MANE 6961:

Adjoints for Scientists and Engineers

Lecture 1

Prof. Hicken
JEC 2036

Course Objectives

MANE 6961, "Adjoints for Scientists and Engineers," aims to help you:

- be able to derive the adjoint equation for any given primal problem and functional;
- use the adjoint for sensitivity analysis and output error estimation; and,
- implement and solve adjoint problems in software.

Instructor

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Prerequisites

To take this course, your previous course work should have included

- multivariate and vector calculus,
- ordinary and partial differential equations,
- numerical methods, and
- programming.

If you are missing one of these, you might be able to get by...

Course Texts

No required text(s)

Supplemental References:

- C. Lanczos, *"Linear Differential Operators,"* SIAM, 1996
- J. L. Lions, *"Optimal Control of Systems Governed by Partial Differential Equations,"* Springer-Verlag, 1971
- A. Borzi and V. Schulz, *"Computational Optimization of Systems Governed by Partial Differential Equations,"* SIAM, 2012

Grading Breakdown

There are four major assignments/projects that will make up the bulk of your grade

- $100\% = 4\times\ 25\%$
- Each will require extensive programming
- I will expect a LaTeX'ed report for each

I will introduce the first assignment next class.

Class Policies

See the syllabus for further details.

Late Assignments: 10% penalty if submitted within 24hrs; 25% penalty if submitted within a week; 100% penalty otherwise.

Please read the Academic Integrity statement in the syllabus:

- first violation = grade of zero on assignment
- second violation = grade of F in the course

Motivation

Applications

In science and engineering, we frequently encounter problems for which we need to determine parameters in a system that is governed by a partial differential equation (PDE).

- simulation-based design optimization
- PDE-constrained inverse problems

Let's consider some concrete examples...

Example 1: drag minimization

Find the airfoil shape that minimizes drag subject to the incompressible Navier-Stokes equations

Example 1: drag minimization (cont.)

Example 2: inverse problem in elastography

Find the shear modulus such that computed displacements are close, in some sense, to a set of measured displacements.

Example 2: inverse problem in elastography (cont.)

Problem Characteristics

Both the above examples share the same basic characteristics.

1. There are a (potentially) large number of parameters that must be determined; in some applications the parameters may be infinite dimensional.
2. The problems are governed by a PDE constraint.

Gradient descent is the most efficient means of solving these types of problems, due to the large number of parameters; however,
how do we find the gradient?

Generic Problem

To answer the above question, let's consider a more general (abstract) problem.

$$\begin{aligned} \min_{\alpha,u} \quad & \mathcal{J}(\alpha, u) \\ \text{s.t.} \quad & \mathcal{R}(\alpha, u) = 0 \end{aligned}$$

where

- $\alpha \in \mathbb{R}^n$ parameter vector to be determined,
- $u \in \mathbb{R}^s$ is the state,
- $\mathcal{J}$ is the objective, or cost function; and
- $\mathcal{R}$ is the state equation.

Generic Problem (cont.)

In order to use a gradient-based method to solve the problem, we need the gradient:

Generic Problem (cont.)

Generic Problem (cont.)

Generic Problem (cont.)

Take-away message

We only need one adjoint for each $\mathcal{J}$ to get the gradient with respect to any number of parameters, including infinite-dimensional parameters.

The reason for this is that

$$\frac{D\mathcal{J}}{D\alpha} = \frac{\partial \mathcal{J}}{\partial \alpha} + \psi^T \frac{\partial \mathcal{R}}{\partial \alpha}$$

involves only (relatively cheap) products.

What's next?

There is not much more to say regarding the algebraic case, but there are a whole host of questions that arise if we dig deeper:

- What does $\partial\mathcal{R}/\partial u$ mean when $\mathcal{R}$ is a PDE?
- What is $(\partial\mathcal{R}/\partial u)^T$ mean when $\mathcal{R}$ is a PDE?
- What role do boundary conditions in the adjoint?
- How does one compute ψ in practice when there are thousands or millions of state equations?
- Does this work for time dependent problems?

This course aims to answer these questions and more.