Shape Optimization: Theory and Numerics

Maths en herbe – IHES

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Canonical Example: The isoperimetric problem

⋆ Find the shortest curve enclosing a given area.

$$\min_{|\Omega|=c} \operatorname{Per}(\Omega).$$

⋆ Equivalently: Find the greatest area that can be enclosed by a curve of given length.

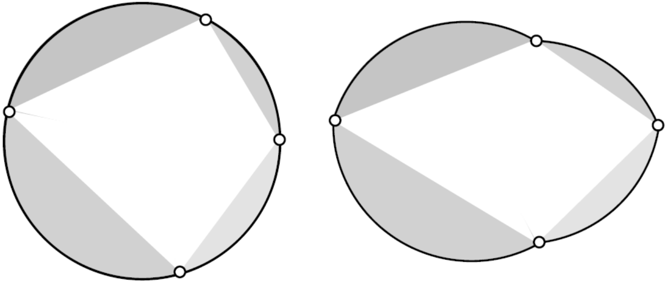
$$\max_{\operatorname{Per}(\Omega)=c} |\Omega|.$$

Questions:

- A solution exists? Is it regular?
- Find it!

⋆ Steiner's proof (1838): (he in fact tried to give at least five proofs for this problem)

- Pick four points on the boundary
- If the quadrilateral is not cyclic then its area can be increased without modifying the perimeter



- Therefore, any shape which is not a disk can be improved!
- **Conclusion:** the disk solves the isoperimetric problem.

⋆ There's a gap in the argument above!

⋆ Other proofs: Fourier series, symmetrization, optimality conditions, etc.

Existence of a solution is important!

Theorem. *Among all curves of a given length, the circle encloses the greatest area.*

Proof. For any curve that is not a circle, there is a method (given by Steiner) by which one finds a curve that encloses greater area. Therefore the circle has the greatest area. ■

Theorem. *Among all positive integers, the integer 1 is the largest.*

Proof. For any integer that is not 1, there is a method (to take the square) by which one finds a larger positive integer. Therefore 1 is the largest integer. ■

Direct method in the calculus of variations: non-trivial here

- Find a minimizing/maximizing sequence $f(x_n) \to \inf f$ (what topology?)
- **Compactness:** Find a converging subsequence: $x_n \to x^*$
- **Continuity:** Prove that f is (semi) continuous: $\lim f(x_n) = f(x^*)$.

What is the best shape of an ice cube?

⋆ Ideally we would like to maximize the contact region between the ice cube and the liquid

$$\max_{|\Omega|=c} \operatorname{Per}(\Omega).$$

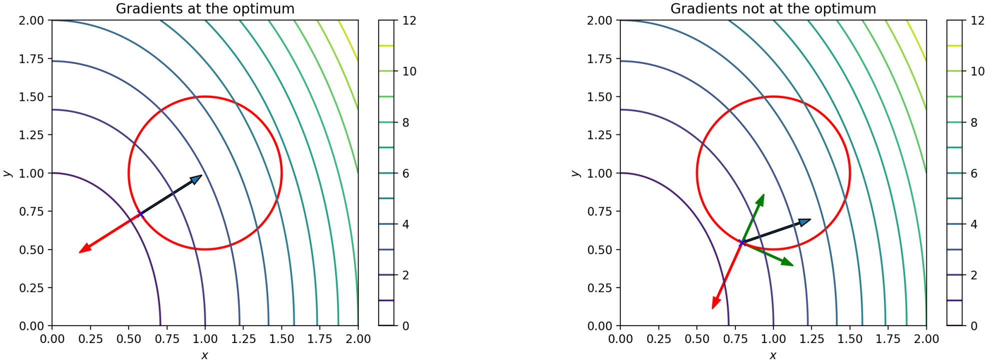
Question: Do we have existence of an optimal shape in this case?

Recalling basic Optimality conditions

$f, g : X \to \mathbb{R}$

$\star$ $\min f(x)$ (unconstrained): x^* solution $\Longrightarrow \nabla f(x^*) = 0.$

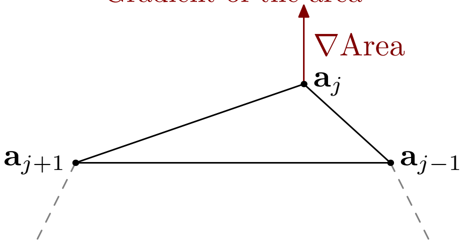
$\star$ $\min\limits_{g(x)=0} f(x)$ (constrained): x^* solution $\Longrightarrow \nabla f(x^*) = \lambda \nabla g(x^*).$



$$\min_{|P|=c} \operatorname{Per}(P)$$

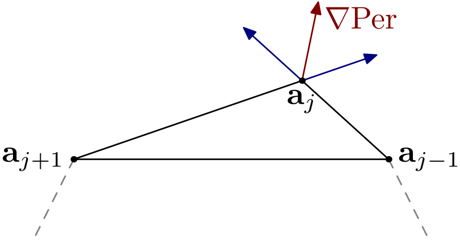
Existence of solutions: "immediate" (classical compactness arguments)
Optimality conditions: $\nabla \operatorname{Per}(P) = \lambda \nabla \operatorname{Area}(P)$

Gradient of the area



$\star$ collinear with height in $\Delta \mathbf{a}_{j-1}\mathbf{a}_j\mathbf{a}_{j+1}$

Gradient of the perimeter



$\star$ collinear with bisector in $\Delta \mathbf{a}_{j-1}\mathbf{a}_j\mathbf{a}_{j+1}$

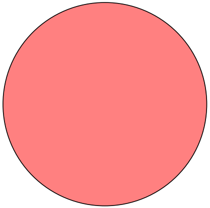
In the end: optimality conditions imply that P is the regular n-gon.

Solution to the isoperimetric problem

$$\min_{|\Omega|=c} \operatorname{Per}(\Omega).$$

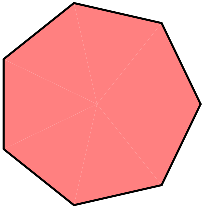
Ω: General Shape

$\star$ the solution is the disk



Ω: n-gon

$\star$ the solution is the regular n-gon



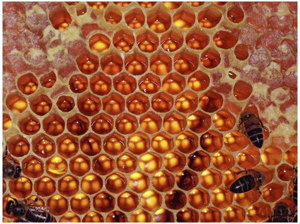
Heuristic argument

If the optimal shape **among general shapes** is the disk then, when restricting to n-gons **the regular one should be optimal**.

$$\min_{\Omega \in \mathcal{A}} J(\Omega)$$

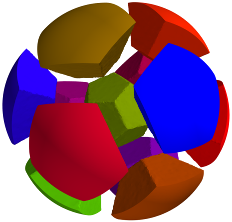
Theoretical aspects

⋆ existence, regularity
⋆ shape derivative
⋆ **find optimal shapes**
⋆ qualitative properties



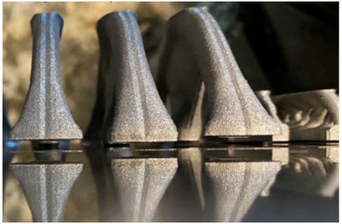
Numerical aspects

⋆ choice of discretization
⋆ efficient computations
⋆ new theoretical ideas
⋆ **solve theoretical gaps**



Practical aspects

⋆ industrial problems
⋆ modelization
⋆ simulation
⋆ **MMOF team–CMAP**



Eigenvalues

$A \in \mathbb{R}^{d\times d}$, symmetric, positive definite: $x^T Ax > 0$ for $x \neq 0$.

Spectral theorem

There exists an orthonormal basis of $\mathbb{R}^d$ made of eigenvectors of $(v_i)_{i=1}^d$ of A corresponding to eigenvalues

$$0 < \lambda_1 \leq \lambda_2 \leq ... \leq \lambda_d.$$

- ⋆ eigenvectors characterize invariant subspaces of A
- ⋆ why are they interesting?

Applications

Knowing the spectrum is good for:

- Solving linear systems $Ax = b$:

$$b = \sum_{i=1}^{d} \beta_i v_i \Longrightarrow x = \sum_{i=1}^{d} \frac{\beta_i}{\lambda_i} v_i$$

- Solving systems of Ordinary Differential Equations $\frac{\partial U}{\partial t} + AU = 0, U(0) = u_0$

$$u_0 = \sum_{i=1}^{d} \beta_i v_i \Longrightarrow U(t) = \sum_{i=1}^{d} \beta_i \exp(-\lambda_i t) v_i.$$

Decay rate in the worst case: $\exp(-\lambda_1 t) v_1$
To have a small decay rate we need a small λ_1.

Laplace operator

⋆ Dimension 1: $\Delta u := u''$

⋆ Dimension 2: $\Delta u := \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2}$

⋆ Dimension 3: $\Delta u := \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} + \dfrac{\partial^2 u}{\partial z^2}$

Heat equation: $q : [0,T] \times \Omega \to \mathbb{R}$, $\dfrac{\partial q}{\partial t} - \Delta q = 0$, $q(0,x) = q_0(x)$, $q(t,x) = 0$ for $x \in \partial\Omega$.

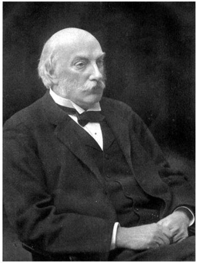
⋆ The Laplacian with Dirichlet boundary conditions has a sequence of eigenvalues $0 < \lambda_1(\Omega) \leq \lambda_2(\Omega) \leq ... \to \infty$ solving the following problems:

$$\begin{cases} -\Delta u_k & = & \lambda_k(\Omega) u_k & \text{in } \Omega \\ u_k & = & 0 & \text{on } \partial\Omega. \end{cases}$$

⋆ if $q_0 = \sum_{k\geq 1} \beta_k u_k$ then $q(t,x) = \displaystyle\sum_{k \geq 0} \beta_k e^{-\lambda_k(\Omega) t} u_k(x)$.

⋆ The heat is best preserved when for *large* t when $\lambda_1(\Omega)$ is minimal

[Lord Rayleigh, *Theory of sound*, Second Edition, p.339, first published in 1877]



210. We have seen that the gravest tone of a membrane, whose boundary is approximately circular, is nearly the same as that of a mechanically similar membrane in the form of a circle of the same mean radius or area. If the area of a membrane be given, there must evidently be some form of boundary for which the pitch (of the principal tone) is the gravest possible, and this

$$-\Delta u = \lambda u, \ u \in H_0^1(\Omega)$$

$$0 < \lambda_1(\Omega) \le \lambda_2(\Omega) ...$$

Rayleigh quotients: $\lambda_k(\Omega) = \min_{S_k \subset H_0^1(\Omega)} \max_{\phi \in S_k \setminus \{0\}} \frac{\int_\Omega |\nabla \phi|^2 dx}{\int_\Omega \phi^2 dx}$

Scaling: $\lambda_k(t\Omega) = \lambda_k(\Omega)/t^2$.

Monotonicity: $\Omega_1 \subset \Omega_2 \Rightarrow \lambda_k(\Omega_1) \ge \lambda_k(\Omega_2)$

Multiplicity: if Ω is connected then $\lambda_1(\Omega) < \lambda_2(\Omega)$

Optimizing Eigenvalues - Drums

Lord Rayleigh - *The Theory of Sound* (1877)

The Drum

The shape that minimizes the area of a membrane at given frequency is the disk.

Faber-Krahn (1920-1923)

The disk minimizes $\lambda_1(\Omega)$ at fixed area

$$\begin{cases} -\Delta u = \lambda_1(\Omega) u & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

Symmetryzation

Steiner symmetrization: consider a direction L

- rearrange all slices of Ω with hyperplanes orthogonal to L into segments centered on L
- for $u : \Omega \to \mathbb{R}$ the Steiner symmetrization consists in performing a Steiner symmetrization for all its level sets

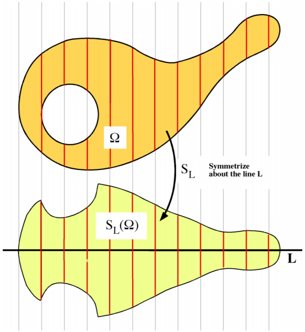


photo: [Treibergs, *Steiner Symmetrization and Applications*]

Motivation for performing symmetrizations

Some properties:

$$|\Omega| = |\Omega^*|, \int_\Omega u^2 = \int_{\Omega^*} (u^*)^2 \text{ and } \int_\Omega |\nabla u|^2 \geq \int_{\Omega^*} |\nabla u^*|^2$$

Important consequence. Symmetrization decreases the first eigenvalue at fixed volume

$$\lambda_1(\Omega) = \inf_{u \in H_0^1(\Omega), u \neq 0} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^2} = \frac{\int_\Omega |\nabla u_1|^2}{\int_\Omega u_1^2} \geq \frac{\int_{\Omega^*} |\nabla u_1^*|^2}{\int_{\Omega^*} (u_1^*)^2} \geq \lambda_1(\Omega^*)$$

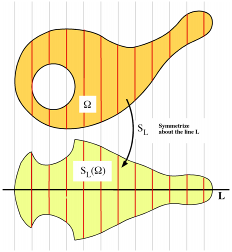
Minimizing the first Dirichlet-Laplace eigenvalue

$$\begin{cases} -\Delta u = \lambda_1(\Omega) u & \text{in } \Omega \\ u = 0 & \text{on } \partial\Omega \end{cases}$$

Faber-Krahn (1920-1923)

The disk minimizes $\lambda_1(\Omega)$ at fixed area.

⋆ Symmetrization decreases λ_1



Polyà-Szegö Conjecture (1920-1923)

The regular n-gon minimizes $\lambda_1(\Omega)$ among n-gons of fixed area.

⋆ An optimal n-gon exists [Henrot, *Extremum problems for eigenvalues*].
⋆ Cases $n \in \{3, 4\}$ solved by Polyà and Szegö.
⋆ Proofs based on Steiner symmetrization.

What is known?

Up to re-scalings the following problems are equivalent:

$$\min_{|\Omega|=\pi,\ \Omega\in\mathcal{P}_n} \lambda_1(\Omega), \qquad \min_{\Omega\in\mathcal{P}_n} |\Omega|\lambda_1(\Omega), \qquad \min_{\Omega\in\mathcal{P}_n} \Big(\lambda_1(\Omega)+|\Omega|\Big)$$

⋆ $n = 3$: the **equilateral triangle** is the minimizer
Proof: A sequence of Steiner symmetrizations w.r.t the mediatrix of the sides converges to the equilateral triangle.

⋆ $n = 4$: the **square** is the minimizer
Proof: A sequence of three Steiner symmetrizations transforms any quadrilateral into a rectangle.

⋆ $n \geq 5$: (almost) nothing is known

- Steiner symmetrization does not work: the number of sides may increase!

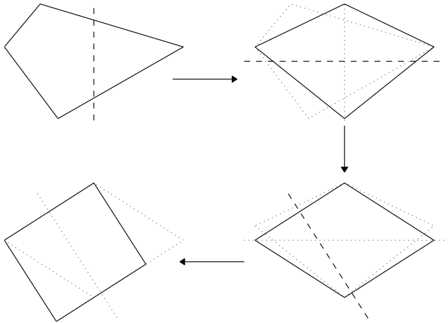


photo: [Henrot, *Extremum problems...*]

Various works on the subject

Numerical evidence:

- [Antunes, Freitas, 06]: derivative free - compute λ_1 on many polygons
- [Bogosel, PhD thesis, 15]: gradient algorithm, confirmation for $n \leq 15$.
- [Dominguez, Nigam, Shahriari, 17]: stochastic optimization, confirmation for $n = 5$

Theory:

- [Fragala, Velichkov, 19]: optimality conditions - different proof for $n = 3$
- [Laurain, 19]: second shape derivative on polygons, Hessian matrix

$$\min_{\Omega \in \mathcal{A}} J(\Omega)$$

Engineering: improve a given shape
Theory: give hints for new theoretical ideas
Prove something:
Easy: show that a shape is not optimal! Find a counterexample.
Hard: show that a **given shape is optimal**!

Derivatives

⋆ a symmetric matrix A is positive definite if all its eigenvalues are positive

Optimality conditions again

If $\nabla f(x^*) = 0$ and $D^2 f(x^*) = \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)$ is positive definite then x^* is a local minimum

⋆ We have a function depending on $2n$ variables (vertex coordinates).

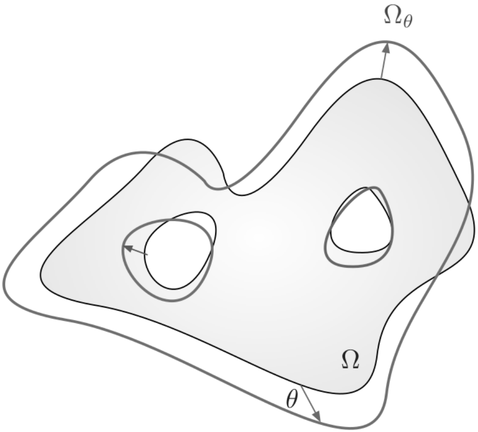
⋆ compute the first and second derivatives of

$$\lambda_1(x_0, y_0, x_1, y_1, ..., x_{n-1}, y_{n-1}).$$

⋆ not straightforward:

$$\text{Coords.} \longrightarrow \text{Shape} \longrightarrow \text{PDE} \longrightarrow \lambda_1$$

Sensitivity analysis: shape derivatives



- ⋆ **objective:** $J : P \mapsto |P|\lambda(P)$ (scale invariant)
- ⋆ λ **simple** $\implies J$ is smooth! [Henrot, Pierre]

- ⋆ $J((I+\theta)(\Omega)) = J(\Omega) + J'(\Omega)(\theta) + o(\|\theta\|)$
- ⋆ **Standard form:** under regularity assumptions we can write $J'(\Omega)(\theta) = \int_{\partial\Omega} \mathbf{f}\ \theta\cdot\mathbf{n}$

Shape derivatives: simple eigenvalues

⋆ a simple eigenvalue λ is differentiable. If u is an associated normalized eigenfunction:

$$\lambda'(\Omega)(\theta) = -\int_{\partial\Omega} \left(\frac{\partial u}{\partial \mathbf{n}}\right)^2 \theta \cdot \mathbf{n} = -\int_{\partial\Omega} |\nabla u|^2 \theta \cdot \mathbf{n}$$

⋆ the formula holds when $u \in H^2(\Omega)$, for example when Ω is **convex** [Grisvard]

⋆ second shape derivative: formulas are known but require additional regularity assumptions on Ω, which are not verified by polygons

Key Idea!

⋆ [Laurain, 19]: do not use the standard form: less regularity is needed

$$\lambda'(\Omega)(\theta) = \int_\Omega \mathbf{S}_1^\lambda : D\theta \text{ with } \mathbf{S}_1^\lambda = [|\nabla u|^2 - \lambda(\Omega)u^2]\,\mathbf{Id} - 2\nabla u \otimes \nabla u$$

⋆ also see [Henrot Pierre, *Shape variation and optimization*, Section 5.9.7]

Second Fréchet shape derivative

⋆ computing the Fréchet derivative w.r.t. ξ we obtain (after some long computations...)

$$\lambda''(\Omega)(\theta,\xi) = \int_\Omega \mathcal{K}^\lambda(\theta,\xi)$$

with

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

where $\dot{u}(\theta)$ and $\dot{u}(\xi)$ are derivatives of u in directions θ and ξ.

⋆ We obtained a new formula valid for Lipschitz domains

⋆ replace θ,ξ with **polygonal perturbations** to obtain the gradient and Hessian.

Theoretical dead end

- Regular n-gon: explicit Hessian depending on the solution of $n+1$ PDEs
- 4 eigenvalues are zero: corresponding to rigid motions and scalings
- Explicit eigenvalues depending on 3 PDEs
- Formulas are so complex that we did not manage to prove theoretically that the eigenvalues are positive!

$\star$ **Goal:** if the remaining $2n-4$ Hessian eigenvalues are strictly positive then local minimality is proved.

$\star$ When theory doesn't help, turn to numerics!

General proof strategy

Given $f : \mathbb{R}^d \to \mathbb{R}$:

Conjecture

x^* is a minimizer of f on $\mathbb{R}^d$

Strategy:

1. Prove that x^* is a local minimizer
2. Find an explicit neighborhood of x^* where local minimality occurs
3. Prove that points far away from x^* are not minimizers
4. Prove that if $f(x) > f(x^*) + \varepsilon$ then $f(x) > f(x^*)$ in a neighborhood of x
5. Use a finite number of numerical computations to conclude.

To **obtain a proof** all numerical computations need to have certified error bounds!
Machine errors need to be accounted for: **interval arithmetics!**

Error accumulation

⋆ floating point arithmetic is used in numerical analysis software
⋆ Using 15 digit precision

$$5.00000000000002 + 6.00000000000003 = 11.0000000000000$$

⋆ We make an error equal to 5×10^{-14}. Small, but not zero.

⋆ **Patriot missile failure:** time was counted in 10ths of seconds: 1/10 not representable exactly in binary. After 100 hours the representation error was 0.342 seconds! Scud missile travels 1.5km/s!

Rigorous Computer Arithmetic

⋆ the result of a numerical computation is not exact: information is lost

Interval arithmetics

⋆ A floating point number is replaced by an interval.

⋆ The output of a sequence of interval operations is an interval guaranteed to contain the exact result

⋆ Specific upwards/downwards rounding procedures are used

⋆ Specialized interval arithmetic software exist: Intlab (Matlab), IntervalArithmetic (Julia), etc.

Examples:

$[2.99, 3.01] + [0.99, 1.01] = [3.98, 4.02]$

$[2.99, 3.01] \times [0.99, 1.01] = [2.9601, 3.0401]$

$[0.99, 1.01]/[2.99, 3.01] = [0.3289, 0.3378]$

Finite elements method

Triangulation, variational formulation, linear system/eigenvalue problem:

$$-\Delta u = f, u \in H_0^1(\Omega) \text{ vs } \int_\Omega \nabla u_h \cdot \nabla v_h = \int_\Omega f_h v_h,\ \forall v_h \in V^h \subset H_0^1(\Omega)$$

⋆ discretization errors: continuous vs discrete solutions: $\|u - u_h\|$

Nobody worries about this

⋆ exact discrete solutions vs solutions obtained via iterative algorithms

⋆ floating point arithmetic errors: meshing, assembly

Explicit error estimates for the Laplacian eigenvalues

⋆ $-\Delta u = \lambda u$, $u \in H_0^1(\Omega)$, Ω polygon

⋆ **piecewise linear** finite elements

Explicit *a priori* error estimates [Liu, Oishi, 13]

- $|\lambda - \lambda_h| \leq C_1 h^2$
- $\|u - u_h\|_{L^2} \leq C_2 h^2$
- $\|\nabla u - \nabla u_h\|_{L^2} \leq C_3 h$
- **Our contribution**: eigenvalues of the Hessian have estimates with error $C_\gamma h^{1-2\gamma}$, $\gamma \in (0, 1/2)$, $C_\gamma \to \infty$ as $\gamma \to 0$.

where C_1, C_2, C_3, C_γ are **explicit** for a given mesh.

⋆ easy to see how to choose h in order to achieve a desired precision

high precision → small h → big discrete linear systems → bad control of machine errors

Local minimality – regular pentagon

- ⋆ Regular pentagon of radius 1: $h = 10^{-4}$, approx 250 million d.o.f
- ⋆ FreeFEM using 200 processors: Cholesky cluster–Institut Polytechnique Paris
- ⋆ explicit estimates–intervals containing the exact result: $q \in [q_h - C_q h^k, q_h + C_q h^k]$
- ⋆ INTLAB gives the bounds for the Hessian eigenvalues
- ⋆ we do not control machine errors in the FEM computations! (future work)
- ⋆ such errors are of size $O(\varepsilon h^{-2})$, $\varepsilon = 2.2 \times 10^{-16}$: in our work $\approx 10^{-8}$
- ⋆ recall that four eigenvalues are zero!

Pentagon			
Eigenvalue	**lower bound**	upper bound	multiplicity
2.568803	2.359297	2.784816	2
8.015038	7.558395	8.460722	2
13.458443	13.012758	13.915086	2

- ⋆ similar results are obtained for $n \in \{6, 7, 8\}$

Computations of optimal size

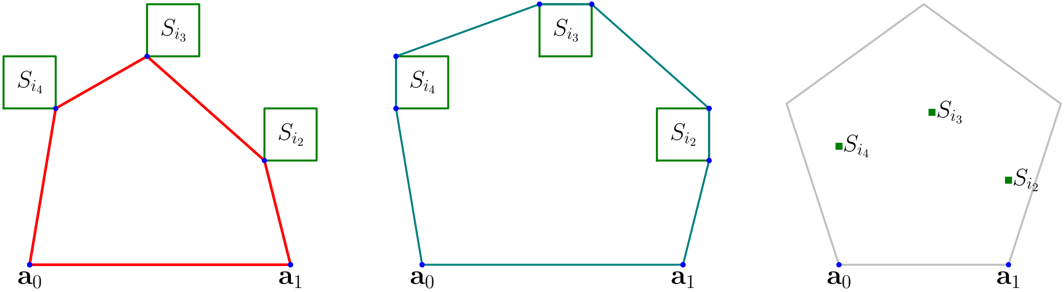
	h	d.o.f.	optimal h	d.o.f
Pentagon	10^{-4}	250 025 001	9.8e-4	$\approx$ 2.6 million
Hexagon	10^{-4}	300 030 001	4.2e-4	$\approx$ 17 million
Heptagon	10^{-4}	350 035 001	1.9e-4	$\approx$ 97 million
Octagon	10^{-4}	400 040 001	1.35e-4	$\approx$ 220 million

$\star$ improving the theoretical estimates should further decrease the size of the computational problems

$\star$ Local minimality+Some Theory $\Longrightarrow$ Explicit local-minimality neighborhood

Finalize the proof

Theorem. Given $n \geq 3$, a finite number of numerical computations solve the conjecture.



⋆ First 2 pictures: lower bound for area and eigenvalue

⋆ if current lower bound for $\lambda_1(P)|P|$ is not good enough, divide the squares sides in half and consider all combinations recursively

⋆ if the recursion does not end we converge to a counterexample!

⋆ Third picture: example of validation of a (really small) region: 262144 computations

Conclusion

Preprint: [Bogosel, Bucur, *On the polygonal Faber-Krahn inequality*, March 2022]

- We propose a new hybrid proof strategy for proving this classical conjecture.
- Local minimality: almost done, with the help of numerical computations.
- Validated numerical computations open the way to new mathematical results unattainable with traditional methods!