Shape Optimization with PDE constraints and Boundary Element Methods by Example
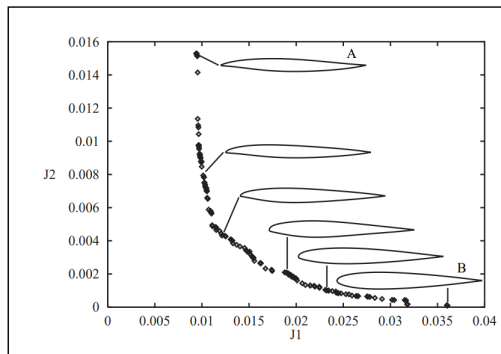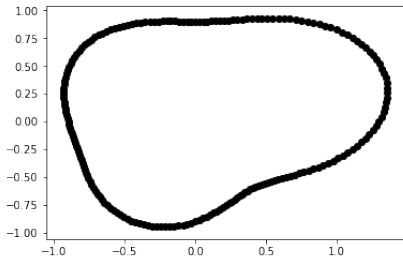
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What is Shape Optimization?

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 $g(\Omega) = c$ $h(\Omega) \leq d$

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

- 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

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

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$$= -B(\Omega) + \lambda_T(T(\Omega) - T_0) + \lambda_V(V(\Omega) - V_0) + \lambda_x \cdot \hat{x}(\Omega)$$

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

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

Formulate integrals involving Ω

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

First Order / Gradient Descent Method

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

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

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

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

Solve by Second Layer Potential

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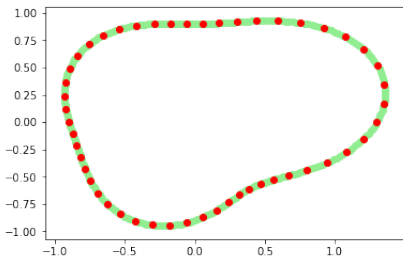
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What is $\sigma(\mathbf{x})$?

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 $\partial\Omega_1, \partial\Omega_2, \ldots, \partial\Omega_n$:

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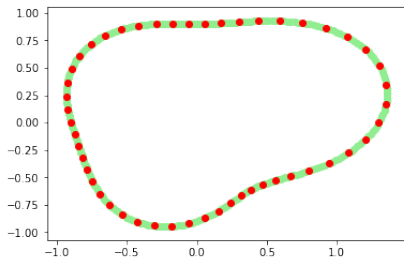\vdots \\
-v(x_n)
\end{bmatrix}
$$

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

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

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

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

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

Back to First Order Gradient Descent

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That completes one iteration of the method. Do it again.
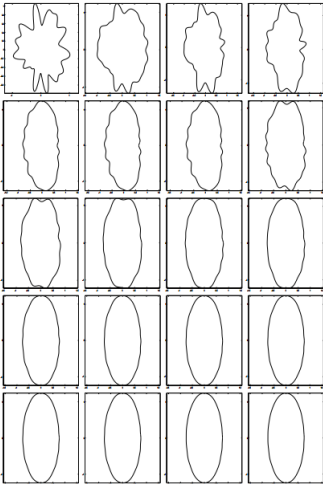
122   K. EPPLER AND H. HARBRECHT

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