# Solution of Linear Algebraic Equations
## (from Numerical Recipes, Ch. 2)

Suppose we want to solve the system of equations:

1) $A\vec{x} = \vec{b}$

Write this out for a 3×3 matrix:

2) $$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

In FORTRAN, $A(I,J) = a_{ij}$, which means that it stores the matrix by columns (first index varies first):

$$A = (a_{11}, a_{21}, a_{31}, a_{12}, a_{22}, a_{32}, a_{31}, a_{32}, a_{33})$$

Now, the system of eqs. in (2) is:

1) $a_{11}x_1 + a_{12}x_2 + a_{13}x_3 = b_1$

2) $a_{21}x_1 + a_{22}x_2 + a_{23}x_3 = b_2$

3) $a_{31}x_1 + a_{32}x_2 + a_{33}x_3 = b_3$

Now, we could solve this system by combining eqs. and eliminating variables, as you are asked to do in Homework 3a. Or, we could solve it formally by multiplying by the inverse of A:

$$\underbrace{A^{-1} A}_{I} \vec{x} = A^{-1} \vec{b}$$

where $I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ = identity matrix.

<u>But</u>, finding the inverse of a matrix is slow. Therefore, we look for other ways to solve the linear system.

Many software libraries are available to solve linear systems:

LINPACK (from Argonne - vectorized on the CRAY)

IMSL

NAG

We will use one from:

<u>Numerical Recipes</u>, W. H. Press et al.

Two general types of methods:

1) Direct
2) Iterative — for large, sparse systems

① ~~Gaussian elimination for~~ Gauss-Jordan elimination

The simplest direct solution method is this. Note that we can:

i) Interchange any two rows of A and the corresponding rows of $\vec{b}$
ii) Replace any row of A by a linear combination of itself & another row, if we do the same to $\vec{b}$
iii) Interchanging columns of A is possible if we simultaneously interchange the corresponding rows of $\vec{x}$.

Strategy: Perform these operations until the matrix A is reduced to the identity matrix

Step 1: Divide row 1 by $a_{11}$:

$$\begin{pmatrix} 1 & \overbrace{\frac{a_{12}}{a_{11}}}^{=a_{12}'} & \overbrace{\frac{a_{13}}{a_{11}}}^{=a_{13}'} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \overbrace{b_1/a_{11}}^{=b_1'} \\ b_2 \\ b_3 \end{pmatrix}$$

Now, subtract the right amount of row 1 from rows 2 + 3 to zero out first column:

$$\begin{pmatrix} 1 & a_{12}' & \cancel{a_{13}} \; a_{13}' \\ 0 & a_{22}-a_{21}\cdot a_{12}' & a_{23}-a_{21}\cdot a_{13}' \\ 0 & a_{32}-a_{31}a_{12}' & a_{33}-a_{31}\cdot a_{13}' \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1' \; \cancel{b_1/a_{11}} \\ b_2 - a_{21} b_1' \\ b_3 - a_{31}\cdot b_1' \end{pmatrix}$$

- Let $a_{22}' = a_{22} - a_{21} a_{12}'$
- Divide row 2 by $a_{22}'$, then zero out column 2 as before
- Repeat for row 3

We're left with:

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1' \\ b_2' \\ b_3' \end{pmatrix}$$

i.e. $x_1 = b_1'$, $x_2 = b_2'$, $x_3 = b_3'$.

<u>Pivoting</u>: Obviously, this method fails if one of the diagonal elements is zero. When this happens, interchange rows (partial pivoting) or rows & columns (full pivoting) to make sure that one divides through by a good number (usually the largest available element).

<u>Speed</u>: $\propto N^3$ ($N$ = # of eqs.)

## (2) Gaussian elimination with back substitution:

Reduce A to an upper (or lower) triangular matrix:

$$\begin{pmatrix} a_{11}' & a_{12}' & a_{13}' \\ 0 & a_{22}' & a_{23}' \\ 0 & 0 & a_{33}' \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1' \\ b_2' \\ b_3' \end{pmatrix}$$

where the primes indicate that these elements do not have their original values. Now use <u>backsubstition</u>:

1) $a_{11}' x_1 + a_{12}' x_2 + a_{13}' x_3 = b_1'$
2) $a_{22}' x_2 + a_{23}' x_3 = b_2'$
3) $a_{33}' x_3 = b_3'$

so

$$x_3 = b_3' / a_{33}'$$

$$x_2 = (b_2' - a_{23}' x_3) / a_{22}'$$

$$x_1 = (b_1' - a_{12}' x_2 - a_{13}' x_3) / a_{11}'$$

<u>Speed</u>: $\propto \frac{1}{3} N^3$

## LU decomposition

Factor A into a product of lower and upper diagonal matrices:

$$A = L \cdot U$$

$$L = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \qquad U = \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}$$

Then, our original equation can be transformed:

$$A \vec{x} = \vec{b}$$

$$L U \vec{x} = \vec{b}$$

Let

$$U \vec{x} \equiv \vec{y}$$

Then solve

1) $L \vec{y} = \vec{b}$
2) $U \vec{x} = \vec{y}$

These systems can be solved by back substitution, as we did for Gaussian elimination.

Write out the matrix multiplication:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = A = L \cdot U = \begin{pmatrix} l_{11} & 0 & 0 \\ l_{12} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{pmatrix} \cdot \begin{pmatrix} u_{11} & u_{12} & u_{13} \\ 0 & u_{22} & u_{23} \\ 0 & 0 & u_{33} \end{pmatrix}$$

This gives us 9 $(= N^2)$ equations for 12 unknowns $(= N^2 + N)$ because the diagonal elements are represented twice.

1) $a_{11} = l_{11} u_{11} + \underbrace{l_{12} u_{21}}_{0} + \underbrace{l_{13} u_{31}}_{0}$

2) $a_{12} = l_{11} u_{12} + \underbrace{l_{12} u_{22}}_{0} + \underbrace{l_{13} u_{23}}_{0}$

$\vdots$

The solution is therefore not unique. But it turns out to be relatively easy to find (by Crout's algorithm). We can specify 3 (or N) of the variables, so we let

$$\boxed{l_{11} = l_{22} = l_{33} = 1}$$

Then, eq. (1) gives:

$$u_{11} = a_{11} / l_{11} = a_{11}$$
$$u_{12} = a_{12}$$
$$u_{13} = a_{13}$$

It can be shown (although I won't do it here) that one can easily find all the elements of $L$ and $U$.

## Ill-conditioned matrices

(see next page)

# Ill-conditioned matrices

A word of warning about solving matrix equations: not all of them are well behaved. Consider the equation(s):

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 6 \\ 3 & 4 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$$

1) $x_1 + 2x_2 + 3x_3 = 1$
2) $2x_1 + 4x_2 + 6x_3 = 2 \qquad (= \text{eq. } 1 \times 2)$
3) $3x_1 + 4x_2 + 5x_3 = 3$

The second equation is just a multiple of the first, so one really only has two eqs. for three unknowns. Mathematically, we say that this matrix is <u>singular</u>.

Now, suppose you have a matrix that is almost singular, but not quite:

$$\begin{pmatrix} 1 & 2 & 3 \\ 2.01 & 4 & 6 \\ 3 & 4 & 5 \end{pmatrix}$$

When you try to solve this problem numerically, you find it is difficult. This matrix is <u>ill-conditioned</u>. It often pays to use double precision on matrices of this type.