\,,$$

$$v \sim \frac{1}{D\lambda_1}\left(\int_\Omega u_1\,dx\right)u_1 + O(\varepsilon)\,.$$

This follows since $\lambda_1 = O(\nu)$ and $\lambda_i = O(1)$ for $i \geq 2$, with $\int_\Omega u_i\,dx = O(\varepsilon)$ for $i \geq 2$ by the Divergence theorem.

Use the asymptotics for λ_1 and the "outer" form for u_1. In 3-lines we get

$$v(x) = E\left[\tau|X(0)=x\right] \sim \frac{|\Omega|}{\pi D}\left[-\log\varepsilon + \log 2 + \pi(R_m(x_1;x_1) - G_m(x;x_1)\right]\,,$$

where R_m and G_m are the surface Neumann G-functions.

For the unit disk, $R_m = (8\pi)^{-1}$ and G_m is known/ For example, if $x_1 = 1$ and $x = 0$, then we readily recover a result of [SSH]:

$$v(0) = E\left[\tau|X(0)=0\right] \sim \frac{|\Omega|}{\pi D}\left[-\log\varepsilon + \log 2 + \frac{1}{4}\right]\,.$$

Eigenvalues in 3-D Domains: Interior Traps I

In a 3-D bounded domain Ω consider

$$\Delta u + \lambda u = 0\,, \quad x \in \Omega \backslash \Omega_p\,; \qquad \int_{\Omega\backslash\Omega_p} u^2\,dx = 1\,,$$
$$\partial_n u = 0 \quad x \in \partial\Omega\,, \quad u = 0\,, \quad x \in \partial\Omega_p\,.$$

Here $\Omega_p = \cup_{i=1}^N \Omega_{\varepsilon_i}$, with $\Omega_{\varepsilon_i} \to x_i$ as $\varepsilon \to 0$ and non-overlapping.

The first eigenvalue has the asymptotics

$$\lambda_1 \sim \frac{4\pi\varepsilon}{|\Omega|}\sum_{j=1}^N C_j - \frac{16\pi^2\varepsilon^2}{|\Omega|}\sum_{j=1}^N\sum_{k=1}^N C_j C_k\,(\mathcal{G})_{jk} + O(\varepsilon^3)\,.$$

Here $(\mathcal{G})_{jk} \equiv G_m(x_j;x_k)$ for $j \neq k$ and $(\mathcal{G})_{jj} \equiv R_m(x_j;x_j)$ where $G_m(x;\xi)$ and $R_m(x;\xi)$ are now the 3-D Neumann G-function.

Also C_j is the electrostatic capacitance of the j^{th} hole defined by

$$\Delta v = 0\,, \quad y \notin \Omega_j = \varepsilon^{-1}\Omega_{\varepsilon_j}\,,$$
$$v = 1\,, \quad y \in \partial\Omega_j\,; \quad v \sim -\frac{C_j}{|y|}\,, \quad |y| \to \infty\,.$$

Eigenvalues in 3-D Domains: Interior Traps II

The matrix $\mathcal{G}$ can be found explicitly when Ω is the unit sphere. By summing series related to Legendre polynomials

$$G_m(x;\xi) = \frac{1}{4\pi|x-\xi|} + \frac{1}{4\pi|x|r'} + \frac{1}{4\pi}\ln\left[\frac{2}{1-|x||\xi|\cos\theta+|x|r'}\right] + \frac{1}{8\pi}\left(|x|^2+|\xi|^2\right) - \frac{13}{20\pi}\,.$$

Here $r' = |x'-\xi|$, where $x' = x/|x|^2$ is the image point and θ is the angle between x and ξ. The regular part $R_m(\xi,\xi)$ is

$$R_m(\xi,\xi) = \frac{1}{4\pi\left(1-|\xi|^2\right)} - \frac{1}{4\pi}\log\left(1-|\xi|^2\right) + \frac{|\xi|^2}{4\pi} - \frac{13}{20\pi}\,.$$

Open: Where are the optimal trap locations x_j for $j = 1,\ldots,N$ inside the unit sphere that maximize the first eigenvalue? For identical traps we need to minimize the explicitly known function $p(x_1,\ldots,x_N) = \sum\sum \mathcal{G}_{jk}$.

Open: What about more general domains such as Ω a cube. Here we need Ewald summation techniques to build the matrix $\mathcal{G}$.

Eigenvalues in 3-D Domains: Boundary Traps

Consider a spherical domain Ω with N-small non-overlapping absorbing boundary patches on an otherwise reflecting boundary.

Open: Where are the optimal locations to put N small patches to maximize the first eigenvalue λ_1?

One might guess that the trap locations that maximize λ_1 are given by the minimum of the discrete energy $\mathcal{F}(x_1, \ldots, x_N)$ defined by

$$\mathcal{F}(x_1, \ldots, x_N) = \sum_{j=1}^{N} \sum_{\substack{k=1 \\ k \neq j}}^{N} \frac{1}{|x_j - x_k|}\,, \quad |x_j| = 1\,.$$

If so, this is a famous discrete optimization problem of finding the minimal discrete energy of "electrons" confined to the boundary of a sphere. This is related to the discovery of Carbon-60 molecules. Long list of references; E. Saff, N. Sloane, A. Kuijlaars etc..

The difficulty with this problem is that the number of local minima grow exponentially with N, and so finding the global minimum is not trivial computationally.

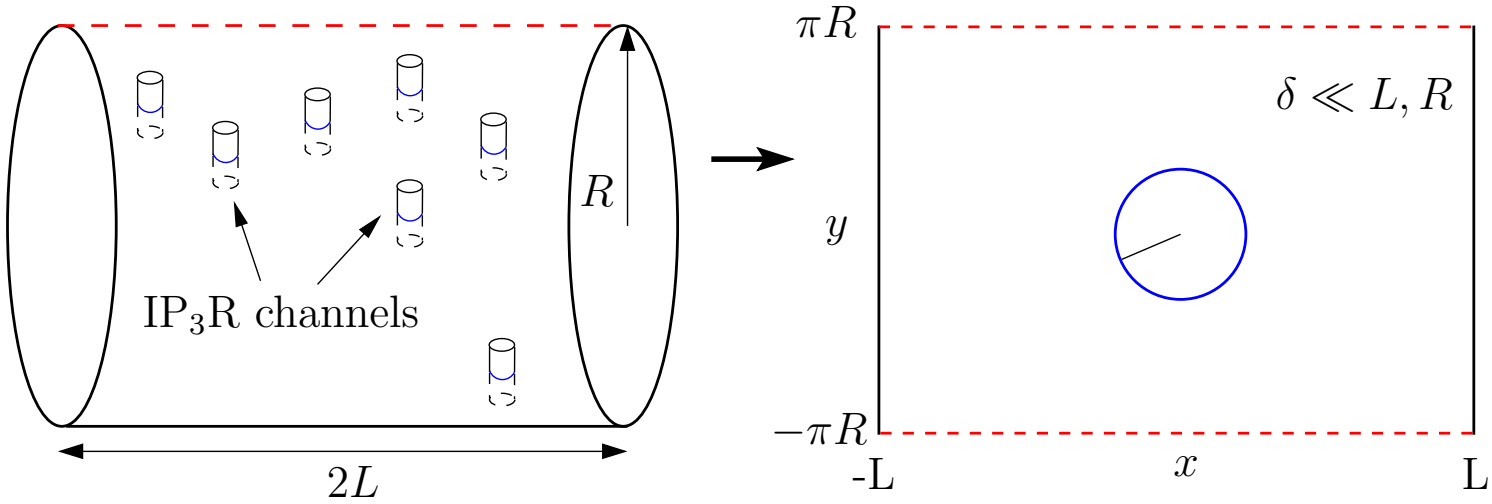
Biomembrane Surface Diffusion With Trap I

Consider the diffusion of proteins on the cylindrical surface (a biomembrane) of length $2L$ and radius R having a small circular trap $\Omega_\delta = |\mathbf{x}| \leq \delta$. The concentration with $\mathbf{x} = (x, y)$, where $|x| < L$ and $|y| < \pi R$, satisfies

$$c_t = D\Delta c\,, \quad \mathbf{x} \in \Omega \backslash \Omega_\delta\,,$$
$$\partial_x c = 0\,, \quad x = \pm L\,; \quad c,\ \partial_y c\,, \quad 2\pi R \text{ periodic in } y\,,$$
$$c = 0\,, \quad \mathbf{x} \in \partial\Omega_\delta\,.$$

Initially, $c(\mathbf{x}, 0) = c_0$. We want to calculate the reaction rate $k(t)$,

$$k(t) = D \int_{\partial\Omega_\delta} \nabla c|_{|\mathbf{x}|=\delta} \cdot \hat{\mathbf{n}}\, dS\,.$$



Biomembrane Surface Diffusion With Trap II

For $t \gg 1$, then $c(\mathbf{x},t) \sim d_0 \phi_0 e^{-\lambda_0 D t}$, where $d_0 = c_0 \int_{\Omega \setminus \Omega_\delta} \phi_0 \, d\mathbf{x}$. Here λ_0 and ϕ_0 are the principal eigenpair of

$$\Delta \phi + \lambda \phi = 0\,, \quad \mathbf{x} \in \Omega\,; \quad \int_\Omega \phi^2 \, d\mathbf{x} = 1\,,$$
$$\partial_x \phi = 0\,, \quad x = \pm L\,; \quad \phi,\ \partial_y \phi\,, \quad 2\pi R \text{ periodic in } y\,,$$
$$\phi = 0\,, \quad \mathbf{x} \in \partial\Omega_\delta\,.$$

The principal eigenvalue has the following asymptotics for $\delta \ll 1$:

$$\lambda_0 \sim \frac{2\pi\nu}{|\Omega|} - \frac{4\pi^2\nu^2}{|\Omega|} R_m(\mathbf{0};\mathbf{0}) + \frac{8\pi^3\nu^3}{|\Omega|}\left([R_m(\mathbf{0};\mathbf{0})]^2 - \frac{G_{m2}(\mathbf{0};\mathbf{0})}{|\Omega_0|} \right)\,.$$

Here $\nu = -1/\log\delta$ and $|\Omega| = 4\pi L R$ is the area of the cylindrical surface. The reaction rate is given by

$$k(t) \sim c_0 D\,|\Omega|\ \lambda_0\, e^{-\lambda_0 D t}\left(1 - \frac{4\pi^2\nu^2}{|\Omega|} G_{m2}(\mathbf{0};\mathbf{0})\right)\,.$$

Biomembrane Surface Diffusion With Trap III

The Neumann Green's function $G_m(\mathbf{x};\mathbf{0})$ with regular part $R_m(\mathbf{0};\mathbf{0})$ satisfy

$$\Delta G_m = \frac{1}{|\Omega|} - \delta(\mathbf{x})\,; \quad \int_\Omega G_m\,d\mathbf{x} = 0\,,$$

$$\partial_x G_m = 0\,, \quad x = \pm L\,; \quad G_m,\ \partial_y G_m\,, \quad 2\pi R \text{ periodic in } y\,,$$

$$G_m(\mathbf{x};\mathbf{0}) \sim -\frac{1}{2\pi}\log|\mathbf{x}| + R_m(\mathbf{0};\mathbf{0}) \quad \text{as } \mathbf{x}\to\mathbf{0}\,.$$

With the same boundary conditions, $G_{m2}(\mathbf{x};\mathbf{0})$ satisfies

$$\Delta G_{m2} = -G_m\,; \quad \int_\Omega G_{m2}\,d\mathbf{x} = 0\,.$$

Clearly, G_m has the Fourier series representation

$$G_m(\mathbf{x};\mathbf{0}) = \frac{2}{|\Omega|}\left(\frac{1}{\pi^2}\sum_{m=1}^{\infty}\frac{\cos(m\pi x)}{m^2} + \frac{R^2}{L^2}\sum_{n=1}^{\infty}\frac{\cos\left(\frac{nL}{R}y\right)}{n^2}\right)$$
$$+\frac{2}{|\Omega|}\sum_{m,n=1}^{\infty}\frac{2\cos(m\pi x)\cos\left(\frac{nL}{R}y\right)}{(m\pi)^2+\left(\frac{nL}{R}\right)^2}.$$

Biomembrane Surface Diffusion With Trap IV

By using Ewald-type summation techniques to extract R_m from the slowly converging doubly-infinite series we calculate

$$R_m(\mathbf{0};\mathbf{0}) = \frac{1}{2\pi}\left(\frac{L}{6R} - \log\left(\frac{L}{R}\right) - 2\sum_{n=1}^{\infty}\log\left(1-e^{-2nL/R}\right)\right).$$

The solution G_{m2} has the Fourier series representation

$$\begin{aligned} G_{m2}(\mathbf{x};\mathbf{0}) &= \frac{2}{|\Omega_0^s|}\left(\sum_{m=1}^{\infty}\frac{\cos(m\pi x)}{(\pi m)^4} + \sum_{n=1}^{\infty}\frac{\cos\left(\frac{nL}{R}y\right)}{\left(\frac{nL}{R}\right)^4}\right) \\ &\quad + \frac{2}{|\Omega_0^s|}\left(\sum_{m,n=1}^{\infty}\frac{2\cos(m\pi x)\cos\left(\frac{nL}{R}y\right)}{\left((m\pi)^2+\left(\frac{nL}{R}\right)^2\right)^2}\right). \end{aligned}$$

Now, $G_2(\mathbf{0},\mathbf{0})$ is readily evaluated by interchanging the infinite summations with the limiting procedure $\mathbf{x}\to\mathbf{0}$, since the resulting infinite series are absolutely convergent. This gives

$$G_{m2}(\mathbf{0};\mathbf{0}) = \frac{1}{4\pi}\left(\frac{1}{45}\frac{L}{R} + \frac{R}{L}\sum_{n=1}^{\infty}\frac{1}{n^2\sinh^2\left(\frac{L}{R}n\right)} + \frac{R^2}{L^2}\sum_{n=1}^{\infty}\frac{\coth\left(\frac{L}{R}n\right)}{n^3}\right).$$

Diffusion of Protein Receptors I

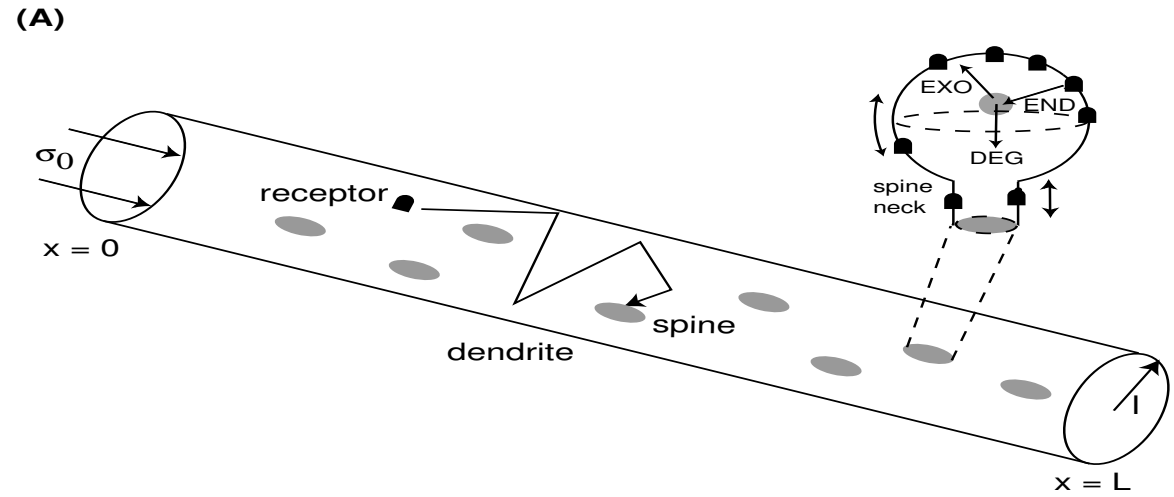
The problem for the diffusion of protein receptors on a cylindrical dendritic membrane $\Omega = \{|x| < L, |y| < 2\pi l\}$, with partially absorbing traps is

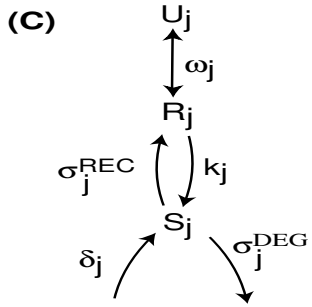
$$U_t = \Delta U\,, \quad \mathbf{x} \in \Omega \backslash \Omega_p\,, \quad \Omega_p = \cup_{j=1}^{N} \Omega_{\varepsilon_j}\,,$$

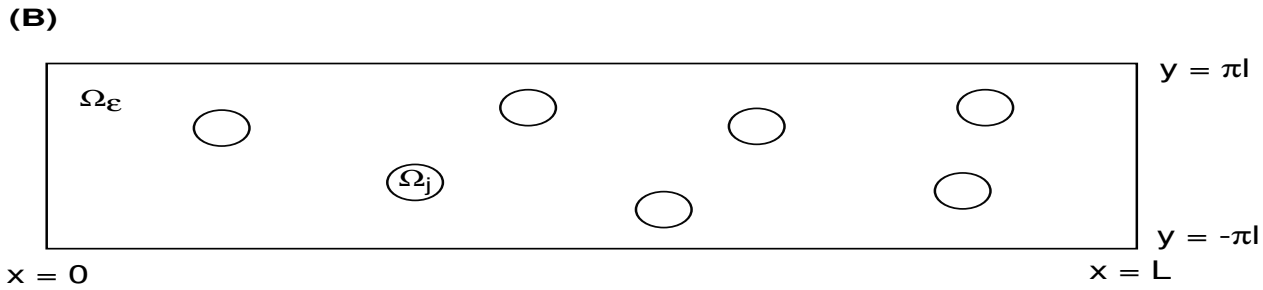
$$\partial_x U(-L, y) = -\sigma\,, \quad \partial_x U(L, y) = 0\,; \quad U\,,\ \partial_y U\,, \quad 2\pi l \text{ periodic in } y\,,$$

$$\varepsilon \partial_n U = -\kappa_j \left(U - T_j\right)\,, \quad \mathbf{x} \in \partial\Omega_{\varepsilon_j}\,, \quad j = 1, \ldots, N\,.$$

Here $\sigma > 0$ models the influx of protein receptors from the soma.







Diffusion of Protein Receptors II

Define the average concentration U_j on the boundary of the j^{th} spine

$$U_j = \frac{1}{2\pi\varepsilon} \int_{\partial\Omega_{\varepsilon_j}} U \, d\mathbf{x} \, .$$

Within each spine $T_j(t)$ and $S_j(t)$ for $j = 1, \ldots, N$ satisfy coupled ODE's of the form

$$T_j' = \mathcal{F}_j \left(T_j, S_j, U_j \right) \, , \qquad S_j' = \mathcal{H}_j \left(T_j, S_j \right) \, .$$

- This model is due to Bressloff and Earnshaw (Phys. Rev. E. (2007), J. Neuroscience (2006)). The 1-D problem was studied by them.
- Calculation of the steady-state solution in terms of σ and the locations of the dendritic spines.
- Stability analysis: couples the stability of ODE's within each spine to the stability problem for the "outer" diffusion equation.
- Time dependent computations?

Diffusion of Protein Receptors III

The 2-D steady-state problem fits in the same framework as the other problems. Define $\mathcal{U}$ by

$$\mathcal{U} = U - U_c(x)\,, \qquad U_c(x) = \frac{\sigma}{2L}(x-L)^2\,.$$

With $\nu = -1/\log\varepsilon$. By using inner-outer matching, $\mathcal{U}$ satisfies

$$\Delta\mathcal{U} = -\frac{\sigma}{L}\,, \quad \mathbf{x}\in\Omega\backslash\Omega_p\,,$$

$$\partial_x\mathcal{U}(\pm L, y) = 0\,; \quad \mathcal{U}\,,\ \partial_y\mathcal{U}\,, \quad 2\pi l \text{ periodic in } y\,,$$

$$\mathcal{U} \sim \nu A_j \log|\mathbf{x}-\mathbf{x}_j| + A_j + U_j - U_c(x_j)\,, \quad \text{as } \mathbf{x}\to\mathbf{x}_j\,.$$

The solution in terms of G_m is $\mathcal{U} = -2\pi\nu\sum_{j=1}^N A_j G_m(\mathbf{x};\mathbf{x}_j) + \chi$. Then, we obtain $2N+1$ equations for the unknowns A_j, U_j and χ:

$$2\pi\nu\sum_{j=1}^N A_j = \frac{\sigma}{L}|\Omega|\,, \quad \text{(Divergence Theorem)}\,,$$

$$(1+2\pi\nu R_{mjj})\,A_j + 2\pi\nu\sum_{i\neq j} A_i G_{mji} = U_c(x_j) - U_j + \chi\,, \quad \text{(Point constraint)}$$

$$2\pi\nu A_j = \kappa_j(U_j - T_j)\,, \quad \text{(BC on each trap)}\,.$$

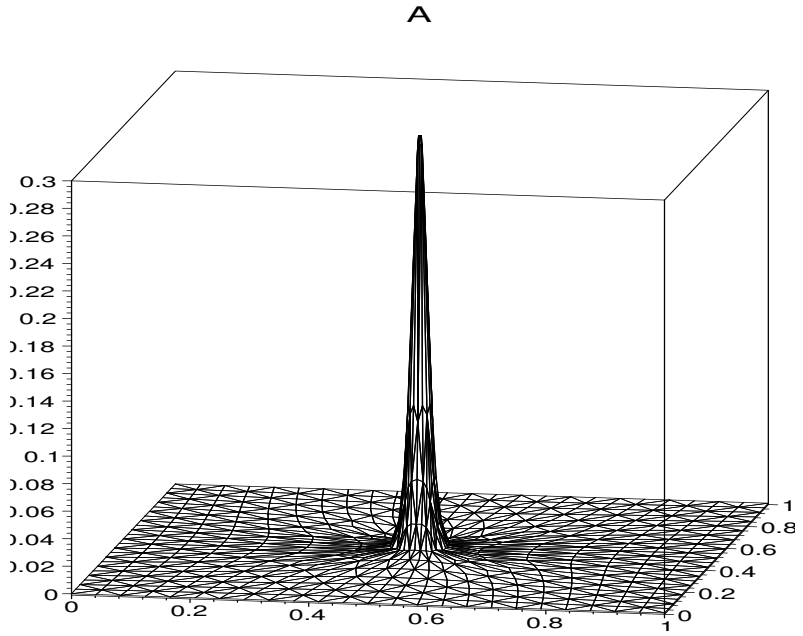
Spot Stability for the GM Model

The activator a and inhibitor h in a 2-D domain Ω, with $\varepsilon \ll 1$ satisfy

$$a_t = \varepsilon^2 \triangle a - a + \frac{a^2}{h}\,, \quad \partial_n a = 0\,, \quad x \in \partial\Omega$$

$$\tau h_t = D \triangle h - h + \varepsilon^{-2} a^2\,, \quad \partial_n h = 0\,, \quad x \in \partial\Omega\,.$$

The problem has no variational structure. There are particle-like solutions for a, called spots, when $\varepsilon \ll 1$. Since a is localized, $\varepsilon^{-1} a^2 \to \sum_{j=1}^{N} S_j \delta(x - x_j)$ in the "outer" region. Hence, the "outer" equilibrium problem for h is solvable by Green's functions.



Spot Stability for the GM model: I

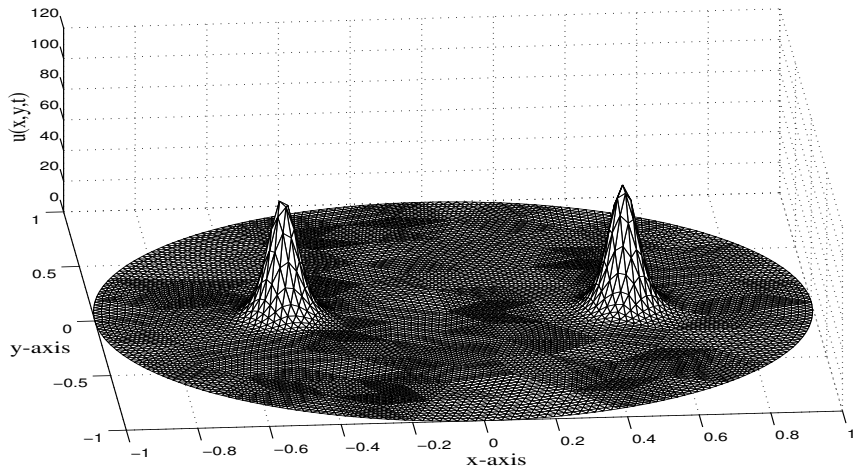
By analyzing a leading order nonlocal eigenvalue problem (NLEP):

Theorem: [Winter, Wei, JNLS 2001] For $\tau = 0$, $\varepsilon \to 0$, and $D \geq O(-\ln \varepsilon)$, an N-spot equilibrium solution is stable on an $O(1)$ time-scale iff

$$D < D_N \sim \frac{|\Omega|}{2\pi\nu N}\,, \qquad \nu \equiv -1/\ln \varepsilon\,.$$

- This leading-order term in a logarithmic expansion predicts that D_N is independent of the spot locations x_j, $j = 1, \ldots, N$.
- We need higher order terms in the logarithmic series for D_N. As for the Neumann eigenvalue problem with traps, we anticipate

$$D_N \sim \frac{|\Omega|}{2\pi\nu N} + F(x_1, \ldots, x_N) + O(\nu)\,, \quad \nu \equiv -1/\ln \varepsilon\,.$$



For a movie showing a spike collapse due to overcrowding click here.

Spot Stability for the GM model: II

Upon including the next term in the logarithmic series for the stability analysis:

Principal Result: [KW, 2006] Let $\tau = 0$, $\varepsilon \to 0$, $D \geq O(\nu^{-1})$ where $\nu \equiv -1/\ln \varepsilon$. Then, an N-spot quasi-equilibrium solution is stable on an $O(1)$ time-scale iff

$$D < D_N \sim \frac{|\Omega|}{2\pi\nu N} + |\Omega| \left(-p(x_1, \ldots, x_N) + \frac{2}{N} \min_{j=1,\ldots,N-1} \boldsymbol{c}_j^t \mathcal{G} \boldsymbol{c}_j \right) + O(\nu) \, .$$

Here $\boldsymbol{e}^t = (1, \ldots, 1)$ and the $\boldsymbol{c}_j$ correspond to an $N-1$ dimensional subspace perpendicular to e: i.e. $\boldsymbol{c}_j^t e = 0$ for with $\boldsymbol{c}_j^t \boldsymbol{c}_j = 1$.

Sketch: Let w be the radially symmetric ground state solution for the spatial profile of the activator. The NLEP problems for $\tau = 0$ are

$$\triangle \Phi - \Phi + 2w\Phi - \chi_j w^2 \frac{\int_{\mathbb{R}^2} w\Phi \, dy}{\int_{\mathbb{R}^2} w^2 \, dy} = \lambda \Phi \, , \quad j = 1, \ldots, N \, ,$$

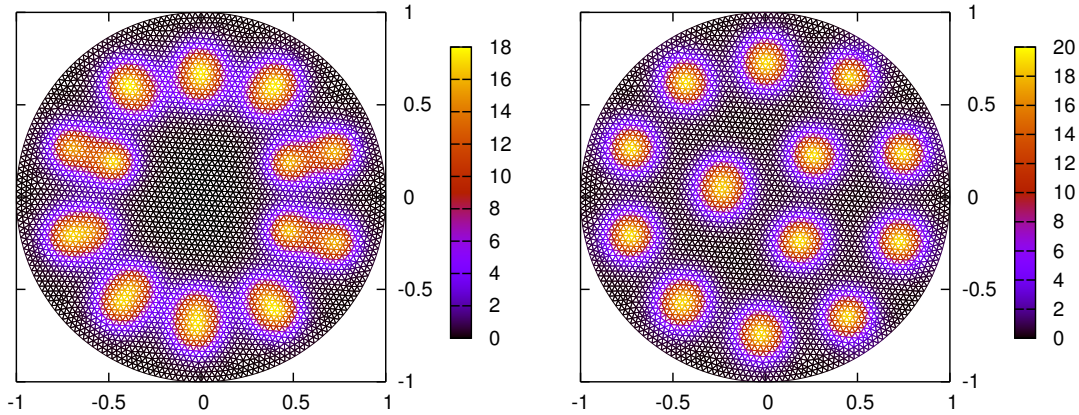
$$\chi_j \equiv \frac{2N\mu_j}{\boldsymbol{e}^t \mathcal{G} \boldsymbol{e}} \, , \qquad \mathcal{C} \boldsymbol{c}_j = \mu_j \boldsymbol{c}_j \, , \qquad \mathcal{C} \equiv I + \frac{2\pi\nu D}{|\Omega|} \boldsymbol{e}\boldsymbol{e}^t + 2\pi\nu\mathcal{G} \, .$$

To calculate the stability threshold set $\min \chi_j = 1$ and solve for $D = D_N$.

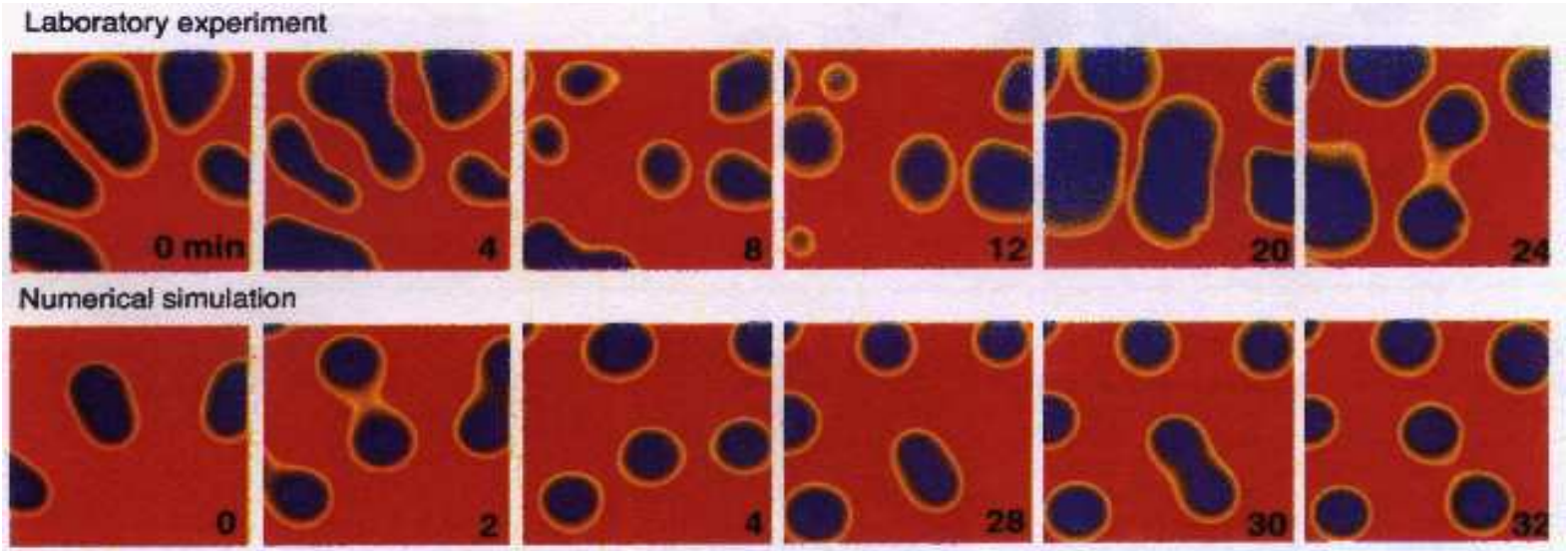
Spot Replication for the Gray-Scott Model: I

$$v_t = \varepsilon^2 \triangle v - v + Auv^2\,, \quad \tau u_t = D \triangle u - (1-u) - uv^2\,.$$

Spot splitting: 2-D GS Model: $A = 3.87$, $D = 1$, $\varepsilon = 0.04$: (Movie)



Exper: FIS Reaction; Numer: GS Model (Swinney et. al. Nature 1994).

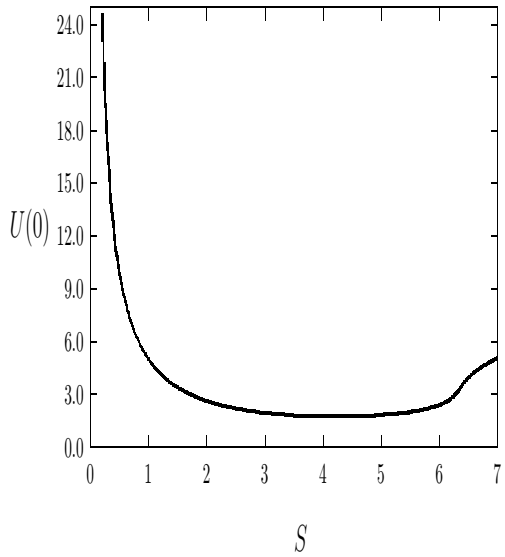


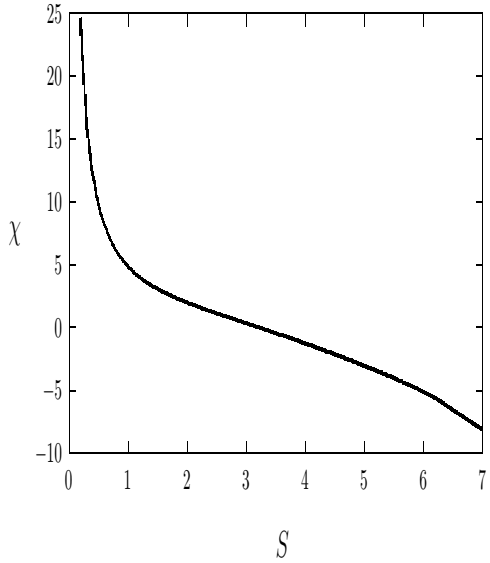
Spot Replication for the Gray-Scott Model: II

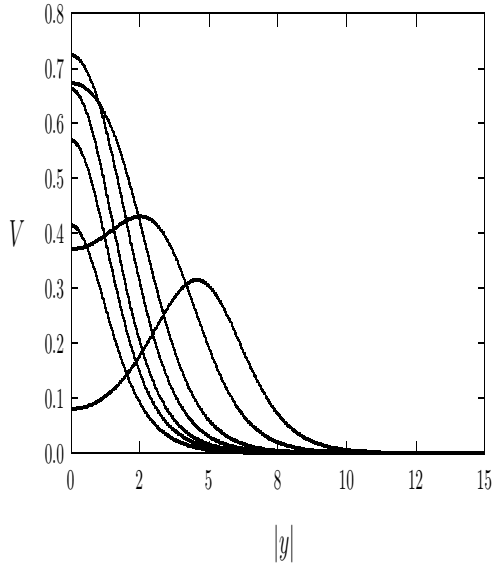
The Core Solution: Near the j^{th} spot we introduce U, V, and y by $u = \frac{\varepsilon}{A\sqrt{D}}U$, $v = \frac{\sqrt{D}}{\varepsilon}V$, and $y = \varepsilon^{-1}(x - x_j)$. The quasi-steady spatial profile for the j^{th} spot, referred to as the core problem, is to look for radially symmetric solutions in $\mathbb{R}^2$ to

$$\Delta_y U - UV^2 = 0\,, \qquad \Delta_y V - V + UV^2 = 0\,,$$
$$V \to 0\,, \quad U \sim S_j \log\rho + \chi(S_j) \quad \text{as} \quad \rho = |y| \to \infty\,.$$

Here $S_j = \int_0^\infty \rho U V^2\, d\rho$ is a parameter, and $\chi(S_j)$ is to be computed. Notice the volcano pattern for V when $S_j > s_v \approx 4.78$.







Spot Replication for the Gray-Scott Model: III

The Outer Problem: In the "outer" region away from the spots, uv^2 is approximated by delta functions. By including all logarithmic terms:

$$\Delta u + \frac{1}{D}(1-u) = \frac{2\pi\nu}{\mathcal{A}} \sum_{j=1}^{N} S_j \delta(x - x_j)\,, \quad x \in \Omega\,; \qquad \partial_n u = 0\,, \quad x \in \partial\Omega$$

$$u \sim \frac{S_j \nu}{\mathcal{A}} \log|x - x_j| + \frac{1}{\mathcal{A}}\left[S_j + \chi(S_j)\nu\right], \quad \text{as } x \to x_j\,, \quad j = 1, \ldots, N\,.$$

Here $\nu = -1/\log\varepsilon$ and A is related to $\mathcal{A}$ by $A \equiv D^{-1/2}\varepsilon(-\log\varepsilon)\mathcal{A}$.

The point constraint gives N nonlinear algebraic equations for S_j:

$$\mathcal{A} = S_j\left(1 + 2\pi\nu R_{jj}\right) + \nu\chi(S_j) + 2\pi\nu \sum_{k\neq j}^{N} S_k G(x_j; x_k)\,, \quad j = 1, \ldots, N\,.$$

Here $R(x;\xi)$ and $G(x;\xi)$ correspond to the Reduced-Wave G-function:

$$\Delta G - \frac{1}{D}G = -\delta(x-\xi)\,, \quad x \in \Omega\,; \qquad \partial_n G = 0\,, \quad x \in \partial\Omega$$

$$G(x,\xi) = -\frac{1}{2\pi}\log|x - x_0| + R(x,\xi)\,.$$

Spot Replication for the Gray-Scott Model: IV

Stability to Angular Perturbations: The stability of the core solution to $e^{im\theta}$ perturbations with $m \geq 2$ is determined by the eigenvalue problem

$$\mathcal{L}_m \Phi - \Phi + 2UV\Phi + V^2 N = \lambda \Phi\,, \quad \Phi \to 0\,, \quad \text{as } \rho \to \infty\,,$$

$$\mathcal{L}_m N - 2UV\Phi - V^2 N = 0\,, \quad N \to 0\,, \quad \text{as } \rho \to \infty\,,$$

$$\mathcal{L}_m \zeta \equiv \zeta'' + \frac{1}{\rho}\zeta' - \frac{m^2}{\rho^2}\zeta\,.$$

Goal: determine critical values s_m of S_j for which we have stability wrt mode $m \geq 2$ iff $S_j < s_m$. Note $N = N(\rho)$ and $\Phi = \Phi(\rho)$.

- We compute numerically that $s_2 \approx 4.31$, $s_3 \approx 5.44$, $s_4 \approx 6.14$. Thus a peanut-splitting instability of the j^{th} spot will occur when its S_j value satisfies $s_2 < S_j < s_3$. This leads to spot self-replication.
- The spot locations evolve dynamically on a slow (in ϵ) time-scale. Thus, each S_j depends not only on the fixed quantities Ω, D, $\mathcal{A}$, but also on all the drifting spot locations x_j.
- Thus, a (local) spot-splitting instability can be triggered at some time during the evolution of the collection of spots.

Spot Replication for the Gray-Scott Model: V

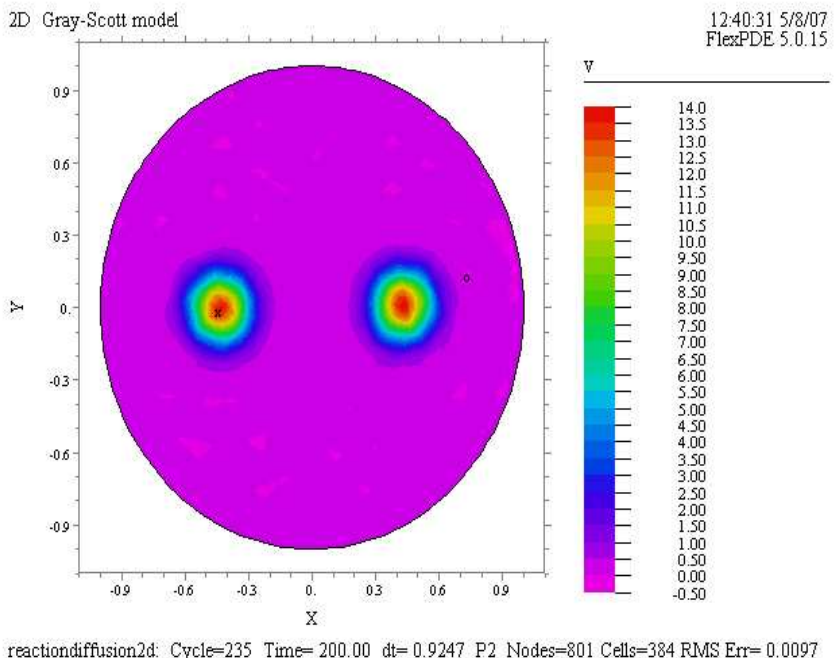
Let Ω be the unit circle and $\tau = 1$. For $N = 1$ and $x_1 = 0$, we get

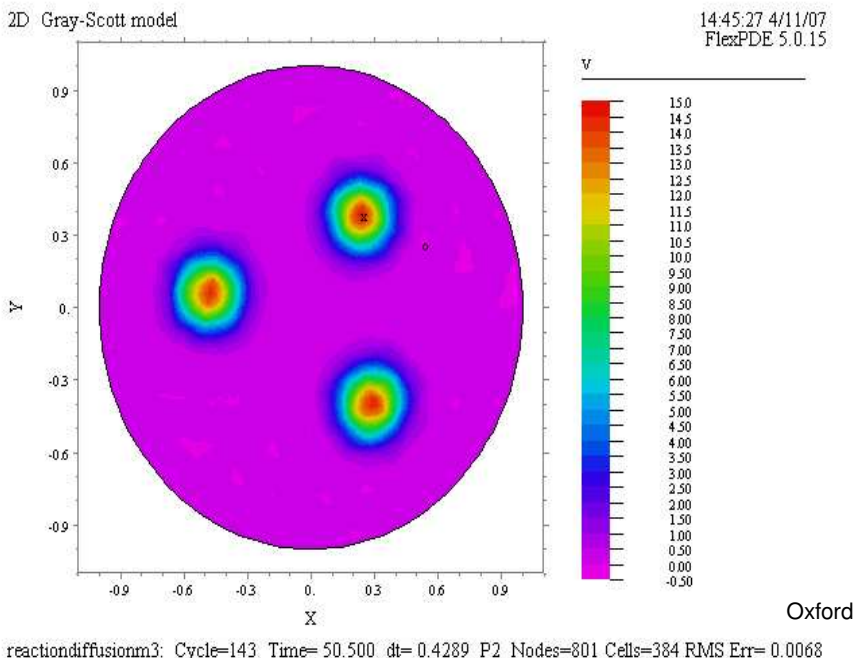
$$R_{11} \equiv R(0;0) = \frac{1}{2\pi}\left[\frac{1}{2}\log D + \log 2 - \gamma - \frac{K_0'(\theta_0)}{I_0'(\theta_0)}\right], \quad \theta_0 = 1/\sqrt{D}\,.$$

Recall that

$$\mathcal{A} = S\left(1 + 2\pi\nu R_{11}\right) + \nu\chi(S)\,.$$

Let $D = 1$ and $\varepsilon = 0.05$. Since $s_2 = 4.31$ and $\chi(s_2) = -1.79$ the spot-splitting threshold is $\mathcal{A}_2 = 5.41$. Similarly $\mathcal{A}_v = 5.79$, and $\mathcal{A}_3 = 6.29$. Full numerics yields a threshold between $\mathcal{A} = 5.6 \sim 5.7$.
(Movie) for $\mathcal{A} = 5.8$. (Movie) for $\mathcal{A} = 7.2$.





Spot Replication for the Gray-Scott Model: VI

- **NLEP Overcrowding Instability** when $A = O\left[\varepsilon\left(-\log\varepsilon\right)^{1/2}\right]$. A positive real eigenvalue leads to spot-annihilation when there are too many.
- **Spot-Splitting Instability** when $A = O\left[\varepsilon(-\log\varepsilon)\right]$ due to an instability of the core solution the angular mode $m = 2$ (peanut-splitting).
- **Annihilation–Creation Attractors** should be possible since the self-replication and NLEP thresholds are so close in 2-D. Nishiura has observed these numerically in a different parameter regime of the GS model. Imagine that for some spots, S_j exceeds splitting threshold for some j. Then spots are created and all the S_j decrease. This gives a smaller effective value of A and we enter NLEP regime, where the spot over-crowding instability occurs. Some spots are destroyed, and the values of S_j increase again.

Spot Replication: Schnakenburg Model I

The Schnakenburg model in Ω with no flux BC on $\partial\Omega$ is

$$\nu_t = \varepsilon^2 \triangle \nu + b - \nu + \mu\nu^2 \,, \quad \mu_t = D_u \triangle \mu + a - \mu\nu^2 \,.$$

Let $\nu = \varepsilon^{-2} v$, $\mu = \varepsilon^2 u$, and $D = \varepsilon^2 D_u$. Then,

$$v_t = \varepsilon^2 \triangle v + b\varepsilon^2 - v + uv^2 \,, \quad \varepsilon^2 u_t = D \triangle u + a - \varepsilon^{-2} uv^2 \,.$$

We neglect the $b\varepsilon^2$ term.

- The Schnakenburg model has been used as a prototype RD model to exhibit the effect of pattern generation by domain growth.
- **1-D Patterns:** I. Barrass, E. Crampin, P. Maini (Bull. Math. Bio. 68, (2006)). Mode transitions due to noise.
- **2-D Spots in a Square:** A. Madzvamuse, P. Maini, A. Wathen, (J. Scientific Computing, 24, (2005)). Numerical evidence of spot-splitting.
- Adiabatically slow domain growth of a square or a circle is equivalent to fixing Ω and decreasing D and ε^2 at the same rate (neglect dilution term).

Spot Replication: Schnakenburg Model II

Goal: Explain Mode-Doubling in 2-D starting from N Spots:

The Core Solution: Near the j^{th} spot we let $u = \frac{1}{\sqrt{D}}U$, $v = \sqrt{D}V$, and $y = \varepsilon^{-1}(x - x_j)$. We obtain the radially symmetric GS core problem in $\mathbb{R}^2$:

$$\Delta_y U - UV^2 = 0\,, \qquad \Delta_y V - V + UV^2 = 0\,,$$
$$V \to 0\,, \quad U \sim S_j \log\rho + \chi(S_j) \quad \text{as} \;\; \rho = |y| \to \infty\,.$$

The Outer Problem: Let $\nu = -1/\log\varepsilon$. The outer problem that accounts for all logarithmic terms is

$$\Delta u = -\frac{a}{D} + \frac{2\pi}{\sqrt{D}}\sum_{j=1}^{N} S_j \delta(x - x_j)\,, \;\; x \in \Omega\,; \quad \partial_n u = 0\,, \quad x \in \partial\Omega$$

$$u \sim \frac{S_j}{\sqrt{D}}\log|x - x_j| + \frac{1}{\sqrt{D}}\left[\frac{S_j}{\nu} + \chi(S_j)\right], \quad \text{as} \;\; x \to x_j\,, \;\; j = 1, \ldots, N\,.$$

The solution in terms of the Neumann G-function is

$$u = -\frac{2\pi}{\sqrt{D}}\sum_{j=1}^{N} S_j G_m(x; x_j) + \frac{u_c}{\sqrt{D}}\,.$$

Spot Replication: Schnakenburg Model III

The point constraints and the div. theorem: $N+1$ equations for S_j and u_c

$$\nu u_c = S_j\left(1+2\pi\nu R_{mjj}\right)+\nu\chi(S_j)+2\pi\nu\sum_{k\neq j}^{N}S_k G_m(x_j;x_k)\,,\quad j=1,\ldots,N\,,$$

$$2\pi\sum_{j=1}^{N}S_j=\frac{a}{\sqrt{D}}|\Omega|\,.$$

- For $N=1$, $S_1=\frac{a|\Omega|}{2\pi\sqrt{D}}$ is independent of G_m, R_m, and x_1. When $S_1>s_2=4.31$, spot-splitting (i.e. mode-doubling) occurs (independent of the spot location x_1) when $|\Omega|$ is sufficiently large.
- For $N>1$, we get $u_c=O(\nu^{-1})$, and so $S_j\sim\mathcal{S}+O(\nu)$. Therefore, to leading order in ν, mode-doubling transitions of N spots will occur (approximately) simultaneously when

$$|\Omega|>\frac{2\pi N s_2\sqrt{D}}{a}\,,\qquad s_2=4.31\,.$$

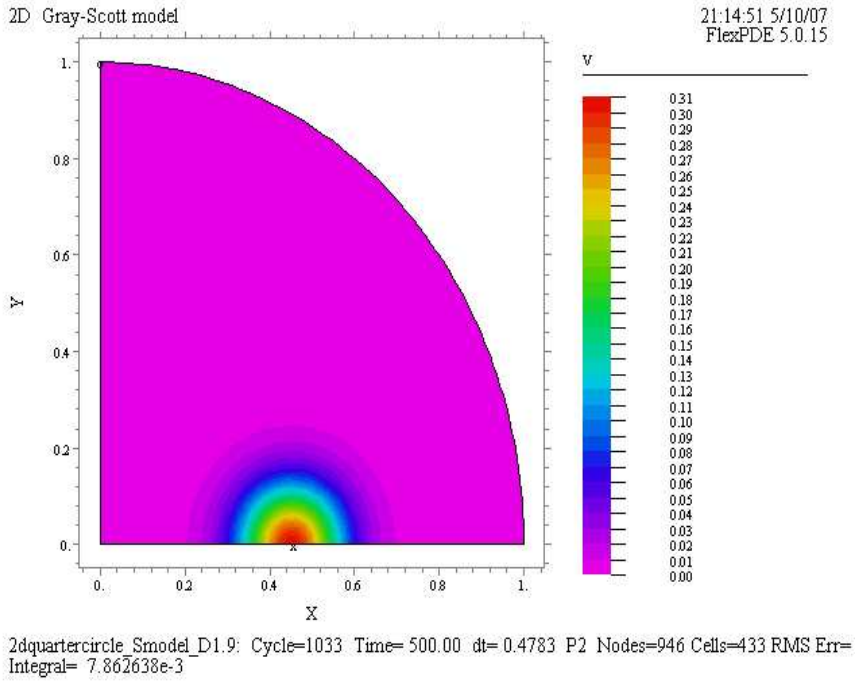
Spot Replication: Schnakenburg Model IV

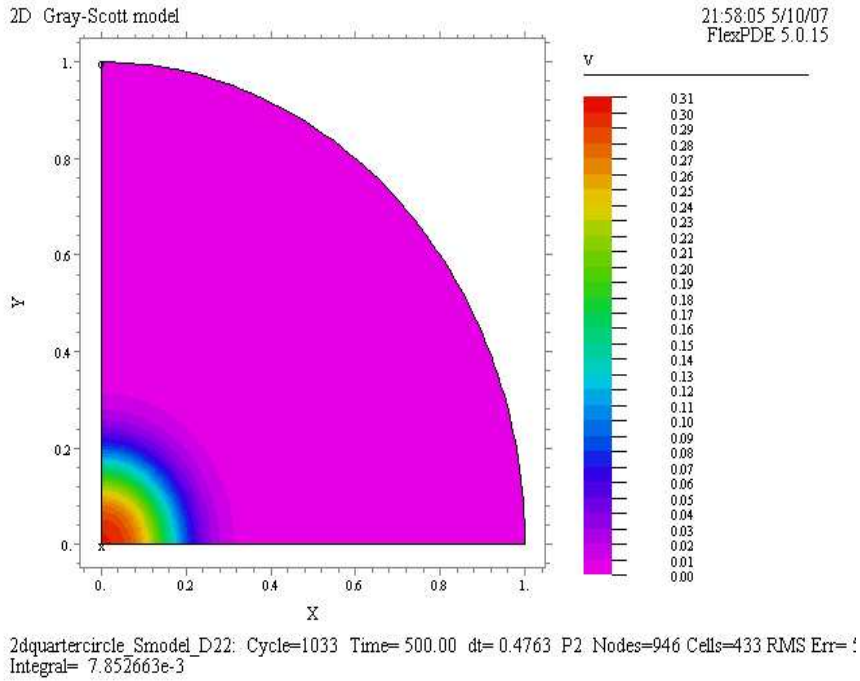
A Simple Example

Let Ω be the unit circle and $a = 4$. Then, starting with one initial spot, a spot-replication event will occur when D crosses below D_2 where

$$D_2 = \left(\frac{a|\Omega|}{2\pi s_2}\right)^2 = \left(\frac{a}{2s_2}\right)^2 = \frac{4}{(4.31)^2} = 0.215\,.$$

Full Numerics: Left: $D = 0.19$ (split). Right: $D_2 = 0.22$ (split).





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Dirichlet Green's Function: Regular Part

Consider the Dirichlet Green's function G_d, with regular part R_d:

$$\triangle G_d = -\delta(x - x_0) \quad x \in \Omega\,; \quad G_d = 0\,, \quad x \in \partial\Omega\,,$$

$$R_d(x, x_0) = G_d(x, x_0) + \frac{1}{2\pi} \log|x - x_0|\,, \qquad \nabla R_{d0} \equiv \nabla R_d(x, x_0)|_{x=x_0}\,.$$

- For a strictly convex domain Ω, $-R_{d0}$ is strictly convex, and thus there is a unique root to $\nabla R_{d0} = 0$. (B. Gustafsson, Duke J. (1990), Caffarelli and Friedman, Duke J. (1985)).
- ∇R_{d0} can be found for certain mappings $f(z)$ of the unit disk as

$$f'(z_0)\nabla R_{d0} = -\frac{1}{2\pi}\left(\frac{z_0}{1 - |z_0|^2} + \frac{f''(\overline{z}_0)}{2f'(\overline{z}_0)}\right)\,.$$

- Let B be the unit disk and $f(z) = \frac{(1-a^2)z}{z^2-a^2}$. Then $f(B)$ is a symmetric nonconvex dumbbell domain for $1 < a < 1 + \sqrt{2}$. Gustafson (1990) proved that $\nabla R_{d0} = 0$ has three roots when $1 < a < \sqrt{3}$.
- Can one derive a similar result for the Neumann Green's function?

An Explicit Formula for ∇R_{m0}

Theorem: (KW) Let $f(z)$ map the unit disk B onto Ω satisfying:

(i) f is analytic and is invertible on $\overline{B}$, with $\overline{f(z)} = f(\overline{z})$.

(ii) f has only simple poles at $z_1, .., z_k$, and f is bounded at ∞.

(iii) $f = g/h$, with $g(z_i) \neq 0$, where g and h are analytic everywhere.

On the image $\Omega = f(B)$, let R_m be the regular part of G_m. Then, at x_0, with $z_0 \in B$ satisfying $x_0 = f(z_0)$,

$$\nabla R_{m0} = \frac{\nabla s(z_0)}{f'(z_0)}, \quad \nabla s(z_0) = \frac{1}{2\pi}\left(\frac{z_0}{1-|z_0|^2} + \frac{f''(\overline{z}_0)}{2f'(\overline{z}_0)}\right)$$

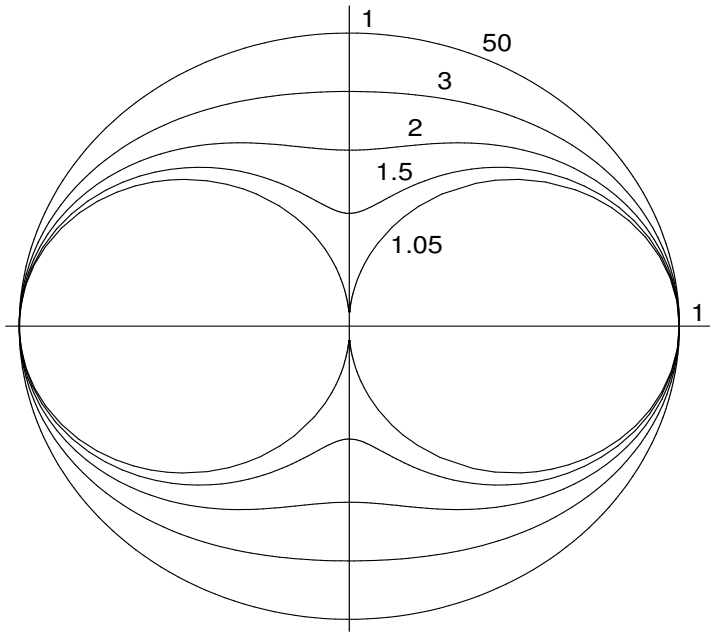
$$- \frac{f'(\overline{z}_0)\left(f(z_0) - f(\frac{1}{\overline{z}_0})\right) + \sum_j \frac{g(z_j)f'(\frac{1}{z_j})}{z_j^2 h'(z_j)}\chi}{2\pi \sum_j \frac{g(z_j)f'(\frac{1}{z_j})}{z_j^2 h'(z_j)}}, \quad \chi = \left(\frac{1}{z_j - \overline{z}_0} + \frac{z_j}{1 - z_j\overline{z}_0}\right)$$

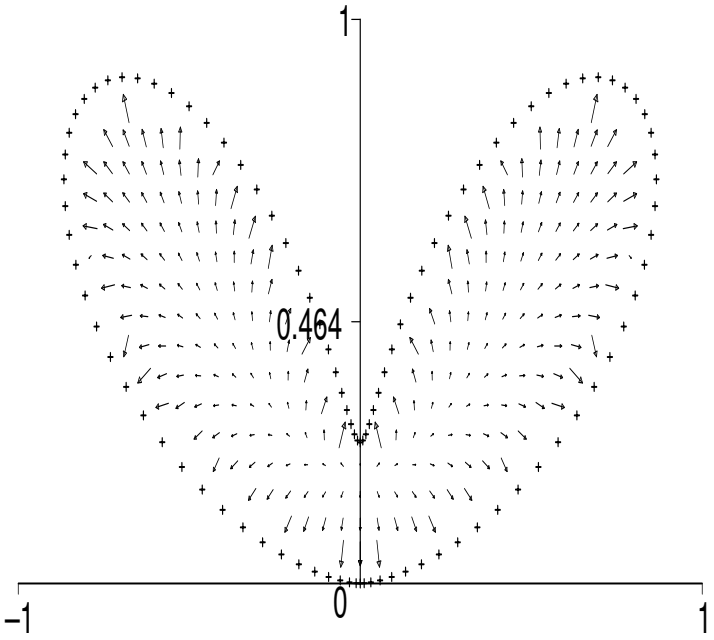
Reference: "Reduced Wave Green's Functions....", Kolokolnikov, MJW, EJAM (2003).

The Zeroes of ∇R_{m0}

Example 1: Let $f(z;a) = \frac{(1-a^2)z}{z^2-a^2}$. Then $f(B)$ is nonconvex for $1 < a < 1+\sqrt{3}$. For any $a > 1$, the complex variable formula can be used to show that $\nabla R_{m0} = 0$ has exactly one root at $z = 0$, which maximizes λ_0 for $\nu \ll 1$. This is qualitatively different than for the Dirichlet problem.

Example 2: A boundary integral computes ∇R_{m0} for other nonconvex symmetric domains. The numerical results give only one root to $\nabla R_{m0} = 0$. The boundary of the domain shown is $(x,y) = (\sin^2 2t + \frac{1}{4}\sin t)(\cos(t), \sin(t)), t \in [0,\pi]$. The vector field ∇R_{m0} has a unique equilibrium at approximately $(0, 0.2)$.





A Non-Uniqueness Result I

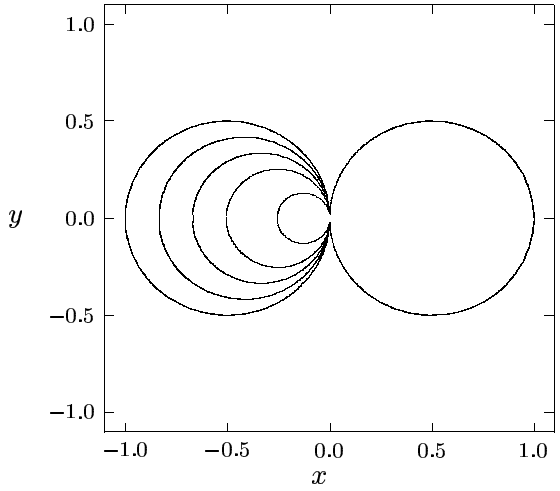
Is there a unique root of $\nabla R_{m0} = 0$ in any simply-connected nonconvex domain? Not necessarily. Let B be the unit ball and $\Omega = f(B)$ where

$$f(z) = -\frac{\kappa z}{(z-a)(z+b)}\,, \quad a = 1+\varepsilon\,, \quad b = 1+\varepsilon\gamma\,,$$

with $\kappa = (a-1)(b+1)$ and $f(1) = 1$. Then, for $\varepsilon \to 0$, the area of Ω is

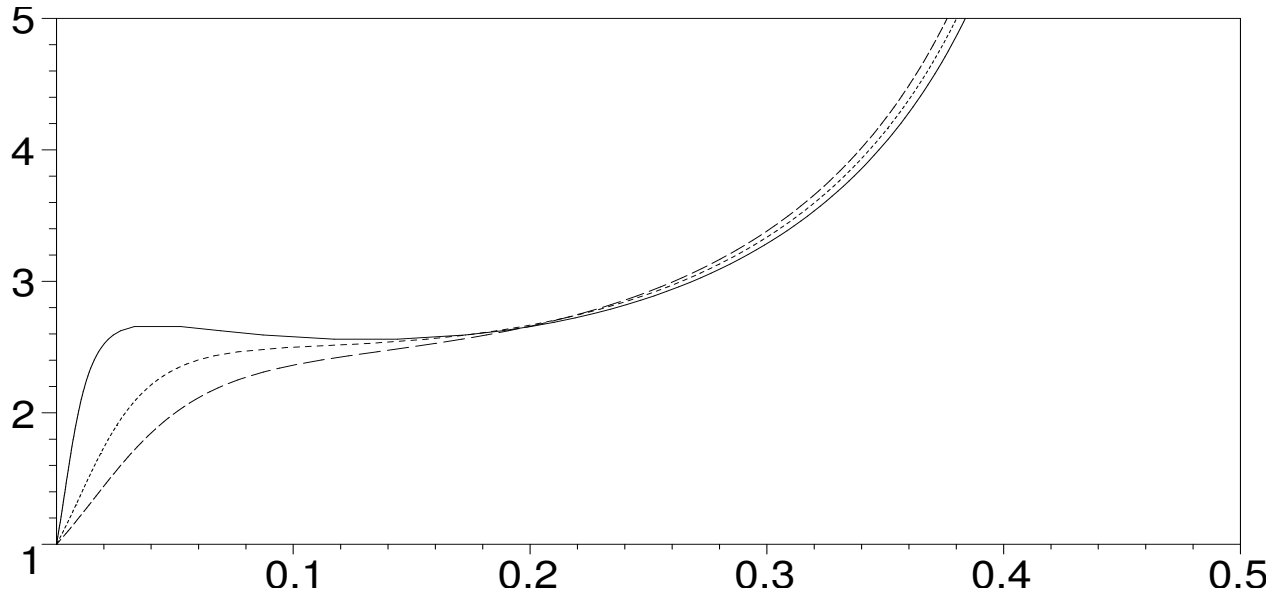
$$|\Omega| \sim \frac{\pi(1+\gamma^2)}{4\gamma^2}\,; \quad \gamma^2 = \text{ratio of area of big lobe to small lobe}$$

Let $\gamma > 1$. For $\varepsilon \to 0$, $\Omega = f(B)$ approaches the union of two circles; a larger circle centred at $(1/2, 0)$ of radius $1/2$, and a smaller circle centred at $(-1/(2\gamma), 0)$ of radius $1/(2\gamma)$. This is an asymmetric dumbbell.



A Non-Uniqueness Result II

- For $\varepsilon \to 0$, $\nabla R_m = 0$ has a unique root except on $1.5966 < \gamma < \sqrt{3}$.
- For a slightly asymmetric dumbbell, where $1 < \gamma < 1.5966$, the optimum place to maximize λ_0 is to put the trap in the channel region of the dumbbell, but shifted slightly towards the largest (right) lobe.
- For $\gamma \gg 1$, where the left lobe of the dumbbell is very small the optimum place to insert the trap is near the centre of the right lobe.
- A saddle-node bifurcation structure for $1.5966 < \gamma < \sqrt{3}$ where λ_0 has two local maxima and a local minimum.



γ^2 vs. x_0 for $\varepsilon = 0.01$ (solid) $\varepsilon = 0.03$ (dotted), and $\varepsilon = 0.05$ (dashed).