A Computer Assisted Proof in Shape Optimization

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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:

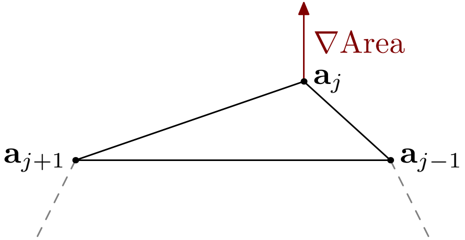
- A solution exists? Is it regular?
- Find it!

Polygonal isoperimetric inequality

$$\min_{\boxed{|P| = c,\ \text{P is an } n\text{-gon}}} \operatorname{Per}(P)$$

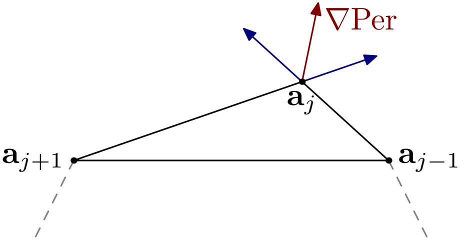
Existence of solutions: "immediate" (classical compactness arguments)
Optimality conditions: $\nabla \operatorname{Per}(P) = \lambda \nabla \operatorname{Area}(P)$

Gradient of the area



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

Gradient of the perimeter



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

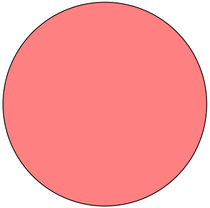
Optimality conditions: gradients are colinear $\implies$ P is the regular n-gon.

Isoperimetric problem: Continuous vs Discrete

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

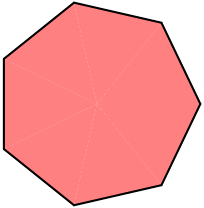
Ω: **General Shape**

$\star$ the solution is the disk



Ω: ***n*-gon**

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



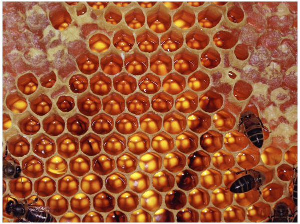
Heuristic argument

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

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

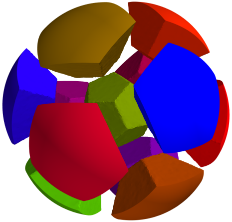
Theoretical aspects

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



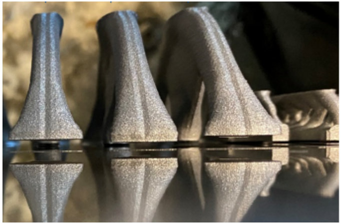
Numerical aspects

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



Practical aspects

⋆ industrial problems
⋆ modelization
⋆ simulation
⋆ optimal design



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

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

- $\star$ eigenvectors characterize invariant subspaces of A
- $\star$ why are they interesting?
- $\star$ they show how multiplication with A changes a vector x along principal directions!

Potential Applications

Knowing the spectrum of A ($Av_i = \lambda_i v_i$) is useful for:

- **Linear systems**: $Ax = b$:

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

- **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:

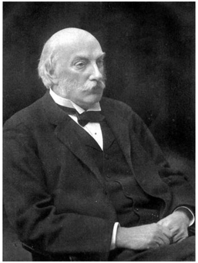
$$\begin{cases} -\Delta u_k & = & \lambda_k(\Omega) u_k & \text{in } \Omega \\ u_k & = & 0 & \text{on } \partial\Omega. \end{cases}$$

⋆ 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

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 - 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

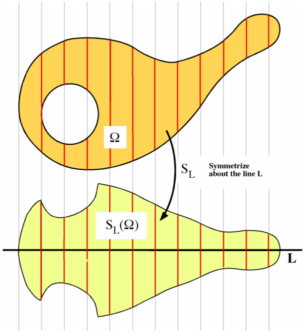


image: [Treibergs, *Steiner Symmetrization and Applications*]

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

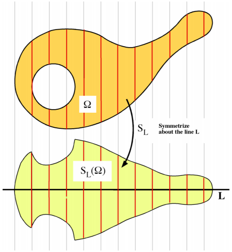
$$\lambda_1(\Omega) = \inf_{u \in H_0^1(\Omega), u \neq 0} \frac{\int_\Omega |\nabla u|^2}{\int_\Omega u^2} = \frac{\int_\Omega |\nabla u_1|^2}{\int_\Omega u_1^2} \geq \frac{\int_{\Omega^*} |\nabla u_1^*|^2}{\int_{\Omega^*} (u_1^*)^2} \geq \inf_{u \in H_0^1(\Omega^*), u \neq 0} \frac{\int_{\Omega^*}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

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

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.

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!

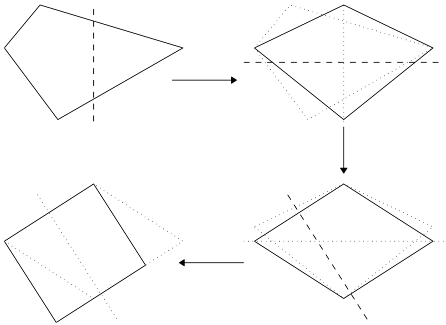


photo: [Henrot, *Extremum problems...*]

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
- [Indrei, 22]: theoretical aspects, identification of a manifold in which the regular polygon is optimal
- [B. Bucur, 22]: appeared in Journal de l'Ecole Polytechnique, 2024.
- [B. Bucur, 24]: hybrid theoretical/numerical proof of local minimality for $n \in \{5, 6\}$

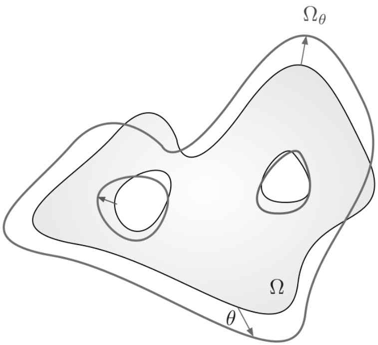
Hybrid proof strategy: use numerical tools when needed

⋆ 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 $n \leq 6$**
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]



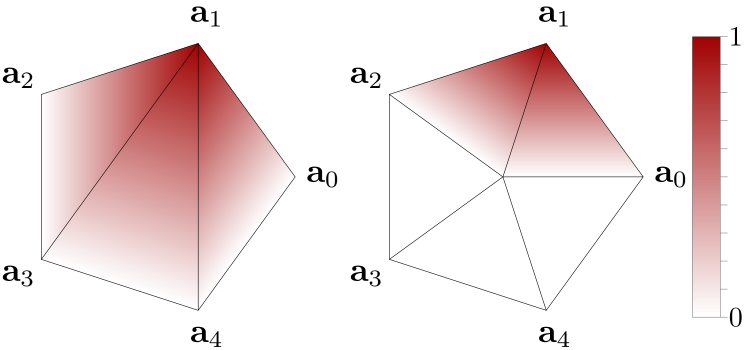
- ⋆ **objective:** $J : P \mapsto |P|\lambda(P)$ (scale invariant)
- ⋆ λ **simple** $\Longrightarrow$ J is smooth! [Henrot, Pierre]

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

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

Polygonal perturbations

- ⋆ for every vertex $\mathbf{a}_i$ consider a vector perturbation $\theta_i \in \mathbb{R}^2$
- ⋆ consider a triangulation of the polygon containing the edges in some triangles



- ⋆ define a $\mathbf{P}_1$ function φ_i on this triangulation by $\varphi_i(\mathbf{a}_j) = \delta_{ij}$ ($\varphi_i = 0$ on interior nodes)
- ⋆ build the vector field $\theta = \sum_{i=1}^n \theta_i \varphi_i \in W^{1,\infty}$

First step: local minimality

- $\star$ 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

- $\star$ We have a function depending on $2n$ variables (vertex coordinates).
- $\star$ compute the first and second derivatives of

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

- $\star$ (not?) straightforward: (chain rule)

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

Local minimality: Key points learned

- Shape derivatives: volumic form is well defined for less regular domains

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

- To obtain the second derivative: simply differentiate the volumic form again - no additional regularity needed
- **Hessian matrix** of $(\mathbf{x}_0, \mathbf{x}_1, ..., \mathbf{x}_{n-1}) \mapsto \lambda_1(P)|P|$ is explicit in terms of $2n+1$ PDEs

Hessian eigenvalues

Local minimality amounts to studying the positivity of the Hessian matrix!

Computing the gradient

⋆ We have

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

the gradient w.r.t. the coordinates of the vertices is given by

$$\nabla\lambda(\mathbf{x}) = \left(\int_\Omega \mathbf{S}_1^\lambda \nabla\varphi_i\right)_{i=1}^n \in \mathbb{R}^{2n}$$

⋆ The regular polygon is a critical point for $|P|\lambda_1(P)$.

Formula for the Hessian matrix

The Hessian matrix $\mathbf{N}^\lambda \in \mathbb{R}^{2n\times 2n}$ of a simple Dirichlet-Laplace eigenvalue with respect to the coordinates of the n-gon is given by the following $n \times n$ block matrix

$$\mathbf{N}^\lambda = (\mathbf{N}^\lambda_{ij})_{1\leq i,j\leq n}$$

where the 2×2 blocks are given by

$$\begin{aligned}\mathbf{N}^\lambda_{ij} = &\int_\Omega (-2DU_jDU_i^T + 2\lambda(\Omega)U_jU_i^T) + \nabla\varphi_j \otimes \mathbf{S}_1^\lambda \nabla\varphi_i + \mathbf{S}_1^\lambda\nabla\varphi_j \otimes \nabla\varphi_i \\ &+ \int_\Omega \left(-|\nabla u|^2 + \lambda(\Omega)u^2\right)\left(2\nabla\varphi_i \odot \nabla\varphi_j\right) \\ &+ 2\int_\Omega (\nabla\varphi_j \cdot \nabla u)(\nabla\varphi_i \otimes \nabla u) + (\nabla\varphi_i \cdot \nabla u)(\nabla u \otimes \nabla\varphi_j) + (\nabla\varphi_i \cdot \nabla\varphi_j)(\nabla u \otimes \nabla u) \\ &- \int_\Omega u^2 \left[\nabla\varphi_j \otimes \left(\int_\Omega \mathbf{S}_1^\lambda \nabla\varphi_i\right) + \left(\int_\Omega \mathbf{S}_1^\lambda\nabla\varphi_j\right) \otimes \nabla\varphi_i\right]\end{aligned}$$

$\star$ $U_i \in H_{0,1}(\Omega)$ solve PDEs depending on u_1, λ_1

Hessian on the regular polygon

⋆ consider a symmetric triangulation defining φ_i
⋆ 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 $\mathbf{M}_{ij}^\lambda$, $0 \leq i,j \leq n-1$ given by

$$\mathbf{M}_{ij}^\lambda = |\Omega| \int_\Omega (-2DU_iDU_j^T + 2\lambda(\Omega)U_iU_j^T) \qquad \text{material derivatives: neg. definite}$$

$$- \lambda(\Omega) \int_\Omega [\nabla\varphi_i \otimes \nabla\varphi_j - \nabla\varphi_j \otimes \nabla\varphi_i] \qquad \text{Hessian of the area}$$

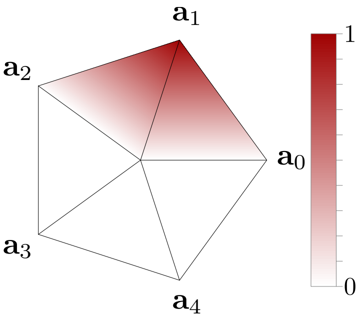
$$+ 2|\Omega| \int_\Omega (\nabla\varphi_i \cdot \nabla\varphi_j)(\nabla u \otimes \nabla u) \qquad \text{positive definite}$$

The regular polygon

- ⋆ consider the Hessian $\mathbf{M}^\lambda$ of $\lambda(\mathbf{x})\text{Area}(\mathbf{x})$
  - four eigenvalues are zero!
  - fixing two vertices: $(2n-4)\times(2n-4)$ submatrix
  - this submatrix is positive definite provided the other $2n-4$ eigenvalues are strictly positive
- ⋆ symmetric triangulation for defining the perturbations
- ⋆ the first eigenfunction has the same symmetries as the regular polygon

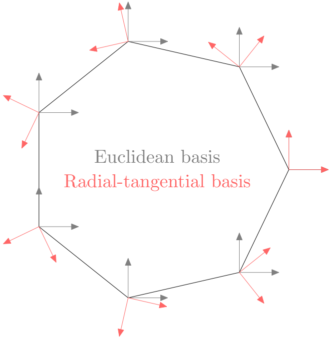
Local minimality: fixing two vertices

Using the stability result, if the $(2n-4)\times(2n-4)$ submatrix has strictly positive eigenvalues, the same will hold in an open, quantified, neighborhood.



Explicit Eigenvalues of the Hessian

⋆ change of basis: normal and tangential coordinates!
⋆ in the new basis the matrix becomes **block circulant**
⋆ characterization of the spectrum in terms of the 2×2 blocks



$\mathbf{M}_0, \mathbf{M}_1, ..., \mathbf{M}_{n-1}$ the blocks of the first line in $\mathbf{M}^\lambda$, $\theta = 2\pi/n$,
$\rho_k = \exp(ik\theta)$

$$\mathbf{B}_{\rho_k} = \mathbf{M}_0 + \mathbf{M}_1(\rho_k \mathbf{R}_\theta) + ... + \mathbf{M}_{n-1}(\rho_k \mathbf{R}_\theta)^{n-1} \in \mathbb{R}^{2\times 2}$$

[G. J. Tee. *Eigenvectors of block circulant and alternating circulant matrices*]

Explicit eigenvalues

The spectrum of $\mathbf{M}^\lambda$ is the union of the spectra of $\mathbf{B}_{\rho_k}$, $0 \le k \le n-1$.

Notation: $a(u,v) = \int_\Omega \nabla u \cdot \nabla v - \lambda_1(\Omega) uv$.

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

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

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

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

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

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

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

Theoretical dead end

- Regular n-gon: explicit Hessian depending on the solution of 3 PDEs
- 4 Hessian eigenvalues are zero: corresponding to rigid motions and scalings
- Formulas complex (depending on 3 PDEs): we did not manage to prove theoretically that the other $2n-4$ eigenvalues are positive!

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

⋆ When theory doesn't help, **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

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

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

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

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

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

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

⋆ toolboxes like INTLAB in Matlab implement these operations rigorously [Rump]

Challenges

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

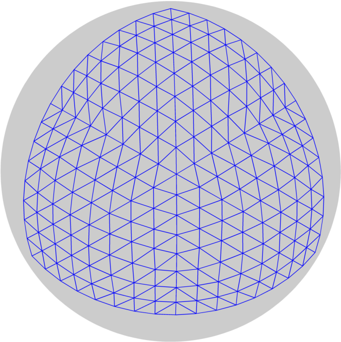
⋆ Use any theoretical and practical tool available to pre-compute information.

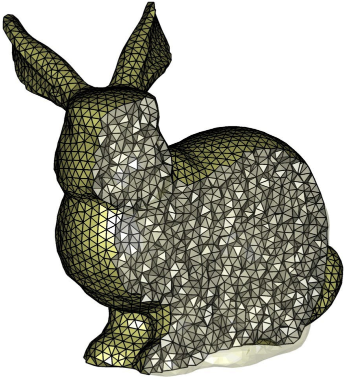
⋆ Nothing can be taken for granted: e.g. one needs to prove that the first eigenvalue found numerically is indeed the first eigenvalue!

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

Approximating solutions to PDEs: finite elements

- 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.





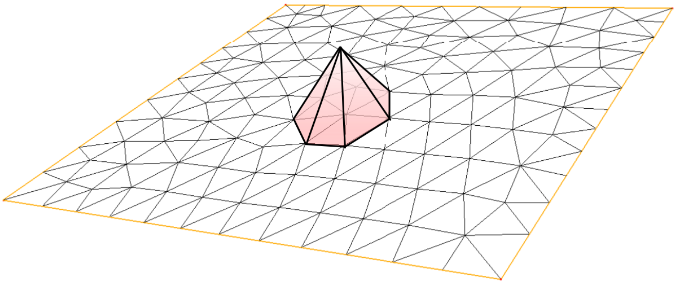
Finite element space

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

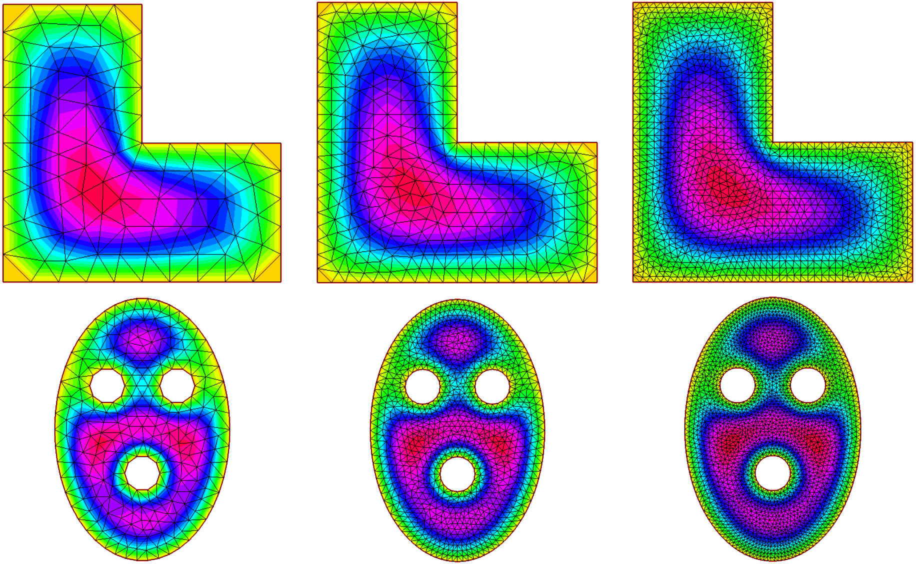
Example

- 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

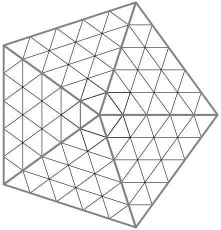
$$\varphi_i(a_j) = 1 \text{ and } \varphi_i(a_j) = 0 \text{ for } i \neq j$$



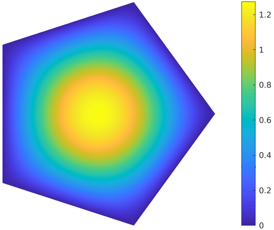
Some examples



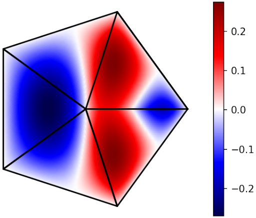
For this problem...



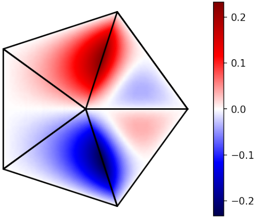
Symmetric mesh



u_1



U^1



U^2

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

Finite elements approximations

Continuous

$$-\Delta u = \lambda u,\ u = 0 \text{ on } \partial\Omega$$

$$-\Delta U = f,\ U = 0 \text{ on } \partial\Omega$$

Finite Elements

Generalized eigenvalue: $Ku = \lambda Mu$

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.

Strategy: $\star$ $a(u,\varphi) = (f,\varphi)_{H^{-1},H^1}$ in $H_0^1(\Omega)$ (continuous problem)
$\star$ $a(v,\varphi) = (f,\varphi)_{H^{-1},H^1}$ in $\mathcal{V}^h$ (same RHS, but discrete; controlled by the interpolation error)
$\star$ $a(v_h,\varphi) = (f_h,\varphi)_{H^{-1},H^1}$ in $\mathcal{V}^h$ (actual FEM solution; continuous vs discrete RHS)

$\star$ easy to see how to choose h in order to achieve a desired precision

Search for an Equilibrium

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

Our contribution

Explicit *a priori* estimates for problems of the form

$$\int_\Omega (\nabla U \cdot \nabla v - \lambda_1(\Omega) U v) = \int_\Omega f v + \int_S g v, \quad \forall v \in H_0^1(\Omega)$$

⋆ S is a union of segments, $g \in H^{1/2}(S)$.

⋆ U is not in H^2 but is piece-wise H^2 [Grisvard]

⋆ Explicit estimate of the form $\|\nabla U - \nabla U_h\|_{L^2(\Omega)} = O(h)$

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

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

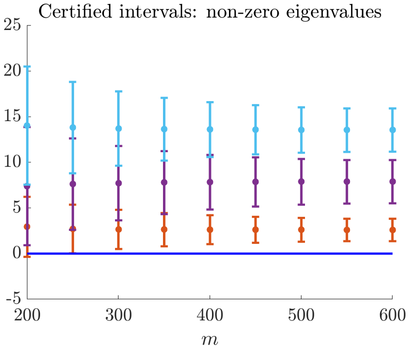
⋆ replace all FEM variables in the formulas and obtain $\mu_h = [\underline{\mu_h}, \overline{\mu_h}]$.

C) Add the a priori estimates.

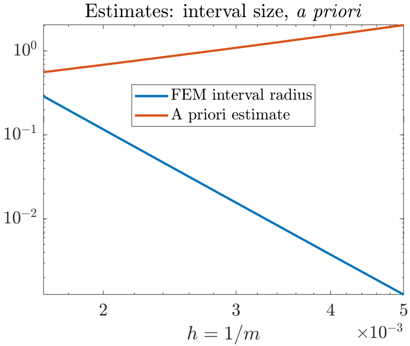
Control errors between continuous and (exact) discrete problems

⋆ 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**.



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.

Comparing with previous results

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	✗	-	-	-	

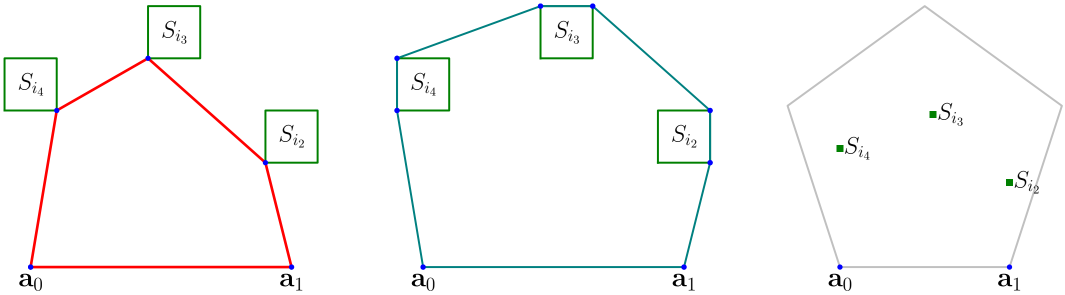
Code for validating local minimality $n \in \{5, 6\}$: `https://github.com/bbogo/PolyaSzego`

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

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!