10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green

Lecture #9: Function Space vs. Real Space Methods for Partial Differential Equations (PDEs).

Practical Utility of Eigen-Analysis
- Stability of Steady States
- Stability of Differential Equations
- Bifurcations
- Correlated Uncertainties

Function Spaces vs. Real Space

$\underline{F}(\underline{x}) = 0$

Broyden, Newton, Trust-Region } Conservation Laws, kinetic equations ➔ $\underline{x}^{soln}$, Equations

Reasonableness Check
Does solution make sense?
- *physically
- *mathematically

If $\underline{x}^{soln}$ is unstable, then in reality $\underline{x}^{soln}$ is useless.
*you converged to the wrong solution

Stability

$\underline{0} = \frac{d\underline{\mathbf{x}}}{dt} = \underline{\mathbf{F}}(\underline{\mathbf{x}})$ is the origin of equation

$$\frac{d\underline{\mathbf{x}}}{dt} = \underline{\mathbf{F}}(\underline{\mathbf{x}}) \qquad \underline{\mathbf{F}}(\underline{\mathbf{x}}) = \underline{\mathbf{F}}(\underline{\mathbf{x}}^{soln}) + \underline{\underline{\mathbf{J}}}(\underline{\mathbf{x}}^{soln})(\underline{\mathbf{x}} - \underline{\mathbf{x}}^{soln}) + \underbrace{\ldots\ldots}_{\text{*neglected higher order terms}}$$

$$\frac{d(\underline{\mathbf{x}} - \underline{\mathbf{x}}^{soln})}{dt} = \frac{d\underline{\mathbf{x}}}{dt}$$

You want eig($\underline{\underline{J}}$) all < 0
If this condition is true, you will find $\underline{x}^{soln}$
If eig($\underline{\underline{J}}$) is positive: unstable state, will go farther away from solution with time.

It is always important to find the Jacobian.
If the eigenvalue of the Jacobian is less than zero, you have found the stable *steady state*.

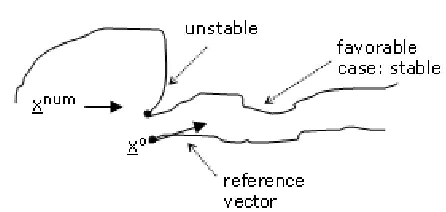

Figure 1. Stable and unstable solutions.

Test to tell if you got the correct solution

$\frac{d\underline{\mathbf{x}}}{dt} = \underline{\mathbf{F}}(\underline{\mathbf{x}}) \qquad \underline{x} = \underline{x}^{o}$

$\underline{w} = \underline{x}(t) - \underline{x}^{ref}(t)$

$\frac{d\underline{\mathbf{x}}}{dt} = \underline{\mathbf{F}}(\underline{\mathbf{x}}) \qquad \underline{x} = \underline{x}^{ref} + \underline{w}$

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$$\frac{d\underline{\mathbf{x}}}{dt} = \frac{d\underline{\mathbf{x}}^{ref}}{dt} + \frac{d\underline{\mathbf{w}}}{dt} = \underline{F}(\underline{x}^{ref} + \underline{w}) = \underline{F}(\underline{x}^{ref}) + \underline{\underline{J}}(\underline{x}^{ref}(t))\cdot\underline{w}$$

→ if eigenvalues are negative, $\underline{w}$ will tend to return to 0

$$\frac{d\underline{\mathbf{w}}}{dt} = \underline{\underline{J}}(\underline{x}^{ref}(t))\cdot\underline{w} + O(\underline{w}^2)$$

If $\underline{\underline{J}} < 0$, you can be pretty confident that you have the right solution.

Stable system always has $\underline{\underline{J}} < 0$; however, there could be unsteady values outside the region analyzed.

Physical Example: If you leave gas on in a room, the situation is metastable, but could blow up with a spark. If the gas is burning, the situation is stable.

There are 2 parts to stability: the equation system and the solver method. Both must be stable in order to find a useful solution.

There are complex mathematical analysis techniques to determine stability that require more information about $\underline{F}(\underline{x})$, but in practice the Jacobian test is usually sufficient.

Bifurcations

In reaction problems, you can always get a steady state solution with a cold system and no conversion. However, if you increase temperature, you can reach a steady state solution where everything reacts. At intermediate temperatures, there is a parameter that governs the extent of reaction.

$$\underline{x} = \begin{pmatrix} \text{conversion} \\ \vdots \end{pmatrix} = \underline{F}(\ldots\ldots\ T_{inlet})$$

$$\underline{F}(\underline{x};T_{inlet}) = 0$$

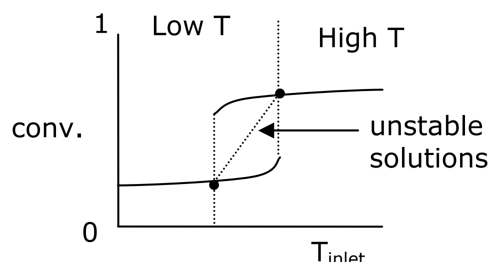


Figure 2. You don't see the unstable solutions in practice, but they exist.

$\underline{F}(\underline{x}^{unstable}) = \underline{0}$

$\underline{\underline{J}}(\underline{x}^{unstable})$ has $\lambda_i = 0$

The boundary between two solution regions is called *bifurcation.*

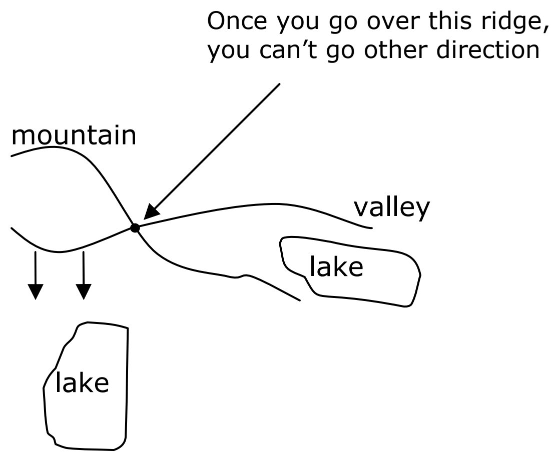
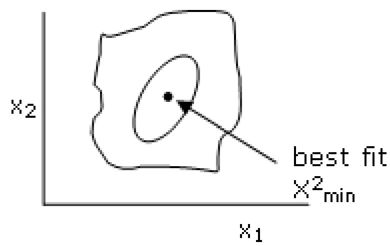


Figure 3. Skiing downhill is analogous to a bifurcation point.

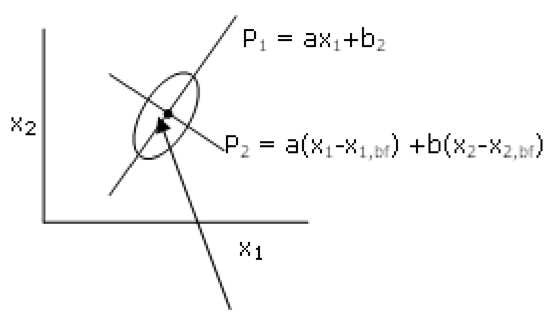
Bifurcation Point

Imagine skiing downhill and you come to a ridge ($\nabla=0$) when you can choose two different directions, but once you go one direction, you can't choose the other.



min X^2 (x_1,x_2) ➔ $\sum\left(\frac{Y_{\text{model}}(\mathbf{x})-Y_{\text{data}}}{\sigma_{\text{data}}}\right)^2$

Figure 4. For small perturbations away from best fit you will get an ellipse. As you get far outside best fit, you will not get ellipse. The shape is nonlinear and irregular.



You can find equations for P_1 and P_2 from the eigenvalues.

Figure 5. Finding the best-fit point.

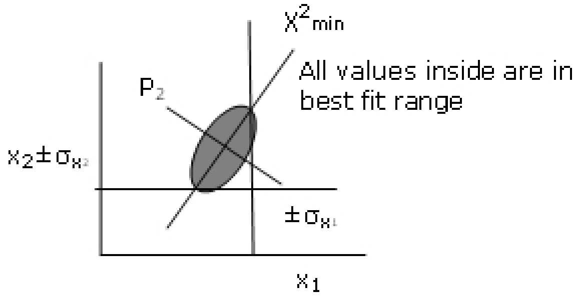


Figure 6. Diagram showing values within the best-fit range.

"Now for the important part of the lecture!"

From homework:

$$-k\frac{dT^2}{dx^2}+H(x)(+g(x)T^2)=0 \qquad x=0\to L$$

$$T(x)=\sum s_n \sin\left(\frac{2\pi nx}{L}\right)+\sum c_n \cos\left(\frac{2\pi nx}{L}\right)$$

$$\text{eigenfunctions}: \frac{d^2}{dx^2}f(x)=\lambda f(x)$$

$$\frac{d^2}{dx^2}\sin\left(\frac{2\pi nx}{L}\right)=-\left(\frac{2\pi n}{L}\right)^2\sin\left(\frac{2\pi nx}{L}\right)$$

$$\int_0^L \sin\left(\frac{2\pi mx}{L}\right)\left[-k\frac{dT^2}{dx^2}+H(x)\right]dx=0$$

$\underline{Z} = (\underline{s},\underline{c})$

Hilbert Space or Function Space

s and c tells us how aligned we are in the Function Space. Function space is good for linear operators or for situations when the eigenfunctions are known for the operator.

$$0=\int \sin\left(\frac{2\pi mx}{L}\right)\left[-k\left(-\sum_n\left(\frac{2\pi n}{L}\right)^2 s_n \sin\left(\frac{2\pi nx}{L}\right)-\sum_n\left(\frac{2\pi n}{L}\right)^2 c_n\cos\left(\frac{2\pi nx}{L}\right)+H(x)\right)\right]dx$$

$$k\left(\frac{2\pi m}{L}\right)^2\left(\frac{L}{2}\right)s_n+\underbrace{\int \sin\left(\frac{2\pi mx}{L}\right)H(x)dx}_{K_m}=0$$

Now you have equations for expansion coefficients: $s_m = \dfrac{-K_m}{k\left(\dfrac{2\pi m}{L}\right)^2 \dfrac{L}{2}}$

You can do the same trick multiplying through by cosine and integrating to get the c_n coefficients. Because $g(x)T^2$ is nonlinear, you will get nonlinear equations with s_m and c_n, if you try that.

On homework you did Finite Differences:

Both methods give an approximate solution

- can make differences smaller and smaller with a finer mesh
- can make function space larger and larger with a bigger basis

Best way to deal with Boundary Conditions:

Set up basis so it is guaranteed to meet the boundary conditions.

However, your solution may not fit ALL boundary condition because it is an approximation that neglected the higher order terms in the expansion (see pg. 1 of this lecture).