Shape Optimization with PDE constraints and Boundary Element Methods by Example

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What is Shape Optimization?

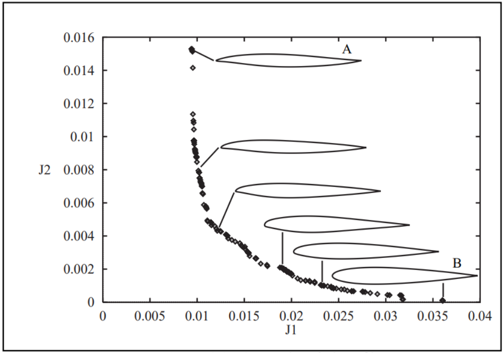


Figure 8.9. *Optimal airfoil profiles.*

- Sizing: Thickness and scale; Shape is constant
- Shape: Topology is constant
- Topology: Example: "How many holes?"

References

- K. Eppler and H. Harbrecht. “Numerical Solution of Elliptic Shape Optimization Problems Using Wavelet-Based BEM”. 2003.
- Y.J. Liu and N. Nishimura. “The Fast Multipole Boundary Element Method for Potential Problems: A tutorial”. 2005.
- J. Haslinger and R.A.E. Makinen. ”Introduction to Shape Optimization: Theory, Approximation, and Computation”. 2003.

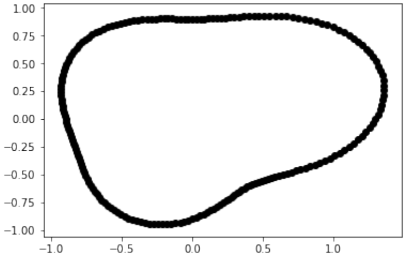
Shape Optimization Problem

Min/Max objective function $f(\Omega)$

subject to constraints $g(\Omega) = c \quad h(\Omega) \leq d$

where Ω is some shape/topology/geometry

Shape Optimization Problem Example



Maximize Bending Rigidity $B(\Omega) = \int_{\Omega} y^2 d\mathbf{x}$

subject to Volume, Torsional Rigidity, Center of Mass constraints

$$V(\Omega) = \int_{\Omega} d\mathbf{x} = V_0 \quad T(\Omega) = 2\int_{\Omega} u(\mathbf{x}) d\mathbf{x} = T_0 \quad \hat{x}(\Omega) = 0$$

where Ω is a 2-D shape and u is a solution to:

$$\Delta u = -2 \text{ on } \Omega \text{ and } u = 0 \text{ on } \partial\Omega$$

The Big Picture

- Formulate/Quantify/Construct the optimization problem
- Iteratively optimize Ω
  - Solve the PDE problem
  - Update Ω
  - Repeat until convergence or termination
- Geometric result and example

Formulate shape Ω

- Given Ω is a 2-D star shape.
- Ω corresponds to $\partial\Omega$
- Let r be a smooth function, treated as a radius of the shape, with $r(0) = r(2\pi)$

$$\partial\Omega = \{(r(\phi)\cos(\phi), r(\phi) sin(\phi)), \phi \in [0, 2\pi]\}$$

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- How do you formulate $r(\phi)$?

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- Choice Made: Fourier series

$$r(\phi) = a_0 + \sum_{i=1}^{\infty} a_i \cos(i\phi) + b_i \sin(i\phi)$$

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- Choice Made: Fourier series + Approximation to $2N + 1$ terms

$$r(\phi) \approx a_0 + \sum_{i=1}^{N} a_i \cos(i\phi) + b_i \sin(i\phi)$$

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$$r(\phi) \approx a_0 + \sum_{i=1}^{N} a_i \cos(i\phi) + b_i \sin(i\phi) \leftrightarrow \{a_0, a_1, b_1, \ldots, a_N, b_N\}$$

Formulate integrals involving Ω

- $r(\phi) \approx a_0 + \sum_{i=1}^{N} a_i \cos(i\phi) + b_i \sin(i\phi)$
- $\hat{x}(\Omega) = \hat{x}(r) \approx \frac{1}{3V(\Omega)} \int_0^{2\pi} (\cos(\phi), \sin(\phi))\, r(\phi)^3 d\phi = (0,0)$
- $B(\Omega) = B(r) \approx \int_\Omega y^2 dx = \frac{1}{4} \int_0^{2\pi} \sin(\phi)^2 r(\phi)^4 d\phi$
- $V(\Omega) = V(r) \approx \int_\Omega dx = \frac{1}{2} \int_0^{2\pi} r(\phi)^2 d\phi$
- $T(\Omega) = T(r) = 2 \int_\Omega u(x) dx =???$

Formulate Lagrangian of Optimization Problem

$$\begin{aligned} L(\Omega, \lambda) &= L(a_0, a_1, b_1, \ldots, a_N, b_N, \lambda_V, \lambda_T, \lambda_x) \\ &= -B(\Omega) + \lambda_T(T(\Omega) - T_0) + \lambda_V(V(\Omega) - V_0) + \lambda_x \cdot \hat{x} \end{aligned}$$

Formulate Lagrangian of Optimization Problem

$$
\begin{aligned}
L(\Omega, \lambda) &= L(a_0, a_1, b_1, \ldots, a_N, b_N, \lambda_V, \lambda_T, \lambda_x) \\
&= -B(\Omega) + \lambda_T(T(\Omega) - T_0) + \lambda_V(V(\Omega) - V_0) + \lambda_x \cdot \hat{x}(\Omega)
\end{aligned}
$$

$$
\begin{aligned}
\nabla L_\Omega(\Omega, \lambda) &= \nabla_{a_0,\ldots,b_N} L(a_0, a_1, b_1, \ldots, a_N, b_N, \lambda_V, \lambda_T, \lambda_x) \\
&= -\nabla B(\Omega) + \lambda_T \nabla T(\Omega) + \lambda_V \nabla V(\Omega) + \lambda_x \cdot \nabla \hat{x}(\Omega)
\end{aligned}
$$

$$
\begin{aligned}
\nabla L_\lambda(\Omega, \lambda) &= \nabla_{\lambda_V,\lambda_T,\lambda_x} L(a_0, a_1, b_1, \ldots, a_N, b_N, \lambda_V, \lambda_T, \lambda_x) \\
&= (T(\Omega) - T_0, V(\Omega) - V_0, \hat{x}(\Omega))
\end{aligned}
$$

Formulate integrals involving Ω

- $\nabla r(\phi) \approx (1, \cos(\phi), \sin(\phi), \cos(2\phi), \sin(2\phi), \ldots, \cos(N\phi), \sin(N\phi))$
- $\nabla \hat{x}(\Omega) = \int_0^{2\pi} \nabla r(\phi)\, (\cos(\phi), \sin(\phi))\, r(\phi)^2 d\phi$
- $\nabla B(\Omega) = \int_0^{2\pi} \nabla r(\phi) \sin^2(\phi) r(\phi)^3 d\phi$
- $\nabla V(\Omega) = \int_0^{2\pi} \nabla r(\phi) r(\phi) d\phi$
- $\nabla T(\Omega) = \int_0^{2\pi} \nabla r(\phi) r(\phi) \left(\frac{\partial u}{\partial n}(\phi)\right)^2 d\phi$

First Order / Gradient Descent Method

For some positive constant c and assuming (Ω_0, λ_0) is "close" to optimal solution (Ω^*, λ^*). For $k = 0, 1, 2, \ldots$:

$$\begin{aligned}\Omega_{k+1} &= \{a_0, a_1, b_1, \ldots, a_N, b_N\}_{k+1} \\ &= \{a_0, a_1, b_1, \ldots, a_N, b_N\}_k - c\nabla_\Omega L(\Omega, \lambda)\end{aligned}$$

$$\lambda_{k+1} = \lambda_k + c\nabla_\lambda L(\Omega, \lambda)$$

Stop iteration if $\nabla_\Omega L(\Omega, \lambda) < \epsilon \approx \mathbf{0}$.

Solving for the stress function u

Need to compute at each iteration for a given Ω:

$$T(\Omega) = 2\int_\Omega u(x)d(x)$$
$$\nabla T(\Omega) = \int_0^{2\pi} \nabla r(\phi) r(\phi) \left(\frac{\partial u}{\partial n}(\phi)\right)^2 d\phi$$

where

$$\Delta u = -2 \text{ on } \Omega$$
$$u = 0 \text{ on } \partial\Omega$$

Conversion to Boundary Integral Equation

For $\mathbf{x} \in \Omega$, let $\mathbf{x} = (x_1, x_2)$ and $q(\mathbf{x}) := (1/4)(x_1^2 + x_2^2)$ where $\Delta q = 1$. By Green's Second Identity:

$$\int_\Omega u(\mathbf{x})d\mathbf{x} = \int_\Omega u(\mathbf{x})\Delta q(\mathbf{x})d\mathbf{x} = -2\int_\Omega q(\mathbf{x})d\mathbf{x} - \int_{\partial\Omega} \frac{\partial u}{\partial n}(\mathbf{s})q(\mathbf{s})d\mathbf{s}$$

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$$= -\frac{1}{8} \int_0^{2\pi} r(\phi)^4 d\phi - \int_{\partial\Omega} \frac{\partial u}{\partial n}(\mathbf{s}) q(\mathbf{s}) d\mathbf{s}$$

Conversion to Laplace Equation

Let $v(\mathbf{x}) := -(1/2)(x_1^2 + x_2^2)$ where $\Delta v = -2$. Deconstruct u:

$$u := v + w$$

such that:

$$u = v + w = 0 \rightarrow w = -v \text{ on } \Omega$$
$$\Delta u = \Delta v + \Delta w = -2 + \Delta w = -2 \rightarrow \Delta w = 0 \text{ on } \partial\Omega$$

Solve for w under Laplace conditions.

Solve by Second Layer Potential

Analytical solution for Laplace Equation:

$$G(\mathbf{x}-\mathbf{y}) = -\frac{1}{2\pi}\log(\mathbf{x}-\mathbf{y})$$

$$\nabla_y G(\mathbf{x}-\mathbf{y})\cdot \mathbf{n_y} = \frac{1}{2\pi(\mathbf{x}-\mathbf{y})}\frac{\langle \mathbf{n_y}, \mathbf{x}-\mathbf{y}\rangle}{(\mathbf{x}-\mathbf{y})}$$

Let double layer potential:

$$D\sigma(\mathbf{x}) = \frac{1}{2\pi}\int_{\partial\Omega}\frac{\langle \mathbf{n_y}, \mathbf{x}-\mathbf{y}\rangle}{\|\mathbf{x}-\mathbf{y}\|^2}\sigma(\mathbf{y})d\mathbf{y}$$

$$w(\mathbf{x}) = D\sigma(\mathbf{x})$$

$$\frac{\partial w}{\partial n}(\mathbf{x}) = D'\sigma(\mathbf{x})$$

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What is $\sigma(\mathbf{x})$?

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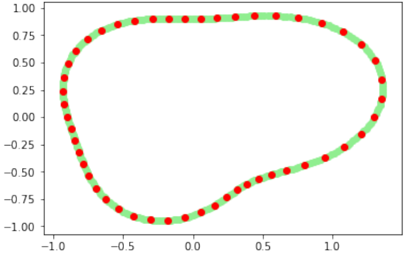
What is $\sigma(\mathbf{x})$?

Discretization of $\partial\Omega$ with Boundary Element Method

Poking the Potato / Solving for $\sigma(x)$

Discretize $\partial\Omega$ into n points: $\mathbf{x_1}, \mathbf{x_2}, \ldots, \mathbf{x_n}$ and boundaries $\partial\Omega_1, \partial\Omega_2, \ldots, \partial\Omega_n$:



$$\begin{bmatrix} \sigma(x_1)/2 + D\sigma(x_1) \\ \sigma(x_2)/2 + D\sigma(x_2) \\ \vdots \\ \sigma(x_n)/2 + D\sigma(x_n) \end{bmatrix} = \begin{bmatrix} & I/2 + D & \end{bmatrix} \begin{bmatrix} \sigma(x_1) \\ \sigma(x_2) \\ \vdots \\ \sigma(x_n) \end{bmatrix} = \begin{bmatrix} -v(x_1) \\ -v(x_2) \\ \vdots \\ -v(x_n) \end{bmatrix}$$

Coming back to Torsion Rigidity...

$$v(\mathbf{x}) = -(1/2)(x_1^2 + x_2^2) \rightarrow \frac{\partial v}{\partial n}(\mathbf{x}) = (-x_1, -x_2) \cdot \mathbf{n_x}$$

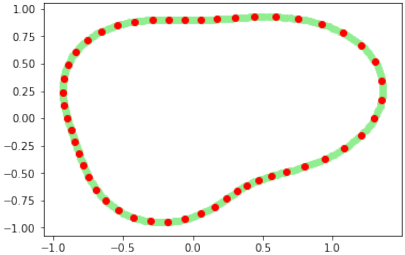
$$w(\mathbf{x}) = D\sigma(\mathbf{x}) \rightarrow \frac{\partial w}{\partial n}(\mathbf{x}) = \frac{\partial D}{\partial n}\sigma(\mathbf{x}) = \frac{\partial D}{\partial \mathbf{x}}\sigma(\mathbf{x}) \cdot \mathbf{n_x}$$

$$u(\mathbf{x}) = v(\mathbf{x}) + w(\mathbf{x}) \rightarrow \frac{\partial u}{\partial n}(\mathbf{x}) = \frac{\partial v}{\partial n}(\mathbf{x}) + \frac{\partial w}{\partial n}(\mathbf{x})$$

$$T(\Omega) = -\frac{1}{8}\int_0^{2\pi} r(\phi)^4 d\phi - \int_{\partial\Omega} \frac{\partial u}{\partial n}(\mathbf{s})q(\mathbf{s})\mathbf{ds}$$

$$\nabla T(\Omega) = \int_0^{2\pi} \nabla r(\phi) r(\phi) \left(\frac{\partial u}{\partial n}(\phi)\right)^2 d\phi$$

Approximating boundary integral equations



$$\int_{\partial\Omega} \frac{\partial u}{\partial n}(\mathbf{s})q(\mathbf{s})\mathbf{ds} = \sum_{k=1}^{n} \int_{\partial\Omega_k} \frac{\partial u}{\partial n}(\mathbf{s})q(\mathbf{s})\mathbf{ds}$$

$$= \sum_{k=1}^{n} \int_{-1}^{1} \frac{\partial u}{\partial n}(\mathbf{s}(t))q(\mathbf{s}(t))|\mathbf{s}'(t)|dt$$

Or any other numerical integration techniques given n observations of $\frac{\partial u}{\partial n}$ over boundary $\partial\Omega$.

Back to First Order Gradient Descent

$$\begin{aligned}\nabla L_\Omega(\Omega, \lambda) &= \nabla_{a_0,\ldots,b_N} L(a_0, a_1, b_1, \ldots, a_N, b_N, \lambda_V, \lambda_T, \lambda_x) \\ &= -\nabla B(\Omega) + \lambda_T \nabla T(\Omega) + \lambda_V \nabla V(\Omega) + \lambda_x \cdot \nabla \hat{x}(\Omega)\end{aligned}$$

$$\begin{aligned}\nabla L_\lambda(\Omega, \lambda) &= \nabla_{\lambda_V,\lambda_T,\lambda_x} L(a_0, a_1, b_1, \ldots, a_N, b_N, \lambda_V, \lambda_T, \lambda_x) \\ &= (T(\Omega) - T_0, V(\Omega) - V_0, \hat{x}(\Omega))\end{aligned}$$

$$\begin{aligned}\Omega_{k+1} &= \{a_0, a_1, b_1, \ldots, a_N, b_N\}_{k+1} \\ &= \{a_0, a_1, b_1, \ldots, a_N, b_N\}_k - c\nabla_\Omega L(\Omega, \lambda)\end{aligned}$$

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$$\begin{aligned}\nabla L_\lambda(\Omega,\lambda) &= \nabla_{\lambda_V,\lambda_T,\lambda_x} L(a_0,a_1,b_1,\ldots,a_N,b_N,\lambda_V,\lambda_T,\lambda_x)\\ &= (T(\Omega)-T_0, V(\Omega)-V_0, \hat{x}(\Omega))\end{aligned}$$

$$\begin{aligned}\Omega_{k+1} &= \{a_0,a_1,b_1,\ldots,a_N,b_N\}_{k+1}\\ &= \{a_0,a_1,b_1,\ldots,a_N,b_N\}_k - c\nabla_\Omega L(\Omega,\lambda)\end{aligned}$$

$$\lambda_{k+1} = \lambda_k + c\nabla_\lambda L(\Omega,\lambda)$$

That completes one iteration of the method. Do it again.

Geometric Results

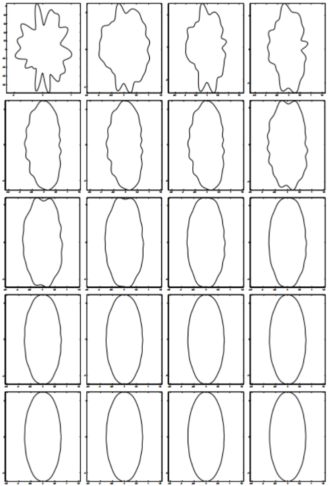

FIGURE 3 Resulting domains with respect to Problem (P2) computed by the Quasi–Newton method for the penalty functional.

Optimal Solution

- If $2\pi T_0 > V_0^2$, then no solution exists.
- Otherwise, the optimal shape Ω^* and Lagrange multiplier λ^* is given by:

$$\Omega^* := x^2 + ay^2 = b$$

where

$$b = \frac{V_0\sqrt{a}}{\pi} \qquad \sqrt{a} = \frac{V_0^2 - \sqrt{V_0^4 - 4\pi^2 T_0^2}}{2\pi T_0}$$

$$\lambda_V^* = \frac{V_0}{\pi\sqrt{a}(1-a)} \qquad \lambda_T^* = -\frac{(1+a)^2}{4a(1-a)} \qquad \lambda_x^* = (0,0)$$

- Optimal value for $B(\Omega^*) = \frac{\pi b^2}{4a^{3/2}}$