Discretized Sensitivities Are Not Derivatives

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Abstract

We consider a steady incompressible two dimensional Navier Stokes problem with a boundary parameterized by α. The flow variables (u, v, p) are implicit functions of α, presumably continuously differentiable. The flow problem is discretized and then solved. We compare the partial derivatives of the discrete flow variables, denoted by $(u^h)_\alpha$, with the discretized sensitivities $(u_\alpha)^h$ and note that these are not equal. We consider the cost of computing each quantity, and then consider situations in which discretized sensitivities might be preferable to partial derivatives; in particular, because convergence rates can be straightforwardly derived. We then consider the efficiency of minimizing a functional $\mathcal{J}(u^h, v^h, p^h)$ using $\mathcal{J}$ only, $\mathcal{J}$ and partial derivatives, $\mathcal{J}$ and discretized sensitivities, or zero finding applied to the discretized sensitivities.

1 Introduction

Consider a physical region Ω over which a set of state variables $u(x)$ are defined. The state variables will be assumed to satisfy a set of state equations $G(u(x), \alpha) = 0$ in the interior of Ω, and some set of boundary conditions $H(u(x), \alpha) = 0$ on the boundary $\partial\Omega$. Here the symbol α represents one or more problem parameters whose values are at the moment unrestricted and unspecified. If a pair of state variables $u(x)$ and parameter values α satisfy the state and boundary conditions, we call that pair *feasible*. We will assume that for any choice of values of α, a unique set of state variables $u(x, \alpha)$ can always be found so that $(u(x, \alpha), \alpha)$ is feasible. Suppose further that there is a functional $J(u(x, \alpha), \alpha)$ which evaluates the "cost" of any feasible pair of state variables and problem parameters. The term "cost" is meant to suggest that the quantity J measures something that we would like to make small. Our only means of affecting the size of J is through our choice of the parameters, and it is a natural goal to seek a set of parameters that achieve the lowest possible value of J.

We may state the following constrained minimization problem:

PROBLEM 1.1 *Find a set of parameter values α^* and a set of state variables $u(x)$ so that*

$$G(u(x), \alpha^*) = 0 \text{ for all } x \text{ in } \Omega, \tag{1}$$

$$H(u(x), \alpha^*) = 0 \text{ for all } x \text{ in } \partial\Omega, \tag{2}$$

$$J(u(x), \alpha^*) \text{ is minimized.} \tag{3}$$

We have already assumed that for any α, there exists a corresponding state variable u, which we denote by $u(x, \alpha)$, so that the pair $(u(x, \alpha), \alpha)$ is feasible. With this assumption, we may in fact treat $u(*, \alpha)$ as an implicit function of α. Hence, we may replace the previous constrained problem by the following equivalent unconstrained minimization problem:

PROBLEM 1.2 *Find a set of parameter values α^* which minimizes:*

$$\mathcal{J}(\alpha) \equiv J(u(x, \alpha), \alpha) \tag{4}$$

Efficient optimization techniques exist for this problem, but they will generally require the evaluation (or more expensive approximation) of the partial derivatives of the cost functional $\mathcal{J}$ with respect to the parameters α. Because of the implicit relationship between the state variables and parameters, these partial derivatives can be computed by the chain rule:

$$\frac{\partial \mathcal{J}}{\partial \alpha} = \frac{\partial J}{\partial u}\frac{\partial u}{\partial \alpha} + \frac{\partial J}{\partial \alpha} \tag{5}$$

The partial derivatives $\frac{\partial J}{\partial u}$ and $\frac{\partial J}{\partial \alpha}$ are usually easy to evaluate exactly; the relationship between the cost and the state variables and parameters is usually explicit and simple. But since the relationship between state variables and parameter is only implicit, the partial derivatives $\frac{\partial u_j}{\partial \alpha_i}$ require differentiating the state and boundary equations and solving the resulting linearized equations at a particular set of state and parameter values.

Especially in discrete computations, it may be easy, given a set of values α, to compute or approximate $u(x, \alpha)$, and hence to evaluate (at least approximately) $\mathcal{J}$, but impossible, impractical, or too expensive to evaluate $\mathcal{J}_\alpha$.

To optimize Problem 1.2 using an algorithm that expects cost functional derivatives J_α, there are a number of ways of handling the need for u_α:

- Approximate u_α using finite differences;
- Replace derivatives by sensitivities;
- Use an automatic differentiation scheme like ADIFOR.

Implicit differentiation of the state equation yields a related, usually linear system for the partial derivatives of the state variables with respect to the parameters:

$$G_u(u, \alpha)u_\alpha = -G_\alpha(u, \alpha) \tag{6}$$

If the partial derivatives of the cost functional with respect to the state variables can be computed, then the chain rule and the state variable partials will now yield a formula for the partials of the cost functional with respect to the parameters.

2 A Parameterized Flow Problem With Costs

We now consider a specific parameterized problem with a cost functional that is to be optimized. The two dimensional physical region is a long channel, open at both ends, with walls which are parallel except for a small bump along the bottom wall. Flow enters the channel from the left with a given profile and exits at the right. The state variables are (u, v, p), the horizontal and vertical velocities and the pressure. The state equations are the steady incompressible Navier Stokes equations:

$$-\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + Re\left(u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial p}{\partial x}\right) = 0 \tag{7}$$

$$-\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) + Re\left(u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial p}{\partial y}\right) = 0 \tag{8}$$

and the incompressible continuity equation:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{9}$$

with suitable boundary conditions that include no slip along the walls:

$$u(x, y) = v(x, y) = 0 \text{ along the walls} \tag{10}$$

3 Optimization Using Derivatives of Discretized Data

4 Optimization Using Discretization of Derivative Data

5 Causes and Effects of Discrepancies

References

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