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 $\mathcal{M}$. As a model problem, suppose we also have a cost functional which we wish to minimize with the form

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

for $j : \mathbb{R} \to \mathbb{R}^{\geq 0}$.

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 then ask for the derivative $\frac{\partial}{\partial \Omega}$ as a boundary motion, or equivalently the directional derivative D_θ in a direction θ. The remainder of this document gives a recipe for this derivative using a technique known as Céa's method, 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.

Unconstrained Shape Derivative

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

Given a known 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, 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 change in the integral comes from the boundary moving to a region where ϕ is larger/smaller (the partial term), as well as the boundary curve getting longer (the curvature term).

These two equations are our primary tools, allowing us to evaluate derivatives 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. For our model Poisson problem, this becomes

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

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

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

As usual with Lagrange multipliers, at any *critical point* of the Lagrangian (denoted here by u^*, p^*, λ^*), the constraints of our original problem are satisfied. E.g, 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 for any Ω, at a corresponding critical point (where the constraints are necessarily satisified), the value of the Lagrangian is exactly the value of the cost functional

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

We can then expand the shape derivative of J in terms of the total derivative of $\mathcal{L}$ as

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

Now, because (u^*, p^*, λ^*) are 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 (u^*, p^*, λ^*), the shape derivative of the unconstrained Lagrangian is exactly the shape derivative of the constrained cost functional. We can then conclude Céa's method by applying our rules for unconstrained shape derivatives from Equations 3 and 4 to $\mathcal{L}$ to yield the shape derivative $D_\theta\mathcal{L} = D_\theta J$.

To apply this method to any particular problem, the primary burden is to define the Lagrangian and find and expression for the values of the Lagrange multipliers at a critical point. The final section below walks through this computation for our model Poisson-constrained problem.

Critical Point of the Model Problem

Recall that the Lagrangian for the model problem is

$$\mathcal{L}(\Omega, u, p, \lambda) := J(\Omega, u) + \int_{\Omega} p(\Delta u - f) + \int_{\partial\Omega} \lambda(u - g). \tag{6}$$

We now determine explicit expressions for the critical point u^*, p^*, λ^* by considering directional derivatives along various directions.

First, let's establish a useful identity. The Laplace operator is not simply self-adjoint on domains with boundary, but by applying Green's formula twice we see that for any two functions a, b

$$\int_{\Omega} a\Delta b = \int_{\Omega} \nabla a \cdot \nabla b - \int_{\partial\Omega} a\frac{\partial b}{\partial n} = \int_{\Omega} b\Delta a - \int_{\partial\Omega} a\frac{\partial b}{\partial n} + \int_{\partial\Omega} b\frac{\partial a}{\partial n}. \tag{7}$$

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

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial u}(v) &= \int_{\Omega} j'(u)v + \int_{\Omega} p\Delta v + \int_{\partial\Omega} \lambda v \\ &= \int_{\Omega} j'(u)v + \int_{\Omega} v\Delta p - \int_{\partial\Omega} p\frac{\partial v}{\partial n} + \int_{\partial\Omega} v\frac{\partial p}{\partial n} + \int_{\partial\Omega} \lambda v \end{aligned}\tag{8}$$

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

$$\frac{\partial \mathcal{L}}{\partial p}(q) = \int_{\Omega} q(\Delta u - f). \tag{9}$$

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

$$\frac{\partial \mathcal{L}}{\partial \lambda}(\mu) = \int_{\partial\Omega} \mu(u - g). \tag{10}$$

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).

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

   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

$$\begin{array}{lllllllll} \Delta u^* & = & f & \text{on} & \Omega & \qquad \Delta p^* & = & -j'(u^*) & \text{on} \quad \Omega \\ u^* & = & g & \text{on} & \partial\Omega & \qquad p^* & = & 0 & \text{on} \quad \partial\Omega \qquad \lambda^* = \frac{\partial p}{\partial n}. \end{array} \tag{11}$$

Now, because the constrained shape derivative of J is exactly the shape derivative of $\mathcal{L}$, we apply the formula for the unconstrained shape derivative to see

$$D_\theta J(\Omega) = D_\theta \mathcal{L}(\Omega, u^*, p^*, \lambda^*) = \int_{\partial\Omega} \left(j(u^*) - \lambda(\frac{\partial u^*}{\partial n} - \frac{\partial g}{\partial n}) \right) \theta \; ds = \int_{\partial\Omega} \left(j(u^*) - \frac{\partial p^*}{\partial n}(\frac{\partial u^*}{\partial n} - \frac{\partial g}{\partial n}) \right) \theta \; ds. \tag{12}$$

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 11, then evaluate the expression above. The process of this derivation can be generalized in several ways, with additional energy terms, boundary conditions, or other PDEs.