10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green
Lecture #5: Introduction to Systems of Nonlinear Equations.

Ill-Conditioning and Condition Numbers

$\underline{\underline{A}} \cdot \underline{x}^{true} = \underline{b}^{true}$

↑ Know exactly ($\underline{\underline{A}}$)

↖ If measurements perfect ($\underline{b}^{true}$)

If one can solve exactly, x^{true} gives the actual flows in a reactor system, for example.

In reality, there are errors in the measurements

$\underline{b} = (\underline{b}^{true} + \delta\underline{b})$, so: $\underline{\underline{A}}(\underline{x}^{true} + \delta\underline{x}) = (\underline{b}^{true} + \delta\underline{b})$

Assume $\underline{\underline{A}}$ is non-singular ($\underline{\underline{A}}$ has an inverse)

$\cancel{\underline{\underline{A}}\underline{x}^{true}} + \underline{\underline{A}}\delta\underline{x} = \cancel{\underline{b}^{true}} + \delta\underline{b} \Rightarrow \underline{\underline{A}}\delta\underline{x} = \delta\underline{b}$

$\delta\underline{x} = \underline{\underline{A}}^{-1}\delta\underline{b}$

$||\delta\underline{x}|| \leq ||\underline{\underline{A}}^{-1}|| \cdot ||\delta\underline{b}||$ $\qquad$ $\text{cond}(\underline{\underline{A}}) = ||\underline{\underline{A}}|| \cdot ||\underline{\underline{A}}^{-1}||$

$$\boxed{\frac{\|\mathbf{b}^{true}\|}{\|\mathbf{A}\|} \leq \|\mathbf{x}^{true}\|}$$

$$\frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}^{true}\|} \leq \|\mathbf{A}^{-1}\| \cdot \|\delta\mathbf{b}\| \cdot \frac{\|\mathbf{A}\|}{\|\mathbf{b}^{true}\|} = \text{cond}(\mathbf{A})\frac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|}$$

$$\frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}^{true}\|} \leq \text{cond}(\mathbf{A})\frac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|} \approx 10^{-2}, 10^{-3}\text{: \# of sig figs in b}$$

if $\text{cond}(\underline{\underline{A}}) = 1$: is what you expect
if $\text{cond}(\underline{\underline{A}}) > 10^4$: no accuracy
Need $\text{cond}(\underline{\underline{A}})$ to be small to bound error

$\text{cond}(\underline{\underline{A}}) \geq 1$ Means error is always amplified.
$\text{cond}(c\underline{\underline{A}}) = \text{cond}(\underline{\underline{A}})$
$\text{cond}(\underline{\underline{A}}) = |\lambda|_{max}/|\lambda|_{min} \rightarrow \text{cond}(\underline{\underline{A}}) \rightarrow \infty$, if $\lambda_i = 0$ $\qquad$ λ: eigenvalue

$$\frac{\|\delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \text{cond}(\mathbf{A})\left(\underbrace{\frac{\delta\mathbf{b}}{\mathbf{b}}}_{\sim 10^{-2}} + \underbrace{\frac{\delta\mathbf{A}}{\mathbf{A}}}_{\sim 10^{-3}} + \varepsilon_{mach}\right)$$

ε_{mach} : machine stores 10^{-15}; still have machine error even when you measure everything perfectly.

Lose ~$\log_{10}(\text{cond}(\underline{\underline{A}}))$ significant figures in $\underline{x}$.

$\underline{\underline{A}}\underline{x}^{soln} = \underline{b}$
just because $\underline{x}$ gives right solution, does not mean you have the true x

What is my tolerance for error?
Have to know this in order to have useful expectations.

You have to know ahead of time which numbers you care about. If $\underline{\underline{A}}$ is singular, model is probably wrong. If $\underline{\underline{A}}$ is not singular and $\text{cond}(\underline{\underline{A}})$ is bad, maybe the scaling is off (different units, for example). Good scaling means that all numbers are within 10^2 of one another. If you know the uncertainties in $\underline{\underline{A}}$, scale so the uncertainties are all similar.

cond($\underline{\underline{A}}$) is the function of physical scenario <u>AND</u> how you scale the equations.

This happens because: $\underset{5\text{ sigs}}{x} + \underset{5\text{ sigs}}{y} = z$ — when you add numbers it depends on order of magnitude

3.1248		3.1248	
$\underline{2.4761}$	while	$\underline{2.4761 \cdot 10^{-11}}$	← these are negligible
5 sig figs		loss of sig figs	

Try to scale the equations by choosing appropriate units

cond($\underline{\underline{A}}$) ~ $4/\varepsilon^2$

$$\begin{pmatrix} 1 & 1+\varepsilon \\ 1-\varepsilon & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1+(1+\varepsilon)\varepsilon \\ \varepsilon \end{pmatrix} \qquad \mathbf{x} = \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix}$$

Gaussian Elimination on an Augmented Matrix

$$\left(\begin{array}{cc|c} 1 & 1+\varepsilon & 1+\varepsilon+\varepsilon^2 \\ 1-\varepsilon & 1 & 1 \end{array}\right) \Rightarrow \left(\begin{array}{cc|c} 1 & 1+\varepsilon & 1+\varepsilon+\varepsilon^2 \\ 0 & \varepsilon^2 & 1-(1+\varepsilon+\varepsilon^2)(1-\varepsilon) \end{array}\right)$$

$1-(1-\varepsilon^3) \approx 0 \approx$ junk, if computer cannot add 1 and ε^3 without loss of accuracy

$\underline{x}_2 = \text{junk}/\varepsilon^2 \approx 0$ [incorrect]

$\underline{x}^{soln} \sim \begin{pmatrix} 1+\varepsilon+\varepsilon^2 \\ 0 \end{pmatrix}$ off by order of ε in small number

If you get warning in MATLAB that cond($\underline{\underline{A}}$) is too high, you should be aware that your solution may be complete nonsense

$$\mathbf{A} = \begin{pmatrix} \bullet & \bullet & \bullet & 0 & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & 0 & 0 \\ \bullet & \bullet & \bullet & \bullet & \bullet & 0 \\ 0 & \bullet & \bullet & \bullet & \bullet & \bullet \\ 0 & 0 & \bullet & \bullet & \bullet & \bullet \\ 0 & 0 & 0 & \bullet & \bullet & \bullet \end{pmatrix}$$

Banded matrix occurs when neighboring numbers affect each other but have little effect on variable far away (i.e. finite difference ODE problems)

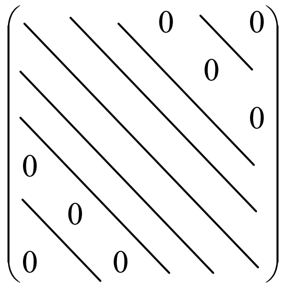
A banded solver ignores the zeros: $O(Nm^2)$ not $O(N^3)$ where "m" is the band width
* saves memory and time

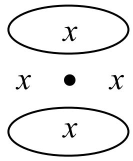
SPARSE

$\underline{\underline{A}}$ = spalloc(M,N,$N_{nonzero}$)
MxN matrix
memory space for up to N nonzero entries

'help sparfun' for more info on sparse matrices

$\underline{\underline{A}}(47, 22)$





Fill-in Problem – Avoid this and maintain symmetrical structure to use SPARSE

In Gauss elimination, the spaces with zeros get filled in and the problem becomes difficult and requires a lot of bandwidth.

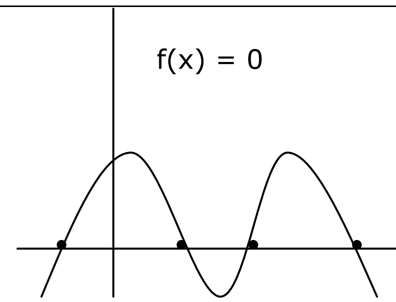
Non-Linear Systems

$F(x) = 0$

$f_1(x,y) = 0$

$f_2(x,y) = 0$

We want (x,y) that is true for f_1 and f_2



1-D problem

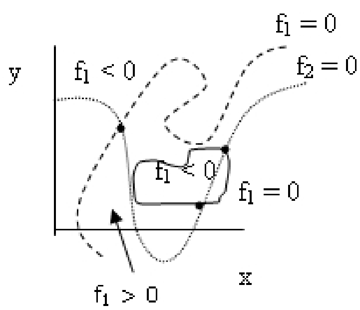


Figure 1. 2-Dimensional problem.

How many solutions?
Impossible to tell.

In our problems (i.e. 20-dimensional), graphical interpretation impossible