10.34, Numerical Methods Applied to Chemical Engineering
Professor William H. Green
Lecture #4: When Algorithms Run Into Problems: Numerical Error; Ill-conditioning, and Tolerances

Homework

- find balance between concise and detailed → manager is audience
- include solutions in word document
- include any issues you had

Factorization

All NxN real matrices can be written: $\underline{\underline{A}} \rightarrow \underline{\underline{P}}^T\underline{\underline{L}}\underline{\underline{U}}$
($\underline{\underline{L}}$: lower triangular, $\underline{\underline{U}}$: upper, $\underline{\underline{P}}$: permutation)

MATLAB is an offshoot of LAPACK (linear algebra package)
- Can download LAPACK from netlib

} Linear algebra is a WELL-DEVELOPED area of study

$\underline{\underline{A}}\underline{x} = \underline{b}$ in MATLAB: $\underline{x} = \underline{\underline{A}} \backslash \underline{b}$ '\' is an "amazing function" – very powerful
* WARNING: do not always know what it's doing

Uniqueness and Existence of Solution

if rank($\underline{\underline{A}}$) = N NxN –- solution exists

if rank($\underline{\underline{A}}$) < N, det($\underline{\underline{A}}$) = 0 -- singular, rank deficient $\underline{\underline{A}}\underline{z} = \underline{0}$, where $\underline{z} \neq \underline{0}$
find additional equation at least one eigenvalue = 0
no inverse: $\underline{z} \neq \underline{\underline{A}}^{-1}*\underline{0}$

$\underline{\underline{A}}\underline{x} = \underline{b}$ does rank($\underline{\underline{A}}$) = rank([$\underline{\underline{A}}$ $\underline{b}$])?
if yes, there is a solution
if yes and rank($\underline{\underline{A}}$)<N, there are an infinite number of solutions

Symmetry

$\underline{\underline{A}}^T = \underline{\underline{A}}$ Also called Hermitian Matrix if all coefficients are real
General Hermitian matrix: transpose and complex-conjugate.
positive definite: $\underline{x}^T\underline{\underline{A}}\underline{x} > \underline{0}$ for all $\underline{x} \neq \underline{0}$ (all eigenvalues are positive)

If symmetric and positive definite: $\underline{\underline{A}} = \underline{\underline{U}}^T\underline{\underline{U}}$; O($N^2$) operation (takes less memory)
$\underline{\underline{L}} = \underline{\underline{U}}^T$ Cholesky factorization: U = chol(A)
if not symmetric/positive definite: 'chol' gives incomplete factorization

Vector Norms

Recall definition of vector norms: $\| \underline{v} \|_p = \left(\sum |v_i|^p \right)^{\frac{1}{p}}$ - vector norm

Matrix Norms

$\| \underline{\underline{A}} \| = \max_{x \neq 0} \frac{\| \underline{\underline{A}} * \underline{x} \|_P}{\| \underline{x} \|_p}$ finds $\underline{x}$ that stretches matrix $\underline{\underline{A}}$ the most

$$\| \underline{\underline{\mathbf{A}}} \|_1 = \max_j \sum_{i=1}^{N} |a_{ij}|$$ add up elements of columns and find biggest value

($\|\underline{\underline{A}}\|_1$ = max column sum)

$$\| \underline{\underline{\mathbf{A}}} \|_\infty = \max_i \sum_{i=1}^{N} |a_{ij}|$$ ($\|\underline{\underline{A}}\|_\infty$ = max row sum)

When p = 1 or ∞, easy to compute matrix norm;
when p is anything else, very complex solution

$\|\underline{\underline{A}}\|_2$ = sqrt(largest eigenvalue of $\underline{\underline{A}}^T\underline{\underline{A}}$) = largest singular value of $\underline{\underline{A}}$

$\|\underline{\underline{A}}\| > 0$ if $\underline{\underline{A}} \neq 0$

$\|c\underline{\underline{A}}\| = |c|\ \|\underline{\underline{A}}\|$

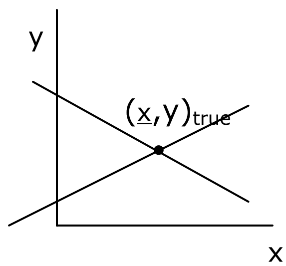
$\|\underline{\underline{A}}+\underline{\underline{B}}\| \leq \|\underline{\underline{A}}\| + \|\underline{\underline{B}}\|$ (triangle inequality)

$\|\underline{\underline{A}}\cdot\underline{\underline{B}}\| \leq \|\underline{\underline{A}}\| \cdot \|\underline{\underline{B}}\|$

$\|\underline{\underline{A}}\bullet\underline{x}\| \leq \|\underline{\underline{A}}\| \cdot \|\underline{x}\|$

Ill-conditioning

$y = m_1 x + b_1$
$y = m_2 x + b_2$



$$\mathbf{A}\begin{pmatrix} x \\ y \end{pmatrix} = \mathbf{b}$$

$$\begin{pmatrix} -m_1 & 1 \\ -m_2 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

Figure 1. As long as the matrix is not singular, there is a solution (intersection).

If $m_1 = m_2$

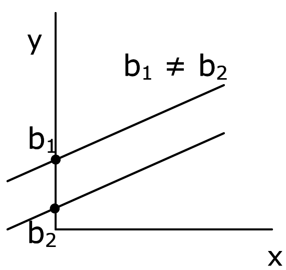


Figure 2. 2 vectors that have no solutions.

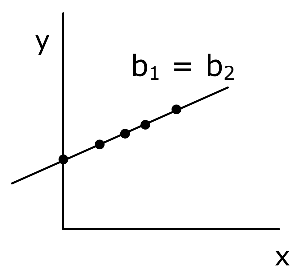


Figure 3. 2 vectors that have an infinite number of solutions.

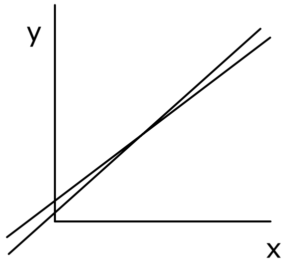


Figure 4. Poor conditioning.

Slopes are very similar: big range of ($\underline{x}$,y) where: $y \approx m_1 x + b_1$
*may be unable to discern difference numerically $y \approx m_2 x + b_2$

$\underline{\underline{A}}^{true} \cdot \underline{x}^{true} = \underline{b}^{true}$
Residual: $r = \underline{b} - \underline{\underline{A}}\underline{x}$
$||r|| <$ tolerance -- "good enough"

Absolute tolerance: # with units defined for specific problem
Relative tolerance: ~# of significant figures, scales with size of characteristic quantity

tolerance: "a" – number (atol)
$\varepsilon||\underline{b}||$ - % (rtol)
$||\Delta x|| < rtol * ||x^{true} + \Delta x||$ - best you can do to being exact
- but you don't know x^{true}

guaranteed

$$||r|| < 2^{N-1} N\varepsilon_{mach}||\underline{\underline{A}}||\ ||\underline{x}|| \qquad \varepsilon_{machine} = \text{usually } 10^{-14}$$

in reality, typically

$$||r|| < N\varepsilon_{mach}||\underline{\underline{A}}||\ ||\underline{x}||$$

Even if matrix is $N = 10^9$, can still achieve an rtol of 10^{-5}

$\underline{\underline{A}}\underline{x}^{sol} \approx \underline{b}$: just because you satisfy the equation, doesn't mean it is the exact solution (ill conditioning)

$\underline{x}^{soln} = \underline{x}^{true} + \Delta x$

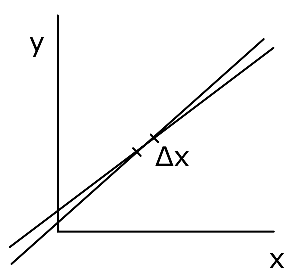


Figure 5. 2 vectors with similar slopes.

$(\underline{\underline{A}} + \delta\underline{\underline{A}})(\underline{x} + \delta\underline{x}) = (\underline{b} + \delta\underline{b})$

$$\frac{\|\delta \mathbf{x}\|}{\|\mathbf{x}\|} < \boxed{\|\mathbf{A}\| \cdot \|\mathbf{A}^{-1}\|} \left(\frac{\|\delta \mathbf{A}\|}{\|\mathbf{A}\|} + \frac{\|\delta \mathbf{b}\|}{\|\mathbf{b}\|} \right)$$

Condition number of $\underline{\underline{A}}$ → cond($\underline{\underline{A}}$)

If the condition number is large, a small change in A or b leads to a large change in $\delta \mathbf{x}$.

If $\underline{\underline{A}}$ is singular, there is no $\underline{\underline{A}}^{-1}$ and cond($\underline{\underline{A}}$) = ∞

Start next time: how scaling affects the condition number