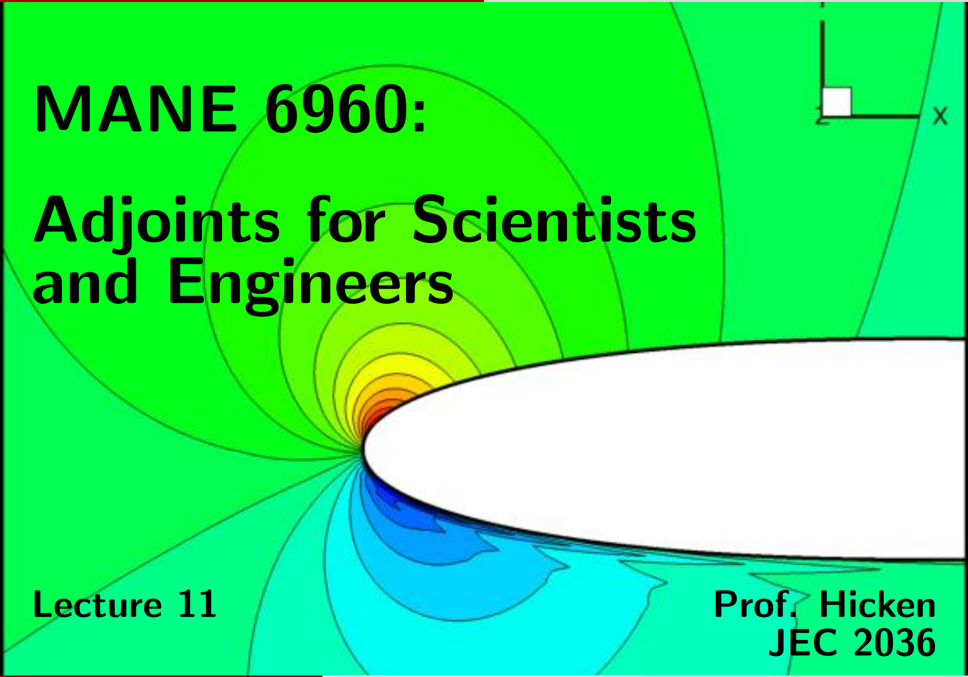

MANE 6960: Adjoints for Scientists and Engineers

Lecture 11

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Lecture Overview

The purpose of this lecture is to review how adjoints can be used to inexpensively compute gradients of functionals.

- We covered this subject in the first lecture, but this will be slightly "deeper dive."
- After this lecture, you will have all the knowledge necessary to complete Assignment 2.

Time permitting, I will also review the forward and reverse mode of algorithmic differentiation, which are useful to know for next lecture.

Direct Sensitivity Method

Direct Sensitivities: Discrete

Throughout this lecture, we will use $\alpha \in \mathbb{R}^n$ to denote parameters that we want to differentiate with respect to.

- α may be a set of shape parameters, a distributed control, or problem parameters like Re or M.

Let $R_h : \mathbb{R}^s \times \mathbb{R}^n \to \mathbb{R}^s$ be a nonlinear state equation, with unique solution $u_h \in \mathbb{R}^s$:

$$R_h(u_h, \alpha) = 0.$$

Furthermore, let $J_h : \mathbb{R}^s \times \mathbb{R}^n \to \mathbb{R}$ be a nonlinear, continuously differentiable function.

Direct Sensitivities: Discrete (cont.)

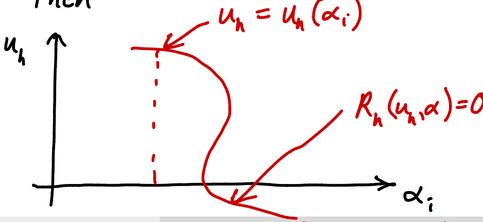
The total derivative of J_h with respect to α_i is

$$\frac{DJ_h}{D\alpha_i} = \frac{\partial J_h}{\partial \alpha_i} + \frac{\partial J_h}{\partial u_h}\frac{Du_h}{D\alpha_i}, \quad i = 1, 2, \ldots, n$$

Treat u_h as an implicit function of α_i via the implicit function theorem.

If R_h is continuously differentiable, and $\partial R_h / \partial u_h$ is invertible, then

$$u_h = u_h(\alpha_i)$$



Direct Sensitivities: Discrete (cont.)

Furthermore

$$\frac{DR_h}{D\alpha_i} = \frac{\partial R_h}{\partial \alpha_i} + \underbrace{\frac{\partial R_h}{\partial u_h}}_{\text{is assumed invertible}} \frac{Du_h}{D\alpha_i} = 0 \leftarrow \text{because } R_h(u_h,\alpha)=0$$

so

$$\boxed{\frac{Du_h}{D\alpha_i} = -\left(\frac{\partial R_h}{\partial u_h}\right)^{-1}\left(\frac{\partial R_h}{\partial \alpha_i}\right) \equiv v_{h,i}}$$

← linearized PDE solution

and

$$\frac{DJ_h}{D\alpha_i} = \frac{\partial J_h}{\partial \alpha_i} + \frac{\partial J_h}{\partial u_h} v_{h,i} \quad , i = 1, 2, .., n$$

Direct Sensitivities: Discrete (cont.)

Definition: Direct Sensitivity Method

The total derivative of J_h with respect to α_i is

$$\frac{DJ_h}{D\alpha_i} = \frac{\partial J_h}{\partial \alpha_i} + \frac{\partial J_h}{\partial u_h} v_{h,i}$$

where $v_{h,i} \in \mathbb{R}^s$ is the direct sensitivity and satisfies

$$\frac{\partial R_h}{\partial u_h} v_{h,i} = -\frac{\partial R_h}{\partial \alpha_i}.$$

- $\partial R_h / \partial \alpha_i$ and $\partial J_h / \partial \alpha_i$ can be obtained using the same method used to compute $\partial J_h / \partial u_h$. (e.g. complex step, coloring, etc)

Direct Sensitivities: Continuous

One can also derive and use a direct sensitivity BVP:

$$\frac{DJ}{D\alpha_i} = J'[\alpha_i] + J'[u]v,$$

where $v \in \mathcal{V}$ satisfies the linear BVP

$$\begin{aligned} N'[u]v &= -N'[\alpha_i], &\qquad \forall x \in \Omega, \\ B'[u]v &= -B'[\alpha_i], &\qquad \forall x \in \Gamma. \end{aligned}$$

Adjoint Sensitivity Method

Adjoint-Based Sensitivities

There are two ways to derive the adjoint sensitivity method. The first, which we saw in the first lecture, is to substitute the direct sensitivity into the derivative, and identify the adjoint with the appropriate product:

$$\begin{aligned}\frac{DJ_h}{D\alpha_i} &= \frac{\partial J_h}{\partial \alpha_i} + \frac{\partial J_h}{\partial u_h} v_h \\ &= \frac{\partial J_h}{\partial \alpha_i} - \underbrace{\frac{\partial J_h}{\partial u_h}\left(\frac{\partial R_h}{\partial u_h}\right)^{-1}}_{\psi^T} \frac{\partial R_h}{\partial \alpha_i}\end{aligned}$$

$$\Longrightarrow \qquad \left(\frac{\partial R_h}{\partial u_h}\right)^T \psi = \left(\frac{\partial J_h}{\partial u_h}\right)^T$$

Lagrangian Approach

The second approach to deriving the adjoint sensitivity method, is to introduce the Lagrangian:

$$L_h(u_h, \psi_h, \alpha) = J_h(u_h, \alpha) - \psi_h^T R_h(u_h, \alpha)$$

- The minus sign is inconsequential
- Since $R_h(u_h, \alpha) = 0$, we have $L_h = J_h$.
- However, this does not imply that $\partial J_h / \partial \alpha = \partial L_h / \partial \alpha$.

The key idea is that L_h should be stationary with respect to changes in ψ_h and u_h.

Lagrangian Approach (cont.)

$$\frac{\partial L_h}{\partial \psi_h} = -R_h(u_h, \alpha) = 0$$

$$\frac{\partial L_h}{\partial u_h} = \frac{\partial J_h}{\partial u_h} - \psi_h^T \frac{\partial R_h}{\partial u_h} = 0$$

and then

$$\frac{\partial L_h}{\partial \alpha_i} = \frac{DJ_h}{D\alpha_i} = \frac{\partial J_h}{\partial \alpha_i} - \psi_h^T \frac{\partial R_h}{\partial \alpha_i}$$

* The Lagrangian approach works well for deriving sensitivities of more general problems (e.g. mesh movement eqns, coupled PDEs, unsteady discretizations)

Lagrangian Approach (cont.)

Definition: Adjoint Sensitivity Method

The total derivative of J_h with respect to α_i is

$$\frac{DJ_h}{D\alpha_i} = \frac{\partial J_h}{\partial \alpha_i} - \psi_h^T \frac{\partial R_h}{\partial \alpha_i}$$

where $\psi_h \in \mathbb{R}^s$ satisfies the discrete adjoint equation

$$\left(\frac{\partial R_h}{\partial u_h}\right)^T \psi_h = \frac{\partial J_h}{\partial u_h}.$$

- The same ψ_h can be reused for all α_i.

solve just one linear system

Continuous or Discrete Adjoint?

Suppose you use the continuous, rather than discrete, adjoint.

- Recall, the continuous-adjoint approach involves finding the adjoint BVP, discretizing it, and solving the resulting discretized problem.

Let $\tilde{\psi}_h$ denote the solution to the discretized adjoint BVP, and define

$$\widetilde{\frac{DJ_h}{D\alpha_i}} = \frac{\partial J_h}{\partial \alpha_i} - \tilde{\psi}_h^T \frac{\partial R_h}{\partial \alpha_i}$$

ψ_h is the discrete adjoint

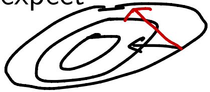
$$= \frac{\partial J_h}{\partial \alpha_i} - \psi_h^T \frac{\partial R_h}{\partial \alpha_i} + (\psi_h - \tilde{\psi}_h)^T \frac{\partial R_h}{\partial \alpha_i}$$

$$= \frac{DJ_h}{D\alpha_i} + \underbrace{(\psi_h - \tilde{\psi}_h)^T \frac{\partial R_h}{\partial \alpha_i}}_{\text{error term}}$$

Continuous or Discrete Adjoint? (cont.)

Therefore, the continuous adjoint approach does not, in general, produce a gradient that is consistent with the exact derivative, $DJ_h/D\alpha$.

- This can cause problems when the continuous adjoint is used with conventional optimization algorithms, which expect accurate derivatives.



On the other hand, Collis and Heinkenschloss [CH02] have shown that the derivative based on the continuous adjoint converges at a faster rate to the true derivative.

$\uparrow$
infinite dimensional

Continuous or Discrete Adjoint? (cont.)

This brings us to one of the advantages of adjoint-consistent discretizations.

If you use an adjoint-consistent method, then you get the best of both worlds: exactness with respect to the finite-dimensional gradient, and optimal convergence to the infinite-dimensional gradient.

Recall, an adjoint consistent discretization satisfies $\tilde{\psi}_n = \psi_n$

thus $$\widetilde{\frac{DJ_n}{D\alpha}} = \frac{DJ_n}{D\alpha}$$

Computing Derivatives: Forward-mode AD

Algorithmic Differentiation

Algorithmic, or automatic, differentiation (AD) is an approach that systematically differentiates the source code.

- It is not symbolic differentiation: we do not get an explicit expression for the function's derivative.
- Instead, for a given set of input (design) variables, $\mathtt{x}$, we get the derivative of the outputs with respect to those inputs at the given values: we get numbers not an expression.

See [GW09] for a comprehensive treatment of the subject.

Algorithmic Differentiation (cont.)

"f" $= J_h$

There are two "modes" of AD.

forward mode: Also called the tangent mode. Computes directional derivatives of the form $(\nabla f)^T p$.

reverse mode: Also called the adjoint mode. Computes (weighted) gradients (∇f).

The forward mode is easier to understand, so we will start there.

Algorithmic Differentiation: forward mode

Consider a simple Julia function that computes

$$f(x_1, x_2) = x_1^2 + x_2 \sin(x_1^2).$$

```julia
function func(x1, x2)
# compute a simple function value
v1 = x1.^2
v2 = x2.*sin(v1)
f = v1 + v2
return f
end
```

- This is a toy example, but it models how we often use intermediate values (`v1` and `v2`) to arrive at the value we want (`f`).

Algorithmic Differentiation: forward mode (cont.)

Suppose we want to compute Df/Dx_1, *at a particular value of* x_1 *and* x_2, using the above code.

- In the code, f does not depend explicitly on x_1.
- To find the desired derivative, we must account for how the intermediate values depend on x_1.
- How? Use the chain rule.

$$\begin{aligned}
\frac{Df}{Dx_1} &= \frac{\partial f}{\partial x_1} \quad + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_1} \quad + \frac{\partial f}{\partial v_2}\frac{Dv_2}{Dx_1} \\
&= \frac{\partial f}{\partial x_1} \quad + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_1} \quad + \frac{\partial f}{\partial v_2}\frac{\partial v_2}{\partial v_1}\frac{\partial v_1}{\partial x_1} \\
&= 0 \quad\quad + (1)(2x_1) \quad + (1)(x_2 \cos(v_1))(2x_1)
\end{aligned}$$

Algorithmic Differentiation: forward mode (cont.)

$$\frac{Df}{Dx_1} = 2x_1 + x_2 \cos(x_1^2) 2x_1$$

- As usual we use Df/Dx_1 to denote the total derivative of f with respect to x_1.
- Similarly, Dv_2/Dx_1 is the total derivative of v_2 with respect to x_1.

Algorithmic Differentiation: forward mode (cont.)

Now the question becomes, how do we implement this in the code?

- A key observation is that the total derivative of the intermediate values with respect to x_1 can be found sequentially as we progress through the function
- That is, we compute the values of Dv_j/Dx_1 together with the value v_j

Algorithmic Differentiation: forward mode (cont.)

Applying the above reasoning, we obtain a new function that computes `f` and `dfdx1`, the total derivative Df/Dx_1.

```
1     function dfunc(x1, x2)
2     # compute a simple function value and its
          derivative w.r.t. x1
3     v1 = x1.^2
4     dv1dx1 = 2.0.*x1 ⟵ diff. line 3
5     v2 = x2.*sin(v1)
6     dv2dx1 = x2.*cos(v1).*dv1dx1 ⟵ diff line 5
7     f = v1 + v2
8     dfdx1 = dv1dx1 + dv2dx1 ⟵ diff line 7
9     return f, dfdx1
10    end
```

Algorithmic Differentiation: forward mode (cont.)

- This example illustrates the forward mode of algorithmic differentiation.
- We have used an implementation of forward mode called source-code transformation.
- In object-oriented languages, the same result can be achieved by defining a new data type that tracks both the function values and their derivatives.

Pros & Cons of Forward-mode AD

ε in FD approx.

- ✓ no truncation error and no h to worry about!
- ✓ the cost of evaluating the differentiated function is only a small factor more than the original code (approximately twice the cost)
- ✗ requires access to the source code
- ✗ computational cost still scales with the # of design variables

Cost is still proportional to the number of design variables, so the advantages over complex-step are minimal.

Kenobi: *That [method] was our last hope.*

Yoda: *No. There is another.*

Exercise

Apply forward-mode to compute the partial derivative $\partial f / \partial x_2$ of the function below.

```
function func(x1, x2)
# compute a simple function value
v1 = x1.^2
v2 = x2.*sin(v1)
f = v1 + v2
return f
end
```

Computing Derivatives:
Reverse-mode AD

Reverse Mode

To understand the reverse mode of AD, we again consider the function

$$\begin{aligned} f(x_1, x_2) &= x_1^2 + x_2 \sin\left(x_1^2\right) \\ &= v_1 + v_2 \end{aligned}$$

where $v_1 = x_1^2$ and $v_2 = x_2 \sin(v_1)$.

The total derivative of f with respect to x_i $(i = 1, 2)$ is

$$\frac{Df}{Dx_i} = \frac{\partial f}{\partial x_i} + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial f}{\partial v_2}\left(\frac{\partial v_2}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial v_2}{\partial x_i}\right)$$

Reverse Mode (cont.)

The forward mode works by evaluating the partial derivatives from right-to-left in the products:

Step 1: $$\frac{Df}{Dx_i} = \frac{\partial f}{\partial x_i} + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial f}{\partial v_2}\left(\frac{\partial v_2}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial v_2}{\partial x_i}\right)$$

Step 2: $$\frac{Df}{Dx_i} = \frac{\partial f}{\partial x_i} + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial f}{\partial v_2}\left(\frac{\partial v_2}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial v_2}{\partial x_i}\right)$$

Step 3: $$\frac{Df}{Dx_i} = \frac{\partial f}{\partial x_i} + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial f}{\partial v_2}\left(\frac{\partial v_2}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial v_2}{\partial x_i}\right)$$

Reverse Mode (cont.)

The reverse mode works by evaluating the partial derivatives from left-to-right in the products:

Step 1: $$\frac{Df}{Dx_i} = \frac{\partial f}{\partial x_i} + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial f}{\partial v_2}\left(\frac{\partial v_2}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial v_2}{\partial x_i}\right)$$

Step 2: $$\frac{Df}{Dx_i} = \frac{\partial f}{\partial x_i} + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial f}{\partial v_2}\left(\frac{\partial v_2}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial v_2}{\partial x_i}\right)$$

Step 3: $$\frac{Df}{Dx_i} = \frac{\partial f}{\partial x_i} + \frac{\partial f}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial f}{\partial v_2}\left(\frac{\partial v_2}{\partial v_1}\frac{\partial v_1}{\partial x_i} + \frac{\partial v_2}{\partial x_i}\right)$$

Reverse Mode (cont.)

To make this work in practice, new variables are introduced in the code that keep track of the total derivatives.

- We will use an overbar on variables to denote the total derivative of f with respect to that variable

$$\bar{f} = \frac{Df}{Df} = 1$$

$$\bar{v}_1 = \frac{Df}{Dv_1} \qquad \bar{v}_2 = \frac{Df}{Dv_2}$$

$$\bar{x}_1 = \frac{Df}{Dx_1} \qquad \bar{x}_2 = \frac{Df}{Dx_2}$$

- $\bar{x}_1$ and $\bar{x}_2$ define the gradient we want

Reverse Mode (cont.)

Recall our Julia implementation:

```
1       function func(x1, x2)
2       # compute a simple function value
3       v1 = x1.^2
4       v2 = x2.*sin(v1)
5       f = v1 + v2
6       return f
7       end
```

- For the reverse mode, we first evaluate lines 3-5
- Then we step backwards through the code, differentiating line by line

Initialize $\bar{f} = 1$, $\bar{v}_1 = 0$, $\bar{v}_2 = 0$, $\bar{x}_1 = 0$, $\bar{x}_2 = 0$.

Reverse Mode (cont.)

```
function func(x1, x2)
# compute a simple function value
v1 = x1.^2
v2 = x2.*sin(v1)
f = v1 + v2
return f
end
```

Differentiating line 5 with respect to the variables that appear on the right (i.e. v_1 and v_2) gives us

$$\bar{v}_2 = \bar{v}_2 + \frac{\partial f}{\partial v_2}\bar{f} = 1$$

$$\bar{v}_1 = \bar{v}_1 + \frac{\partial f}{\partial v_1}\bar{f} = 1$$

Reverse Mode (cont.)

```
function func(x1, x2)
# compute a simple function value
v1 = x1.^2
v2 = x2.*sin(v1)
f = v1 + v2
return f
end
```

Differentiating line 4 with respect to the variables on its right (x_2 and v_1) gives us

$$\bar{v}_1 = \bar{v}_1 + \frac{\partial v_2}{\partial v_1}\bar{v}_2 = 1 + x_2\cos(v_1)$$

$$\bar{x}_2 = \bar{x}_2 + \frac{\partial v_2}{\partial x_2}\bar{v}_2 = \sin(v_1)$$

Reverse Mode (cont.)

```
1       function func(x1, x2)
2       # compute a simple function value
3       v1 = x1.^2
4       v2 = x2.*sin(v1)
5       f = v1 + v2
6       return f
7       end
```

Finally, differentiating line 3 with respect to the variables on its right (x_1) gives us

$$\bar{x}_1 = \bar{x}_1 + \frac{\partial v_1}{\partial x_1}\bar{v}_1 = 2x_1(1 + x_2\cos(v_1))$$

Reverse Mode (cont.)

Thus, in the end we have

$$\frac{Df}{Dx_1} = \bar{x}_1 = 2x_1(1 + x_2\cos(v_1))$$
$$\frac{Df}{Dx_2} = \bar{x}_2 = \sin(v_1)$$

- You can easily verify that these are the correct values for the gradient of f evaluated at (x_1, x_2).
- Putting this into the form of Julia, we get the following…

Reverse Mode (cont.)

```
function dfunc_reverse(x1, x2)
# compute a simple function value and its gradient
v1 = x1.^2
v2 = x2.*sin(v1)
f = v1 + v2
# intialize bar variables
f_bar = 1.0; v2_bar = 0.0; v1_bar = 0.0
x2_bar = 0.0; x1_bar = 0.0;
v2_bar = v2_bar + f_bar # line 5
v1_bar = v1_bar + f_bar # line 5
v1_bar = v1_bar + x2.*cos(v1).*v2_bar # line 4
x2_bar = x2_bar + sin(v1).*v2_bar # line 4
x1_bar = x1_bar + 2.0*x1*v1_bar # line 3
dfdx1 = x1_bar; dfdx2 = x2_bar
return f, dfdx1, dfdx2
end
```

Pros & Cons of Reverse-mode AD

FD ε

- ✓ no truncation error and no h to worry about!
- ✓ the cost of evaluating the differentiated function is only a small factor more than the original code (approximately twice the cost) 4
- ✓ produces the entire gradient at once! (cost is virtually independent of the number of design variables)
- ✗ requires access to the source code

Note: you can only get the gradient of one output at a time, therefore. . .

Important Guideline

Suppose you have a function that takes in n inputs and produces m outputs, and you need the gradient, with respect to all inputs, of all outputs. Generally speaking,

- if $n > m$, use the reverse mode
- if $m > n$, use the forward mode (or complex step)

References

[CH02] Scott S. Collis and Matthias Heinkenschloss, *Analysis of the streamline upwind/Petrov Galerkin method applied to the solution of optimal control problems*, Tech. Report TR02-01, Houston, Texas, 2002.

[GW09] Andreas Griewank and Andrea Walther, *Evaluating derivatives: principles and techniques of algorithmic differentiation*, Society for Industrial & Applied Mathematics ; Cambridge University Press [distributor], 2009.