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Hadamard incomplete sensitivity and shape optimization*

by

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Abstract: The paper discusses incomplete sensitivity evaluations for shape optimization problems. It also shows how reduced order models can be introduced to extend the validity domain of the approach.

Keywords: Hadamard boundary condition, shape optimization, incomplete sensitivity, robustness, multi-criteria, unsteady, turbomachinery.

1. Introduction

For gradient-based shape optimization methods, it is necessary to have an estimation of the derivatives of the discrete cost function with respect to control parameters. When the number of control parameters is large, an adjoint equation is necessary (see Pironneau, 1984; Jameson, 1994, and Giles, 1997). It is tempting to use a discretization of the adjoint equation of the continuous problem; this, however, would not account for the discretization errors of the numerical schemes (like numerical dissipation for instance). Automatic differentiation produces the exact derivatives of the discrete cost function. Moreover, in reverse mode, the cost of this evaluation is independent of the number of control parameters as for a standard adjoint method. But, practical issues remain for large codes.

In multi-criteria optimization sensitivity analysis it is important to discriminate between Pareto points and this even if a gradient free approach is used. Indeed, the knowledge of sensitivity permits to qualify various points of a Pareto front from the point of view of robustness: two points on a Pareto front can be compared if one considers the sensitivity of the functional with respect to the independent variables which are not control parameter. The robust optimum is the one with lowest sensitivity.

Also, sensitivity evaluation is important, because often in simulations information on the uncertainties regarding the results is more important than the results themselves. For instance, it is essential to be able to identify dominant

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independent variables in a system. As these will need more accurate monitoring, precise measurements should be provided for them.

This paper is devoted to the concept of incomplete sensitivity in shape optimization. The aim is to avoid the linearization of the state equation. We will see that sometimes this needs a reformulation of the initial problem.

2. Shape optimization

For the design of a shape S, consider a general situation with a geometrical design or control variable x fixing $S(x)$, auxiliary geometrical parameters $q(x)$ (mesh related information), a state variable $u(q(x))$ solution of some state equation $F(u(q(x))) = 0$ and finally a cost function for optimization $J(x, q(x), u(q(x)))$:

$$J : x \to q(x) \to u(q(x)) \to J(x, q(x), u(q(x))). \tag{1}$$

The derivative of J with respect to x is:

$$\nabla_x J = J_x + J_q q_x + J_u u_q q_x. \tag{2}$$

The major part of the computing time of this evaluation is due to $u_q q_x$ in the last term. The classical approach is by adjoint variable where the last term becomes:

$$J_u u_q q_x = \left(J_u (F_u)^{-1}\right) F_q q_x = v F_q q_x$$

where v is solution of $vF_u = J_u$. But, $F_q q_x = F_x$ equals zero except along the shape where it describes the dependency of the boundary conditions on the shape with respect to shape variations. This remark is central for the development of low complexity computational strategies for the gradient. In particular, it means that if the parameterization is chosen such that $F_x \sim 0$, computing the adjoint variable v is useless. For instance, a typical situation with fluid flows is with zero normal pressure gradient along the shape and admissible shape variation normal to the shape.

3. A model problem

Let us start with a simple model problem. Consider as cost function $J = \epsilon^n u_y(\epsilon)$ and as state equation the following Poisson equation (taking $|\epsilon| << 1$)

$$-u_{yy} = 1, \quad \text{on} \quad]\epsilon, 1[\quad u(\epsilon) = 0, \quad u(1) = 0$$

which has as solution $u(y) = -y^2/2 + (\epsilon + 1)y/2 - \epsilon/2$.
This is a case of a function which has a strong geometrical element and a weak dependence on the geometry via the state u. The gradient of J with respect to ϵ is given by

$$J_\epsilon(\epsilon) = \epsilon^{n-1}(n u_y(\epsilon) + \epsilon u_{y\epsilon}(\epsilon)) = \frac{\epsilon^{n-1}}{2}(-n(\epsilon - 1) - \epsilon).$$

The second term between parenthesis, $-\epsilon$, is the state linearization contribution which is neglected in incomplete sensitivities. We can see that the sign of the gradient is always correct and the approximation is better for large n.

4. Hadamard equivalent boundary condition

Above, we mentioned the normal pressure boundary condition. Another important condition is slip or non penetration condition. The Hadamard slip boundary condition accounts for the effects of small shape deformations on the state and is prescribed on the un-deformed shape x^1 instead of the slip condition on the deformed shape x^2.

Denote by n_1 and n_2 the unit normal on the un-deformed and deformed shapes. On the later the slipping boundary condition reads: $u_2.n_2 = 0$ and on the former, if we suppose that the variations of the geometrical quantities dominate the physical ones:

$$u_2.n_2 \sim u_1.n_1 + u_1.(n_2 - n_1) = 0.$$

This defines an implicit relation for $u_1.n_1$, which can be implemented in an iterative resolution procedure:

$$u_1^{p+1}.n_1 = -u_1^p.(n_2 - n_1).$$

In the same way, an equivalent boundary condition can be derived for the tangential component. These relations give satisfactory results when the shape curvature and the amount of the deformation are not high (see Bardos and Pironneau, 1994, and Mohammadi and Pironneau, 2001) and indicate how incomplete sensitivities can be defined neglecting state variations in shape deformation.

Another interesting situation is when one can express the state in the domain as (denote the shape by y_s):

$$u = w(y - y_s)v(w(y - y_s)). \tag{3}$$

Suppose u must satisfy a homogeneous Dirichlet boundary condition on the shape, then w tends to zero with the distance to the shape $y - y_s$ and v is selected to satisfy the state equations. Now, sensitivity analysis for a functional such as $J = J(y_s, u)$ gives:

$$\nabla_{y_s} J = J_{y_s} + J_u(wv_{y_s} + vw_{y_s}).$$

But, $w(0) = 0$ and one knows the dependency between w and y_w. Therefore, in cases where the near-wall dependency of the solution with respect to the distance to the shape is known, the sensitivity with respect to shape variations normal to the wall can be obtained without linearizing the state equation. Wall functions for fluids give such typical dependencies.

5. Incomplete sensitivities

Continuing the analysis above, we have observed that when the shape is regular, the last term in (2) is small if J is of the form $J(x) = \int_{shape} f(x, q(x))g(u)$. In other words, it should involve a product of state by geometry quantities. In the analysis for the injection condition we have $f = n$ and $g = u$.

A middle path between full linearization of the state equation and incomplete sensitivity is to use a reduced complexity or reduced order model $\tilde{u}(x, u) \sim u(x)$ to provide an inexpensive approximation of the missing term in (2):

$$\nabla_x J = J_x + J_q q_x + J_u \tilde{u}_x \ \frac{u}{\tilde{u}}. \tag{4}$$

Reduced order models can come, for instance, from a reduction in dimension of the state equations as in wall functions (see Mohammadi and Pironneau, 1994). They can also be built through learning, assimilation and identification in parametric or non parametric models (see for example Krige, 1951; Chiles and Delfiner, 1989; Hoel, 1971; Jeong et al., 2005; Kohonen, 1995; Lindman, 1974; Mandic and Chambers, 2001; Spooner et al., 2002, and Veroy and Patera, 2005) using up-to-date techniques to minimize the curse of dimensionality in the sampling needed in building these models (see, for example, Smolyak, 1963; Bungartz and Griebel, 2004; Finkel and Bentley, 1974; Gorban et al., 2007; Jolliffe, 2002, and Kumano et al., 2006).

6. Level set method

Let us make a link between the two previous points and the level set method which is an established technique to represent moving interfaces with a tremendous dedicated literature (see Allaire et al., 2001; Peskin, 1998, and Osher and Sethian, 1998).

A parameterization of a boundary Γ by the level set method is based on the zero-level curve of a function ψ (say the signed Euclidean distance to Γ):

$$\Gamma = \{x \in \Omega \ : \ \psi(x) = 0\}, \qquad \psi(x) = \pm \inf_{y \in \Gamma} |x - y|$$

with the convention of a plus sign if $x \in \Omega$ and minus sign otherwise. Hence

$$\psi|_{\Gamma} = 0, \quad \psi|_{\mathbb{R}^d \setminus \Omega} < 0, \quad \psi_{\Omega} > 0. \tag{5}$$

When the boundary moves with velocity V by a pseudo time step $\delta\zeta$, the shape becomes:

$$\Gamma = \{x \ : \ \psi(\zeta + \delta\zeta, x + V\delta\zeta) = 0\}.$$

This motion can be described by:

$$\frac{\partial \psi}{\partial \zeta} + V \nabla \psi = 0.$$

In the context of optimization we consider $V = \nabla_\psi J \, . \, n$ where the local normal to the iso-contours of ψ is defined by $n = \nabla\psi/|\nabla\psi|$ (where ∇ is with respect to space coordinate). The variation of ψ is then given by

$$\psi_\zeta = -\nabla_\psi J |\nabla\psi|. \tag{6}$$

Decomposition (3) is particularly interesting with a level set parameterization:

$$u = w(\psi)v.$$

Consider a functional of the form:

$$J = J(\psi, u(\psi))$$

with a gradient with respect to ψ given by:

$$\nabla_\psi J = J_\psi + J_u u_\psi$$

with

$$u_\psi = w'v + w(\psi)v_\psi$$

as $w(\psi = 0) = 0$. Incomplete sensitivity $u_\psi = w'v$ is exact in this case and can be extended inside the domain if a low order model is known for v. This gradient is used in (6), but it needs regularity control. On the other hand, the loss of regularity can be useful in topology optimization (see Garreau et al., 2001) as it permits for holes to appear. In Mohammadi (2007) examples of this loss of regularity are shown for constrained shape optimization problems with level set parameterizations.

6.1. Multi-criteria problems

This is a situation where incomplete sensitivity has an edge over full gradient calculation. Suppose p functionals $j_i, i = 1, .., p$ are involved in a design problem (as the one presented below):

$$\min_x j_1(u(x)), \quad \text{such that} \quad j_j(u(x)) = 0, \quad j = 2, .., p.$$

The low-complexity of incomplete sensitivity permits to avoid use of penalty in $J = \sum_i \alpha_i j_i$. Indeed, to get J' we evaluate individual incomplete sensitivities j'_i and use a projection over the subspace orthogonal to constraints: $\{(.., j'^{\perp}_j, ..), j \neq i\}$. For instance, one can use:

$$\tilde{j}'_i = j'_i - \sum_{j \neq i} (j'_i, j'_j) j'_j$$

then $J' = \tilde{j}'_{i_{max}}$ where $i_{max} = Argmin_i \|\tilde{j}'_i\|$. With a full gradient this would have implied calculating an adjoint variable for each of the constraints $v_i F_u = (j_i)_u$.

7. Application

An important class of functionals concerns the aerodynamic force on the shape along an arbitrary direction s:

$$J = \int_{shape} [T \cdot n] \cdot s \, d\sigma \tag{7}$$

with $T = p\,I - \nu(\nabla u + \nabla u^T)$ the Newtonian stress tensor. This enters the validity domain of incomplete sensitivities.

We present the application of incomplete sensitivity concept to the design of axial blades under geometric and state constraints. Two quantities define the blade functioning: the flow rate Q and the pressure rise $\triangle p$ between in and outlet boundaries. The optimization is necessary to improve the fan performances while maintaining strong constraints such as low axial packaging and low sound level emitted. The fan efficiency is defined as:

$$\eta = \frac{Q \triangle p}{\Omega T_r} \tag{8}$$

where $T_r = \int_{shape} r\,[T \cdot n] \cdot e_\theta \, d\sigma$ is the torque and Ω the rotation rate. The problem of interest is therefore to minimize the torque T_r at given Q, Ω and volume. We would like also to increase Δp. Ω is an independent variable and is given. The volume constraint can be transformed into a boundary integral by denoting $\vec{X} = (x, y, z)^t$:

$$V = \int_\Omega 1 dv = \int_\Omega \frac{1}{3} \nabla.(\vec{X}) dv = \int_{\partial\Omega} \vec{X}.\vec{n} d\sigma.$$

But, Q and Δp are not defined on the shape and are therefore outside the application domain of incomplete sensitivity. Q is easy to enforce through the inlet velocity conditions, which can be frozen during the design. Δp, on the other hand, needs more workout to maintain. This is a typical situation where the original problem is not in the application domain of incomplete sensitivity, but can be brought in using the state equations, here the Navier-Stokes system for incompressible flows.

Consider a computation domain with the boundary in three parts: inlet Γ_i, outlet Γ_o and solid wall Γ_w. Using Stokes formula for the steady momentum equation we have:

$$\int_\Gamma (u(u.n) + T.n) d\sigma = 0.$$

A first classical approximation is to neglect viscous effects at inlet and outlet boundaries. Then, using periodicity conditions for lateral boundaries we have:

$$\int_{\Gamma_i} u(u.n) d\sigma + \int_{\Gamma_o} u(u.n) d\sigma + \int_{\Gamma_i} pn d\sigma + \int_{\Gamma_o} pn d\sigma + \int_{\Gamma_w} T n_w d\sigma = 0. \tag{9}$$

Let us denote mean value quantities at inlet and outlet boundaries by u_i, u_o, p_i, p_o. The inlet and outlet boundaries have the same length L. From the continuity equation ($\nabla.u = 0$) and due to periodicity on lateral boundaries and slip condition on the shape, we have $u_i.n_i = -u_o.n_i$.

The first component (along x axis) of (9) is therefore reduced to:

$$\triangle p = p_o - p_i = -C_x \frac{1}{2} \rho_\infty |u_\infty|^2 \frac{c}{L} \tag{10}$$

where $C_x = C_d \cos(\beta) - C_l \sin(\beta)$ is the horizontal aerodynamic force. Hence, the pressure difference between inlet and outlet boundaries can be expressed through the horizontal aerodynamic force on the blade, which is a boundary integral making possible the application of incomplete sensitivities.

This analysis has been used for blade design for geometries provided by Valeo Motors and Actuators (see Stanciu et al., 2002, and Mohammadi and Pironneau, 2001) where one observes an increase in both efficiency and pressure rise together with a decrease in torque. This makes us confident of the fact that the analysis above linking pressure rise to aerodynamic coefficients is valid, making possible the use of incomplete sensitivity in this design. In some situations, however, the geometrical derivative of the drag functional can be zero, as it is shown in a recent paper for the compressible Navier-Stokes equations in bounded domains (see Plotnikov and Sokolowski, 2010).

8. Time dependent problems

Another situation, where incomplete sensitivities bring a real relief, is for time-dependent applications. In these situations, incomplete sensitivities enable for real time sensitivity definition in the sense that the state and the sensitivities are available simultaneously without the need for solving a backward in time adjoint problem. This avoids the difficulty of intermediate states storage. Indeed, unlike in steady applications, where intermediate states can be replaced by the converged state, reducing the storage to one state, in time dependent problems one cannot make this simplification.

We distinguish two situations: when the control is stationary and when the control is time-dependent. A shape optimization problem for unsteady flows is in the first class, while an active flow control problem belongs to the second.

The problem of shape optimization for unsteady flows can be formulated as:

$$\min_{S \in O_{ad}} J(S, \{u(t, q(S)), t \in [0, T]\}) \tag{11}$$

where the state $u(t, q(S))$ varies in time, but not S. The cost function involves the state over a given time interval $[0, T]$ through, for instance:

$$J(S) = \frac{1}{T} \int_0^T j(S, q(S), u(t, q(S)))dt \tag{12}$$

where j involves instantaneous pressure based lift or drag coefficients:

$$C_d(t) = \frac{1}{\rho_\infty |\vec{u}_\infty|^2} \int_S (\vec{u}_\infty . \vec{n}) p(t, q(S)) ds,$$
$$C_l(t) = \frac{1}{\rho_\infty |\vec{u}_\infty|^2} \int_S (\vec{u}_\infty^\perp . \vec{n}) p(t, q(S)) ds,$$

where ρ_∞ and $\vec{u}_\infty$ denote reference density and velocity vector taken for external flows as far field quantities.

The gradient of J is the averaged instantaneous gradient:

$$J'(S) = \frac{1}{T} \int_0^T j'(S, q(S), u(t, q(S))) dt$$
$$= \frac{1}{T} \int_0^T (j_S + j_q q_S) + \frac{1}{T} \int_0^T j_u u_S.$$

We need to accumulate the gradient over the period $[0, T]$. The first term is the incomplete sensitivity. In case full gradient is required, then an adjoint problem is required to compute the remaining terms.

Shape optimization for unsteady flows has numerous applications. For instance, noise reduction as the radiated noise is linked to lift and drag time fluctuations.

8.1. Model problem

Let us present the incomplete sensitivity analysis on another model problem for unsteady situations. Consider the following time dependent state equation for $u(y, t), \quad -S \leq y \leq S, \quad t \geq 0$ in a infinite channel of width $2S$:

$$u_t - u_{yy} = F(S, y, t), \quad u(S, t) = u(-S, t) = 0, \tag{13}$$

with

$$F(S, y, t) = -\varepsilon\omega \sin(\omega t)(S^2 - y^2) + 2(1 + \varepsilon \cos(\omega t))$$

inducing small perturbation in time around a parabolic solution if $\varepsilon << 1$.

Indeed, the exact solution for this equation is:

$$u(y, t) = (S^2 - y^2) f(t), \qquad f(t) = (1 + \varepsilon \cos(\omega t)).$$

And consider a functional of the form:

$$j(S, t) = S^m u_y(y = S, t), \quad m \in \mathbb{N}^* \tag{14}$$

involving instantaneous state quantities. The sensitivity with respect to S is:

$$j_S(S, t) = m S^{m-1} u_y(S, t) + S^m u_{yS}(S, t). \tag{15}$$

The first term is the "instantaneous incomplete sensitivity".

As we have:

$$u_y(S,t) = -2Sf(t), \quad \text{and} \quad u_{y_S}(S,t) = -2f(t).$$

one can express the different contribution in (15):

$$j_S(S,t) = mS^{m-1}(-2Sf(t)) + S^m(-2f(t)).$$

Comparing with $-2(m+1)S^m f(t)$, one sees that the approximation of the gradient based on this incomplete sensitivity is accurate and its precision increases with m. Most important, the incomplete sensitivity has always the right sign. It is obvious that the analysis still holds if the functional involves a time integral:

$$J(S,T) = \int_{(0,T)} S^m u_y(y = S,t)\ dt.$$

Now, if the functional involves an integral over the domain:

$$J(S,T) = \int_{(0,T)\times(-S,S)} j(y,t)\ dt\ dy$$

one can still make the analysis above and see the importance of different contributions:

$$J_S(S,T) = \int_{(0,T)\times(-S,S)} (mS^{m-1}u_y(S,t) + S^m u_{y_S}(y,t))\ dt\ dy + \int_{(0,T)} [S^m u_y(y,t)]_{\pm S}\ dt.$$

Again, an incomplete evaluation of the sensitivity is accurate because $u_{y_S} = 0$. One also notices that if m is odd, the last integral vanishes, even though this integral is cheap to get as it does not involve any state sensitivity with respect to S.

Anyway, incomplete sensitivity is efficient but it only holds for special functionals.

Let us now give an example where the control depends on time as well. This is a buffeting control problem using Hadamard equivalent boundary conditions and incomplete sensitivities. We consider the flow at transonic regime over an airfoil. At this regime, the wake unsteadiness forces the shock to move up and down on the upper surface of the airfoil (details of the case are given in Mohammadi and Pironneau, 2001). We would like to provide active control by an injection/suction devices placed at mid-chord on the upper and lower surfaces. The amount of injection/suction is defined using instantaneous incomplete sensitivity for $J = (C_l)_t$ which aims at removing lift fluctuations. These are set to zero outside the support of the control:

$$\delta S(t) = -\rho \nabla J(t)\ \chi_C$$

where shape variations are linked to injection/suction by the Hadamard approximation:

$$u.n(t+\delta t) = -u.\delta n(t) + \frac{\delta S(t)}{\delta t}.n(t)$$

where $n(t)$ is the normal to the shape at time t and $\delta n(t)$ is the variation of the normal. It is shown that with this definition of control based on an injection defined through incomplete sensitivity evaluation the buffeting can be removed. The approach has an extra advantage as it also tells where control devices should be placed as sensitivity is instantaneously available everywhere along the shape.

9. Concluding remarks

Hadamard incomplete sensitivity concept has been described. As this is reduced order modelling, it has limitations and only applies to special functionals. These must involve product of state by geometry quantities and should be defined over the support of the control parameters (i.e. shape for a shape optimization problem). Aerodynamic coefficients are in this class. It has been shown how to reformulate the initial problem when not entering this validity domain. Again, this is not always possible, but when it is so, it permits to access sensitivity at zero cost. Beyond this, incomplete sensitivities are really helpful for time dependent problems (not reported here) and for multi-criteria situations avoiding the calculation of one adjoint by functional.

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