Céa's Method for PDE-constrained shape optimization

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Consider a PDE-constrained shape optimization problem with governing PDE such as the Poisson equation

$$\begin{array}{rcll} \Delta u & = & f & \text{on} \quad \Omega \\ u & = & g & \text{on} \quad \partial\Omega \end{array} \tag{1}$$

where the domain of interest Ω is a subset of some larger domain $\mathcal{M}$ (for example, perhaps $\mathcal{M} = \mathbb{R}^n$). As a model problem, suppose we also have a cost functional which we wish to minimize with the form

$$J(\Omega) := \int_\Omega j(u(x))\, dx \tag{2}$$

where u is the solution to Equation 1 on Ω and $j : \mathbb{R} \to \mathbb{R}_{\geq 0}$ is a pointwise cost functional, such as $j(u) = u^2$.

In such a setting, we consider the optimization variable to be the choice of domain Ω, and seek an optimal $\Omega \subset \mathcal{M}$ which minimizes J. We will typically solve such problems using iterative descent schemes, so the primary challenge is to state the *shape derivative* of J with respect to changes in Ω.

Any perturbation of Ω can be modeled as an outward normal motion of the boundary $\theta : \partial\Omega \to \mathbb{R}$. We can then consider the derivative $\frac{\partial}{\partial\Omega} J$, i.e. how much $J(\Omega)$ changes due to the motion of its boundary. Equivalently, the directional derivative $D_\theta J$ gives the change in $J(\Omega)$ due to a particular boundary motion θ. The remainder of this document gives a recipe for D_θ using a technique known as Céa's method [1], which leverages Lagrange multipliers. For the sake of brevity, we'll avoid mentioning the relevant function spaces, but be warned that these details are nontrivial. Additionally, note that the particular form of the constraint and cost function above are merely for illustrative purposes in this document; the strategy followed here can be applied to a broad range of problems.

Notationally, in all of the integrals below we'll drop the dx and implicitly integrate with respect to the volume element of Ω or $\partial\Omega$ as appropriate.

Unconstrained Shape Derivative

To begin, consider an *unconstrained* shape derivative. We present these equations without derivation, because geometrically they are very intuitive.

Given a fixed function $\phi : \mathcal{M} \to \mathbb{R}$ (which is independent of Ω)

$$D_\theta \int_\Omega \phi = \int_{\partial\Omega} \phi\,\theta. \tag{3}$$

Geometrically, if we grow our integration domain Ω, the change in the integral is determined by the amount of "stuff" passing under the expanding boundary. Recall that θ denotes a boundary motion of Ω in the outward normal direction.

Similarly, the shape derivative of a boundary integral is given by

$$D_\theta \int_{\partial\Omega} \phi = \int_{\partial\Omega} \left(\frac{\partial \phi}{\partial n} + \kappa \phi \right) \theta \tag{4}$$

where κ denotes the curvature of $\partial\Omega$.

Geometrically, the first partial term corresponds to the boundary moving to a region where ϕ is larger or smaller. The second κ term corresponds to the boundary getting longer: in general the length of a curve moving in its normal direction at unit speed will change at a rate κ.

These two equations are our primary tools, allowing us to evaluate shape derivatives of integrals over a function ϕ with respect to a change in the integration domain Ω. However, they do not account for constraints as in PDE-constrained problems, so we will now use Lagrange multipliers to convert the constrained problem to an unconstrained problem so that we may apply these relationships.

Lagrange Multipliers and the Shape Derivative

To express our problem in the usual language of Lagrange multipliers, we expand the optimization to explicitly include u as an unknown, along with a corresponding PDE constraint. Rather than $J(\Omega)$, we now write $J(\Omega, u)$ to indicate that J is defined for any choice of u. For our model Poisson problem, this becomes

$$\min_{\Omega, u} J(\Omega, u) \qquad \text{such that} \qquad \begin{array}{rcll} \Delta u & = & f & \text{on} \quad \Omega \\ u & = & g & \text{on} \quad \partial\Omega. \end{array}$$

Now, we can generally introduce Lagrange multipliers which encode the constraints. The particular form of these multipliers will depend on the PDE and boundary conditions of interest. For our model problem we introduce two Lagrange multipliers $p : \mathcal{M} \to \mathbb{R}$ and $\lambda : \partial\Omega \to \mathbb{R}$, with the corresponding Lagrangian

$$\mathcal{L}(\Omega, u, p, \lambda) := J(\Omega, u) + \int_\Omega p(\Delta u - f) + \int_{\partial\Omega} \lambda(u - g). \tag{5}$$

using integral may be = 0 but each point difference may not be 0, weak ?

As usual with Lagrange multipliers, the constraints of our original problem are satisfied at any critical point of the Lagrangian (u^*, p^*, λ^*). For example, if $\frac{\partial \mathcal{L}}{\partial p} = 0$, then we must have that $\Delta u - f = 0$, and thus the Poisson constraint is satisfied.

Notice that if $(\Omega, u^*, p^*, \lambda^*)$ is a critical point, the value of the Lagrangian is exactly the value of the cost functional

$$\mathcal{L}(\Omega, u^*, p^*, \lambda^*) = J(\Omega),$$

and the constraints are satisified by definition. We can then expand the shape derivative of J in terms of the total derivative of $\mathcal{L}$ as

$$\frac{\partial}{\partial\Omega} J(\Omega) = \frac{d}{d\Omega} \mathcal{L}(\Omega, u^*(\Omega), p^*(\Omega), \lambda^*(\Omega)) = \frac{\partial \mathcal{L}}{\partial\Omega} + \frac{\partial \mathcal{L}}{\partial u}\frac{\partial u^*}{\partial\Omega} + \frac{\partial \mathcal{L}}{\partial p}\frac{\partial p^*}{\partial\Omega} + \frac{\partial \mathcal{L}}{\partial \lambda}\frac{\partial \lambda^*}{\partial\Omega}.$$

Because $(\Omega, u^*, p^*, \lambda^*)$ is a critical point of the Lagrangian, this expression greatly simplifies. The partial derivatives with respect to these functions are all zero by definition, and we have

$$\frac{\partial}{\partial\Omega} J(\Omega) = \frac{\partial \mathcal{L}}{\partial\Omega} + \cancelto{0}{\frac{\partial \mathcal{L}}{\partial u}}\frac{\partial u^*}{\partial\Omega} + \cancelto{0}{\frac{\partial \mathcal{L}}{\partial p}}\frac{\partial p^*}{\partial\Omega} + \cancelto{0}{\frac{\partial \mathcal{L}}{\partial \lambda}}\frac{\partial \lambda^*}{\partial\Omega} = \frac{\partial \mathcal{L}}{\partial\Omega}(\Omega, u^*, p^*, \lambda^*).$$

Thus, at a critical point $(\Omega, u^*, p^*, \lambda^*)$, the shape derivative of the unconstrained Lagrangian is exactly the shape derivative of the constrained cost functional. Therefore, applying our rules for unconstrained shape derivatives from Equations 3 and 4 to $\mathcal{L}$ will yield the shape derivative $D_\theta \mathcal{L} = D_\theta J$. The final section below walks through this computation for our model Poisson-constrained problem, first finding expressions for the Lagrange multipliers at a critical point, then evaluating their unconstrained shape derivative.

Critical Point of the Model Problem

Recall that the Lagrangian for the model problem is given in Equation 5. We now determine explicit expressions for the critical point u^*, p^*, λ^* on a domain Ω by considering directional derivatives along various carefully-chosen directions.

First, let's establish a useful identity. On a domain without boundary, the Laplace operator is simply self-adjoint, i.e. $\int_\Omega a\Delta b = \int_\Omega b\Delta a$. More generally, on a domain with boundary we can apply Green's formula twice to see that for any two functions a, b we have

$$\int_\Omega a\Delta b = \int_\Omega \nabla a \cdot \nabla b - \int_{\partial\Omega} a\frac{\partial b}{\partial n} = \int_\Omega b\Delta a - \int_{\partial\Omega} a\frac{\partial b}{\partial n} + \int_{\partial\Omega} b\frac{\partial a}{\partial n}. \tag{6}$$

Note that the signs in this expression depend on the sign convention for the Laplace operator; throughout this document we use the positive-definite Laplacian common in geometry.

We now evaluate the partial derivatives of $\mathcal{L}(\Omega, u, p, \lambda)$ with respect to u, p, and λ. We use notation like $\frac{\partial\mathcal{L}}{\partial u}(v)$ to denote the derivative of $\mathcal{L}$ with respect to u only, evaluated at (Ω, u, p, λ) along the direction $du = v$ to yield a scalar.

The derivative of $\mathcal{L}$ with respect to u in a direction v is given by

$$\begin{aligned} \frac{\partial\mathcal{L}}{\partial u}(v) &= \int_\Omega j'(u)v + \int_\Omega p\Delta v + \int_{\partial\Omega} \lambda v \\ &= \int_\Omega j'(u)v + \int_\Omega v\Delta p - \int_{\partial\Omega} p\frac{\partial v}{\partial n} + \int_{\partial\Omega} v\frac{\partial p}{\partial n} + \int_{\partial\Omega} \lambda v. \end{aligned} \tag{7}$$

Here we have used $j'(u)$ to denote the ordinary derivative of a pointwise function (e.g. if $j(u) = u^2$, $j'(u) = 2u$). The derivative of $\mathcal{L}$ with respect to p in a direction q is given by

$$\frac{\partial\mathcal{L}}{\partial p}(q) = \int_\Omega q(\Delta u - f). \tag{8}$$

The derivative of $\mathcal{L}$ with respect to λ in a direction μ is given by

$$\frac{\partial\mathcal{L}}{\partial \lambda}(\mu) = \int_{\partial\Omega} \mu(u - g). \tag{9}$$

At a critical point, we must have that the directional derivative vanishes along *all* directions, and thus each of the directional derivative expressions above must vanish for *all* choices of (v, q, μ). We can now consider some carefully chosen directions to determine the values of (u^*, p^*, λ^*).

1. Consider $\frac{\partial\mathcal{L}}{\partial p}(q)$ for q with $q = 0$ on $\partial\Omega$.

$$\frac{\partial\mathcal{L}}{\partial p}(q) = 0 = \int_\Omega q(\Delta u - f) \quad \Longrightarrow \quad \Delta u^* = f \quad \text{on} \quad \Omega.$$

2. Consider $\frac{\partial\mathcal{L}}{\partial \lambda}(\mu)$ for any μ.

$$\frac{\partial\mathcal{L}}{\partial \lambda}(\mu) = 0 = \int_{\partial\Omega} \mu(u - g) \quad \Longrightarrow \quad u^* = g \quad \text{on} \quad \partial\Omega.$$

3. Consider $\frac{\partial \mathcal{L}}{\partial u}(v)$ for v with $v = 0$ and $\frac{\partial v}{\partial n} = 0$ on $\partial\Omega$ (delta distributions on the interior are one possible such choice of v).

$$\frac{\partial \mathcal{L}}{\partial u}(v) = 0 = \int_{\Omega} j'(u)v + \int_{\Omega} v\Delta p \cancelto{0}{- \int_{\partial\Omega} p\frac{\partial v}{\partial n} + \int_{\partial\Omega} v\frac{\partial p}{\partial n} + \int_{\partial\Omega} \lambda v} \quad \Longrightarrow \quad \Delta p^* = -j'(u)$$

Now that we know $\Delta p^* = -j'(u)$, the first two integrals will cancel to 0 in all subsequent expressions.

4. Consider $\frac{\partial \mathcal{L}}{\partial u}(v)$ for v with $\frac{\partial v}{\partial n} = 0$

$$\frac{\partial \mathcal{L}}{\partial u}(v) = 0 = \cancelto{0}{\int_{\Omega} j'(u)v + \int_{\Omega} v\Delta p} - \cancelto{0}{\int_{\partial\Omega} p\frac{\partial v}{\partial n}} + \int_{\partial\Omega} v\frac{\partial p}{\partial n} + \int_{\partial\Omega} \lambda v \quad \Longrightarrow \quad \lambda^* = \frac{\partial p}{\partial n}$$

Now that we know $\lambda^* = \frac{\partial p}{\partial n}$, the second two boundary integrals will cancel to 0 in all subsequent expressions.

5. Consider $\frac{\partial \mathcal{L}}{\partial u}(v)$ for general v.

$$\frac{\partial \mathcal{L}}{\partial u}(v) = 0 = \cancelto{0}{\int_{\Omega} j'(u)v + \int_{\Omega} v\Delta p} - \int_{\partial\Omega} p\frac{\partial v}{\partial n} + \cancelto{0}{\int_{\partial\Omega} v\frac{\partial p}{\partial n} + \int_{\partial\Omega} \lambda v} \quad \Longrightarrow \quad p^* = 0 \quad \text{on} \quad \partial\Omega.$$

In summary, for any fixed Ω the unique critical point in the other unknowns of the Lagrangian $\mathcal{L}(\Omega, u, p, \lambda)$ is given by

$$\begin{array}{rclll} \Delta u^* & = & f & \text{on} & \Omega \\ u^* & = & g & \text{on} & \partial\Omega \end{array} \qquad \begin{array}{rclll} \Delta p^* & = & -j'(u^*) & \text{on} & \Omega \\ p^* & = & 0 & \text{on} & \partial\Omega \end{array} \qquad \lambda^* = \frac{\partial p}{\partial n}. \tag{10}$$

Because the constrained shape derivative of J is exactly the shape derivative of $\mathcal{L}$, we apply the formulas for the unconstrained shape derivative to $\mathcal{L}$ and get

$$D_\theta J(\Omega) = D_\theta \mathcal{L}(\Omega, u^*, p^*, \lambda^*) = \int_{\partial\Omega} \left(j(u^*) - \lambda\left(\frac{\partial u^*}{\partial n} - \frac{\partial g}{\partial n}\right) \right) \theta \; ds = \int_{\partial\Omega} \left(j(u^*) - \frac{\partial p^*}{\partial n}\left(\frac{\partial u^*}{\partial n} - \frac{\partial g}{\partial n}\right) \right) \theta \; ds. \tag{11}$$

This expression gives the shape derivative for the PDE-constrained problem. To evaluate the shape derivative of $J(\Omega)$ at any given domain Ω, we first compute (u^*, p^*, λ^*) according to Equation 10, then evaluate the expression above. Equipped with this derivative, we can (for instance) perform L_2 gradient descent on $J(\Omega)$ by iteratively evaluating the shape derivative and stepping the boundary of Ω in the outward normal direction with velocity given by the shape derivative.

This method demonstrates a general procedure for evaluating shape derivatives: first defining the Lagrangian, and then finding expressions for the values of the Lagrange multipliers at a critical point and taking their unconstrained shape derivative. The process can be generalized in several ways, with additional energy terms, boundary conditions, or other PDEs.

References

[1] Jean Céa. 1986. Conception optimale ou identification de formes, calcul rapide de la dérivée directionnelle de la fonction coût. *RAIRO-Modélisation mathématique et analyse numérique* (1986).