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, 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 Pieric derive the adjoint solution analytically for the quasi-one-dimensional Euler equations. In [14] Arian and Lollo 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,
\[ R(U, h) = -\frac{d}{dx}(hF) + \frac{dh}{dx}P = 0 \]  

(1)

with \( h \) being the channel height, \( U \) the vector of conserved variables, \( F \) the convective fluxes and the source term modeling the channel area variation. The vectors \( U, F \) and \( P \) are defined by,

\[ U = (\rho, \rho u, E)^T, \quad F = (\rho u, \rho u^2 + p, (E + p)u)^T, \quad P = (0, p, 0)^T \]  

(2)

with \( \rho \) being the density, \( p \) the pressure, \( E \) the total internal energy per unit volume and \( u \) the velocity.

For the transonic flow configuration we impose the total enthalpy and total pressure at the inlet of the domain and the static pressure at its outlet. For the supersonic cases total enthalpy, total pressure and the Mach number are imposed at the inlet.

2.2. Numerical discretization

We discretize the integral form of (1) by finite volumes with first order accuracy

\[ R_i = \frac{1}{\Delta x} \left[ h_{i+\frac{1}{2}} F_{i+\frac{1}{2}} - h_{i-\frac{1}{2}} F_{i-\frac{1}{2}} \right] + \frac{h_{i+\frac{1}{2}} - h_{i-\frac{1}{2}}}{\Delta x} P_i \]  

(3)

The interface flux is calculated according to Osher’s scheme [16]:

\[ F_{i+\frac{1}{2}}(U_l, U_r) = \frac{F(U_l) + F(U_r)}{2} - \int_{U_l}^{U_r} |A|dU \]  

(4)

with \( A \) being the Jacobian of the flux function. The integral path used in the above formulation is taken along the right eigenvectors of \( A \). The solution is approximated with piecewise constant data, hence the initial states of the Riemann problem coincide with the cell averages \( U_l = U_i \) and \( U_r = U_{i+1} \) resulting in a first order scheme.

The solution of Eq. (3) is found via a Newton method which uses a multigrid preconditioned Krylov subspace solver [17] for the linearized problem.

2.3. Finite dimension design space

We choose to solve the problem in a finite design space. The channel height, \( h(x) \), is composed of a seed height function, \( h_0(x) \), perturbed by a sum of \( N \) fixed shape basis functions, \( h_i(x) \), with the coefficients, \( a_i \), serving as the design variables:

\[ h(x) = h_0(x) + \sum_{i=1}^{N} a_i h_i(x). \]  

(5)

The channel’s seed shape, \( h_0(x) \), depicted in Fig. 1, is defined on the domain \( \Omega = [-1, 1] \), as follows: \( h_0(x) = 2 \) for \(-1 \leq x < -1/2\), \( h_0(x) = 1 + \sin^2(\pi x) \) for \(-1/2 \leq x < 1/2\), and \( h_0(x) = 2 \) for \( 1/2 < x \leq 1\).

We choose cubic B-Splines for the basis, \( h_i(x) \). Cubic B-Splines are widely used in applications and specifically in aerospace engineering. Another reason for using B-Splines is that for this study it will be useful to localize the effect of the shock wave on the Hessian and cubic B-Splines are local functions. In [14] it is shown that the perturbation of the shape must be regular enough at the shock location for the gradient and the Hessian to exist. B-splines satisfy these regularity requirements.

The B-splines basis functions are uniformly distributed starting after the throat and in the diverging part of the nozzle. The support of the basis functions \( h_i(x) = B_i^3(x) \) is compact, and it is non-zero only between the collocation points \( i - 2 \) and \( i + 2 \).

Fig. 1. The unperturbed nozzle.
and \( i + 2 \). The collocation points of such splines are \( N = 10 \) in the test cases hereafter, and they are uniformly distributed between 1/10 and 1/2, which is the interval where the geometry is perturbed.

3. Smoothness of the objective function under shocked flow

In the following we study the smoothness of the objective function under shocked flow conditions. The functionals considered are the pressure matching and the pressure minimization integrals (the latter is related with drag):

\[
I_p = \int_{-1}^{1} \frac{1}{2} (p - \bar{p})^2 \, dx \quad \text{and} \quad I_{pm} = \int_{-1}^{1} p \, dx \tag{6}
\]

The integrals are computed to a first order accuracy, that is summing piecewise constant data. The flow conditions for the cases presented below (shocked flow) are total pressure \( p^0 = 2 \) and total enthalpy \( H^0 = 4 \) at the inlet, static pressure \( p = 1.6 \) at the outlet. This choice of parameters and the initial shape guarantees the flow to be transonic and that it contains a shock at \( x = 1.14 \).

3.1. The pressure minimization problem

In Fig. 2(a) the pressure integral objective is plotted against \( x_2 \) (the second design variable) in the range \([-0.025:0.025]\). The variable \( x_2 \) is chosen since it has the strongest effects on the shock position. The objective function is plotted for three different resolution levels of the flow solution, by factors of 4: 256, 1024, and 4096 grid points. The sampling of \( x_2 \) has been chosen in order to resolve each oscillation with 10 computations as can be seen in the following. For the finest grid the range of \( x_2 \) is sampled with 1600 computations, for the medium grid 400 computations have been performed and for the coarsest grid 100 computations were sufficient in order resolve the oscillations.

Note that the resolution of the design space does not change, only that of the state variable. The curves seem to be converging to an asymptotic curve represented by the 4096 line. Although the curves look smooth, high frequency oscillations are present, as it can be seen from the derivative information.

In Fig. 2(b) and (c) the first and second derivatives of the objective function with respect to \( x_2 \) are depicted, respectively. They are calculated by second-order finite differences.

The non-smooth parts in the second derivative correspond to shock crossing grid points. As the grid refines, the oscillations become of higher and higher frequency. The wavelength of the oscillations, \( \Delta x_2 \), is decreasing by a factor of 4 as the grid refines by that same factor.

3.2. The pressure matching problem

The behavior observed for the pressure minimization objective function is exacerbated for the pressure matching objective. Fig. 2(d) depicts the objective as a function of the second design variable. Fig. 2(e) and (f) depict the first and second derivatives of the objective with respect to \( x_2 \), respectively. As before, the non-smooth parts in the second derivative correspond to shock crossing grid points. The finer the grid resolution the more oscillations are observed. Fig. 2(f) gives a glimpse of what can happen to the Hessian for design optimization problems that contain shocks, or moving discontinuities in general. Not only the frequency of the oscillations increases with grid resolution (as in the pressure minimization case), but here also the amplitude increases dramatically.

We stress that the behavior seen in Fig. 2(f) was validated by comparing a finite difference method with a term-by-term construction of the Hessian (as described in Section 5). The wild oscillations corresponding to the finest mesh (with 4096 points) should not be confused with truncation or numerical errors. These are the true second derivatives of the discrete objective functional!

Since the problem of interest is typically posed in the continuous level, and the discrete level comes as an approximation of the continuous problem, such behavior of the Hessian is clearly undesirable. In other words the discrete Hessian is not consistent with the continuous Hessian. In this case, the continuous behavior of the second derivative is closer to the coarse mesh approximation. The finer the mesh is, the further the discrete Hessian values are from the continuous one. We conclude that for transonic flow with shocks it may be more useful to approximate the Hessian on a coarse mesh; by doing that we will obtain a more accurate approximation for less CPU, two desired properties. Using the fine Hessian in this case will be counter productive and possibly lead to failure of the minimization process. Note that quasi-Newton will also be problematic here since the first derivative oscillates wildly (Fig. 2(e)). In practice, smoothing of the gradient should be considered or using the continuous adjoint approach. Another strategy is employed in Section 7, and consists in neglecting some terms in the Hessian.

3.3. Discussion: discontinuity movement on a grid

In the following we provide a simple example where we argue that the problem arises from the discrete representation of the data on a finite grid. We isolate the effect of a discontinuity moving over the grid from the numerical solution of a partial
differential equation. In order to demonstrate the effect of shock moving relative to a grid, we present an ideal case not involving a partial differential equation. Let

\[
\phi(x, \alpha, \beta) = \frac{1}{2} + \frac{1}{2} \tanh \left( \beta \frac{x - \alpha}{\Delta x} \right)
\]
This function models a discontinuity smoothed over a fixed number of grid points. The parameter \( x \) plays the role of a design variable and \( \beta \) determines the shock sharpness.

To model the pressure matching functional, we choose to examine:

\[
I(\alpha, \beta) = \int_{-1}^{1} \frac{1}{2} (\phi(x, \alpha, \beta) - 4)^2 \, dx
\]  

(8)

The integral appearing in the functional (8) is computed on a uniform grid of spacing \( \Delta x \) using a first order scheme. A higher order integration scheme does not alter the results.

Different numerical integration schemes lead to smoother or sharper shocks. This effect is hence modeled via the parameter \( \beta \). However, a shock capturing scheme will capture a shock over at least three grid points. More diffusive schemes result in smoother shocks. Two scenarios are studied, sharp and smooth discontinuities, as demonstrated in Fig. 3. Sharp corresponds to \( \beta = 2 \), and smooth corresponds to \( \beta = 1 \). When \( \beta = 2 \) the discontinuity is smeared on about 3 grid points, and when \( \beta = 1 \) on about 5 grid points. In the limit of large \( \beta \), \( I(\alpha, \beta) \) is a linear function of \( \alpha \). In this limit the exact first derivative is a constant, the second is zero. On the contrary, in Fig. 3 we observe large oscillations in the numerical first and second derivatives that are due to the abrupt change of slope and curvature taking place when the discontinuity goes through a given grid point. This is due to the representation of the data on a finite grid. For example, to get a constant first derivative with respect to \( \alpha \) in accordance with the exact result, the representation of the smoothed delta function in the vicinity of the shock should be the same while the delta function is translating. But this is of course not the case. For the second derivative this is even more severe since (the second derivative of \( \phi \) with respect to \( \alpha \)) has a large oscillation of zero average at the continuous level. But zero average at the discrete level cannot be granted as the shock moves. Also, the finer the grid, the wilder are the oscillations.

4. Analysis of the sensitivities and adjoint for shocked flow

For shockless flow the sensitivities are smooth, i.e., the solution varies continuously with a perturbation in the design variables. For shocked flow this dependence is also smooth for design variables that correspond to perturbations away from the shock. However, we find that the sensitivities behave like a delta function at the shock, when the support of the relevant design variable overlaps the shock location. The manifestation of the delta function in the discrete level is of a form of a spike at the shock location which increases without bound as the grid refines. This is consistent with the continuous level for which it can be shown that the sensitivity is equal to the delta function at the shock (the derivative of a Heaviside function equals a delta function).

In Section 4.1 we present the numerical setup used to calculate the sensitivities and the adjoint solution. In Section 4.2 we validate the numerical solution by comparing with the exact one for supersonic flow. In Section 4.3 the sensitivities are studied at the vicinity of the shock, and in Section 4.4 the discrete adjoint solution is obtained and validated against the continuous exact solution.

4.1. Calculation of the discrete sensitivities and adjoint

The core information needed for computing sensitivities and adjoint is the exact Jacobian of the numerical scheme. This is achieved by differentiating the approximate Riemann solver employed with respect to the conservative variables by hand in order to provide the building blocks \( \partial \mathbf{F}^f / \partial \mathbf{U} \) (see Eq. (4)). We write the Jacobian as

\[
\mathbf{J} = \mathbf{L} + \mathbf{D} + \mathbf{U}
\]  

(9)

Let \( \mathbf{L}_i \) be the lower block of \( \mathbf{J} \) pertinent to the \( i \)th grid point. Hence

\[
\mathbf{L}_i = \frac{\partial \mathbf{R}_i}{\partial \mathbf{U}_{i-1}} = \frac{h_{i+\frac{1}{2}}}{\Delta x} \frac{\partial \mathbf{F}_{i+\frac{1}{2}}}{\partial \mathbf{U}_{i-1}}
\]  

(10a)

and similarly

\[
\mathbf{D}_i = \frac{\partial \mathbf{R}_i}{\partial \mathbf{U}_i} = \frac{1}{\Delta x} \left[ \frac{h_{i+\frac{1}{2}}}{\Delta x} \frac{\partial \mathbf{F}_{i+\frac{1}{2}}}{\partial \mathbf{U}_i} - \frac{h_{i+\frac{1}{2}}}{\Delta x} \frac{\partial \mathbf{F}_{i-\frac{1}{2}}}{\partial \mathbf{U}_i} \right] + \frac{h_{i+\frac{1}{2}} - h_{i-\frac{1}{2}}}{\Delta x} \frac{\partial \mathbf{P}_i}{\partial \mathbf{U}_i}
\]  

(10b)

\[
\mathbf{U}_i = \frac{\partial \mathbf{R}_i}{\partial \mathbf{U}_{i+1}} = -\frac{h_{i+\frac{1}{2}}}{\Delta x} \frac{\partial \mathbf{F}_{i+\frac{1}{2}}}{\partial \mathbf{U}_{i+1}}
\]  

(10c)

In what follows we denote with \( L = \mathbf{J} \) the Jacobian and with \( L^* = \mathbf{J}^\top \) the adjoint operator in order to use the same nomenclature as in [14].

The sensitivity equation reads

\[
\frac{d \mathbf{U}}{dx_i} = \mathbf{f}_i = -\frac{\partial \mathbf{R}}{\partial x_i}
\]  

(11)
The right hand side, that contains the derivative of the residuals (3) with respect to the design variables, $a_i$, can be expressed analytically using the relationship between the channel height and the design variables given by (5). Hence the value of $f_i$ at the $j$th grid point is given by,

$$
(f_i)_{j} = \frac{1}{\Delta x} \left[ h_i(x_{j-\frac{1}{2}}) F_{j-\frac{1}{2}} - h_i(x_{j+\frac{1}{2}}) F_{j+\frac{1}{2}} \right] + \frac{h_i(x_{j+\frac{1}{2}}) - h_i(x_{j-\frac{1}{2}})}{\Delta x} P_i
$$

(12)
with $h(x)$ being the corresponding shape function evaluated at $x$.

The adjoint equation is given by,

$$ L^* v = - \frac{\partial I}{\partial \mathbf{U}} $$

(13)

The right hand side can be expressed exactly on the discrete level by hand differentiation of Eq. (6). All derivations have been cross-checked by finite-differences and Automatic Differentiation using TAPENADE [18] (see also http://tapenade.inria.fr:8080/tapenade/index.jsp).

Once the analysis problem is converged (CFD), the Jacobian $L$ is computed as described above, an LU factorization is performed using the LAPACK library. Then the same LU factorization is used to solve the $N$ sensitivity equations. Its transpose is easily formed and used for the adjoint equation.

4.2. Validation of the sensitivities $dU/dh$ for supersonic flow away from the throat

For supersonic flow conditions we have the exact solution in the form of $dU/dh$ where $h$ represents the nozzle’s shape [14]. It should be remarked that $dU/dh$ is, strictly speaking an operator. In this specific case it can be locally plotted as a derivative. In Fig. 4 a comparison with analytical results from [14] is presented for the same flow conditions. The numerical solution is obtained by using 100 shape functions between $[-1,+1]$ and the problem is discretized with 4096 cells. Sensitivities are computed and divided by the shape function $dh/dx$. All the 100 sensitivities are collapsed into one plot $dU/dh$. Consequently for given abscissa $x$ three numerical curves can be found. They correspond to the three shape functions whose support cover this point. The slightly different values can be explained by the fact that the different shape functions perturb differently the neighborhood of $x$.

4.3. Sensitivities for shocked flows

The transonic flow configuration has been investigated using 4096 grid points and ten shape functions. In Fig. 5 a sample of the sensitivities, $d\rho/dx_k$, is plotted where $x_k$ is the $k$th design variable, for $k = 4, 7, 10$. We obtain a delta function behavior.

Fig. 4. $dU/dh$ for supersonic flow; lines numerical, circles analytical.
for \( dp/d\alpha_7 \) as the corresponding shape function covers the shock position. The value of this spike is of \( O(1000) \) but the figure has been chopped in order to illustrate other details. The value increases as the grid is refined.

However, we also find that in the discrete level perturbing some of the design variables for which their support does not overlap with the shock, results in some spikes at the shock (see Fig. 5 the first and third plots corresponding to the 4th and 10th design variables). We find that the size of these spikes decreases as the mesh is refined. The peaks observed in the first and third plots of Fig. 5, at the shock location, are an effect of the change in numerical dissipation induced by the shape perturbation away from the shock.

Summarizing, we find that at the shock the discrete results are consistent with the continuous analysis by refining the grid systematically and observing that the discrete result approach the continuous one in a careful grid convergence study.

### 4.4. Adjoint solution for shocked flow

In the following we numerically compute the adjoint solution for the pressure minimization case. The adjoint is computed in the fully discrete approach by taking the transposed Jacobian of the numerical scheme as the adjoint operator. Unlike the sensitivity solutions, in the adjoint case the solution is smooth at the shock. At the throat there is a logarithmic singularity at the continuous level. The numerical adjoint solution matches the exact solution as demonstrated in Fig. 6. As the mesh refines the log singularity of the exact solution at the throat is recovered. In the continuous limit it is necessary to put an adjoint boundary condition at the shock for the adjoint problem to be well posed [19]. However, at the discrete level no such condition is necessary to implement even as the mesh is refined. The numerical viscosity used here is consistent with the inviscid limit in the sense that it vanishes at the limit of infinitely fine mesh. We speculate that, when consistent with the inviscid limit, even a small numerical viscosity compensates the lack of boundary condition. Although the continuous adjoint solution did make use of a boundary condition at the shock and the discrete solution did not, the two solutions are consistent as demonstrated in Fig. 6. This issue warrants a much deeper mathematical study that is beyond the scope of this paper.

![Fig. 5. Sensitivities of the density \( \rho \) with respect to the 4th, 7th and 10th design variables in transonic flow conditions (with a shock).](image-url)
5. Hessian derivation, implementation, and consistency

5.1. The matrix representation of the Hessian: \(O(N + 1)\) linear solutions

The mathematical derivation of two Hessian representations is detailed in [14] and is reported here for sake of completeness. We give here only the details necessary for discussing the Hessian representation that is used in this work. The first representation in [14] relies on the adjoint-sensitivities and therefore comes with a computational cost of \(O(2N + 1)\) linear solutions. The representation used in the current work has a matrix format that can be decomposed into at most 8 sub-terms. The cost of the matrix representation is only \(O(N + 1)\) linear solutions and therefore seems to be advantageous over the adjoint-sensitivity method.

The formal expression for the element \((i,j)\) of the Hessian is given by:

\[
\Pi(i,j) = \frac{d^2 I}{dx_i dx_j} = \int_A \left[ \left( \frac{dv}{dx_i} \right)^T \left( \frac{df_i}{dx_j} \right) \right] dx
\]

where

\[
f_i = -\frac{\partial R(\rho, u, p)}{\partial x_i}
\]

and the residual \(R\) is defined in Eq. (1).

Each of the two terms in the integrand of Eq. (14) is simplified and rearranged in a matrix form of the Hessian as explained briefly in the following.

5.1.1. The term \(\frac{dv}{dx_j}(\frac{df_i}{dx_j})^T\)

It can be shown that \(f_i\) is equal to

\[
f_i = \left( \frac{\partial h_i}{\partial x} p - \frac{d}{dx} (h_i F) \right).
\]

where the vectors \(P\) and \(F\) are defined in Eq. (2). The derivative of \(f_i\) is computed explicitly from Eq. (16):

\[
\frac{df_i}{dx_j} = -\frac{d}{dx_j} \frac{\partial R}{\partial x_i} = -\frac{\partial R^2}{\partial x_i \partial x_j} \frac{\partial}{\partial U} \frac{\partial R}{\partial x_i} \frac{dU}{dx_j} = -\frac{\partial L}{\partial x_i} \frac{dU}{dx_j}
\]

where the second derivative with respect to \(x\) can be eliminated, since the residual \(R\) is linear in the design variables:

\[
\frac{\partial R^2}{\partial x_i \partial x_j} = 0.
\]

5.1.2. The term \((\frac{dv}{dx_j})^T f_i\)

The adjoint sensitivity term is derived by first considering the sensitivity equation:

\[
\frac{\partial R}{\partial U} \frac{dU}{dx_i} + \frac{\partial R}{\partial x_i} = 0
\]
In terms of the sensitivities we can write,

\[ f_i = -\frac{\partial R}{\partial x_i} = L \frac{dU}{dx_i} \]

Therefore,

\[ \int_\Omega \left( \frac{d\nu}{dx_j} \right)^T f_i dx = \int_\Omega \left( \frac{d\nu}{dx_j} \right)^T L \frac{dU}{dx_i} dx. \]

Taking the adjoint of the right-hand-side integrand we get (using the identity, \( L \frac{\partial U}{\partial x_j} = -\frac{\partial}{\partial x_i} v - \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_i} v + \frac{\partial}{\partial x_j} \frac{\partial}{\partial x_i}, \) see [14]),

\[ \int_\Omega \left( \frac{d\nu}{dx_j} \right)^T f_i dx = \int_\Omega \left( \frac{d\nu}{dx_j} \right)^T L \frac{dU}{dx_i} dx = \int_\Omega dU^T \left( \frac{\partial^2}{\partial x_i^2} - \left( \frac{\partial L}{\partial x_i} \frac{dU}{dx_j} + \frac{\partial L}{\partial x_j} \right) \right) dx \]

\[ \text{(18)} \]

5.1.3. The Hessian in matrix form

Substituting relations (17) and (18) in (14) and rearranging terms, the Hessian can be represented in the following matrix-vector form:

\[ \Pi(i,j) = \int_\Omega \left[ \frac{dU}{dx_i} \frac{dU}{dx_j} \right]^T \left\{ \left[ \begin{array}{ccc} \frac{\partial L}{\partial x_i} & 0 & 0 \\ 0 & \frac{\partial L}{\partial x_j} & 0 \\ 0 & 0 & \frac{\partial L}{\partial x_i} \end{array} \right] - v \otimes \left[ \begin{array}{c} \frac{\partial L}{\partial x_i} \\ \frac{\partial L}{\partial x_j} \\ \frac{\partial L}{\partial x_i} \end{array} \right] \right\} \left[ \begin{array}{c} \frac{dU}{dx_i} \\ \frac{dU}{dx_j} \\ 1 \end{array} \right] dx \]

\[ \text{(19)} \]

The notation \( \otimes \) is introduced in order to clarify the application of the operators in the integrand on the sensitivities and adjoint variables. It should be interpreted as follows:

\[ v \otimes \frac{\partial L}{\partial x_j} \frac{dU}{dx_i} = \frac{\partial L}{\partial x_i} \left( \frac{dU}{dx_j} \right) - v \cdot \left[ \frac{\partial L}{\partial x_i} \frac{dU}{dx_j} \right] \]

where the parenthesis \( A(x) \) denotes the action of an operator \( A \) on \( x \), and the dot \( \cdot x \) denotes a dot product between \( v \) and \( x \).

The cost of computing the terms composing the matrix representation of the Hessian consists of solving \( N \) linear sensitivity equations, and \( 1 \) additional adjoint equation; all together \( \sqrt{N} + 1 \) linear equations. As in the adjoint-sensitivity method, the terms \( L_{x_i} \) and \( L_{x_j} \) need to be computed as well. Although the matrix approach seems to have an advantage over the adjoint-sensitivity approach with regards to computational cost, we suspect that the former is likely to be more delicate in practice for flows with shocks, based on the following argument. In the Hessian representation given by Eq. (19) the terms \( dU/\partial x_i \) and \( dU/\partial x_j \) contain a delta function at the shock, while the terms \( \partial L/\partial x_i \) \( \partial L/\partial x_j \) \( \partial L/\partial U \) \( \partial L/\partial p \) \( \partial U \) contain a Heaviside function. As mentioned before the adjoint variable, \( v \), is continuous at the shock. The numerical implementation of Eq. (19) may be more delicate compared to that of Eq. (14) since some of the terms involve multiplication of delta functions at the shock. This is not the case for the adjoint-sensitivity Hessian representation (as discussed in [14]).

5.2. Numerical implementation of the Hessian in matrix form

The matrix form of the Hessian for the 1-D Euler equations (as given in Eq. (19)) was computed, term by term, in the discrete level. It was also computed analytically in the continuous level, based on [14], and a systematic comparison was made for both the shockless and shocked cases, for the pressure matching and pressure integral objectives.

Sensitivities and adjoint solutions have been calculated as described in Section 4. Four terms need to be computed; \( \frac{\partial^2}{\partial x_i \partial x_j} \) (for the pressure minimization problem), \( \frac{\partial^2}{\partial x_i^2} \) \( \frac{\partial^2}{\partial x_i \partial x_j} \) \( \frac{\partial^2}{\partial x_j^2} \). The first term can be easily computed analytically. The second and third terms are just the transpose of each other, and can be obtained by differentiating Eq. (10). The resulting formulas are identical to (10) with each \( h_{ij} \) replaced by \( h_{ij}(x_{ij}) \), the \( j \)th shape function evaluated at the corresponding abscissa.

Finally the action of \( \frac{\partial L}{\partial x_i} \) on the sensitivities is approximated by second order finite differences. We interpret the symbol \( \frac{\partial L}{\partial x_i} \) as the gradient of the adjoint in the space of the state variables. Hence its application on a vector can be interpreted as a directional derivative times a step size.

Let \( \epsilon_m \) be the machine epsilon. The approximation writes as follows:

\[ \frac{\partial L}{\partial U} \left( \frac{dU}{dx_j} \right) \approx \frac{1}{2 \sqrt{\epsilon_m}} \left[ \left. \frac{\partial L}{\partial U} \right| \left( U + \sqrt{\epsilon_m} \frac{dU}{dx_j} \right) - \left. \frac{\partial L}{\partial U} \right| \left( U - \sqrt{\epsilon_m} \frac{dU}{dx_j} \right) \right] \]

\[ \text{(20)} \]
5.3. Consistency for shockless flow

In this subsection we demonstrate the convergence of the discrete Hessian to the continuous one for shockless flow. In order to simulate shockless flow the following boundary conditions were set; total enthalpy and total pressure at the inlet are 4 and 2, respectively, the inlet Mach number was set to equal 3, resulting in a shockless, purely supersonic flow.

For shockless flow the numerical results indicate that the discrete Hessian is consistent with the continuous one, for both objective functionals. As the mesh refines the discrete quantity converges to the continuous one as demonstrated in Fig. 7.

The relative error is defined by

\[ \text{RelErr} = \frac{\|H - H_c\|}{\|H_c\|} \]

where \( H_c \) denoted the continuous (exact) Hessian, and the norm is measured as the largest singular value of the given matrix.

5.4. Consistency for shocked flow

In order to simulate shocked flow the following boundary conditions were set; total enthalpy and total pressure at the inlet are 4 and 2, respectively, and the static pressure at the outlet was set to 1.6. The resulting flow is transonic with a strong shock at \( x = 1.14 \) with a Mach number varying between \( M = 0.3 \) at the inlet and \( M = 1.6 \) before the shock.

For shocked flow we find two properties that are dramatically different from the shockless case. Firstly, when examining the infinite norm of the different terms of the Hessian in shocked flow, all appear to be important, none can be claimed to be dominant systematically (more details are discussed in Section 6). Secondly, we find that for shocked flow there is an issue with consistency of the discrete limit with the continuous solution. Recall that some elements in the sensitivity matrix \( Q = dU/dx \) contain a delta function in the continuous level, and a large spike in the discrete level (a spike that increases unboundedly as the number of mesh points increases).

In Fig. 7(b) the relative discretization errors of the discrete Hessian compared with the continuous one, are plotted for the pressure minimization and pressure matching problems for shocked flow. The values calculated have been verified by comparing them to the actual second derivative of the functional computed numerically by finite differences (see Fig. 2(c) and (f)). In the pressure minimization case the discrete Hessian has a trend of converging toward the continuous one, with grid refinement. On the other hand the Hessian of the pressure matching problem starts to depart from the continuous one beyond some grid refinement level. That behavior is a result of non-smoothness in the discrete objective functional due to the shock as discussed in Section 3. The convergence observed for the pressure minimization case for shocked flow must be judged carefully. It is due to the particular choice of the design variables \( \alpha = 0 \) (for the dependency of the functional on \( \alpha_2 \) see Fig. 2(c)). For values of \( \alpha \neq 0 \) oscillations are present and hence convergence to the continuous solution cannot be attained in general.

6. The behavior of the different terms composing the Hessian in its matrix representation

In the following we study numerically the role of different terms in the matrix representation of the Hessian for the two objective functions, for both shockless and shocked flow. We consider the following three terms:

6.1. Definition of \( T_1 \): the objective term

\[
T_1 \equiv \int_{\Omega} \begin{bmatrix}
\frac{du}{dx} \\
1
\end{bmatrix} \begin{bmatrix}
\frac{\alpha^T}{\alpha^T} \\
0
\end{bmatrix} \begin{bmatrix}
\frac{dU}{dx} \\
1
\end{bmatrix} dx
\]

(21)
6.2. Definition of $T_2$: the first-order Lagrange term

$$T_2 \equiv \int_{\Omega} \left[ \frac{\partial u}{\partial x_i} \right]^T (-v) \otimes \left[ \begin{array}{c} 0 \\ \frac{\partial u}{\partial x_i} \\ 0 \end{array} \right] \frac{\partial u}{\partial x_i} \, dx$$  \hspace{1cm} (22)$$

6.3. Definition of $T_3$: the second-order Lagrange term

$$T_3 \equiv \int_{\Omega} \left[ \frac{\partial u}{\partial x_i} \right]^T (-v) \otimes \left[ \begin{array}{c} \frac{\partial^2 u}{\partial x_j \partial x_i} \\ 0 \\ 0 \\ \frac{\partial u}{\partial x_i} \end{array} \right] \, dx$$  \hspace{1cm} (23)$$

$T_1$ contains the second partial derivative of the integrand which defines the functional. In order to compute $T_2$ the partial derivative of the adjoint and linearized problem with respect to the design variables must be determined. $T_3$ contains the partial derivative of the adjoint operator with respect to the state variables. It is the most difficult term to compute numerically.

In Fig. 8 the infinite norm of the different terms normalized by the norm of the exact Hessian is plotted. It can be noticed that for shockless flows the dominant term is $T_2$, whereas $T_1$ and $T_3$ are about one order of magnitude smaller. For shocked flow both $T_1$ and $T_3$ grow with the number of grid points. The slopes observed in Fig. 8(b) and (c) indicate that the growth rate is proportional to the number of grid points. Further it can be noticed the the proportionality factor is equal in the case of the pressure minimization functional but is slightly different for the inverse problem. $T_2$ does not grow with grid refinement and asymptotically behaves like $\|T_2\|/\|H_c\| = \mathcal{O}(1)$.

This behavior of the different terms provides some guideline for approximating the analytic Hessian. It can be deduced that, for this particular case, $T_2$ is the dominant term and there is no need to compute $T_3$ for shockless flows.

For shocked flows, we observe that again $T_2$ is a good candidate for approximating the Hessian. Furthermore, we deduce that $T_1$ and $T_3$ cannot be separated in the case of shocked flows as they balance each other. This implies that if $T_3$ is neglected also $T_1$ must be neglected. We observe that for the pressure minimization functional $T_1 + T_3$ converges towards a finite value.

Fig. 8. $\|T_i\|/\|H_i\|$ vs number of grid points for different objective functions and different flows.
as \( T_1 + T_2 + T_2 \) and \( T_2 \) are finite. On the other hand, for the pressure matching problem \( T_1 + T_3 \) grows with the number of grid points and become the dominant contribution to the numerical Hessian.

7. Recommended approximations to the exact Hessian

Approximations to the exact Hessian are needed for the following reasons

i. \( T_3 \) might be very difficult to compute in industrial codes.

ii. The numerical Hessian is not consistent with the continuous Hessian.

In the following \( H_i \) denotes some approximate Hessian matrix, whereas \( H_c \) is the continuous Hessian and \( H_e \) is the numerical Hessian. A first approximation is to use

\[
H_1 \equiv T_2
\]

The previous section gave some evidence that this might be a fruitful approach.

Another approach is to regularize \( T_1 \) and \( T_3 \) in the case of a shocked flow. This is achieved by excluding the neighborhood of the shock from the integrations (21) and (23). Let us denote with \( \Omega_{sh} = [x_{sh} - e : x_{sh} + e] \)

\[
H_2 \equiv T_2 + \int_{\Omega_{sh}} \left[ \begin{array}{c} \frac{\partial U}{\partial x} \\ 1 \end{array} \right]^T \left( \begin{array}{cc} \frac{\partial^2 \mathbf{F}}{\partial x^2} & 0 \\ 0 & 0 \end{array} \right) - \mathbf{v} \otimes \left( \begin{array}{c} \frac{\partial U}{\partial x} \\ 0 \end{array} \right) \right] \left[ \begin{array}{c} \frac{\partial U}{\partial x} \\ 1 \end{array} \right] dx
\]

The results are presented in Fig. 9. It can be seen that \( H_1 \) is a good approximation for both objective functions and for shockless and shocked flows. Typical errors are about 10% which is acceptable since the Hessian is used as a preconditioner for a Newton’s method and as such does not need to be exact. \( H_2 \) performs better than \( H_1 \) in the case of the inverse problem, but the gain seems not worth computing \( T_3 \).

![Fig. 9](image-url)
8. Conclusions

In this work we study the effect of a discontinuity in the state variables on the Hessian computation. Aerodynamic shape optimization under transonic flow is an example of a practical problem of great interest that falls into that category. These type of problems as practiced in industry are immensely complex and therefore it is very difficult to understand how shocks in the flow affect the optimization problem. We therefore chose a much simpler problem that still contains some of the difficulties encountered in the industrial applications; optimization governed by the quasi-one-dimensional Euler equations under transonic flow conditions were a strong shock occurs. We believe that the results presented in this paper are general and do not depend on the choice of Oscher scheme. In order to support that claim we included a simple study that demonstrates the oscillatory behavior when a discontinuity is moving relative to a grid (see Section 3.3) In [14] that problem was studied in detail in the continuous level where exact solutions can be obtained. However, the discrete level introduces properties that do not exist in the continuous level. In this work we analyze and implement the methods introduced in [14] in the discrete level. We find that shocks in the flow field, or in general discontinuities in the state variables, introduce phenomena that do not exist in the continuous level and can alter the results significantly. In the following we summarize our findings.

We show evidence of an objective functional that can be smooth in the continuous level and yet be non-smooth in the discrete level. A change in some of the design variables causes the shock to move relative to the discrete mesh. When a discontinuity is crossing a grid point the objective function changes slope and curvature in a discontinuous manner. These changes can be very large and they are purely a discrete effect. We find that resolving the design surface accurately can exacerbate that effect making grid refinement counter productive for the purpose of computing the discrete sensitivities. These effects are stronger the higher the order of the discrete sensitivities and can result with some of the discrete Hessian terms oscillating wildly.

Next we compute the discrete Hessian using the matrix formulation that require both the adjoint and sensitivities. For shockless flow the discrete Hessian is consistent with the continuous one for both objective functionals. However, for shocked flow consistency breaks down beyond a certain grid resolution; below that resolution the discrete does seem to converge to the continuous. That phenomena is expected based on the behavior of the first order sensitivities for shocked flow. For the 1-D Euler equations, we find that the consistency breakdown occurs much earlier for the pressure matching case than for the pressure minimization objective.

We observe that what may seem paradoxically, in shocked flow the more accurately the discrete Hessian is resolved the less useful it is for the purpose of optimization acceleration (Newton method).

We study the effect of approximating the continuous Hessian by eliminating some of the terms. Neglecting terms is a strategy that can work for shockless flow but we find that when a strong shock is present special care in choosing what term to neglect is necessary. For shockless flow we find that neglecting the objective functional term \(T_1\) or the \(\frac{\partial^2}{\partial^2 x} \) term \(T_3\) results in an excellent approximation for the Hessian. For shocked flow we find that the Hessian is computed with reasonable accuracy if only \(T_2\) is kept. Higher accuracy is achieved by including all the terms and by removing the shock from the computation of the relevant integrals. Whether the gain in accuracy is worth the effort of computing \(T_3\) remains questionable.

Based on this study we recommend to compute the Hessian on a coarse mesh or by the \(H_1\) approximation. That would have a double effect of consuming less CPU while having a more effective preconditioner for a Newton method. Computing the Hessian only on the coarse mesh can be a very effective strategy especially for multigrid optimization methods. Smoothing the gradients may be fruitful if an approach based on finite difference of gradients is chosen (also in the case of quasi-Newton).

Finally, we observe that for large 3D aerospace applications under transonic flow, the shocks distribute among thousands of computational cells. In addition these shocks are smeared due to artificial dissipation. As a result of these two effects we speculate that the oscillations reported in this work may not be observed at all in some cases, or will be milder. However, we think that this issue must be further studied as the risk for oscillations exists and can result in non-convergence or convergence to a local minima.

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References


