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The effect of shocks on second order sensitivities for the quasi-one-dimensional Euler equations

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ABSTRACT

The effect of discontinuity in the state variables on optimization problems is investigated on the quasi-one-dimensional Euler equations in the discrete level. A pressure minimization problem and a pressure matching problem are considered. We find that the objective functional can be smooth in the continuous level and yet be non-smooth in the discrete level as a result of the shock crossing grid points. Higher resolution can exacerbate that effect making grid refinement counter productive for the purpose of computing the discrete sensitivities. First and second order sensitivities, as well as the adjoint solution, are computed exactly at the shock and its vicinity and are compared to the continuous solution. It is shown that in the discrete level the first order sensitivities contain a spike at the shock location that converges to a delta function with grid refinement, consistent with the continuous analysis. The numerical Hessian is computed and its consistency with the analytical Hessian is discussed for different flow conditions. It is demonstrated that consistency is not guaranteed for shocked flows. We also study the different terms composing the Hessian and propose some stable approximation to the continuous Hessian.

1. Introduction

Aerodynamic optimization problems that arise in airplane design are typically large scale and highly ill-conditioned. Such problems are slow to converge without Hessian information. First order sensitivities and the adjoint method are fundamental for gradient based optimization. They are being used by all modern Computational Fluid Dynamics (CFD) codes that have a design optimization capability. In the most typical setting, given a geometry and a set of design variables that describe changes to the geometry, the optimal design process involves repeated solutions of the flow problem, followed by the adjoint solution (first order sensitivities), which are inputs to an optimization step that modifies the geometry. The state-of-the-art practice is to use the adjoint method to compute the gradient, and quasi-Newton method to accelerate the convergence. Quasi-Newton approximates the Hessian (or its inverse) by a low rank update method (rank-2 in most cases), taking the identity matrix to be the initial guess. That choice corresponds to having the gradient as the initial search direction in the optimization process. In industrial aerodynamic design the number of design variables is in the hundreds, and there are not enough resources for more than $O(10)$ global optimization iterations, resulting in poor convergence. Therefore, we think that a better approximation of the Hessian is essential to achieve fast convergence. Such an approximation can serve as the initial guess for a quasi-Newton method.

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In [1] Betts et al. studied the benefits of having second order sensitivity information, obtained by a finite-difference method, on the convergence properties of drag minimization problem for an airfoil geometry in 2D. The conclusions were that having the Hessian provides significant performance benefits. When there is a large set of inequality constraints the benefits are even more significant since the optimizer identifies the active set of constraints earlier, a major source of slow convergence for such problems.

In Sherman et al. [2] four formulations for computing the Hessian for CFD applications using sensitivity and adjoint methods are introduced. The authors then apply these formulations using automatic-differentiation (AD) and a hand-differentiated incremental iterative method that are interwoven to produce a hybrid scheme. The study results in accurate Hessian calculation but not efficient from computational perspective. More recently Ghate and Giles [3] investigated the AD approach and provide more details on efficient implementation of the method.

Other approaches include analysis of the Hessian using local mode analysis [4,5], sparse approximations [6], direct construction [7], and approximations by neglecting various terms in the direct construction [8]. A more extensive review of the field of aerodynamic optimization and its challenges can be found in [9].

Papadimitriou and Giannakoglou [8] introduce a Hessian approximation for inverse design problems subject to the Navier–Stokes equations in which the terms that depend on the adjoint variables are neglected allowing an essentially "free" Hessian approximation when the sensitivities are available (see [8] and references therein). The resulting approximation is tested in 2D for an inverse design problem and Mach numbers up to 0.5 (shockless flow). The authors show that the approximation is effective and indeed the Hessian results in a significant convergence improvement over standard quasi-Newton methods. The neglected terms contains the second order Jacobian which can be challenging to compute in most CFD codes. These terms can be approximated using a finite-difference method or automatic differentiation, but that can increase the computational burden significantly.

In Zervogiannis et al. [10] the authors extend their work and study a total pressure loss minimization of a non-rotating cascade airfoil for turbomachinery design application and include the second order Jacobian term. In that study it was found that "some terms that were insignificant for the inverse design case have an important effect".

It is difficult to generalize these conclusions and to predict the scenario for strongly non-linear flows.

In [11] Matsuzawa and Hafez propose a shock treatment in the framework of adjoint shape optimization governed by the compressible Euler equations. The authors state that since the gradient is highly oscillatory around the shock, it must be smoothed out. In the present work it is clearly shown how the oscillatory behavior arises. In the case of a mass functional, there is no discontinuity in the functional integrand, and therefore there is no oscillatory behavior of the gradient and the optimum is reached without difficulties. Bardos and Pironneau [12,13] showed that the linearized compressible Euler equations in presence of shocks are well defined in a generalized function setting. On the other hand in [14] it is shown that the pressure matching functional is not differentiable when the target pressure and the actual pressure have a coinciding shock.

An ideal test case to study the effect of shocks on the optimization problem is the quasi-one-dimensional Euler equations. In [15] Giles and Pierce derive the adjoint solution analytically for the quasi-one-dimensional Euler equations. In [14] Arian and Iollo derive the sensitivities as well as the Hessian analytically for the minimization problems governed by the quasi-one-dimensional Euler equations. A pressure minimization problem and a pressure matching inverse problem were considered. The flow sensitivity, adjoint sensitivity, gradient, and Hessian were calculated exactly using a direct approach that is specific to the model problems. For the pressure minimization problem it was found that the Hessian exists and it contains elements with significantly larger values around the shock location. In addition, two formulations for calculating the Hessian were proposed and implemented for the given problems. Both methods can be implemented in industrial applications.

In this work we compute the Hessian numerically for two objective functions for inviscid flow modeled by the quasi-one-dimensional Euler equations in a nozzle geometry. The objective functions are pressure matching and the integral of the pressure over the nozzle length. We study the smoothness of the objective functions under shocked flow conditions, as well as the consistency of the adjoint solution, the sensitivities and the Hessian with the continuous ones. We also conduct a systematic study of the relative importance of each term composing the Hessian for different flow conditions and objective functions in order to derive a stable approximation. These issues represent the paradigm of the problems encountered in the design of aerodynamic components at transonic speeds. Hence, the analysis of this model problem is a preliminary and crucial step for the development of efficient optimization methods for complex aerodynamic configurations of interest.

The paper is organized as follows. In Section 2 we define the equations of motion and the design space. In Section 3 the effect of shocks on the smoothness of the objective function is discussed. In Section 4 the first order flow sensitivities and adjoint solution are studied for shocked flows. In Section 5 the consistency of the numerical Hessian is investigated. In Section 6 the significance of the different terms composing the Hessian in its matrix representation is studied. In Section 7 we discuss our findings for recommended approximations to the exact Hessian. Final conclusions are made in Section 8.

2. Formulation

2.1. Equations of motion

The quasi-1d steady compressible Euler equations in differential form are given by,