Constrained Single-Step One-Shot Method with Applications in Aerodynamics

Nicolas R. Gauger\textsuperscript{1),2)}

\textsuperscript{1)} German Aerospace Center (DLR) Braunschweig Institute of Aerodynamics and Flow Technology Numerical Methods Branch (C\textsuperscript{2}A\textsuperscript{2}S\textsuperscript{2}E)

\textsuperscript{2)} Humboldt University Berlin Department of Mathematics
Collaborators

• HU Berlin: A. Griewank, A. Hamdi, E. Özkaya, A. Plocke

• DLR: C. Ilic

• Uni Paderborn: A. Walther

• Uni Trier: V. Schulz, S. Schmidt
Problem Statement

Goal: \[ \min_{u} f(y,u) \quad \text{s.t.} \quad c(y,u) = 0, \]
where \( y \) and \( u \) are the state and design variables.

Given fixed point iteration \( y_{k+1} = G(y_k,u) \) (e.g. pseudo-time stepping) to solve PDE \( c(y,u) = 0. \)

Assumptions:

- \( \frac{\partial c}{\partial y} \) always invertible. IFT \( \Rightarrow \) given \( u \), \( \exists! y \) s.t. \( c(y,u) = 0. \)
- \( G, f \in C^{2,1}. \)
- \( G \) contractive: \( \|G_y(y,u)\| = \|G^T_y(y,u)\| \leq \rho < 1 \)
One-Shot approach

\[ L(y, \bar{y}, u) = f(y, u) + (G(y, u) - y)^T \bar{y} \]
\[ = N(y, \bar{y}, u) - y^T \bar{y} \]

shifted Lagrangian

Stationary point:

\[ \begin{align*}
L_{\bar{y}} &= G(y, u) - y = 0 \\
L_y &= N_y(y, \bar{y}, u)^T - \bar{y} = 0 \\
L_u &= N_u(y, \bar{y}, u)^T = 0
\end{align*} \]

One-step one-shot (step \(k+1\)):

\[ \begin{align*}
y_{k+1} &= G(y_k, u_k) \quad \text{primal update} \\
\bar{y}_{k+1} &= N_y(y_k, \bar{y}_k, u_k)^T \quad \text{dual update} \\
u_{k+1} &= u_k - B_k^{-1} N_u(y_k, \bar{y}_k, u_k)^T \quad \text{design update}
\end{align*} \]

Aims: Choose \(B\) such that:

- Convergence of \((OS)\).
- Bounded retardation.
Bounded retardation

Jacobian of the extended iteration:

\[
J_* = \left. \frac{\partial (y_{k+1}, \bar{y}_{k+1}, u_{k+1})}{\partial (y_k, \bar{y}_k, u_k)} \right|_{(y^*, \bar{y}^*, u^*)} = \begin{pmatrix} G_y & 0 & G_u \\ N_{yy} & G_y^T & N_{yu} \\ -B^{-1} N_{uy} & -B^{-1} G_u^T & I - B^{-1} N_{uu} \end{pmatrix}
\]

Whenever we can define \( B \) such that

\[
\frac{1 - \rho(G_y)}{1 - \hat{\rho}(J_*)} < \text{const}
\]

we have bounded retardation.
Necessary condition for contractivity

Eigenvalues of $J_*$ are the zeros of the equation

$$\det((\lambda - 1)B + H(\lambda)) = 0$$

where

$$H(\lambda) = \left(-G_u^T(G_y^T - \lambda I)^{-1}, I\right)\begin{pmatrix} N_{yy} & N_{yu} \\ N_{uy} & N_{uu} \end{pmatrix}\left(-(G_y - \lambda I)^{-1}G_u \right).$$

Necessary (but not sufficient) condition for contractivity:

$$B = B^T > 0 \quad \text{and} \quad B > \frac{1}{2} H(-1).$$

[Griewank, 2006]
Remark:

Deriving (sufficient) conditions on $B$ for $J^*$ to have a spectral radius smaller than 1 has proven difficult. Instead, we look for descent on the augmented Lagrangian

$$L^a (y, \bar{y}, u) := \frac{\alpha}{2} \| G(y, u) - y \|^2 + \frac{\beta}{2} \left\| N_y (y, \bar{y}, u)^T - \bar{y} \right\|^2 + \left( N - \bar{y}^T y \right),$$

where $\alpha > 0$ and $\beta > 0$.
Correspondence condition

The full gradient of $L^a$ is given by

$$\begin{bmatrix}
\nabla_y L^a \\
\nabla_y L^a \\
\nabla_u L^a
\end{bmatrix} = -Ms(y, \bar{y}, u), \quad \text{where} \quad s(y, \bar{y}, u) = \begin{bmatrix}
G(y, u) - y \\
N_y (y, \bar{y}, u)^T - \bar{y} \\
- B^{-1} N_u (y, \bar{y}, u)^T
\end{bmatrix}$$

and

$$M = \begin{bmatrix}
\alpha(I - G_y^T), -I - \beta N_{yy}, 0 \\
- I, \beta(I - G_y), 0 \\
- \alpha G_u^T, - \beta N_{yu}^T, B
\end{bmatrix}.$$
Correspondence condition

Consequence (Correspondence condition):
There is a 1-1 correspondence between the stationary points of $L^a$ and the roots of $s$ if

$$\det[\alpha\beta(I - G_y^T)(I - G_y) - I - \beta N_{yy}] \neq 0,$$

for which it is sufficient that

$$\alpha\beta(1 - \rho)^2 > 1 + \beta\|N_{yy}\|.$$  

[Hamdi, Griewank, 2008]
Descent condition

**Theorem (Descent condition):**

\( s(y, \bar{y}, u) \) is a descent direction for all large positive \( B \)

if and only if

\[
\alpha \beta (I - \frac{1}{2} (G_y + G_y^T)) > (I + \frac{\beta}{2} N_{yy})(I - \frac{1}{2} (G_y + G_y^T))^{-1} (I + \frac{\beta}{2} N_{yy}),
\]

which is implied by

\[
\sqrt{\alpha \beta} (1 - \rho) > 1 + \frac{\beta}{2} \|N_{yy}\|.
\]

- Satisfied for \( \beta = \frac{2}{c}, \quad \alpha = \frac{2c}{(1 - \rho)^2} \) with \( c = \|N_{yy}\| \).

**Theorem:** A suitable \( B \) is given by:

\[
B = \alpha G_u^T G_u + \beta N_{yu}^T N_{yu} + N_{uu}.
\]

[Hamdi, Griewank, 2008]
One-step one-shot
Aerodynamic shape design

Descent for \( \beta = \frac{2}{c} \), \( \alpha = \frac{2c}{(1-\rho)^2} \) with \( c = \| N_{yy} \| \).

(In practice choose \( c = 1, \quad \Rightarrow \quad \beta = 2, \quad \alpha >> 1. \))

A suitable \( B \) is given by \( B = \alpha G_u^T G_u + \beta N_{yu}^T N_{yu} + N_{uu} \).

Instead BFGS updates for the Hessian

\[
\nabla_u^2 L^a = \underbrace{\alpha G_u^T G_u + \beta N_{yu}^T N_{yu} + N_{uu}}_{B} + \underbrace{\alpha (G - y)^T G_u}_{\rightarrow 0} + \underbrace{\beta (N_y^T - \bar{y})^T N_{yu}}_{\rightarrow 0}.
\]

The gradient \( \nabla_u L^a = \alpha (G - y)^T G_u + \beta (N_y - \bar{y})^T N_{yu} + N_u \)

is evaluated by Algorithmic Differentiation (AD).
One-step one-shot
Aerodynamic shape design

- Transonic case: RAE 2822 at $Ma = 0.73$ with $\alpha = 2^\circ$
- Cost function: drag ($cd$)
- $\tau_{ij}$ (2D Euler) + mesh deformation + parameterization
- First and second derivatives by AD tool ADOL-C
- Geometric constraint: constant thickness
- Camberline/Thickness decomposition, 20 Hicks-Henne coefficients define camberline
Automatic Differentiation of Entire Design Chain

- Adjoint version of entire design chain by ADOL-C
- TAUij (2D Euler) + mesh deformation + parameterization

\[
\frac{dC_D}{dP} = \frac{\partial C_D}{\partial m} \cdot \frac{\partial m}{\partial (dx)} \cdot \frac{\partial (dx)}{\partial x_{\text{new}}} \cdot \frac{\partial x_{\text{new}}}{\partial P} \quad \text{and} \quad \frac{\partial (dx)}{\partial x_{\text{new}}} = \frac{\partial (x_{\text{new}} - x_{\text{old}})}{\partial x_{\text{new}}} = Id
\]

TAUij_AD meshdefo_AD defgeo_AD
One-step one-shot

Drag reduction
- RAE 2822, $M = 0.73$, $\alpha = 2.0^\circ$
- inviscid flow, mesh 161x33 cells
- 20 design variables (Hicks-Henne)
- One-step one-shot

Flow Solver: TAUij
- Compressible Euler
- Explicit RK-4
- Multigrid
- Implicit residual smoothing

Graphs showing flow characteristics and optimization iterations.
Primal compared to coupled iteration

Retardation-Factor = 4

[Özkaya, Gauger, 2008]
Treatment of lift constraint by penalty multiplier method

\[ \min_u C_D(y, u) \quad s.t. \quad C_L \geq C_{L, target} \quad and \quad y = G(y, u) \]

Penalty function for lift:
\[ h = (C_{L, target} - C_L), \quad h \leq 0 \]

Redefine objective function:
\[ f = C_D + \lambda h \]

min \[ C_D(y, u) + \lambda h \quad ; \quad h \to 0 \]

Update the penalty parameter in each one-shot step \( k \):
\[ \lambda_{k+1} = \lambda_k (1 + ch), \quad c > 0 \]
\[ h > 0 \quad \Rightarrow \quad \lambda \uparrow, \quad h < 0 \quad \Rightarrow \quad \lambda \downarrow \]

A good starting value is:
\[ \lambda_0 = \frac{\| \nabla_u C_D \|}{\| \nabla_u h \|} \]
Constrained One-Step One-Shot

Drag reduction by constant lift
- RAE 2822, $M = 0.73$, $\alpha = 2.0^\circ$
- inviscid flow, mesh 161x33 cells
- 40 design variables (Hicks-Henne)
- One-step one-shot

Flow Solver: TAUij
- Compressible Euler
- Explicit RK-4
- Multigrid
- Implicit residual smoothing

Cp Distribution

Airfoil Shape
Primal compared to coupled iteration

Retardation-Factor = 6

[Gauger, Plocke, 2008]
History of Penalty Multiplier

[Gauger, Plocke, 2008]
Extension to Navier-Stokes (ELAN Code)

Flow Solver: ELAN (TU Berlin)
- 3D Navier-Stokes (RANS)
- incompressible with pressure correction
- multiblock
- k-ω (Wilcox) turbulence model (and others)
- Fortran (20,000 lines)

AD Tool: TAPENADE (INRIA)
- source to source
- reverse for first derivatives
- tangent on reverse for second derivatives
Drag reduction with lift constraint
- NACA 4412
- Re = 1.000.000, $\alpha$=5.1°
- RANS
- k-$\omega$ (Wilcox) turbulence model
- 300 surface mesh points

Approaches for Optimization
- one-shot method
- entire design chain differentiated
- gradient smoothing
- penalty multiplier method

Extension to Navier-Stokes (ELAN Code)
Drag reduction with lift constraint

- NACA 4412
- \( \text{Re} = 1,000,000, \; \alpha = 5.1^\circ \)
- RANS
- \( k-\omega \) (Wilcox) turbulence model
- 300 surface mesh points

Approaches for Optimization

- one-shot method
- entire design chain differentiated
- gradient smoothing
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Drag reduction with lift constraint

- NACA 4412
- \( Re = 1.000.000, \quad \alpha = 5.1^\circ \)
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5% drag reduction

Approaches for Optimization

- one-shot method
- entire design chain differentiated
- gradient smoothing
- penalty multiplier method

[Özkaya, Gauger, 2009]
Thanks for your attention!