Towards a numerical proof of Polya's conjecture

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1. Description of the Problem

Consider the Dirichlet-Laplace eigenvalue problem:

$$\begin{cases} -\Delta u = \lambda u & \text{in } \Omega, \\ \quad u = 0 & \text{on } \partial\Omega. \end{cases} \qquad 0 < \lambda_1(\Omega) \le \lambda_2(\Omega) \le \dots \le \lambda_k(\Omega) \dots + \infty. \tag{1}$$

The classical Faber-Krahn inequality states that under a volume constraint the first eigenvalue is minimized when Ω is a ball.

Pólya and Szegö have conjectured a polygonal version of this inequality [1, page 158]. Precisely, let denote by $\mathcal{P}_n$ the family of n-gons in $\mathbb{R}^2$ and for every $n \ge 3$ consider the problem

$$\min_{P \in \mathcal{P}_n, |P| = \pi} \lambda_1(P). \tag{2}$$

Pólya-Szegö Conjecture (1951). *The unique solution to problem* (2) *is the regular polygon with n sides and area π.*

The conjecture holds true for $n = 3$ and $n = 4$. A proof can be found, for instance, in [3] as straightforward applications of the Steiner symmetrization principle. However, Steiner symmetrization techniques do not work for $n \ge 5$ since the number of vertices could possibly increase. In [2] a new approach is proposed which works in the case of triangles, establishing that equilateral triangles are the only critical points for the first eigenvalue.

It is quite easy to prove the existence of an optimal n-gon (with angles different from π, see for instance [3, Chapter 3]). However, it is not even known that this polygon has to be convex! Meanwhile, many numerical experiments have been performed for small values of n, suggesting the validity of the conjecture.

Objectives

- Prove that local minimality of the regular polygon can be reduced to a single certified numerical computation.
- For each $n \ge 5$, the complete proof of the conjecture can formally be reduced to a finite number of numerical computations.

2. First and Second order shape derivatives

The shape derivatives of a simple eigenvalue of (1) are well known when Ω is smooth. It is well established that a simple eigenvalue is shape differentiable even when Ω is not smooth, but the boundary integral formula $\lambda'(\Omega)(V) = -\int_{\partial\Omega} (\partial_n u)^2 V \cdot n$ is only valid if the corresponding eigenfunction u belongs to $H^2(\Omega)$. This is true when Ω is convex, but it is not clear how to find a similar formula when Ω is not smooth.

In order to circumvent such problems, inspired by [4], we compute the distributed volumic formulas for the shape derivatives. Writing the shape derivatives as volume integrals only requires Lipschitz regularity and therefore these formulas are valid in the case of polygons.

First, let us recall the notion of material derivative. For $\theta \in W^{1,\infty}$ denote $\dot{u}(\theta)$ the Frechet derivative of the solution of the eigenvalue problem on $(\mathbf{Id} + \theta)(\Omega)$ transported back to Ω. It is classical that $\dot{u}(\theta) \in H^1_0(\Omega)$ verifies:

$$\int_\Omega \nabla \dot{u}(\theta) \cdot \nabla v - \lambda(\Omega) \int_\omega \dot{u}(\theta) v = -\int_\Omega (\operatorname{div}\theta\, \mathbf{Id} - D\theta - D\theta^T) \nabla u \cdot \nabla v + \lambda'(\Omega)(\theta) \int_\Omega uv + \lambda(\Omega) \int_\Omega uv \operatorname{div}\theta.$$

with the normalization condition $\int_\Omega 2u\dot{u}(\theta) + u^2 \operatorname{div}\theta\, dx = 0$.

Recall the following tensor calculus aspects:

- $a \otimes b$ is the second order tensor of two vectors $(a \otimes b)_{ij} = a_i b_j$
- $a \odot b = \frac{1}{2}(a \otimes b + b \otimes a)$ is the symmetric outer product.
- $a \cdot b$ is the usual scalar product
- $\mathbf{S} : \mathbf{T} = \sum_{i,j=1}^n S_{ij} T_{ij}$ is the matrix dot product.
- $(a \otimes b)c = (c \cdot b)a$ and $\mathbf{S} : (a \otimes b) = a \cdot \mathbf{S} b$.

Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain and $\theta, \xi \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$. Let λ be a simple eigenvalue of the Dirichlet Laplacian and u an associated L^2-normalized eigenfunction.

Theorem: First shape derivative

The distributed shape derivative of λ is given by

$$\lambda'(\Omega)(\theta) = \int_\Omega \mathbf{S}_1^\lambda : D\theta\, dx$$

with $\mathbf{S}_1^\lambda = (|\nabla u|^2 - \lambda(\Omega) u^2)\, \mathbf{Id} - 2\nabla u \otimes \nabla u$. If, in addition, $u \in H^2(\Omega)$, the corresponding boundary expression is

$$\lambda'(\Omega)(\theta) = -\int_{\partial\Omega} |\nabla u|^2 \theta \cdot \mathbf{n}\, d\sigma.$$

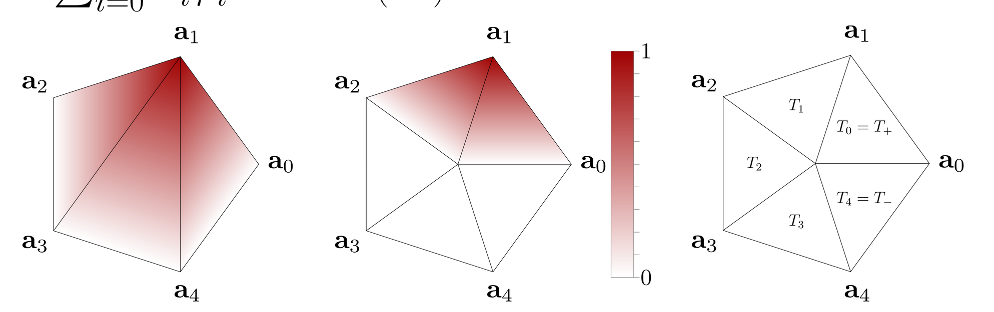
Theorem: Second shape derivative

The second order distributed Fréchet derivative is given by $\lambda''(\Omega)(\theta, \xi) = \int_\Omega \mathcal{K}^\lambda(\theta, \xi)$ with

$$\begin{aligned} \mathcal{K}^\lambda(\theta, \xi) = & -2\nabla \dot{u}(\theta) \cdot \nabla \dot{u}(\xi) + 2\lambda(\Omega) \dot{u}(\theta) \dot{u}(\xi) \\ & + \mathbf{S}_1^\lambda : (D\theta \operatorname{div}\xi + D\xi \operatorname{div}\theta) \\ & + \left(-|\nabla u|^2 + \lambda u^2\right) (\operatorname{div}\xi \operatorname{div}\theta + D\theta^T : D\xi) \\ & + 2(D\theta D\xi + D\xi D\theta + D\xi D\theta^T) \nabla u \cdot \nabla u \\ & - \left[\lambda'(\Omega)(\theta) \operatorname{div}\xi + \lambda'(\Omega)(\xi) \operatorname{div}\theta\right] u^2. \end{aligned}$$

where $\dot{u}(\theta)$ and $\dot{u}(\xi)$ are the material derivatives in directions θ, ξ, respectively.

The previous result is valid for all Lipschitz domains Ω and Lipschitz vector fields ξ, η. Denote the vertices of the polygon by $\mathbf{a}_i \in \mathbb{R}^2$, $i = 0, ..., n-1$. For each vertex consider the vector perturbation $\theta_i \in \mathbb{R}^2$, $i = 0, ..., n-1$. Consider a triangulation $\mathcal{T}$ of Ω such that the edges of the polygon are complete edges of some triangles in this triangulation (like in [4]). Define the globally Lipschitz functions φ_i for $0 \le i \le n-1$ that are piecewise affine on each triangle of $\mathcal{T}$. Several choices are possible as in the figure below. Then, we build a global perturbation of $\mathbb{R}^2$ given by $\theta = \sum_{i=0}^{n-1} \theta_i \varphi_i \in W^{1,\infty}(\mathbb{R}^2)$.



With this in mind we quickly find formulas for the gradient of λ with respect to the vertices.

Theorem: Gradient

The gradient of a simple Dirichlet-Laplace eigenvalue when Ω is a polygon with coordinates $\mathbf{x}$ is given by

$$\nabla \lambda(\mathbf{x}) = \left(\int_\Omega \mathbf{S}_1^\lambda \nabla \varphi_i \right)_{i=0,\dots,n-1}.$$

If $u \in H^2(\Omega)$ then $\nabla \lambda(\mathbf{x}) = \left(-\int_{\partial\Omega} |\nabla u|^2 \varphi_i \mathbf{n} \right)_{i=0,\dots,n-1}$, where $\mathbf{n}$ is the outer unit normal vector.

Before writing the Hessian matrix we decompose the material derivative equation. Following the notation in [4], we introduce the functions $U_i \in H^1_0(\Omega, \mathbb{R}^2)$, $i = 0, ..., n-1$ such that $\dot{u}(\theta) = \sum_{i=0}^{n-1} \theta_i \cdot U_i$. We obtain that $\forall v \in H^1_0(\Omega)$

$$\int_\Omega (DU_i \nabla v - \lambda(\Omega) U_i v)\, dx = \int_\Omega -(\nabla \varphi_i \otimes \nabla u) \nabla v + 2(\nabla u \odot \nabla v) \nabla \varphi_i\, dx + \int_\Omega \mathbf{S}_1^\lambda \nabla \varphi_i \int_\Omega uv\, dx + \lambda(\Omega) \int_\Omega uv \nabla \varphi_i\, dx. \tag{3}$$

with normalization $\int_\Omega 2uU_i + u^2 \nabla \varphi_i\, dx = 0$.

Plugging these into the second distributed shape derivative formula gives the expression of the Hessian matrix for a simple eigenvalue λ. We do not write the formula here, since it is huge. However, when Ω is a regular polygon and the triangulation is symmetric we obtain a much simplified formula.

Theorem: Hessian for regular polygon

In the case where Ω is a regular n-gon and the triangulation $\mathcal{T}$ defining φ_i is symmetric the Hessian matrix of $\lambda(\Omega)|\Omega| = \mathcal{A}(\mathbf{x})\lambda(\mathbf{x})$ in terms of the coordinates of the polygon has the 2×2 blocks $\mathbf{M}_{ij}^\lambda$, $0 \le i, j \le n-1$ given by

$$\begin{aligned} \mathbf{M}_{ij}^\lambda = |\Omega| \int_\Omega & (-2DU_i DU_j^T + 2\lambda(\Omega) U_i U_j^T) \\ & - \lambda(\Omega) \int_\Omega [\nabla \varphi_i \otimes \nabla \varphi_j - \nabla \varphi_j \otimes \nabla \varphi_i] \\ & + 2|\Omega| \int_\Omega (\nabla \varphi_i \cdot \nabla \varphi_j)(\nabla u \otimes \nabla u). \end{aligned}$$

One may note that the normalization condition for U_i does not influence the final formula so we might just pick the simpler orthogonality condition $\int_\Omega U_i u = 0$.

In the following * denotes quantities associated to the regular polygon. We prove that the Hessian matrix varies continuously in a quantitative way with respect to perturbations of the vertices.

Theorem: Geometric stability of the Hessian

There exist $C, q > 0$ such that for every polygon $P \in \mathcal{P}_n$ satisfying $|\mathbf{a}_i \mathbf{a}_i^*| \le \varepsilon \le \varepsilon_0$, $i = 1, \dots, n$ we have

$$\|\mathbf{M}_{ij}^\lambda - (\mathbf{M}_{ij}^\lambda)^*\|_\infty \le C\varepsilon^q.$$

Therefore, proving that the Hessian matrix for the regular polygon has non-negative eigenvalues is enough to conclude that regular polygons are local minima.

3. Computing the eigenvalues of the Hessian

The Hessian matrix is explicit in terms of u and U_i, but in this form it does not give information about its eigenvalues. It is possible to change the basis so that the Hessian becomes **block circulant**: $\mathbf{H}_\lambda = \mathbf{P}^T \mathbf{M}_\lambda \mathbf{P}$ where $\mathbf{P} = (\mathbf{P}_{ij})_{1 \le i,j \le n}$ is a 2×2 block matrix with $\mathbf{P}_{jj} = \begin{pmatrix} \cos(j-1)\theta & -\sin(j-1)\theta \\ \sin(j-1)\theta & \cos(j-1)\theta \end{pmatrix}$. In this case it is classical that the eigenvalues and eigenvectors of $\mathbf{H}_\lambda$ can be obtained by looking at some particular 2×2 matrices.

Denote with $\mathbf{M}_0, \mathbf{M}_1, ..., \mathbf{M}_{n-1}$ the blocks of the first line in $\mathbf{M}_\lambda$ and $\theta = 2\pi/n$. Then for $\rho_k = \exp(ik\theta)$ a root of unity of order n we have

$$\mathbf{B}_{\rho_k} = \mathbf{M}_0 + \mathbf{M}_1(\rho_k \mathbf{R}_\theta) + \dots + \mathbf{M}_{n-1}(\rho_k \mathbf{R}_\theta)^{n-1},$$

where $\mathbf{R}_\tau = \begin{pmatrix} \cos\tau & -\sin\tau \\ \sin\tau & \cos\tau \end{pmatrix}$. The spectrum of $\mathbf{H}_\lambda$ is the union of the spectra of the matrices $\mathbf{B}_{\rho_k}, k = 0, ..., n-1$. Denote $a(u, v) = \int_\Omega (\nabla u \cdot \nabla v - \lambda(\Omega) uv)$ and $\mathbb{P}_n$ the regular polygon with radius 1. Then we obtain the following:

Theorem: Eigenvalues of the Hessian

For $0 \le k \le n-1$ we have $\mathbf{B}_{\rho_k} = \begin{pmatrix} \alpha_k & i\gamma_k \\ -i\gamma_k & \beta_k \end{pmatrix}$ with

$$\alpha_k = \frac{2n(1-\cos(k\theta))}{\sin\theta} \int_{T_0} (\partial_x u)^2 - 2|\mathbb{P}_n| a(U_0^1, \sum_{j=0}^{n-1} \cos(jk\theta)(\cos(j\theta) U_j^1 + \sin(j\theta) U_j^2))$$

$$\beta_k = \frac{2n(1-\cos(k\theta))}{\sin\theta} \int_{T_0} (\partial_y u)^2 - 2|\mathbb{P}_n| a(U_0^2, \sum_{j=0}^{n-1} \cos(jk\theta)(-\sin(j\theta) U_j^1 + \cos(j\theta) U_j^2))$$

$$\begin{aligned} \gamma_k &= -2|\mathbb{P}_n| a(U_0^1, \sum_{j=0}^{n-1} \sin(jk\theta)(-\sin(j\theta) U_j^1 + \cos(j\theta) U_j^2)) \\ &= 2|\mathbb{P}_n| a(U_0^2, \sum_{j=0}^{n-1} \sin(jk\theta)(\cos(j\theta) U_j^1 + \sin(j\theta) U_j^2)) \end{aligned}$$

and the eigenvalues of $\mathbf{B}_{\rho_k}$ are given by

$$\mu_{2k} = 0.5(\alpha_k + \beta_k - \sqrt{(\alpha_k - \beta_k)^2 + 4\gamma_k^2}), \mu_{2k+1} = 0.5(\alpha_k + \beta_k + \sqrt{(\alpha_k - \beta_k)^2 + 4\gamma_k^2}).$$

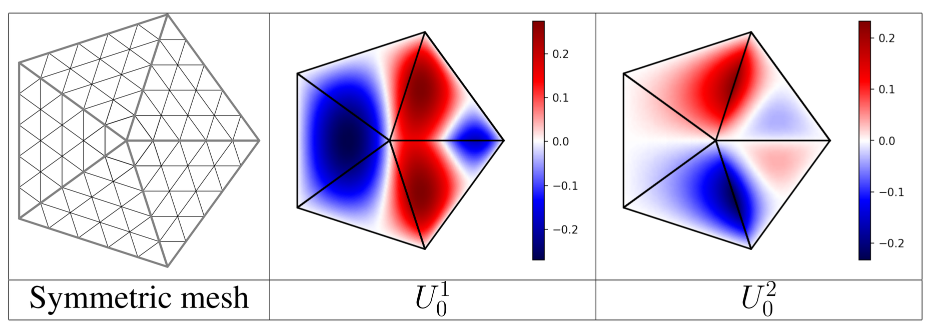
Some remarks:

- on a symmetric mesh with the symmetric choice of φ_j, the eigenvalues for the Hessian matrix of $\lambda(\mathbf{x})\mathcal{A}(\mathbf{x})$ can be explicitly expressed in terms of u_1, U_0^1, U_0^2.
- when $k = 0$ we have $\mathbf{B}_{\rho_k} = 0$
- when $k = 1$ we have $\alpha_1 = \beta_1 = \gamma_1$ (something similar holds for $k = n-1$)
- we explicitly show that vectors corresponding to translations, rotations and scalings are eigenvectors of the Hessian matrix $\mathbf{M}^\lambda$ for the zero eigenvalue.
- it is enough to prove that all other $2n-4$ eigenvalues are strictly positive in order to conclude local minimality.

4. Numerical Results

Although formulas are explicit, we were not able to prove theoretically the positivity of the eigenvalues of $\mathbf{M}^\lambda$. It is nonetheless possible to compute these eigenvalues numerically and to asses their positivity. We use FreeFEM with $\mathbf{P}_1$ finite elements.

- Explicit error bounds exist for approximations of λ_1 and u_1 in therms of the mesh size h.
- We provide explicit *a priori* error bounds for solutions of (3). This is extremely delicate since the right hand side is not in L^2, which means that U_i is not in $H^2(\Omega)$.
- We obtain **explicit error bounds** for the eigenvalues of $\mathbf{M}^\lambda$ of order $O(h^{1-2\gamma})$ for every $\gamma \in (0, 1/2)$.
- Numerical computations (with up to 4×10^8 d.o.f) allow us to conclude **local minimality** of the regular polygon for $n \in \{5, 6, 7, 8\}$. Simulations with up to 200 processors are made on the Cholesky server at IP Paris.
- We do not take into account **roundoff errors** that come from working in floating point precision. However, it is generally agreed that these errors are **smaller than the discretization errors**.



Symmetric mesh | U_0^1 | U_0^2

5. Towards a complete proof of the conjecture

Theorem: bound on diameter

Let $n \ge 3$. There exists a value $D_n > 0$ such that if $P \in \mathcal{P}_n$, $|P| = \pi$ and $\operatorname{diam}(P) > D_n$ then P is not optimal for (2).

- The local minimality and the stability of the Hessian imply that no other local minimum exists close enough to the regular polygon.
- The region between the regular polygon and the "large diameter" polygons can be explored using a finite number of validated numerical simulations.

In this way, the proof of the conjecture is reduced to a finite number of validated numerical computations.

References

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