Progress in the Usage of Inexact Linearizations in Piggy-back Iterations for Adjoint Computation

E. Padway
Corresponding author: emmett.padway@nianet.org

National Institute of Aerospace, Hampton, VA, USA.

Abstract: In this abstract, we present improvements in computing steady-state adjoint-based sensitivities using inexact linearizations of fixed-point iterations used to solve the nonlinear problem. This method guarantees convergence of the adjoint solution, provided that the solution the of the nonlinear primal problem converges. The method is enhanced by introducing a nonlinear update tolerance and an automatic nonlinear constraint tolerance to allow for cheaper and more robust sensitivity computation as well as cheaper design algorithms.

Keywords: Optimization, Adjoint Methods, Fixed-point Iterations.

1 Introduction

In aerodynamic shape optimization, gradient based approaches are used to solve the minimization problem:

$$\min_{D} L(u(D), D), \text{ s.t. } R(u(D), D) = 0. \tag{1}$$

L is the objective function (such as lift or drag), R is the residual operator (the error in the discretized form of the governing equations), u is the conservative variable vector, and D is the design variable vector. The classic approach is that of partial differential equation (PDE) constrained optimization –also known as the nested approach – in which the PDE is solved at each iteration and the sensitivities about the converged state are used to change the design variables to generate a new design. The sensitivity equation is

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} + \frac{\partial L}{\partial u}\frac{du}{dD}, \tag{2}$$

where an expression for $\frac{du}{dD}$ is required for the sensitivity to be computed. Since the nested approach proceeds off the assumption that $R = 0$, we can say that

$$\left[\frac{\partial R}{\partial u}\right]\frac{du}{dD} + \frac{\partial R}{\partial D} = 0. \tag{3}$$

Substituting equation for $\frac{du}{dD}$ into the sensitivity equation yields

$$\frac{dL}{dD} = \frac{\partial L}{\partial D} - \frac{\partial L}{\partial u}\left[\frac{\partial R}{\partial u}\right]^{-1}\frac{\partial R}{\partial D}, \tag{4}$$

We then define an adjoint variable $\mathbf{\Lambda}$ according to the equation below

$$\left[\frac{\partial R}{\partial u}\right]^T \mathbf{\Lambda} = -\left[\frac{\partial L}{\partial u}\right]^T, \tag{5}$$

which scales with the number of objective functions rather than the number of design variables. The other approach to the optimization problem is often referred to as the one-shot approach [1], in which the PDE, the adjoint system and the design problem are solved in tandem:

$$\begin{aligned} u^{k+1} &= N(u^k, D), \\ \Lambda^{k+1} &= B(u^k, \Lambda^k, D), \\ D^{k+1} &= D^k + F(u^k, \Lambda^k, D^k). \end{aligned} \tag{6}$$

Where $N(u^k, D)$ is a fixed-point iteration meant to drive $R(u^k, D)$ to 0, B is an operator which in the context of "piggy-back" iterations is defined to be $L_u + N_u \Lambda^k$, and F is a preconditioner to guarantee convergence for the coupled iterations. Much of the previous work on these piggy-back iterations used explicit iterations of the form

$$N(u^k, D) = u^k + \frac{\Delta t}{vol} R(u^k), \tag{7}$$

where Δt and vol were the local time step and volume respectively. The differentiation of such a fixed-point iteration is straight-forward and work on implicit iterations of the form

$$N(u^k, D) = u^k - \left[P_k\right]^{-1} R(u^k), \tag{8}$$

where P_k is an approximate residual Jacobian is less common due to the need to differentiate the approximate inversion of the P_k matrix. In order to address the differentiation of the approximate matrix inverse previous work looks at the use of inexact linearizations in the context of coupling only the PDE constraint and adjoint equations [2]. The approximate linearizations are the Newton-Chord linearization and the inexact-quasi-Newton linearization and are defined as

$$\begin{aligned} \frac{\partial \left[P_k\right]^{-1}}{\partial u}_{NC} &= 0, \\ \frac{\partial \left[P_k\right]^{-1}}{\partial u}_{IQN} &= \left[P_k\right]^{-1} \frac{\partial \left[P_k\right]}{\partial u} \left[P_k\right]^{-1}. \end{aligned} \tag{9}$$

These methods showed desirable convergence behaviors in both mathematical proof and numerical experiment, in that the error due to such approximations decreases at the same rate as the solution of the PDE itself. We will apply the piggy-back iterations to convergent iterations only in order to decrease the computational expense of such techniques. Specifically we define a contraction at each iteration k, where ρ^k is defined as $\rho^k = \left\|R(u^{k-1})\right\| / \left\|R(u^k)\right\|$, and for $\rho^k < \tau_\rho$ the adjoint iteration is performed. To restrict the adjoint iterations only to convergent iterations, we can set $\tau_\rho = 1.0$, in this work we also augment this control by automatically performing the adjoint computation for iterations where $\left\|R(u^k)\right\| \leq 1e - 12$ regardless of the convergence behavior of the nonlinear problem at that iteration. In the full paper we will combine this with an adaptive tolerance controller and with the work on inexactly constrained linearizations [3] so that we may lower the cost of the design process.

2 Preliminary Results

We use the case of a NACA0012 airfoil in $Mach = .7$ and $\alpha = 2^o$ in compressible inviscid flow for verification and preliminary results. We compare the sensitivities, the expense (measured by time taken to solve the adjoint problem), and the number of nonlinear iterations (out of 300) skipped for the adjoint solution methods. The choice to skip certain iterations is not harmful to the accuracy of the final sensitivities and decreases the cost with both inexact linearizations becoming more economical than the steady-state adjoint solution method.

	Design Variable 1	Design Variable 2	Time (s)	n_{skip}
Complex	-0.4507974688123841	0.4465241035044418	N/A	N/A
NC($\tau_\rho = \infty$)	-0.450797468**910912**	0.446524103**534101**	163.16	0
NC($\tau_\rho = .9$)	-0.450797468**777518**	0.446524103**463391**	96.97	120
IQN($\tau_\rho = \infty$)	-0.4507974688**99974**	0.4465241035**30128**	187.09	0
IQN($\tau_\rho = .9$)	-0.450797468**767427**	0.446524103**460009**	112.68	120
Steady State	-0.450797468**918543**	0.4465241035**35613**	116.43	N/A

Table 1: Comparison of sensitivities computed by various methods

3 Final Paper

In the final paper, we will complete a study about the impact of the nonlinear iteration tolerance as well as an automated tolerance controller as we believe the choice of a constant value of τ_ρ is undesirable. We will use the results of these investigations to guide our choices in the inexactly constrained design methodology in the final paper.

References

[1] S. Gunther, N. Gauger, and Q. Wang, 2016. "Simultaneous single-step one-shot optimization with unsteady PDEs", Journal of Computational and Applied Mathematics, Volume 294.

[2] E. Padway and D. Mavriplis, "Inexact Linearization of Fixed Point Iterations in the Piggy-Back Iterations of the One-Shot Adjoint" AIAA Paper 2022-1613, AIAA SciTech 2022 Forum, 3-7 January 2022, San Diego & Online.

[3] D. Brown and S. Nadarajah, 2018. "Inexactly constrained discrete adjoint approach for steepest descent-based optimization algorithms", Numerical Algorithms, 78(3).