Sensitivity Analysis for Chaotic, Turbulent Flows

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Outline

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Sensitivity Analysis Methods compute derivatives of outputs with respect to inputs.

With the adjoint, we go backwards in time to find the sensitivity of outputs to inputs.

The computational cost of the Adjoint method DOES NOT scale with the number of gradients computed.
Adjoint Flow-Field
Sensitivities propagate upstream

From Wang and Gao, 2012
Sensitivity Analysis Applications
Aerodynamic Shape Optimization

From Jameson 2004
Sensitivity Analysis Applications
Error Estimation and Mesh Adaptation

From Venditti and Darmofal, 2003
Sensitivity Analysis Applications

Other Applications

- Flow Control
- Uncertainty Quantification
- and many more...

From University of Miami CCS
High Fidelity Model Issue

As computers become more powerful, high fidelity turbulence models such as LES will become increasingly popular.

High fidelity models capture the chaotic nature of turbulent flows.

However, traditional sensitivity analysis methods break down when applied to chaotic fluid flows.
Chaotic, Turbulent Flow-fields
Unsteady Wakes

From E. Nielsen
Motivation

Chaotic, Turbulent Flow-fields

Aeroacoustics

LEFT: From E. Nielsen RIGHT: From TU Berlin
Motivation

Chaotic, Turbulent Flow-fields

Mixing

From J. Larsson, Stanford University
Traditional Forward Sensitivity Analysis

- Interested in the long time averaged quantity $J$, governed by a system of equations $f$ with some design parameter(s) $s$:

$$\bar{J} = \int_0^T J(u, s) dt, \quad \frac{\partial u}{\partial t} = f(u, s)$$

- Solve the tangent equation for $\nu = \frac{\partial u}{\partial s}$:

$$\frac{\partial \nu}{\partial t} = \frac{\partial f}{\partial u} \nu + \frac{\partial f}{\partial s}$$

- Compute the sensitivity of $\bar{J}$ to $s$:

$$\frac{d\bar{J}^T}{ds} = \int_0^T \frac{\partial J}{\partial u} \nu + \frac{\partial J}{\partial s} dt$$
Main Issue

- For chaotic systems, this does not work, because:

\[
\frac{d\bar{J}\infty}{ds} \neq \lim_{T \to \infty} \frac{d\bar{J}^T}{ds}
\]

- This is because the tangent solution \( v \) diverges for chaotic systems. Counter-intuitively, increasing \( T \) can exacerbate this divergence.

- Adjoint sensitivity analysis breaks down for a similar reason.

- This property of chaotic systems has been shown by Lea et al. for the Lorenz Attractor.

- This problem exists for chaotic PDEs as well.
Chaotic KS Equation Solution

\[
\frac{\partial u}{\partial t} = -u \frac{\partial u}{\partial x} - \frac{1}{R} \frac{\partial^2 u}{\partial x^2} - \frac{\partial^4 u}{\partial x^4}
\]

\( R = 2.0 \) for Chaos in space and time.
Objective Function

\[ J^T = \frac{1}{T} \int_0^T \frac{\partial u}{\partial t} dt \]
Both Tangent and Adjoint solutions diverge exponentially for the KS equation.
NACA 0012 Airfoil Vorticity Contours
Mach 0.1, Angle of Attack 20°, $Re = 10000$
NACA 0012 Airfoil Vorticity Contours
Mach 0.1, Angle of Attack 20°, Re = 10000
Drag Coefficient Time History

Aperiodicity indicates that the flow is chaotic
A chaotic system has at least three different modes.
- An unstable mode, associated with a positive Lyapunov Exponent.
- A stable mode, associated with a negative Lyapunov Exponent.
- A neutrally stable mode, associated with a zero Lyapunov Exponent.

The unstable mode is responsible for the divergence of the tangent and adjoint equations.
Least Squares Sensitivity Method: The Basics (cont’d)

- Solve for stable modes forwards in time and solve unstable modes backward in time to prevent divergence of tangent and adjoint solutions.
- This solution is called the "Shadow Trajectory" (Wang, 2012) and is the least divergent tangent solution.
- Find the shadow trajectory by solving the following linearly contrained, least squares problem:

$$\min_{\eta,v(t), 0 < t < T} \|v\|_2, \quad \text{s.t.} \quad \frac{\partial v}{\partial t} = \frac{\partial f}{\partial u} v + \frac{\partial f}{\partial d} + \eta f, \quad 0 < t < T$$
Divergent and Shadow trajectories for the Lorenz Attractor.
LSS as a "Black Box"

\[ \bar{J} = \int_0^T J(u, s) \, dt, \quad \frac{\partial u}{\partial t} = f(u, s) \]

**Inputs:**
- Forward Solution: \( u_i \)
- Design Variable(s): \( s \)
- Operator values \( f_i \)
- Operator design parameter sensitivity \( \frac{\partial f_i}{\partial s_i} \)
- Objective Function Sensitivity: \( \frac{\partial J}{\partial u_i} \)
- Objective Function Sensitivity: \( \frac{\partial J}{\partial s_i} \)
- Jacobian matrices: \( \frac{\partial f_i}{\partial u_i} \)

**Outputs:**
- Sensitivities: \( \frac{d\bar{J}}{ds} \)
The KKT matrix is a large, symmetric block matrix, where each block is $n$ by $n$ for an $n$ state system. Total size is $2mn + n + 1$ by $2mn + n + 1$ for $m$ time steps. For a discretization with a five element stencil, there are approximately $23mn$ non-zero elements in the matrix.

For the Airfoil simulation shown earlier the KKT matrix would be $3.2 \times 10^9$ by $3.2 \times 10^9$ with $3.7 \times 10^{10}$ non-zero elements.
Multigrid Elimination

- New method to reduce memory usage when solving the LSS KKT system.
- Gaussian Elimination conducted like 1D Multigrid.
- Eliminate every 2nd equation, reduce the system from $2mn + n + 1$ to $n + 1$ equations.
- No need to save coefficients on every grid.
- Potentially Parallelizable.
- Method can be used to solve any unsteady system and its adjoint simultaneously.
The KKT matrix is symmetric indefinite, so it becomes singular on coarser grids due to poor scaling.

Instead, conduct ME on the KKT system’s Schur Complement, which is SPD (ignoring the constraint equation).

Original System:

\[
\begin{bmatrix}
I & B^T \\
B & 0
\end{bmatrix}
\begin{bmatrix}
v \\
\lambda
\end{bmatrix} = -
\begin{bmatrix}
0 \\
b
\end{bmatrix}
\]

Schur Complement:

\[BB^T \lambda = b\]
Elimination Scheme

Fine Grid Equations

\[
L_{i-1} \lambda_{i-2} + D_{i-1} \lambda_{i-1} + U_{i-1} \lambda_i + f_{i-1} \eta = b_{i-1} \quad (1)
\]
\[
L_i \lambda_{i-1} + D_i \lambda_i + U_i \lambda_{i+1} + f_i \eta = b_i \quad (2)
\]
\[
L_{i+1} \lambda_i + D_{i+1} \lambda_{i+1} + U_{i+1} \lambda_{i+2} + f_{i+1} \eta = b_{i+1} \quad (3)
\]
Elimination Scheme

Coarse Grid Equation

\[ L_I \lambda_{i-2} + D_I \lambda_i + U_I \lambda_{i+2} + f_I \eta = b_I \]

Where:

\[ L_I = -L_i D_{i-1}^{-1} L_{i-1} \]
\[ D_I = -L_i D_{i-1}^{-1} U_{i-1} + D_i - U_i D_{i+1}^{-1} L_{i+1} \]
\[ U_I = -U_i D_{i+1}^{-1} U_{i+1} \]
\[ f_I = -L_i D_{i-1}^{-1} f_{i-1} + f_i - U_i D_{i+1}^{-1} f_{i+1} \]
\[ b_I = -L_i D_{i-1}^{-1} b_{i-1} + b_i - U_i D_{i+1}^{-1} b_{i+1} \]

A similar method is used to restrict the constraint equation and the equation for the long-time averaged gradient of interest.
LSS and ME applied to the Lorenz Equations

Lorenz Equations:

\[
\frac{dx}{dt} = s(y - x), \quad \frac{dy}{dt} = x(r - z) - y, \quad \frac{dz}{dt} = xy - bz
\]

Long time averaged z gradients computed by LSS/ME:

\[
\frac{d\bar{z}}{ds} = 0.1545, \quad \frac{d\bar{z}}{dr} = 0.9709, \quad \frac{d\bar{z}}{db} = -1.8014
\]

Gradients computed by finite difference/linear regression:

\[
\frac{d\bar{z}}{ds} = 0.16 \pm 0.02, \quad \frac{d\bar{z}}{dr} = 1.01 \pm 0.04, \quad \frac{d\bar{z}}{db} = -1.68 \pm 0.15
\]
Avoiding inverting Matrices

- ME can be implemented so that no Jacobian matrices need to be inverted.

- Consider the following system:

\[
\begin{pmatrix}
D_1 & U_1 & 0 \\
L_2 & D_2 & U_2 \\
0 & L_3 & D_3 \\
\end{pmatrix}
\begin{pmatrix}
\lambda_1 \\
\lambda_2 \\
\lambda_3 \\
\end{pmatrix}
= 
\begin{pmatrix}
b_1 \\
b_2 \\
b_3 \\
\end{pmatrix}
\]

- The system is restricted using ME:

\[A\lambda_2 = b\]

with:

\[A = -L_2D_1^{-1}U_1 + D_2 - U_2D_3^{-1}L_3\]

\[b = -L_2D_1^{-1}b_1 + b_2 - U_2D_3^{-1}b_3\]
Avoiding inverting Matrices (cont’d)

- This system can be solved iteratively, using some preconditioner $P$:

  $$P\Delta x = b - Ax_k, \quad x_{k+1} = x_k + \Delta x$$

  Where $x_k$ is the value of $\lambda_2$ after $k$ iterations.

- Decompose $Ax_k$ into three parts:

  $$Ax_k = -L_2D_1^{-1}U_1x_k + D_2x_k - U_2D_3^{-1}L_3x_k = \alpha + \beta + \gamma$$
Avoiding inverting Matrices (cont’d)

Consider $\alpha$:

$$-L_2 D_1^{-1} U_1 x_k = \alpha$$

Compute $y_k = U_1 x_k$:

$$-L_2 D_1^{-1} y_k = \alpha$$

Next, define $z_k = D_1^{-1} y_k$. Iteratively solve:

$$D_1 z_k = y_k$$

Use the result to compute $\alpha$:

$$\alpha = -L_2 z_k$$

This idea can be applied to a much larger system and allows ME to be conducted without inverting any Jacobian matrices.
Conclusion

- Traditional sensitivity analysis methods are unable to compute sensitivities of long-time averaged quantities in CFD simulations.
- The LSS method could compute these quantities in an efficient manner if applied with Multigrid elimination.

Future Work
- Further develop and implement ME without inverting Jacobians, ideally in C, C++ or Fortran.
- Apply LSS/ME to the KS equation.
- Validate LSS on aerodynamic test cases.
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