MANE 6960:

Adjoints for Scientists and Engineers

Lecture 23

Prof. Hicken
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Adjoints and chaotic dynamics

You may have the impression that, other than some implementation details, you can apply the adjoint to any problem and expect useful results.

This turns out to be false.

As we shall see, when applied to chaotic problems, the adjoint fails to produce useful results.

- Recall that a chaotic dynamical system is one that is sensitive to parameter changes; e.g. turbulent flows.

Adjoints and chaotic dynamics (cont.)

In this lecture, we will derive and analyze the adjoint of the incompressible Navier-Stokes (NS) equations.

- The NS equations are frequently used to model turbulent flows.
- We will show that the solution to the NS equation is bounded in the L^2 norm, but. . .
- Surprisingly, the L^2 norm of the adjoint is not bounded.

The Adjoint of the incompressible Navier-Stokes Equations

The Incompressible Navier-Stokes

Recall that the incompressible Navier-Stokes equations are given by the following IBVP:

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} - \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j} = 0, \quad \forall x \in \Omega, t \in [0, T],$$

$$\frac{\partial u_j}{\partial x_j} = 0, \quad \forall x \in \Omega, t \in [0, T], \tag{NS}$$

where $u = (u_1, u_2, u_3)^T$ is the velocity and p is the pressure.

- we use the Einstein summation convention;
- density has been absorbed into the pressure;
- ν is the nondimensional kinematic viscosity (i.e. the Reynolds number).

The Incompressible Navier-Stokes (cont.)

The PDEs in (NS) are supplemented with the following boundary and initial conditions:

$$
\begin{aligned}
B_0(u) &\equiv u = 0, & \forall x \in \Gamma, t \in [0, T], \\
B_\infty(u) &\equiv u - u_\infty = 0, & \forall x \in \Gamma_\infty, t \in [0, T], \\
u(0, x) &\equiv u_0(x), & \forall x \in \Omega,
\end{aligned}
$$

where Γ denotes the surface of some geometry (e.g. an aircraft), Γ_∞ is a far-field boundary.
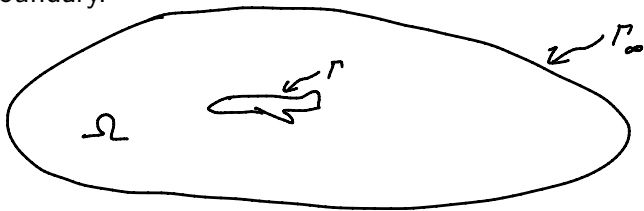
The Incompressible Navier-Stokes (cont.)

To facilitate the derivation of the adjoint equation, we define the following spatial operators:

$$N_i(u, p) \equiv u_j \frac{\partial u_i}{\partial x_j} + \frac{\partial p}{\partial x_i} - \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}$$

$$N_p(u, p) \equiv \frac{\partial u_j}{\partial x_j}$$

So,

$$\frac{\partial u_i}{\partial t} + N_i(u, p) = 0$$

$$N_p(u, p) = 0$$

Conservation of Kinetic Energy

Before we investigate the adjoint of (NS), we will first show that the fluid's kinetic energy can only increase due to boundary contributions.

In the present context, we define the kinetic energy as

$$\mathsf{k} = \frac{1}{2} u_j u_j.$$

$$= \frac{1}{2} \sum_{j=1}^{3} u_j u_j$$

Conservation of Kinetic Energy (cont.)

Multiplying the momentum equation by u_i (with the implied sum over i), and integrating over the domain, we find

$$\int_\Omega u_i \frac{\partial u_i}{\partial t}\, d\Omega + \int_\Omega u_i u_j \frac{\partial u_i}{\partial x_j}\, d\Omega$$

$$+ \int_\Omega u_i \frac{\partial p}{\partial x_i}\, d\Omega - \int_\Omega \nu u_i \frac{\partial^2 u_i}{\partial x_j \partial x_j}\, d\Omega = 0.$$

$$\Rightarrow \int_\Omega \frac{\partial}{\partial t}\left(\frac{1}{2} u_i u_i\right) d\Omega \;+\; \int_\Omega \frac{\partial}{\partial x_j}\left(u_j \,\frac{1}{2} u_i u_i\right) d\Omega$$

$$+ \int_\Omega \frac{\partial}{\partial x_i}\left(p\, u_i\right) d\Omega \;-\; \int_\Omega \nu \frac{\partial}{\partial x_j}\left(u_i \frac{\partial u_i}{\partial x_j}\right) d\Omega \;+\; \int_\Omega \nu \frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}\, d\Omega \;= 0$$

Conservation of Kinetic Energy (cont.)

In the above, I have used $\frac{\partial u_j}{\partial x_j} = 0$.

e.g. $\frac{\partial}{\partial x_j}\left(u_j \frac{1}{2} u_i u_i\right) = \frac{1}{2} u_i u_i \cancel{\frac{\partial u_j}{\partial x_j}}^{0} + \frac{1}{2} u_i u_j \frac{\partial u_i}{\partial x_j} + \frac{1}{2} u_i u_j \frac{\partial u_i}{\partial x_j}$

Continuing, we will make use of the B.C. $u = 0 \quad \forall x \in \Gamma$, and $\frac{\partial u_i}{\partial x_j} \longrightarrow 0$ as $\|\vec{x}\| \longrightarrow \infty$

$$\frac{\partial}{\partial t} \int_{\Omega} \left(\frac{1}{2} u_i u_i\right) d\Omega + \int_{\Gamma_\infty} \left(\frac{1}{2} u_i u_i\right)(u_j n_j) d\Gamma$$

$$+ \int_{\Gamma_\infty} p(u_j n_j) d\Gamma + \int_{\Omega} \nu \frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j} d\Omega = 0$$

Conservation of Kinetic Energy (cont.)

To summarize, the time rate of change of the total kinetic energy in the domain is

$$\frac{d}{dt}\int_{\Omega}\mathsf{k}\,d\Omega = -\int_{\Gamma_{\infty}}\mathsf{k}(u_i n_i)\,d\Gamma - \int_{\Gamma_{\infty}}p(u_i n_i)\,d\Gamma - \underbrace{\int_{\Omega}\nu\frac{\partial u_i}{\partial x_j}\frac{\partial u_i}{\partial x_j}\,d\Omega}_{-\text{ve}\quad\forall\ u_i}.$$

Thus, the total kinetic energy can only change due to

- convective transport of kinetic energy through Γ_{∞};
- pressure work on Γ_{∞}; and,
- viscous dissipation.

Drag functional

While our final conclusions will not depend strongly on the choice of functional, it is helpful to choose a particular functional in order to keep things more concrete.

We will use the force on Γ in the x direction which is given by

$$J(u,p) = \int_{\Gamma} \left(p\delta_{1j} - \nu \frac{\partial u_1}{\partial x_j} \right) n_j \, d\Gamma.$$

$$\delta_{ij} = \left\{ \begin{array}{l} 1, \ i = j \\ 0, \ i \neq j \end{array} \right. \qquad\qquad \delta_{ij} = I$$

Linearized Navier-Stokes

As usual, it is helpful to begin the derivation of the adjoint by first linearizing the PDE(s). Below, we differentiate the spatial parts of the conservation of mass and momentum equations with respect to u_i and p in the directions v_i and q, respectively:

$$N_i'[u_i]v_i = \quad v_i \, \frac{\partial u_i}{\partial x_i} \quad + \quad u_j \, \frac{\partial v_i}{\partial x_j} \quad - \quad \nu \frac{\partial^2 v_i}{\partial x_j \, \partial x_j} \qquad \text{(no sum } i\text{)}$$

$$N_i'[u_k]v_k = \quad v_k \, \frac{\partial u_i}{\partial x_k} \qquad\qquad\qquad \overleftarrow{\quad} \; (k \neq i)$$

$$\qquad\qquad\qquad\qquad\qquad\qquad\qquad (no\ sum\ k)$$

$$N_i'[p]q = \quad \frac{\partial q}{\partial x_i}$$

$$N_p'[u_i]v_i = \quad \frac{\partial v_i}{\partial x_i} \qquad\qquad\qquad\qquad (no\ \ sum\ i)$$

Adjoint Operators

Next, we derive the (spatial) Green's extended identity and, thus, the adjoint operators:

$$\int_\Omega \psi_i \left(v_j \frac{\partial u_i}{\partial x_j} + u_j \frac{\partial v_i}{\partial x_j} - \nu \frac{\partial^2 v_i}{\partial x_j \partial x_j} \right) d\Omega$$

$$+ \int_\Omega \psi_i \left(\frac{\partial q}{\partial x_i} \right) d\Omega + \int_\Omega \phi \frac{\partial v_i}{\partial x_i} d\Omega$$

Adjoint Operators (cont.)

For the first two terms we find

$$\int_\Omega \left(\Psi_i \, v_j \, \frac{\partial u_i}{\partial x_j} \;+\; \Psi_i \, u_j \, \frac{\partial v_i}{\partial x_j} \right) d\Omega$$

used $\frac{\partial u_j}{\partial x_j} = 0$

$$= \int_\Omega v_i \left[\Psi_j \, \frac{\partial u_j}{\partial x_i} \;-\; u_j \, \frac{\partial \Psi_i}{\partial x_j} \right] d\Omega$$

$$+ \int_{\Gamma \cup \Gamma_\infty} \Psi_i \, v_i \, (u_j \, n_j) \, d\Gamma$$

Adjoint Operators (cont.)

For the viscous term we get

$$- \int_\Omega \nu \, \Psi_i \frac{\partial^2 v_i}{\partial x_j \, \partial x_j} \, d\Omega \; = \; - \int_\Omega \nu \, \frac{\partial}{\partial x_j} \left(\Psi_i \, \frac{\partial v_i}{\partial x_j} \right) d\Omega$$

$$+ \int_\Omega \nu \left(\frac{\partial \Psi_i}{\partial x_j} \right) \left(\frac{\partial v_i}{\partial x_j} \right) d\Omega$$

$$= - \int_\Omega v_i \, \nu \, \frac{\partial^2 \Psi_i}{\partial x_j \, \partial x_j} \, d\Omega \; - \int_{\Gamma \cup \Gamma_\infty} \nu \, \Psi_i \, \frac{\partial v_i}{\partial x_j} \, n_j \, d\Gamma$$

$$+ \int_{\Gamma \cup \Gamma_\infty} \nu \, v_i \, \frac{\partial \Psi_i}{\partial x_j} \, n_j \, d\Gamma$$

Adjoint Operators (cont.)

Finally, for the "pressure" terms we find

$$\int_{\Omega} \psi_i \frac{\partial q}{\partial x_i} \, d\Omega \quad + \int_{\Omega} \phi \frac{\partial v_i}{\partial x_i} \, d\Omega$$

$$= \int_{\Omega} \frac{\partial}{\partial x_i} \left(\psi_i \, q \right) d\Omega \quad - \int_{\Omega} q \frac{\partial \psi_i}{\partial x_i} \, d\Omega$$

$$\quad + \int_{\Omega} \frac{\partial}{\partial x_i} \left(\phi \, v_i \right) d\Omega \quad - \int_{\Omega} v_i \frac{\partial \phi}{\partial x_i} \, d\Omega$$

$$= -\int_{\Omega} q \frac{\partial \psi_i}{\partial x_i} \, d\Omega \quad -\int_{\Omega} v_i \frac{\partial \phi}{\partial x_i} \, d\Omega \quad + \int_{\Gamma \cup \Gamma_\infty} q \, \psi_i \, n_i \, d\Omega \quad + \int_{\Gamma \cup \Gamma_\infty} \phi \, v_i \, n_i \, d\Omega$$

Adjoint Operators (cont.)

Definition: Adjoint PDEs for the NS

The adjoint PDEs corresponding to the incompressible Navier-Stokes and a boundary-based functional are

$$-\frac{\partial \psi_i}{\partial t} - u_j \frac{\partial \psi_i}{\partial x_j} + \psi_j \frac{\partial u_j}{\partial x_i} - \frac{\partial \phi}{\partial x_i} - \nu \frac{\partial^2 \psi_i}{\partial x_j \partial x_j} = 0,$$

$$\frac{\partial \psi_j}{\partial x_j} = 0. \tag{ADJ}$$

To get the above, I grouped integrals containing v_i and q separately

Adjoint Operators (cont.)

Some notes about the adjoint PDEs:

- The adjoint vector field $\psi = (\psi_1, \psi_2, \psi_3)^T$ is also divergence-free.
- The adjoint scalar field ϕ acts like the pressure to enforce the divergence-free condition on ψ.

Adjoint Boundary Conditions

$$\text{match} \atop \text{with} \quad -\int_{\Gamma \cup \Gamma_\infty} \psi^T \begin{pmatrix} \nu\, \nabla v_1 \cdot n \\ \nu\, \nabla v_2 \cdot n \\ \nu\, \nabla v_3 \cdot n \end{pmatrix}$$

Differentiating the x-force functional we find:

$$\text{match with} \atop \int_{\Gamma \cup \Gamma_\infty} q\, (\psi_1, \psi_2, \psi_3) \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}$$

$$J'[u]v = -\int_\Gamma \nu \frac{\partial v_1}{\partial x_j} n_j \, d\Gamma, \; = -\int_\Gamma (1,0,0) \begin{pmatrix} \nu\nabla v_1 \cdot n \\ \nu\nabla v_2 \cdot n \\ \nu\nabla v_3 \cdot n \end{pmatrix} d\Gamma$$

$$J'[p]q = \int_\Gamma q n_1 \, d\Gamma. \; = \int_\Gamma q(1,0,0) \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix} d\Gamma$$

Matching these terms with the appropriate terms in the extended Green's identity, we obtain the following adjoint boundary conditions:

$$\psi(t,x) = (1,0,0)^T, \qquad \forall x \in \Gamma, t \in [0,T],$$

$$\psi(t,x) = (0,0,0), \qquad \forall x \in \Gamma_\infty, t \in [0,T].$$

Analysis of the Navier-Stokes Adjoint

Energy-Stability Analysis of the Adjoint

We want to investigate the stability of the Navier-Stokes adjoint IBVP.

- We will use the "energy" method, which is the same approach we applied to study the nonlinear (kinetic-energy) stability of the Navier-Stokes equation.
- Here, "energy" refers to the L^2 norm of the adjoint field, not to some physical energy.

Energy-Stability Analysis of the Adjoint (cont.)

We replace t with $\tau = T - t$ in first equation in (ADJ), multiply the result by ψ_i, and integrate over Ω:

$$\int_\Omega \psi_i \frac{\partial \psi_i}{\partial \tau} \, d\Omega - \int_\Omega \psi_i u_j \frac{\partial \psi_i}{\partial x_j} \, d\Omega + \int_\Omega \psi_i \psi_j \frac{\partial u_j}{\partial x_i} \, d\Omega$$

$$- \int_\Omega \psi_i \frac{\partial \phi}{\partial x_i} \, d\Omega - \int_\Omega \nu \psi_i \frac{\partial^2 \psi_i}{\partial x_j \partial x_j} \, d\Omega.$$

The time term simplifies to

$$\int_\Omega \psi_i \frac{\partial \psi_i}{\partial \tau} \, d\Omega = \frac{\partial}{\partial \tau} \int_\Omega \frac{1}{2} \psi_i \psi_i \, d\Omega = \frac{1}{2} \frac{\partial}{\partial \tau} \| \psi \|_\Omega^2$$

Energy-Stability Analysis of the Adjoint (cont.)

The second, advection term becomes

again, I used $\frac{\partial u_j}{\partial x_j} = 0$

$$-\int_\Omega \psi_i u_j \frac{\partial \psi_i}{\partial x_j}\, d\Omega = -\int_\Omega \frac{\partial}{\partial x_j}\left(u_j \tfrac{1}{2} \psi_i \psi_i\right) d\Omega = -\int_{\Gamma \cup \Gamma_\infty} \tfrac{1}{2}\psi_i \psi_i \left(u_j n_j\right) d\Omega$$

$$= 0 \qquad (\text{why ?})$$

The third term ~~becomes~~ *is*

$$\int_\Omega \psi_i \psi_j \frac{\partial u_j}{\partial x_i}\, d\Omega = \int_\Omega \begin{bmatrix} \psi_1, & \psi_2, & \psi_3 \end{bmatrix} \begin{bmatrix} \dfrac{\partial u_1}{\partial x_1} & \dfrac{\partial u_1}{\partial x_2} & \dfrac{\partial u_1}{\partial x_3} \\[2mm] \dfrac{\partial u_2}{\partial x_1} & \dfrac{\partial u_2}{\partial x_2} & \dfrac{\partial u_2}{\partial x_3} \\[2mm] \dfrac{\partial u_3}{\partial x_1} & \dfrac{\partial u_3}{\partial x_2} & \dfrac{\partial u_3}{\partial x_3} \end{bmatrix} \begin{bmatrix} \psi_1 \\[1mm] \psi_2 \\[1mm] \psi_3 \end{bmatrix} d\Omega$$

Energy-Stability Analysis of the Adjoint (cont.)

The pressure term simplifies to
$$\frac{\partial \psi_i}{\partial x_i} = 0$$

$$-\int_{\Omega} \psi_i \frac{\partial \phi}{\partial x_i} \, d\Omega = -\int_{\Omega} \frac{\partial}{\partial x_i} (\psi_i \, \phi) d\Omega \;\; = -\int_{\Gamma \cup \Gamma_{\infty}} \phi \; \psi_i \, n_i \, d\Gamma$$

Recall
$$\psi = (1,0,0) \quad \text{on} \quad \Gamma$$
$$\psi = (0,0,0) \quad \text{on} \quad \Gamma_{\infty}$$

Finally, the viscous term becomes

$$-\int_{\Omega} \nu \psi_i \frac{\partial^2 \psi_i}{\partial x_j \partial x_j} \, d\Omega = -\int_{\Omega} \nu \frac{\partial}{\partial x_j} \left(\psi_i \, \frac{\partial \psi_i}{\partial x_j} \right) d\Omega + \int_{\Omega} \nu \, \frac{\partial \psi_i}{\partial x_j} \frac{\partial \psi_i}{\partial x_j} \, d\Omega$$

$$= -\int_{\Gamma \cup \Gamma_{\infty}} \nu \, \psi_i \, \frac{\partial \psi_i}{\partial x_j} \, d\Omega + \int_{\Omega} \nu \, \frac{\partial \psi_i}{\partial x_j} \, \frac{\partial \psi_i}{\partial x_j} \, d\Omega$$

Energy-Stability Analysis of the Adjoint (cont.)

The L^2 energy of the NS adjoint obeys the following ODE:

$$\frac{d}{dt} \int_\Omega \frac{1}{2} \psi_i \psi_i \, d\Omega = - \int_\Omega \psi_i \frac{\partial u_j}{\partial x_i} \psi_j \, d\Omega - \nu \int_\Omega \frac{\partial \psi_i}{\partial x_j} \frac{\partial \psi_i}{\partial x_j} \, d\Omega$$

$$+ \int_\Gamma \left(\phi \delta_{1j} + \nu \frac{\partial \psi_1}{\partial x_j} \right) n_j \, d\Omega.$$

- We will ignore the boundary-integral term subsequently, since it involves terms linear in the adjoint, while the other terms are quadratic.

Energy-Stability Analysis of the Adjoint (cont.)

Ignoring boundary contributions, the adjoint energy is controlled by two terms:

- The production term: $-\int_{\Omega} \psi_i \frac{\partial u_j}{\partial x_i} \psi_j \, d\Omega$.
- The dissipation term: $-\nu \int_{\Omega} \frac{\partial \psi_i}{\partial x_j} \frac{\partial \psi_i}{\partial x_j} \, d\Omega$.

The dissipation term is non-positive for all adjoint fields (Why?), so this term will decrease the adjoint energy

The production term is more subtle...

First, decompose the velocity gradient tensor into symmetric and skew-symmetric parts:

$$\frac{\partial u_j}{\partial x_i} = \underbrace{\frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right)}_{e_{ij}} + \underbrace{\frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} - \frac{\partial u_i}{\partial x_j}\right)}_{r_{ij} \text{ rotation tensor}}$$

Energy-Stability Analysis of the Adjoint (cont.)

The rotation tensor does not contribute to energy growth/diss of ψ:

$$\psi_i \, r_{ij} \, \psi_j \;=\; \psi_j \, r_{ji} \, \psi_i \;=\; -\underbrace{\psi_j \, r_{ij} \, \psi_i}_{=} \;=\; 0$$
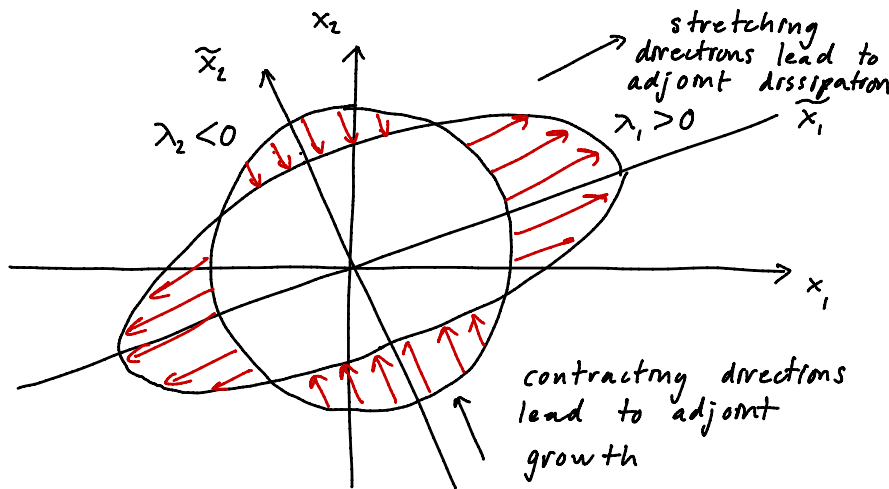
Next, we decompose the strain-rate tensor into principle axes; so

$$-\psi_i \, \frac{\partial u_j}{\partial x_i} \, \psi_j = -\psi_i \, e_{ij} \, \psi_j = -\sum_{i=1}^{3} \lambda_i \, \widetilde{\psi}_i^{\,2}$$

ψ expressed in principle axes-coords

eigenvalues of e_{ij}

# Energy-Stability Analysis of the Adjoint (cont.)

Energy-Stability Analysis of the Adjoint (cont.)

Thus, the L^2 energy of the adjoint may decrease, stabilize, or grow, depending on the relative magnitude of the production and dissipation terms:

- For low Re flows (steady and laminar), the dissipation term will tend to dominate and the adjoint will be bounded;

- For moderate Re flows that are periodic, the two terms will balance;

- For high Re (turbulent) flows, the production term will dominate and the adjoint will grow exponentially in (reverse) time.

Energy-Stability Analysis of the Adjoint (cont.)
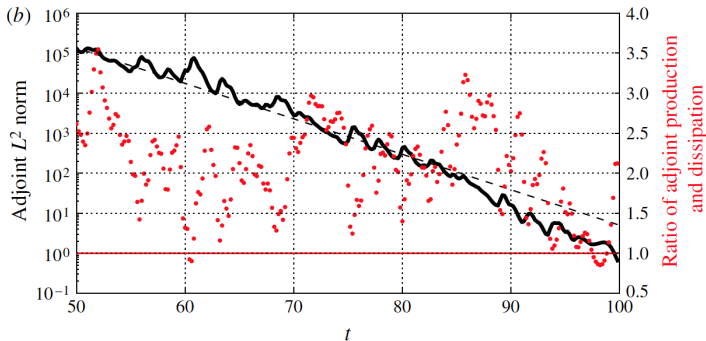
L^2 norm of the drag-adjoint for the flow around a cylinder at Re=500 (black line). The red dots are the ratio of the production and dissipation terms.[WG13]

References

[WG13] Qiqi Wang and Jun-Hui Gao, *The drag-adjoint field of a circular cylinder wake at Reynolds numbers 20, 100 and 500*, Journal of Fluid Mechanics **730** (2013), 145–161.