A Computer Assisted Proof in Shape Optimization

Beniamin Bogosel

Aurel Vlaicu University, Arad, Romania

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joint work with Dorin Bucur

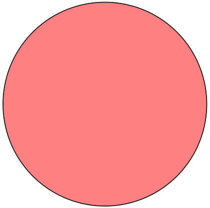
1. Shape Optimization and Dirichlet Laplacian Eigenvalues
2. Hybrid proof strategy
3. Numerical computations

Isoperimetric problem: Continuous vs Discrete

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

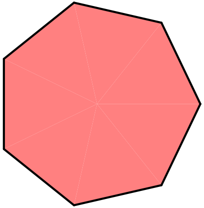
Ω: **General Shape**

⋆ the solution is the disk



Ω: ***n*-gon**

⋆ the solution is the regular n-gon

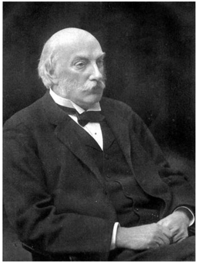


Heuristic argument

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

Optimization of spectral quantities with respect to the domain

[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

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

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

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

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

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

Optimizing Eigenvalues with repspect to the Domain Geometry

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

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

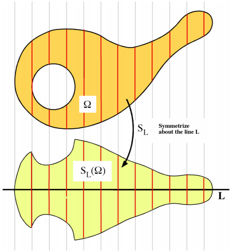
Minimizing the first Dirichlet-Laplace eigenvalue

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

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.

⋆ $n \geq 5$: numerical evidence, no proofs yet

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

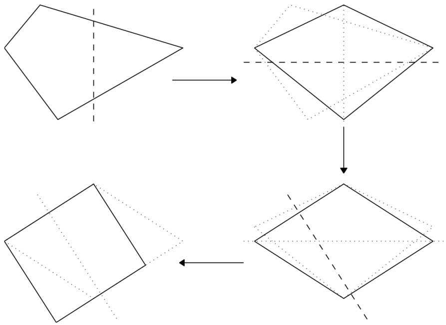


photo: [Henrot, *Extremum problems...*]

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:

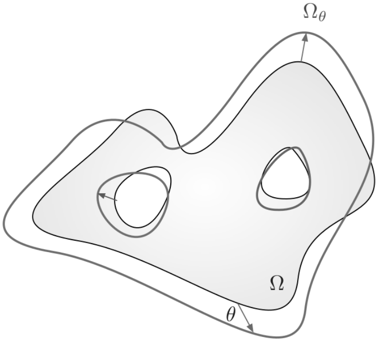
- [Fragala, Velichkov, 19]: optimality conditions - different proof for $n = 3$
- [Laurain, 19]: second shape derivative on polygons, Hessian matrix
- [Indrei, 22]: theoretical considerations
- [B. Bucur, 22]: appeared in Journal de l'Ecole Polytechnique, 2024.
- [B. Bucur, 24]: hybrid theoretical/numerical proof of local minimality for $n \in \{5, 6\}$

Hybrid proof strategy: use numerical tools when needed

⋆ the optimization variables are **the coordinates of the polygon**
⋆ **finite dimensional optimization problem** - classical optimality conditions

1. Explicit computation of the Hessian matrix of $P \mapsto \lambda_1(P)|P|$
2. **Proof of the local minimality** of the regular n-gon: **numerical proof for** $n \in \{5, 6\}$
3. Computation of a neighborhood around the regular polygon where minimality occurs
4. Analytic estimate for geometric features of an optimal polygon
5. Reduce the conjecture for a given $n \geq 5$ to a finite number of certified numerical computations.

[B., Bucur, *On the polygonal Faber-Krahn inequality*, Journal de l'Ecole Polytechnique, 2024]



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

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

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

$$\lambda''(\Omega)(\theta,\xi) = \text{... involved but explicit}$$

First step: local minimality

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

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

$$\text{Coords.} \longrightarrow \underbrace{\text{Shape} \longrightarrow \text{PDE} \longrightarrow \lambda_1}_{\text{shape derivative}}$$

Theorem: Eigenvalues of the Hessian

For $0 \leq k \leq n-1$ we have $\mathbf{B}_{\rho_k} = \begin{pmatrix} \alpha_k & i\gamma_k \\ -i\gamma_k & \beta_k \end{pmatrix}$ with $a(u,v) = \int_{\mathbb{P}_n} \nabla u \cdot \nabla v - \lambda_1 uv$

$$\alpha_k = \frac{2n(1-\cos(k\theta))}{\sin\theta} \int_{T_0} (\partial_x \mathbf{u_1})^2 - 2|\mathbb{P}_n| a(\mathbf{U_0^1}, \sum_{j=0}^{n-1} \cos(jk\theta)(\cos(j\theta)\mathbf{U_j^1} + \sin(j\theta)\mathbf{U_j}^2))$$

$$\beta_k = \frac{2n(1-\cos(k\theta))}{\sin\theta} \int_{T_0} (\partial_y \mathbf{u_1})^2 - 2|\mathbb{P}_n| a(\mathbf{U_0}^2, \sum_{j=0}^{n-1} \cos(jk\theta)(-\sin(j\theta)\mathbf{U_j}^1 + \cos(j\theta)\mathbf{U_j}^2))$$

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

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

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

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

Everything depends on three PDEs

⋆ Regular n-gon: explicit Hessian depending on the solution of 3 PDEs

$$\int_{\mathbb{P}_n} \nabla u_1 \cdot \nabla v = \lambda_1 \int_{\mathbb{P}_n} u_1 v, \forall v \in H_0^1(\mathbb{P}_n)$$

$$a(U^1, v) = \int_{\mathbb{P}_n} (\nabla u_1 \cdot \nabla \varphi)\partial_x v + \int_{\mathbb{P}_n} (\nabla v \cdot \nabla \varphi)\partial_x u_1 - \frac{2\lambda_1}{n} \int_{\mathbb{P}_n} u_1 v, \forall v \in H_0^1(\mathbb{P}_n)$$

$$a(U^2, v) = \int_{\mathbb{P}_n} (\nabla u_1 \cdot \nabla \varphi)\partial_y v + \int_{\mathbb{P}_n} (\nabla v \cdot \nabla \varphi)\partial_y u_1, \forall v \in H_0^1(\mathbb{P}_n)$$

$$\int_{\mathbb{P}_n} U^i u_1 = 0, \ i = 1, 2$$

with $a(u, v) = \int_{\mathbb{P}_n} \nabla u \cdot \nabla v - \lambda_1 uv$

Theoretical dead end

⋆ 4 Hessian eigenvalues are zero: corresponding to rigid motions and scalings

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

⋆ Theoretical results unavailable for now, **turn to numerics**!

⋆ **Questions**:

- how to do numerics rigorously? (apart from exact arithmetic)
- how can numerical simulations be used in a mathematical proof?

Error accumulation

⋆ floating point arithmetic is used in numerical analysis software

⋆ Using double precision (machine epsilon = `2.2204e-16`)

$$5.00000000000002 + 6.00000000000003 = 11.0000000000000$$

⋆ Small error, but not zero.

GAO/IMTEC-92-26, *Patriot Missile Defense: Software Problem Led to System Failure at Dhahran, Saudi Arabia*

⋆ **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!

Can we blindly trust numerical computations?

[S. Rump, *Verification methods: Rigorous results using floating-point arithmetic*, Acta Numerica, *Intlab*], [W. Tucker, *Validated numerics*]

$$f(x,y) = 333.75y^6 + x^2(11x^2y^2 - y^6 - 121y^4 - 2) + 5.5y^8 + x/(2y)$$

$\tilde{x} = 77617, \tilde{y} = 33096$. Evaluating $f(\tilde{x},\tilde{y}) \approx -0.8273960599$.
Symbolic computation: $f(\tilde{x},\tilde{y}) = -2 + \tilde{x}/(2\tilde{y})$.

$$\begin{aligned} 5.5\tilde{y}^8 &= +7917111340668961361101134701524942848 \\ 333.75\tilde{y}^6 + \tilde{x}^2(11\tilde{x}^2\tilde{y}^2 - \tilde{y}^6 - 121\tilde{y}^4 - 2) &= -7917111340668961361101134701524942850 \end{aligned}$$

Matlab computation: $f(\tilde{x},\tilde{y}) =$ `-1.1806e+21`. Wrong result, no warning!

vs. interval arithmetic computation

Intlab computation: $f(\tilde{x},\tilde{y}) =$ `1.0e+021*[ -5.9030, 4.7224]` Useless, but correct!

Reliable computing: Interval arithmetic

$\star$ floating point arithmetic is reliable (when used correctly): BUT a floating point computation is **not a proof**

$\star$ interval arithmetic replaces floating point numbers x with intervals $[x]$.

$\star$ operations on intervals are defined such that $\tilde{x} \in [x], \tilde{y} \in [y] \Longrightarrow \tilde{x} * \tilde{y} \in [x] * [y]$

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

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

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

$\star$ toolboxes like INTLAB in Matlab implement these operations rigorously [Rump]

Challenges

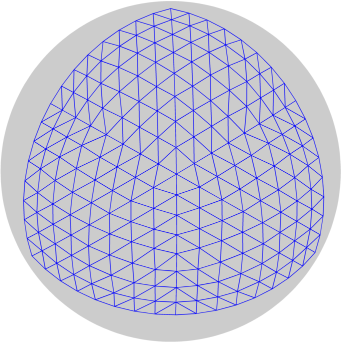
$\star$ many operations $\longrightarrow$ large intervals $\longrightarrow$ useless results

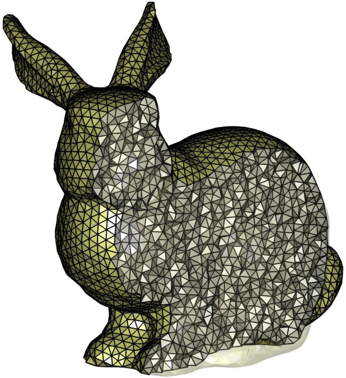
$\star$ Use any theoretical and practical tool available to pre-compute information.

$\star$ Nothing can be taken for granted: e.g. one needs to prove that the first/second eigenvalue found numerically is indeed the first/second eigenvalue!

Goal: Show that a Hessian eigenvalue $\mu = \mathcal{F}(\lambda_1, \nabla u_1, \nabla U^1, \nabla U^2)$ is strictly positive.

- The domain D is discretized using a mesh $\mathcal{T}_h$ which consists of a partitions in triangles in 2D or tetrahedra in 3D.
- The parameter h which indicates the convergence of the method is typically related to the size of the mesh elements.





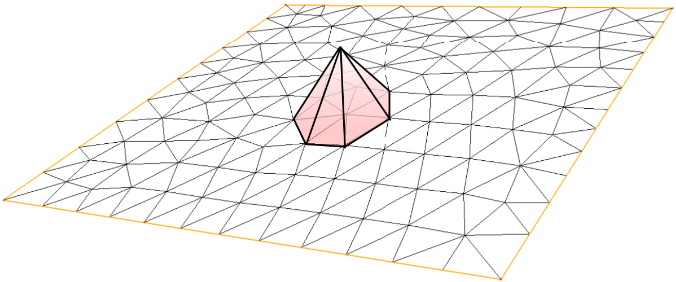
Finite element space

A basis $\{\varphi_1, ..., \varphi_{N_h}\}$ of finite element functions is introduced on the mesh $\mathcal{T}_h$

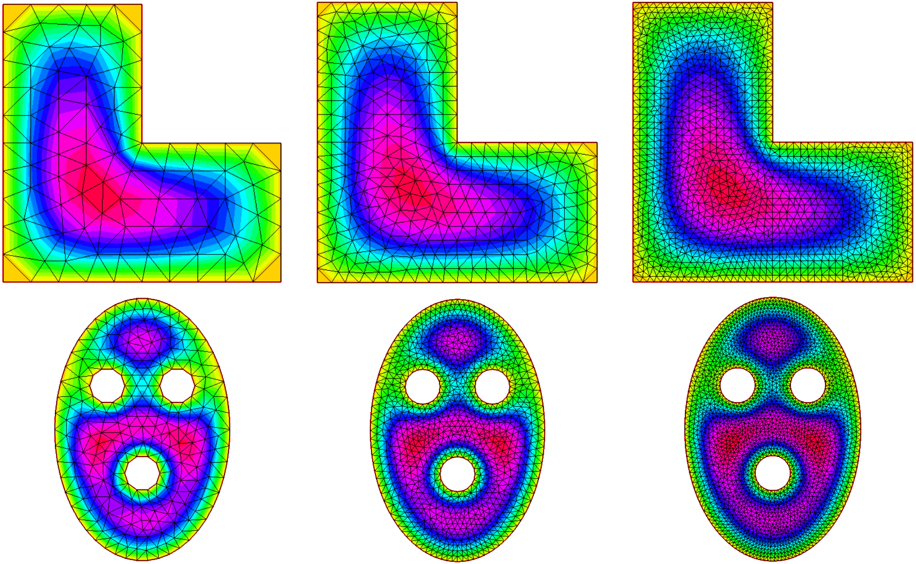
Example

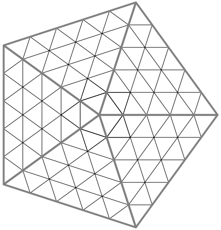
- N_h is the number of vertices $a_1, ..., a_{N_h}$ of the mesh
- For each $i = 1, ..., N_h$, φ_i is affine on each triangle $T \in \mathcal{T}_h$ and

$$\varphi_i(a_j) = 1 \text{ and } \varphi_i(a_j) = 0 \text{ for } i \neq j$$

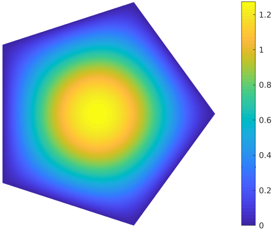


Some examples

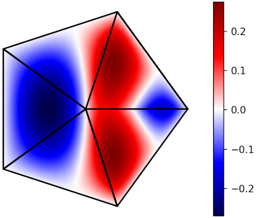




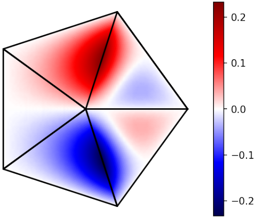
Symmetric mesh



u_1



U^1



U^2

- $\star$ $m =$ number of mesh nodes on the ray $(0,0) \longrightarrow (1,0)$
- $\star$ mesh size parameter $h = 1/m$
- $\star$ as $h \to 0$ computations become more and more precise(?), but more costly!

Continuous	**Finite Elements**
$-\Delta u = \lambda u,\ u = 0$ on $\partial\Omega$	Generalized eigenvalue: $Ku = \lambda Mu$
$-\Delta U = f,\ U = 0$ on $\partial\Omega$	Linear system: $KU = F$

Sources of error:

a) Contiuous to discrete. Quantity of interest $\in [\mu_0 - Ch, \mu_0 + Ch]$, explicit constant C.

Nobody worries about this...

b) Errors when solving the discrete problems (eigenvalue, linear systems)
c) Errors coming from floating point computations

A priori estimates: continuous vs (exact) discrete solutions

$\mathbf{P}_1$ finite elements: simple, explicit estimates

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

- $|\lambda - \lambda_h| \leq C_1 h^2$
- $\|u - u_h\|_{L^2} \leq C_2 h^2$
- $\|\nabla u - \nabla u_h\|_{L^2} \leq C_3 h$ (interpolation error dominates $\|\nabla(u - \Pi_{1,h} u)\|_{L^2} \leq Ch|u|_{H^2}$)

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

⋆ **Our contribution:** Explicit $O(h)$ estimate for the other PDEs involved in the computations

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

Search for an Equilibrium

high precision $\rightarrow$ small h $\rightarrow$ big discrete linear systems $\rightarrow$ bad control of machine errors

Study of the discrete problems

$Ku = \lambda Mu$: K is the rigidity matrix, M the mass matrix

1. Compute K, M explicitly: limit the number of computations leads to smaller intervals
2. Residual based estimations: floating point computation (cheap), residual estimation using interval matrices, find intervals guaranteed to contain generalized eigenvalues
3. Identify the first eigenvalue: is simple and corresponds to positive eigenvector, test if the interval enclosure contains zero or not
4. Identify the second eigenvalue: difficult in general
   - show the second eigenvalue is double (symmetric mesh)
   - we have $\lambda_2 = \lambda_3 < \lambda_1(B_1) \approx 26.31$: check that the interval enclosure for the second eigenvalue verifies this to validate it
5. Similar ideas apply for solutions of discrete linear systems

In the end: discrete eigenvalues, first eigenvector, solutions to all discrete linear systems are found including interval enclosures

Example: first eigenvalue

1. The discrete problem. $Ku = \lambda Mu$

$\star$ compute a floating point approximation of the generalized eigenpair $(\tilde\lambda, \tilde x)$

$\star$ evaluate the residual using **interval arithmetics**: $r = K\tilde x - \tilde\lambda M\tilde x$

$\star$ we can show that $[\tilde\lambda - f(r), \tilde\lambda + f(r)]$ contains one eigenvalue of the discrete problem

$\star$ if $\tilde\lambda$ is simple then $[\tilde x - g(r), \tilde x + g(r)]$ contains an associated eigenvector

$\star$ how do we know we approximated λ_1? We check if the eigenvector is non-negative: the intervals found above should not contain zero.

2. Adding the a priori estimates

$\star$ $[\tilde\lambda - f(r) - Ch^2, \tilde\lambda + f(r) + Ch^2]$ contains an eigenvalue for the continuous problem

$\star$ $[\tilde x - g(r) - Ch, \tilde x + g(r) + Ch]$ contains the eigenfunction for the continuous problem

$\star$ previous considerations show that this is indeed the first eigenpair

Remark: The precision obtained is dominated by "the largest" among the approximation of rounding errors in the discrete problem and the *a priori* estimate.

Conflicting interests: h small $\implies Ch^2$ small; h big $\implies f(r)$ small

Example: second eigenvalue

1. The discrete problem. $Ku = \lambda Mu$

⋆ the second eigenvalue of the discrete problem for to a symmetric mesh is at least double.

⋆ compute the approximation in floating point for the second eigenvalue: how do we know it's the second discrete one?

2. Look at the continuous problem

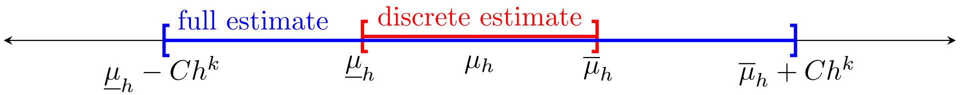
⋆ the regular n-gon with unit radius is inscribed in the unit disk B_1.

⋆ $\lambda_k(\mathbb{P}_n) \geq \lambda_k(B_1)$. Therefore $[0, \lambda_4(B_1)]$ contains **at most three** eigenvalues of $\mathbb{P}_n$

⋆ For h small enough (quantifiable) there are at most three discrete eigenvalues in $[0, \lambda_4(B_1)]$.

⋆ Check that the second discrete eigenvalue we found verifies the bound above: this shows that it is indeed the second one.

Remark: We exploit the connection with the continuous problem: cost efficient solution even for fine meshes/large matrices. Otherwise, other techniques exist in the literature.



⋆ the quantity to be approximated is computed using some numerical method μ_h

⋆ using theoretical estimates and interval arithmetic we find bounds for the discrete quantity $[\underline{\mu}_h, \overline{\mu}_h]$.

- computations might involve: computing integrals, solving linear systems, solving eigenvalue problems

⋆ *a priori* estimates are added regarding the difference between discrete approximation and the continuous quantity

Validation strategy

A) Solve the FEM problems using interval arithmetics.

Control machine errors for the discrete problems

⋆ solve in floating point; validate afterwards (INTLAB, residual)

⋆ explicit assembly – all triangles in the mesh are congruent

⋆ modify `verifyeig` in INTLAB: replace matrix inversion with 3 verified linear systems

B) Compute the eigenvalues of the Hessian matrix.

Interval arithmetic is used in all computations

⋆ replace all FEM variables in the formulas and obtain $\mu_h = [\underline{\mu_h}, \overline{\mu_h}]$.

C) Add the a priori estimates.

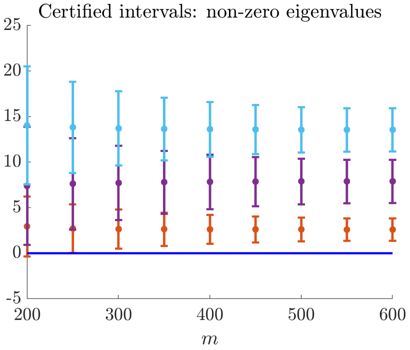
Control errors between continuous and (exact) discrete problems

⋆ use optimal interpolation constants: mesh contains congruent triangles

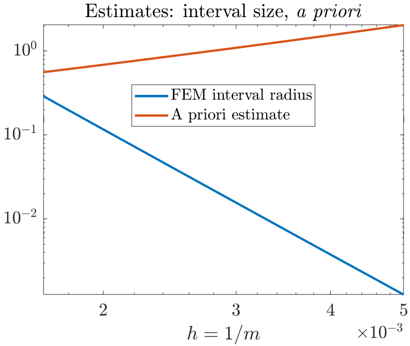
⋆ the actual eigenvalue μ is guaranteed to belong to $[\underline{\mu_h} - Ch, \overline{\mu_h} + Ch]$

If $2n - 4$ of the intervals obtained are contained in $(0, +\infty)$ the **proof of local minimality succeeds**.

Computations for the regular pentagon



Certified intervals, $m = 1/h$



FEM error vs interval radius

- ⋆ Hessian has three pairs of double eigenvalues
- ⋆ Proof of local minimality succeeds! (also works for $n = 6$)
- ⋆ Bottleneck for $n \geq 7$: intervals become too large. FEM estimates need to be improved or more precise methods are needed.

n	[B. Bucur, JEP, 24]			[B. Bucur, preprint, 24]			
	h	DoF	Intervals	$h = 1/m$	m	DoF	Intervals
5	9.8e-4	2.5 million	✗	0.0040	250	156876	✓
6	4.2e-4	17 million	✗	0.0026	380	434341	✓
7	1.9e-4	97 million	✗	-	-	-	
8	1.35e-4	220 million	✗	-	-	-	

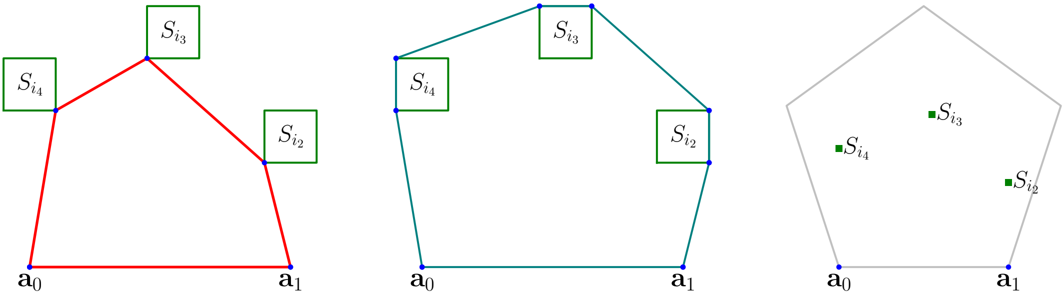
Code for validating local minimality $n \in \{5, 6\}$:
`https://github.com/beniamin-bogosel/PolyaSzego`

A finite number of computations can solve the problem

- Local minimality+ some theory: local minimality neighborhood around the regular n-gon (one validated computation)
- Theoretical results: exclude polygons which are far from the regular one (diameter, inradius, minimal edge length, geometric properties)
- Cover the remaining region with a series of validated numerical computations.

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 successfully we converge to a counterexample!

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

Conclusion

Paper: [B., Bucur, *On the polygonal Faber-Krahn inequality*, Journal de l'Ecole Polytechnique – Mathématiques, 2024]

Preprint: [B., Bucur, *Polygonal Faber-Krahn inequality: Local minimality via validated computing*, 2024] `https://arxiv.org/abs/2406.11575`

- We propose a new hybrid proof strategy for proving this classical conjecture.
- Local minimality: done using interval arithmetic for $n \in \{5, 6\}$
- Validated numerical computations open the way to new mathematical results hard to obtain using purely theoretical methods!

Thank you for your attention!