



MANE 6961:

Adjoint for Scientists and Engineers

Lecture 7

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Lecture Objective

Many physical systems are modelled using nonlinear boundary-value problems. Furthermore, the quantity of interest in such systems is often a nonlinear functional that depends on the solution of the (nonlinear) BVP.

This motivates the generalization of the concept of an adjoint to nonlinear problems, which is the topic we will begin to discuss in this lecture.

Nonlinear Boundary-Value Problems

In this lecture, and those that follow, we will be concerned with the generic nonlinear BVP defined below:

$$\begin{aligned} N(u) &= 0, & \forall x \in \Omega, \\ B(u) &= 0, & \forall x \in \Gamma. \end{aligned} \tag{*}$$

- N is a nonlinear differential operator
- B is a nonlinear boundary operator

Examples:

Nonlinear Functionals

In addition, we will consider generic nonlinear functionals of the form

$$\begin{aligned} J(u) &= \int_{\Omega} g(u) \, d\Omega + \int_{\Gamma} c(C(u)) \, d\Gamma \\ &= (g(u), 1)_{\Omega} + (c(C(u)), 1)_{\Gamma}. \end{aligned}$$

- $g(u)$ is a nonlinear function of u
- $C(u)$ is a nonlinear boundary operator
- $c(C(u))$ is a nonlinear boundary function

Fréchet and Gâteaux Derivatives

Motivation

Recall the definition of the discrete adjoint from the first lecture:

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

This suggests that we will need to differentiate N , B , and J with respect to u , in order to generalize the adjoint BVP to nonlinear problems.

But what is the meaning of $\partial N / \partial u$ when N is a nonlinear operator and u is a function, i.e. an infinite-dimensional vector?

Motivation (cont.)

The problem with using the usual derivative in the context of functions can be appreciated by trying to apply the definition of a partial derivative.

For a function $J_h : \mathbb{R}^n \rightarrow \mathbb{R}$, the i th partial derivative w.r.t. u_h is given by

$$\frac{\partial J_h}{\partial u_{h,i}} = \lim_{\epsilon \rightarrow 0} \frac{J_h(u_h + e_i \epsilon) - J_h(u_h)}{\epsilon}$$

where

$$(e_i)_j = \begin{cases} 1, & \text{if } j = i \\ 0, & \text{if } j \neq i \end{cases}$$

Motivation (cont.)

Defining e_i becomes problematic when $u \in \mathcal{V}$, i.e. when \mathcal{V} is a function space and u is infinite-dimensional.

We need a more general definition for a derivative with respect to a function.

Fréchet Derivative

Definition: Fréchet Derivative

Let \mathcal{V} and \mathcal{W} be two Banach spaces, and let $\mathcal{U} \subset \mathcal{V}$ be an open subset. The function $N : \mathcal{U} \rightarrow \mathcal{W}$ is Fréchet differentiable at $u \in \mathcal{U}$ if

$$\lim_{v \rightarrow 0} \frac{\|N(u+v) - N(u) - N'[u]v\|_{\mathcal{W}}}{\|v\|_{\mathcal{V}}} = 0,$$

for some bounded linear operator $N'[u] : \mathcal{V} \rightarrow \mathcal{W}$, which we call the Fréchet derivative of N at u .

- Banach space: a complete, normed vector space.

Fréchet Derivative (cont.)

I used the nonlinear differential operator, N , in the Fréchet derivative definition, but I just as easily could have used B or J . The only difference in the present context is the range space.

- For N , \mathcal{W} is a function space, for example, the space of functions with bounded 2-norms on Ω , i.e. $L^2(\Omega)$.
- For B , \mathcal{W} is the space of bounded functions on Γ .
- For J , $\mathcal{W} = \mathbb{R}$.

Gâteaux Derivative

The Fréchet derivative definition is not very helpful in practice. Instead, I usual rely on the directional derivative to compute the Fréchet derivative.

Definition: Directional (Gâteaux) Derivative

Let \mathcal{V} and \mathcal{W} be two Banach spaces. The directional, or Gâteaux, derivative of the function $N : \mathcal{U} \subset \mathcal{V} \rightarrow \mathcal{W}$ at $u \in \mathcal{U}$ in the direction $v \in \mathcal{U}$ is

$$D_v N(u) = \lim_{\epsilon \rightarrow 0} \frac{N(u + \epsilon v) - N(u)}{\epsilon}$$

Gâteaux Derivative (cont.)

Why is the directional derivative useful?

If N is Fréchet differentiable at u (which we will assume), then the directional derivative of N exists at u in all directions v ,¹ and

$$N'[u]v = D_v N(u).$$

This is analogous to the finite-dimensional formula $(\nabla f) \cdot v = D_v f$

Furthermore, we have the following practical formula:

$$D_v N(u) = \left[\frac{d}{d\epsilon} N(u + \epsilon v) \right]_{\epsilon=0}.$$

¹The converse is not true; the directional derivative can exist in all directions, but N may not be Fréchet differentiable.

Exercise

Determine the Fréchet derivative of the functional

$$J(u) = \int_{\Omega} (\nabla u) \cdot (\nabla u) d\Omega.$$

Exercise (cont.)

Exercise

Determine the Fréchet derivative of the nonlinear operator

$$N(u) = u \frac{\partial u}{\partial x}.$$

Exercise (cont.)

Deriving the Adjoint BVP for Nonlinear Problems

Green's Identity, revisited

With Fréchet differentiation in our toolbox, we can now derive the adjoint for nonlinear BVPs and functionals.

First, we will need to identify the relevant terms in the extended Green's identity:

$$(\psi, Lu)_{\Omega} - (u, L^* \psi)_{\Omega} = (Cu, B^* \psi)_{\Gamma} - (Bu, C^* \psi)_{\Gamma}.$$

For the nonlinear BVP, we have

- $L \rightarrow N'[u]$;
- $B \rightarrow B'[u]$; and
- $C \rightarrow C'[u]$.

Green's Identity, revisited (cont.)

Definition: Adjoint Operators of Nonlinear BVPs

Consider the nonlinear boundary value problem (\star) , and assume that N and B are Fréchet differentiable for all $u \in \mathcal{U} \subset \mathcal{V}$. Then we have the following identity:

$$(\psi, N'[u]v)_{\Omega} - (v, N'[u]^*\psi)_{\Omega} = \\ (C[u]'v, B'[u]^*\psi)_{\Gamma} - (B'[u]v, C'[u]^*\psi)_{\Gamma}, \quad \forall v, \psi \in \mathcal{U},$$

where $N'[u]^*$ denotes the adjoint differential operator, and $B'[u]^*$ denotes the adjoint boundary-condition operator.

Adjoint BVP

We now have a means of finding the adjoint differential and boundary operators; however, in order to define the adjoint BVP we also need the boundary values and source term.

To this end, we need the Fréchet derivative of the functional $J(u)$:

$$J'[u]v = \int_{\Omega} g'[u]v \, d\Omega + \int_{\Gamma} c'[Cu]C'[u]v \, d\Gamma.$$

Then we can make the following associations with the linear adjoint problem:

- $g \rightarrow g'[u]$;
- $c \rightarrow c'[Cu]$; and
- $C \rightarrow C'[u]$.

Adjoint BVP (cont.)

Definition: Adjoint Problem (nonlinear BVP)

Let u be the solution to the nonlinear BVP (\star) , and consider the nonlinear functional $J(u)$ defined earlier. Then the associated adjoint boundary-value problem is

$$\begin{aligned} N'[u]^* \psi &= g'[u], & \forall x \in \Omega, \\ B'[u]^* \psi &= c'[Cu], & \forall x \in \Gamma. \end{aligned} \tag{Adj}$$

Connection to Sensitivity Analysis

We conclude by demonstrating that the adjoint problem (Adj) is precisely the one we want for sensitivity analysis (we will delve into this topic more in a few lectures).

Consider a nonlinear BVP and functional that depends on a parameter $\alpha \in \mathbb{R}^n$:

$$J(u, \alpha) = \int_{\Omega} g(u, \alpha) d\Omega + \int_{\Gamma} c(C(u), \alpha) d\Gamma$$

Connection to Sensitivity Analysis (cont.)

Connection to Sensitivity Analysis (cont.)

Connection to Sensitivity Analysis (cont.)

References