MANE 6960:

Adjoints for Scientists and Engineers

Lecture 3

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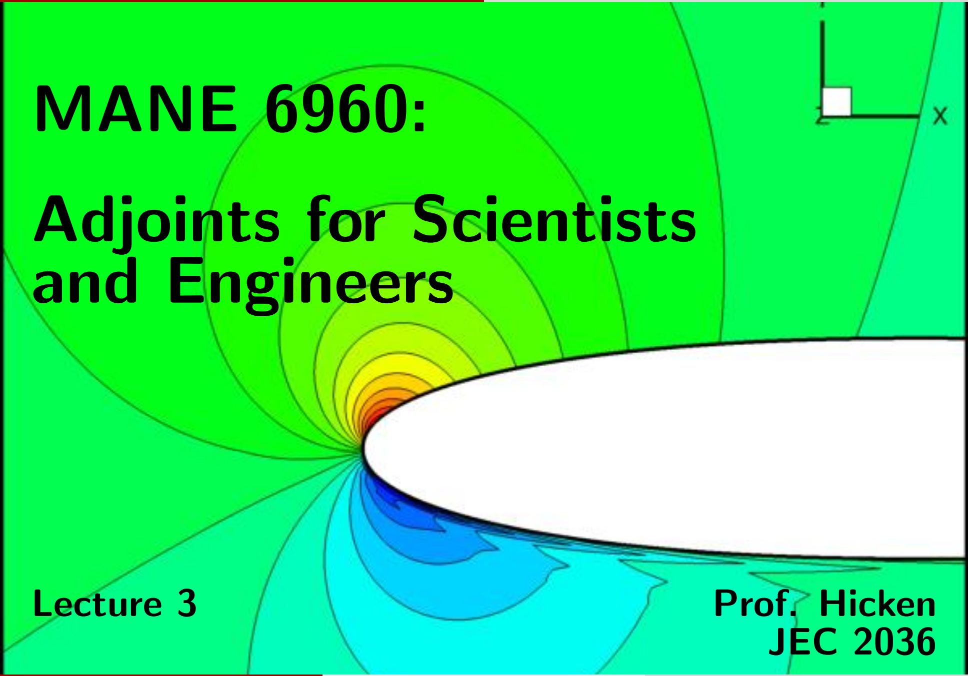


Adjoint Boundary Conditions and Compatibility

Review

Recall that, in the discrete case, we can compute the gradient of a function, $J_h(\alpha, u_h)$, with respect to α in one of two ways:

$$\begin{aligned} \text{Direct:} \quad \frac{DJ_h}{D\alpha} &= \frac{\partial J_h}{\partial \alpha} + \frac{\partial J_h}{\partial u_h}\frac{Du_h}{D\alpha} \\ \text{Adjoint:} \quad \frac{DJ_h}{D\alpha} &= \frac{\partial J_h}{\partial \alpha} + \psi^T \frac{\partial R_h}{\partial \alpha}. \end{aligned}$$

The adjoint approach has the distinct advantage that we only need to solve one adjoint equation (a linear system of equations) to obtain the gradient with respect to any number of variables α.

Review (cont.)

We would like to understand the adjoint approach in the continuous case, where we have a partial differential equation (PDE) rather than an algebraic equation.

To this end, we need to find the analog of the discrete adjoint equation, i.e.

$$L_h^T \psi_h = g_h,$$

in the continuous case.

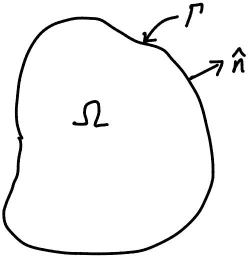
- last lecture we found the adjoint operator, L^*
- this lecture we will derive the adjoint boundary conditions

Generic Linear PDE

To simplify the analysis, we will continue to assume the PDE is linear.

More specifically, we will consider the generic, linear boundary-value problem (BVP)

$$\begin{aligned} Lu &= f, \qquad \forall x \in \Omega, \\ Bu &= b, \qquad \forall x \in \Gamma. \end{aligned}$$



- Ω is the domain of the PDE
- $\Gamma = \partial\Omega$ is the boundary of Ω
- $f \in L^2(\Omega)$ is the source term
- $b \in L^2(\Gamma)$ are the boundary values

Generic Linear PDE (cont.)

In the above boundary-value problem, B is a boundary operator:

- like L, but defined over the boundary Γ
- builds linear combinations of u and its derivatives
- may change from one part of Γ to another

Examples of B:

Laplace:

$$Bu = u, \quad \forall x \in \Gamma_D$$

$$Bu = (\vec{\nabla} u)\cdot\hat{n} = n_x \frac{\partial u}{\partial x} + n_y \frac{\partial u}{\partial y}, \quad \forall x \in \Gamma_N$$

Euler:

$$B\vec{v} = \vec{v}\cdot\hat{n}, \quad \forall x \in \Gamma_{wall}$$

Generic Linear Functional

Suppose we have solved the above boundary-value problem for u. Now we want to use u to evaluate a functional.

Definition: Functional (real-valued)

A functional, J, is a mapping from a function space V over the reals to a real-valued scalar. This is denoted

$$J : V \to \mathbb{R}.$$

Example: Lift, Drag, total heat flux, total energy

Generic Linear Functional (cont.)

As with the PDE, we will assume the functional is linear in u. Thus, the most general form of linear functional on Ω is

$$J(u) = (g, u)_\Omega + (c, Cu)_\Gamma$$

- recall that $(u, v)_\Omega \equiv \int_\Omega uv \, d\Omega$
- similarly, $(u, v)_\Gamma \equiv \int_\Gamma uv \, d\Gamma$

Why not $J = (g, Gu)_\Omega + (c, Cu)_\Gamma$

$$= \underbrace{(G^* g, u)_\Omega + \text{boundary terms}}_{\text{same form as above}}$$

Generic Linear Functional (cont.)

Thus,

$$(c, Cu)_\Gamma = \int_\Gamma c(Cu)\, d\Gamma.$$

- C is a differential boundary operator, analogous to B
- $c \in L^2(\Gamma)$ is a weighting function

Example of C:

$$Cu = (\vec{\nabla} u) \cdot \hat{n} = n_x \frac{\partial u}{\partial x} + n_y \frac{\partial u}{\partial y}$$

Compatibility

It turns out that we are not free to choose the operator C freely.

Definition: Compatibility [Har07, Lan61]

Let $J(u) = (g, u)_\Omega + (c, Cu)_\Gamma$ be a functional, and let u be the solution to the boundary-value problem

$$\begin{aligned} Lu &= f, \qquad \forall x \in \Omega, \\ Bu &= b, \qquad \forall x \in \Gamma. \end{aligned} \tag{$\star$}$$

Then J is compatible with ($\star$) if

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

Compatibility (cont.)

Notice that the compatibility condition is Green's extended identity, but with some new operators introduced in the boundary terms.

Why should we care about compatibility?

The compatibility condition tells us what the adjoint boundary conditions should be. . .

aka Green's extended identity

Compatibility (cont.)

To see this, subtract $(\psi, \overbrace{Lu - f}^{\text{from PDE}}) = 0$ from the functional (in the following, remember that $(u, v) = (v, u)$ for any inner product):

$$
\begin{aligned}
J(u) &= (g, u)_\Omega + (c, Cu)_\Gamma \\
&= (g, u)_\Omega + (c, Cu)_\Gamma - (\psi, \overbrace{Lu - f}^{=0})_\Omega \\
&= (g, u)_\Omega + (c, Cu)_\Gamma - (\psi, Lu)_\Omega + (\psi, f)_\Omega \qquad \text{, by linearity of } (,)_\Omega \\
&= (u, g)_\Omega + (c, Cu)_\Gamma \\
&\qquad - \overbrace{\left[(u, L^*\psi)_\Omega + (Cu, B^*\psi)_\Gamma - (Bu, C^*\psi)_\Gamma\right]}^{\text{Green's extended}} + (\psi, f)_\Omega \\
&= (f, \psi)_\Omega + (b, C^*\psi)_\Gamma - (u, L^*\psi - g)_\Omega - (Cu, B^*\psi - c)_\Gamma
\end{aligned}
$$

This is true for any ψ, at this point

Compatibility (cont.)

We can eliminate u from the functional if ψ satisfies

$$\begin{aligned} L^*\psi &= g, \qquad &\forall x \in \Omega, \\ B^*\psi &= c, \qquad &\forall x \in \Gamma. \end{aligned} \tag{Adj}$$

Then we have the following duality:

$$\begin{aligned} J(u) &= (g, u)_\Omega + (c, Cu)_\Gamma \\ &= (f, \psi)_\Omega + (b, C^*\psi)_\Gamma \\ &= J(\psi) \end{aligned}$$

Compatibility (cont.)

This duality gives us an inexpensive means of computing the gradient, as desired.

To see this, suppose that $f = f(\alpha)$ and $b = b(\alpha)$ where $\alpha \in \mathbb{R}^n$ are parameters. Then

$$\frac{D}{D\alpha} J(\psi) = \left(\frac{\partial f}{\partial \alpha}, \psi \right)_{\Omega} + \left(\frac{\partial b}{\partial \alpha}, C^* \psi \right)_{\Gamma}$$

Contrast this with

$$\frac{D}{D\alpha} J(u) = \left(g, \frac{Du}{D\alpha} \right)_{\Omega} + \left(c, C \frac{Du}{D\alpha} \right)$$

where $Du/D\alpha$ requires the solution of n linear PDEs.

Adjoint Problem

Definition: Adjoint Problem (linear BVP)

Let $J(u) = (g, u)_\Omega + (c, Cu)_\Gamma$ be a functional, and let u be the solution to the linear boundary-value problem $(\star)$. Then the associated adjoint boundary-value problem is

$$\begin{aligned} L^*\psi &= g, \qquad \forall x \in \Omega, \\ B^*\psi &= c, \qquad \forall x \in \Gamma, \end{aligned} \tag{Adj}$$

and the adjoint-based functional is

$$J(\psi) = J(u) = (f, \psi)_\Omega + (b, C^*\psi)_\Gamma.$$

Adjoint Problem (cont.)

Notice the roles of the various operators and functions:

	primal	**adjoint**
BVP PDE operator	L	L^*
BVP boundary op.	B	B^*
J boundary op.	C	C^*
source	f	g
J volume weight	g	f
boundary value	b	c
J boundary weight	c	b

related via Green's extended identity

Exercise

Consider the Poisson's equation in one dimension:

$$Lu = \frac{d}{dx}\left(\nu \frac{du}{dx}\right) = f, \qquad \forall x \in [0,1]$$

$$Bu = \begin{cases} u, & x = 0 \\ \frac{du}{dx}, & x = 1 \end{cases} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

where $\nu(x) > 0$ is a spatially varying diffusion coefficient.

1. What are L^* and B^*?
2. What form can $J(u)$ take?
3. What is the adjoint problem based on the above?

Exercise (cont.)

Use integration by parts to find Green's extended identity (and thereby L^*, B^*, C, C^*):

$$(\psi, Lu)_\Omega = \int_\Omega \psi \frac{d}{dx}\left(\nu \frac{du}{dx}\right) d\Omega$$

$$= \int_\Omega \frac{d}{dx}\left(\psi \nu \frac{du}{dx}\right) d\Omega - \int_\Omega \left(\frac{d\psi}{dx}\right) \nu \left(\frac{du}{dx}\right) d\Omega$$

$$= \left[\psi \nu \frac{du}{dx}\right]\Big|_{x=0}^{1} - \int_\Omega \frac{d}{dx}\left(\frac{d\psi}{dx} \nu u\right) d\Omega$$

$$+ \int_\Omega \frac{d}{dx}\left(\nu \frac{d\psi}{dx}\right) u \, d\Omega$$

Exercise (cont.)

$$(\psi, Lu)_\Omega = \underbrace{\int_\Omega u \frac{d}{dx}\left(\nu \frac{d\psi}{dx}\right) d\Omega}_{(u, L^* \psi)_\Omega}$$

$$+ \underbrace{\left(\psi \nu \frac{du}{dx}\right)\bigg|_{x=1}}_{-(Bu, C^*\psi)_\Gamma} \underbrace{- \left(\psi \nu \frac{du}{dx}\right)\bigg|_{x=0}}_{+(Cu, B^*\psi)_\Gamma}$$

$$\underbrace{- \left(\frac{d\psi}{dx} \nu u\right)\bigg|_{x=1}}_{+(Cu, B^*\psi)_\Gamma} \underbrace{+ \left(\frac{d\psi}{dx} \nu u\right)\bigg|_{x=0}}_{-(Bu, C^*\psi)_\Gamma}$$

Exercise (cont.)

$$(Bu, C^* \psi)\big|_{x=0} = \underbrace{(u)}_{Bu} \underbrace{\left(-\nu \frac{d\psi}{dx}\right)}_{C^*\psi}\Bigg|_{x=0}$$

$$(Bu, C^* \psi)\big|_{x=1} = \underbrace{\left(\frac{du}{dx}\right)}_{Bu} \underbrace{\left(-\nu \psi\right)}_{C^*\psi}\Bigg|_{x=1}$$

$$(Cu, B^* \psi)\big|_{x=0} = \underbrace{\left(-\nu \frac{du}{dx}\right)}_{Cu} \underbrace{\left(\psi\right)}_{B^*\psi}\Bigg|_{x=0}$$

$$(Cu, B^* \psi)\big|_{x=1} = \underbrace{\left(-\nu u\right)}_{Cu} \underbrace{\left(\frac{d\psi}{dx}\right)}_{B^*\psi}\Bigg|_{x=1}$$

Exercise (cont.)

1)

$$L^* \psi = \frac{d}{dx}\left(\nu \frac{d\psi}{dx}\right)$$

$$B^* \psi = \begin{cases} \psi, & x=0 \\ \frac{d\psi}{dx}, & x=1 \end{cases}$$

This problem is self adjoint: primal and adjoint BVP use same operators

Exercise (cont.)

2) Functional can look like

$$\boxed{J(u) = \int_\Omega g\, u\, d\Omega - c_0 \upsilon \frac{du}{dx}\bigg|_{x=0} - c_1 \upsilon u\bigg|_{x=1}}$$

Cannot have (for example)

$$J(u) = c_1 \frac{du}{dx}\bigg|_{x=1}$$

But $du/dx = 0$ is a know boundary value!

so use it!

Exercise (cont.)

3) Functional provides source and boundary values to adjoint BVP:

$$L^* \psi = \frac{d}{dx}\left(\nu \frac{d\psi}{dx}\right) = g \quad , \quad \forall\, x \in [0,1]$$

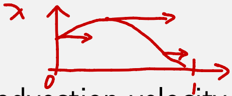
$$B^* \psi\big|_{x=0} = \psi(0) = c_0$$

$$B^* \psi\big|_{x=1} = \frac{d\psi}{dx}(1) = c_1$$

Exercise

Consider the linear advection equation in one dimension:

$$Lu = \frac{d}{dx}(\lambda u) = f, \qquad \forall x \in [0, 1]$$
$$Bu = u(0) = b$$



where $\lambda(x) > 0$ is the spatially varying advection velocity.

1. What are L^* and B^*?
2. What form can $J(u)$ take?
3. What is the adjoint problem based on the above?

Exercise (cont.)

As before, we use integration by parts to get Green's identity (and, hence, L^*, B^*, C, C^*):

$$(\psi, Lu)_\Omega = \int_\Omega \psi \frac{d}{dx}(\lambda u)\, d\Omega$$

$$= \int \frac{d}{dx}(\psi \lambda u)\, d\Omega - \int \lambda \frac{d\psi}{dx} u \, d\Omega$$

$$= [\psi \lambda u]\Big|_{x=0}^{1} - \int \lambda \frac{d\psi}{dx} u \, d\Omega$$

Exercise (cont.)

Continuing,

$$(\psi, Lu)_\Omega = \overbrace{\int u\left(-\lambda \frac{d\psi}{dx}\right) d\Omega}^{(u,\, L^*\psi)_\Omega}$$

$$\underbrace{+ \; (\psi \lambda u)\Big|_{x=1}}_{(Cu,\, B^*\psi)_\Gamma}$$

$$\underbrace{- \; (\psi \lambda u)\Big|_{x=0}}_{-(Bu,\, C^*\psi)_\Gamma}$$

Exercise (cont.)

1) $$L^* \psi = -\lambda \frac{d\psi}{dx}$$

$$(Bu, C^*\psi)\big|_{x=0} = \underbrace{(u)}_{Bu}\big|_{x=0}\underbrace{(\lambda\psi)}_{C^*\psi}\big|_{x=0}$$

$$(Cu, B^*\psi)\big|_{x=1} = \underbrace{(\lambda u)}_{Cu}\big|_{x=1}\underbrace{(\psi)\big|_{x=1}}_{B^*\psi}$$

$$\therefore \quad B^*\psi = \psi(x=1)$$

Exercise (cont.)

2) Functional can take the form

$$J(u) = \int_\Omega g u \, d\Omega + c_1 (\lambda u)\big|_{x=1}$$

Functional should not include boundary terms at inlet; but, again, we know u at inlet, $x=0$, so we could write

$$J(u) = \int_\Omega g u \, d\Omega + c_1 (\lambda u)\big|_{x=1} + c_0 \lambda b$$

Also, note that functional cannot use derivative at boundary (for compatibility)

Exercise (cont.)

3) The adjoint problem is given by the BVP

$$-\lambda \frac{d\psi}{dx} = g \quad , \quad \forall x \in \underbrace{[0,1]}_{\Omega}$$

$$\psi(1) = c_1$$

"flow" is reversed, so BC is at outlet of primal problem

Exercise (cont.)

References

[Har07] Ralf Hartmann, *Adjoint consistency analysis of discontinuous Galerkin discretizations*, SIAM Journal on Numerical Analysis **45** (2007), no. 6, 2671–2696.

[Lan61] Cornelius Lanczos, *Linear Differential Operators*, D. Van Nostrand Company, Limited, London, England, 1961.