Numerical Methods in Engineering

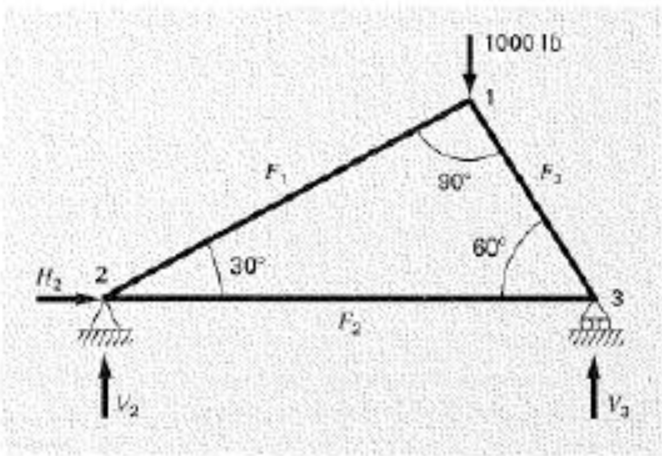
System of linear equations

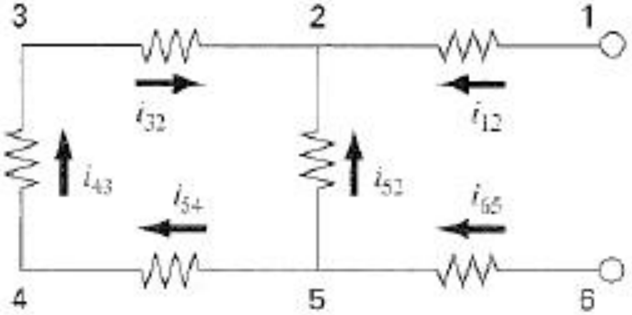
Linear algebraic equations

- An equation of the form $ax+by=c$ is called a linear equation in x and y variables.
- $ax+by+cz=d$ is a linear equation in three variables, x, y, and z.
- Thus, a linear equation in n variables is

  $a_1x_1+a_2x_2+ \ldots +a_nx_n = b$
- A system of linear equations consists of n number of these equations and a solution of such system consists n number of real numbers.

Engineering Problems





Noncomputer methods for solving systems of linear equations

- Linear algebra provides the tools to solve such systems of linear equations.
- For small number of equations ($n \leq 3$) linear equations can be solved readily by simple techniques such as “method of elimination.”
- Nowadays, easy access to computers makes the solution of large sets of linear algebraic equations possible and practical.

Solving system of linear algebraic Equations

There are many ways to solve a system of linear equations:

Graphical method
Cramer's rule
Method of elimination

For $n \leq 3$

Computer methods

Gauss elimination

LU decomposition

Gauss-Seidel

Graphical Method (n=2; mostly)

- This plot method is used for two equations (linear system)
- X_2 is a function of X_1.
- plot X_1 vs. X_2 for each equation "plot the slope and the intercept"
- the solution is the intersection of the two lines

- For two equations:

$$a_{11}x_1 + a_{12}x_2 = b_1$$
$$a_{21}x_1 + a_{22}x_2 = b_2$$

- Solve both equations for x_2:

$$\begin{cases} x_2 = \dfrac{b_1 - a_{11}x_1}{a_{12}} = -\left(\dfrac{a_{11}}{a_{12}}\right)x_1 + \dfrac{b_1}{a_{12}} \\ x_2 = \dfrac{b_2 - a_{21}x_1}{a_{22}} = -\left(\dfrac{a_{21}}{a_{22}}\right)x_1 + \dfrac{b_2}{a_{22}} \end{cases} \Rightarrow \quad x_2 = (\text{slope})x_1 + \text{intercept}$$

- Plot x_2 vs. x_1 on rectilinear paper, the intersection of the lines present the solution.

The graphical method can be used for n=3 (3 equations), but beyond, it will be very complex to determine the solution.

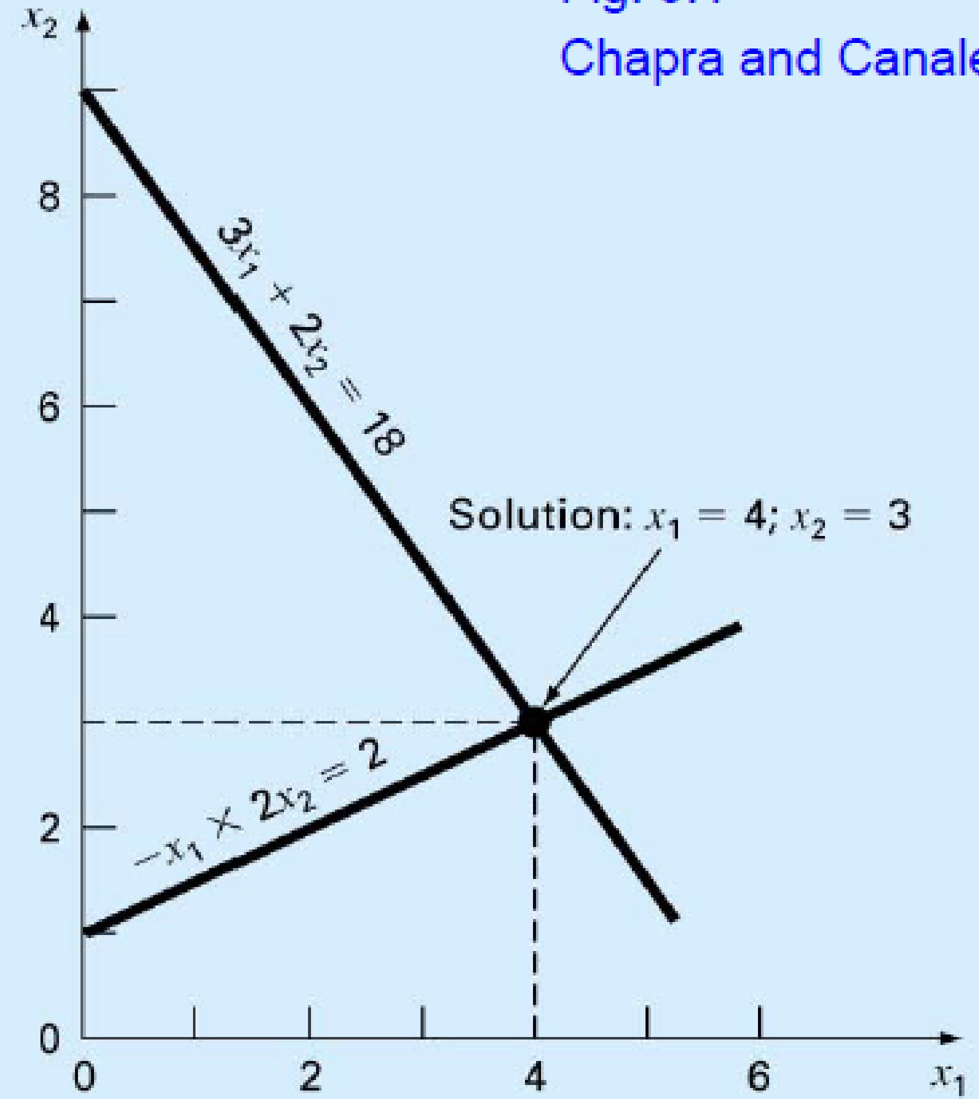


Fig. 9.1
Chapra and Canale

However, this technique is very useful to visualize the properties of the solutions:

- No solution
- Infinite solutions
- ill-conditioned system (the slopes are too close)

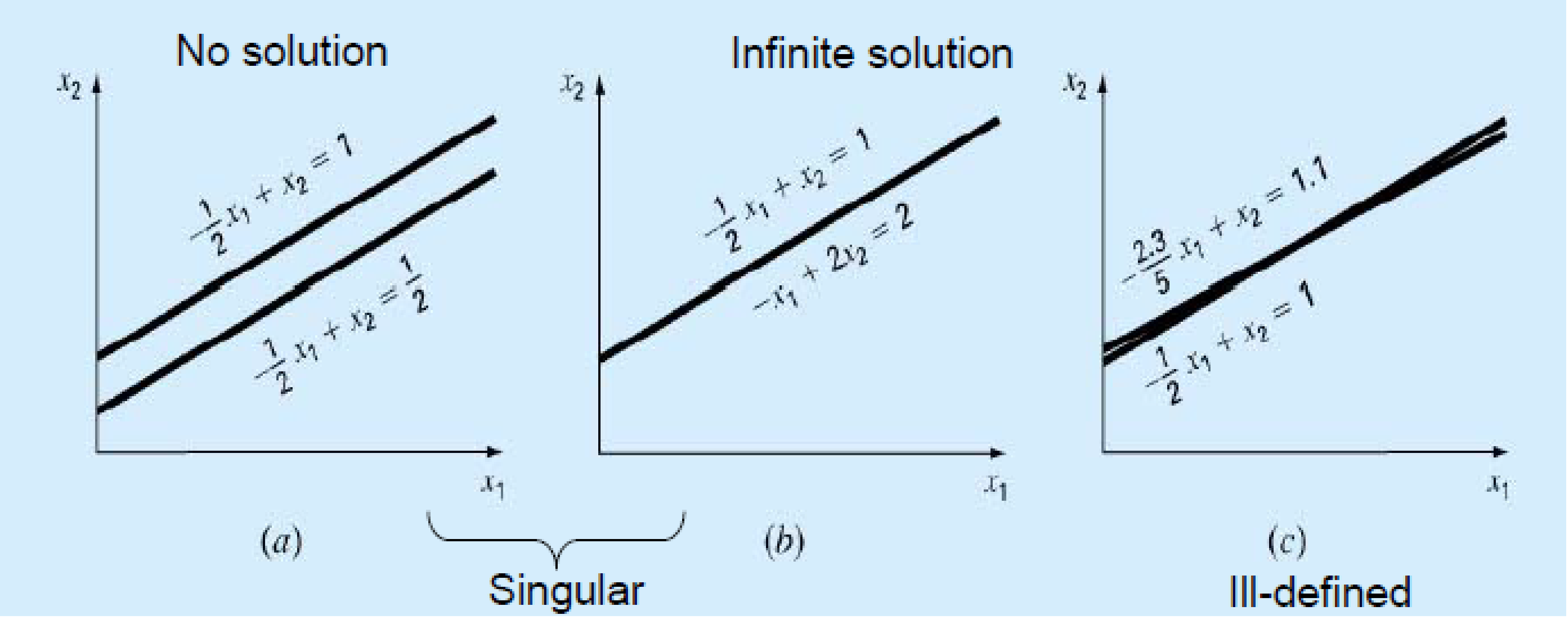


Figure 9.2Chapra and Canale

Determinants and Cramer's Rule

Gabriel Cramer (July 31, 1704 - January 4, 1752) was a Swiss mathematician, born in Geneva. He showed promise in mathematics from an early age. At 18 he received his doctorate and at 20 he was co-chair of mathematics.

- A system of linear equations can be written in matrix form:

$$[A]\{x\} = \{B\}$$

- Where [A] is the coefficient matrix:

$$[A] = \begin{bmatrix} a_{11} a_{12} \\ a_{21} a_{22} \end{bmatrix} \qquad [A] = \begin{bmatrix} a_{11}\ a_{12}\ a_{13} \\ a_{21}\ a_{22}\ a_{23} \\ a_{31}\ a_{32}\ a_{33} \end{bmatrix}$$

Determinants and Cramer's Rule

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}, \quad D = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \quad D = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}\begin{bmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{bmatrix} - a_{12}\begin{bmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{bmatrix} + a_{13}\begin{bmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{bmatrix}$$

Cramer's Rule

Given a 2x2 system of equation;

$$[A]\{x\}=\{B\}$$

$$[A]=\begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix}$$

$$\det(\mathrm{A}) = \begin{vmatrix} a_{11} a_{12} \\ a_{21} a_{22} \end{vmatrix} = a_{11}a_{22} - a_{12}a_{21} \neq 0$$

$$x_1 = \frac{\begin{vmatrix} b_1 & a_{12} \\ b_2 & a_{22} \end{vmatrix}}{\det(A)}$$

$$x_2 = \frac{\begin{vmatrix} a_{11} & b_1 \\ a_{21} & b_2 \end{vmatrix}}{\det(A)}$$

Cramer's Rule

For a 3x3 system of equation;

$$[A]\{x\} = \{B\}$$

$$[A] = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

- *Cramer's rule :*

$$x_1 = \frac{\begin{vmatrix} b_1 & a_{12} & a_{13} \\ b_2 & a_{22} & a_{23} \\ b_3 & a_{32} & a_{33} \end{vmatrix}}{\det(A)} \qquad x_2 = \frac{\begin{vmatrix} a_{11} & b_1 & a_{13} \\ a_{21} & b_2 & a_{23} \\ a_{31} & b_3 & a_{33} \end{vmatrix}}{\det(A)} \qquad x_3 = \frac{\begin{vmatrix} a_{11} & a_{12} & b_1 \\ a_{21} & a_{22} & b_2 \\ a_{31} & a_{32} & b_3 \end{vmatrix}}{\det(A)}$$

Cramer‘s rule

- Advantage: systematic
- Disadvantage: very time consuming ! (even for computers)

Method of Elimination

- The basic strategy is to successively solve **one of the equations** of the set for **one of the unknowns** and to eliminate that variable from the remaining equations by substitution.

- The elimination of unknowns can be extended to systems with more than two or three equations; however, the method becomes extremely tedious to solve by hand.

Method of Elimination

To illustrate this well known procedure, let us take a simple system of equations with two equations:

$$\begin{cases} a_{11}x_1 + a_{12}x_2 = b_1 \\ a_{21}x_1 + a_{22}x_2 = b_2 \end{cases}$$

Step I. We multiply (1) by a_{21} and (2) by a_{11}, thus

$$\begin{cases} a_{11}a_{21}x_1 + a_{12}a_{21}x_2 = b_1a_{21} \\ a_{11}a_{21}x_1 + a_{11}a_{22}x_2 = b_2a_{11} \end{cases}$$

Common factor

By subtracting

$$a_{11}a_{22}x_2 - a_{12}a_{21}x_2 = b_2a_{11} - b_1a_{21}$$

Method of Elimination

Therefore;

$$x_2 = \frac{a_{11}b_2 - a_{21}b_1}{a_{11}a_{22} - a_{12}a_{21}}$$

Step II. And by replacing in the above equations:

$$x_1 = \frac{a_{22}b_1 - a_{12}b_2}{a_{11}a_{22} - a_{12}a_{21}}$$

Note

Compare the to the Cramer's law… it is exactly the same.

The problem with this method is that it is very time consuming for a large number of equations. Not systematic.

Computer algorithm for solving systems of equations

(Naïve) Gauss elimination

LU decomposition

Gauss-Seidel

Naive Gauss Elimination

Naïve$\rightarrow$ it does not avoid the problem of dividing by zero. This point has to be taken into account when implementing this technique on computers.

Extension of method of elimination to large sets of equations by developing a systematic scheme or algorithm to eliminate unknowns and to back substitute.

As in the case of the solution of two equations, the technique for n equations consists of two phases:

(Forward elimination)
Manipulated the equations to eliminate one unknown. We solved for the other unknown

(Back substitution)
We back-substituted it in one of the original equations to solve for other unknowns.

Gauss Elimination

Carl Friedrich Gauss (Gauß) (30 April 1777 – 23 February 1855) was a German mathematician and scientist of profound genius who contributed significantly to many fields, including number theory, analysis, differential geometry, geodesy, magnetism, astronomy and optics. Sometimes known as "the prince of mathematicians" and "greatest mathematician since antiquity", Gauss had a remarkable influence in many fields of mathematics and science and is ranked as one of history's most influential mathematicians.

Ref: Wikipedia

Naive Gauss Elimination
Similar to Elimination of Unknowns

Basic algorithm

1. Forward Elimination of Unknowns
   Reduce the coefficient matrix [A] to an **upper triangular system**
2. Eliminate x_1 from the 2^{nd} to n^{th} Eqns.
3. Eliminate x_2 from the 3^{rd} to n^{th} Eqns.
4. Continue process until the n^{th} equation has only 1 non-zero coefficient

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix} \rightarrow \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a''_{33} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b'_1 \\ b'_2 \\ b''_3 \end{Bmatrix}$$

Illustration

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

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

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

Forward Elimination

Eliminate x_1 from equation (2): Multiply (1) by a **factor** (a_{21}/a_{11}), then subtract the result from (2)

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

$$-\left(\frac{a_{21}}{a_{11}}a_{11}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \frac{a_{21}}{a_{11}}a_{13}x_3 = \frac{a_{21}}{a_{11}}b_1\right)$$

$$\left(a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right)x_2 + \left(a_{23} - \frac{a_{21}}{a_{11}}a_{13}\right)x_3 = b_2 - \frac{a_{21}}{a_{11}}b_1$$

$$a'_{22}x_2 + a'_{23}x_3 = b'_2 \quad (2')$$

Illustration

Forward Elimination

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

Pivot Equation

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

Elimination Row

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

Eliminate x_1 from equation (2). Multiply (1) by a_{21}/a_{11}, then subtract the result from (2)

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

$$-\left(\frac{a_{21}}{a_{11}}a_{11}x_1 + \frac{a_{21}}{a_{11}}a_{12}x_2 + \frac{a_{21}}{a_{11}}a_{13}x_3 = \frac{a_{21}}{a_{11}}b_1\right)$$

Pivot element

$$\left(a_{22} - \frac{a_{21}}{a_{11}}a_{12}\right)x_2 + \left(a_{23} - \frac{a_{21}}{a_{11}}a_{13}\right)x_3 = b_2 - \frac{a_{21}}{a_{11}}b_1$$

$$a'_{22}x_2 + a'_{23}x_3 = b'_2 \quad (2')$$

Illustration

Forward Elimination

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

$$+ a'_{22}x_2 + a'_{23}x_3 = b'_2 \quad (2')$$

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

Elimination Row

Eliminate x_1 from equation (3). Multiply (1) by a_{31}/a_{11}, then subtract the result from (3)

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

$$-\left(\frac{a_{31}}{a_{11}}a_{11}x_1 + \frac{a_{31}}{a_{11}}a_{12}x_2 + \frac{a_{31}}{a_{11}}a_{13}x_3 = \frac{a_{31}}{a_{11}}b_1\right)$$

$$\left(a_{32} - \frac{a_{31}}{a_{11}}a_{12}\right)x_2 + \left(a_{33} - \frac{a_{31}}{a_{11}}a_{13}\right)x_3 = b_3 - \frac{a_{31}}{a_{11}}b_1$$

$$a'_{32}x_2 + a'_{33}x_3 = b'_3 \quad (3')$$

Illustration

Forward Elimination

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

$$+ a'_{22}x_2 + a'_{23}x_3 = b'_2 \quad (2')$$ Pivot Equation

$$+ a'_{32}x_2 + a'_{33}x_3 = b'_3 \quad (3')$$ Elimination Row

Eliminate x_2 from equation (3'). Multiply (2') by a'_{32}/a'_{22}, then subtract the result from (3')

$$a'_{32}x_2 + a'_{33}x_3 = b'_3$$

$$-\left(\frac{a'_{32}}{a'_{22}}a'_{22}x_2 + \frac{a'_{32}}{a'_{22}}a'_{23}x_3 = \frac{a'_{32}}{a'_{22}}b'_2\right)$$

$$\left(a'_{33} - \frac{a'_{32}}{a'_{22}}a'_{23}\right)x_3 = b'_3 - \frac{a'_{32}}{a'_{22}}b'_2$$

$$a''_{33}x_3 = b''_3 \quad (3'')$$

Illustration

After the Forward Elimination step

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 &= b_1 \quad (1) \\
+ a'_{22}x_2 + a'_{23}x_3 &= b'_2 \quad (2') \\
+ a''_{33}x_3 &= b''_3 \quad (3'')
\end{aligned}
$$

Backwards substitution:

$$x_3 = \frac{b''_3}{a''_{33}}$$

From (2')

$$x_2 = \frac{b'_2 - a'_{23}x_3}{a'_{22}}$$

From (1)

$$x_1 = \frac{b_1 - a_{12}x_2 - a_{13}x_3}{a_{11}}$$

Backwards substitution:

In general, the last equation should reduce to:

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

Numerical problems
Pitfalls of Gauss Elimination Methods

- ***Division by zero***

  It is possible that during both elimination and back-substitution phases a division by zero can occur.

$$\begin{cases} 0x_1 + 4x_2 + 5x_3 = 8 \\ 7x_1 + 3x_2 + 1x_3 = 5 \\ 2x_1 + 1x_2 + 5x_3 = 7 \end{cases}$$

Here we have a division by zero if we replace in the above formula for Gauss elimination (the same thing will happen if we use a very small number). The *pivoting technique* has been developed to avoid this problem.

Pitfalls of Gauss Elimination Methods

- ***Round-off errors***

The large number of equations to be solved induces a propagation of the errors. A rough rule of thumb is that round-off error may be important when dealing with 100 or more equations.

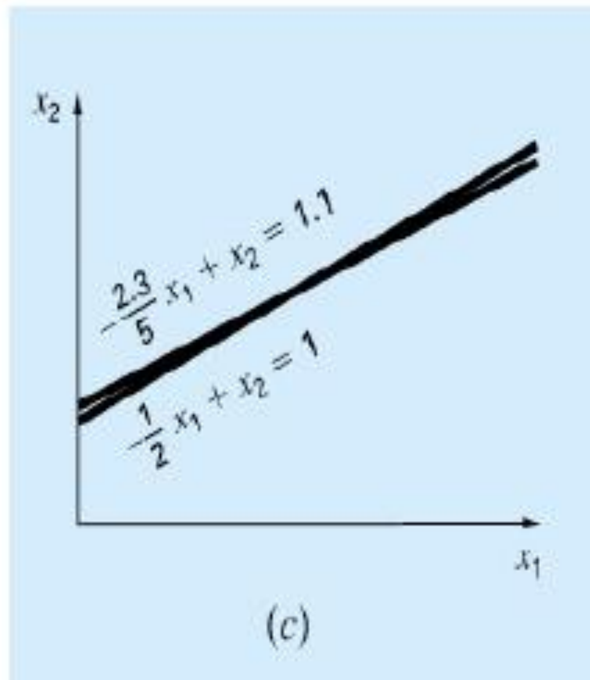
Always substitute your answers back into the original equations to check whenever a substantial errors has occurred

Pitfalls of Gauss Elimination Methods

- ***ill-conditioned systems***

Systems where small changes in coefficients result in large changes in the solution. It happens when two or more equations are nearly identical, resulting a wide ranges of answers to approximately satisfy the equations.

Round off errors can induce small changes in the coefficients, these changes can lead to large solution errors



Techniques for Improving Solutions

• Use of more significant figures. however, this has a price (computational time, memory, …)

• Pivoting

• Scaling

Pivoting

If a pivot element is zero, normalization step leads to division by zero. The same problem may arise, when the pivot element is close to zero. Division by zero or small numbers can be avoided:

a) Before Gauss forward elimination, find largest element (absolute value) in the first column
b) Reorder the equations so that the largest element is the pivot element
c) Repeat for each elimination step (i.e. 2nd application would find the largest element (absolute value) in the 2nd column (below the 1st equation) and seek the largest magnitude pivot element

Partial pivoting. Switching the rows so that the largest element is the pivot element.

Complete pivoting. Searching for the largest element in all rows and columns then switching. But is rarely used because it adds complexity to the program.

Example

$$2x_1 - 6x_2 - x_3 = -38$$
$$-3x_1 - x_2 + 7x_3 = -34$$
$$-8x_1 + x_2 - 2x_3 = -20$$

Solve using Gauss Elimination with partial pivoting

$$\begin{bmatrix} 2 & -6 & -1 & -38 \\ -3 & -1 & 7 & -34 \\ -8 & 1 & -2 & -20 \end{bmatrix}$$

First, we pivot by switching row 1 and 3

$$\begin{bmatrix} -8 & 1 & -2 & -20 \\ -3 & -1 & 7 & -34 \\ 2 & -6 & -1 & -38 \end{bmatrix}$$

Multiply row 1 by (-3/8) and subtract from row 2 to eliminate a_{21}

$$\begin{bmatrix} -8 & 1 & -2 & -20 \\ 0 & -1.375 & 7.75 & -26.5 \\ 2 & -6 & -1 & -38 \end{bmatrix}$$

Multiply row 1 by (2/-8) and subtract from row 3 to eliminate a_{31}

Example

$$\begin{bmatrix} -8 & 1 & -2 & -20 \\ 0 & -1.375 & 7.75 & -26.5 \\ 0 & -5.75 & -1.5 & -43 \end{bmatrix}$$

we pivot by switching row 2 and 3

$$\begin{bmatrix} -8 & 1 & -2 & -20 \\ 0 & -5.75 & -1.5 & -43 \\ 0 & -1.375 & 7.75 & -26.5 \end{bmatrix}$$

Multiply row 2 by (-1.375/-5.75) and subtract from row 3 to eliminate a_{32}

$$\begin{bmatrix} -8 & 1 & -2 & -20 \\ 0 & -5.75 & -1.5 & -43 \\ 0 & 0 & 8.108696 & -16.2174 \end{bmatrix}$$

Check:

$$2(4) - 6(8) - (-2) = -38$$

$$-3(4) - (8) + 7(-2) = -34$$

$$-8(4) + (8) - 2(-2) = -20$$

Backward substitution:

$$x_3 = \frac{-16.2174}{8.108696} = -2$$

$$x_2 = \frac{-43 - (-1.5)(-2)}{-5.75} = 8$$

$$x_1 = \frac{-20 - (-2)(-2) - 1(8)}{-8} = 4$$

Scaling

It is important to use unites that lead to the same order of magnitude for all the coefficients (exp: voltage can be used in mV or MV).

We have seen that adding and subtracting of numbers with very different magnitudes can result in Round-off error

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Scale all rows so that the maximum coefficient value in any row is one

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Note: Scaling by very large numbers can potentially introduce RO error

Suggestion:
Employ scaling only to make a decision regarding pivoting
Comparison & row switching are not subject to RO error
Complete solution using original coefficients

Scaling

Scaling – helps make pivoting decisions

$$3x_1 + 70{,}000x_2 = 40{,}000$$
$$-x_1 + 0.2x_2 = 3$$

$$\Big\downarrow \text{ scale}$$

$$0.0000428x_1 + 1x_2 = 0.5714$$
$$-x_1 + 0.2x_2 = 3$$

$$\Big\downarrow \text{ Pivot}$$

$$-x_1 + 0.2x_2 = 3$$
$$0.0000428x_1 + 1x_2 = 0.5714$$

Summary

- Graphical methods
- Cramer‘s rule
- Naive Gauss elimination
- Gauss elimination with partial pivoting

Variation of Gauss Elimination (Gauss-Jordan

When an unknown is eliminated it is eliminated from all equations, not just subsequent ones (Diagonal matrix results)
All rows are normalized by their pivot element
Identity matrix result

[A] is augmented
$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \end{array}\right]$$

$$[I]\{x\} = \{b'\}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} b'_1 \\ b'_2 \\ b'_3 \end{Bmatrix}$$

Almost identical to Gauss elimination but, more operations are required
No back substitution step

LU decomposition

In Gauss elimination, we consider an augmented matrix combining [A] and {b} to solve the system

$$\left[\begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \end{array}\right]$$

Gauss elimination becomes inefficient when solving equations with the same coefficients for [A] but with different b's.

LU decomposition separates the time consuming elimination of [A] from the manipulation of {b}

Hence, the decomposed [A] could be used with several {b} 's in an efficient manner.

→ What is LU decomposition?

LU decomposition

LU decomposition is based on the fact that any square matrix [A] can be written as a product of two matrices as:

$$[A]=[L][U]$$

where [L] is a lower triangular matrix and [U] is an upper triangular matrix.

In other words, [A] is factored or “decomposed into lower [L] and upper [U] triangular matrices.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ . & 1 & 0 \\ . & . & 1 \end{bmatrix} \cdot \begin{bmatrix} . & . & . \\ 0 & . & . \\ 0 & 0 & . \end{bmatrix}$$

→ How can we get the LU decomposition of a Matrix?

LU decomposition from Gauss elimination

Gauss algorithm: replaces

$$Ax - b = 0$$

by

$$Ux - d = 0$$

where U is an upper diagonal matrix.

Operator form: what is the matrix T which does the same ?

$$T(Ax - b) = Ux - d$$

Gaussian Elimination

The matrix

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

is replaced by:

$$\widetilde{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} - ca_{11} & a_{22} - ca_{12} & a_{23} - ca_{13} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

We can write this operation in the form of

$\widetilde{A} = T_{21}(-c)A$ where $T_{21}(-c)$ is a matrix

The Gauss operator

- A Gauss elimination step can be written as:

$$\begin{bmatrix} 1 & 0 & 0 \\ -c & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} - ca_{11} & a_{22} - ca_{12} & a_{23} - ca_{13} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

We have found a matrix $T_{21}(-c)$ which, when multiplying the matrix A , does the operation subtracting c times lines one from line 2

Gaussian Elimination

Let us apply the theorem to a 3X3 matrix. First step of the Gauss elimination algorithm is the elimination of the a_{21} coefficient

$$\begin{bmatrix} 1 & 0 & 0 \\ -\dfrac{a_{21}}{a_{11}} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} - \dfrac{a_{21}}{a_{11}} a_{11} & a_{22} - \dfrac{a_{21}}{a_{11}} a_{12} & a_{23} - \dfrac{a_{21}}{a_{11}} a_{13} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & \tilde{a}_{22} & \tilde{a}_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

Gaussian Elimination

Next step is the elimination of the a_{31} coefficient.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\dfrac{a_{31}}{a_{11}} & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & \tilde{a}_{22} & \tilde{a}_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & \tilde{a}_{22} & \tilde{a}_{23} \\ a_{31} - \dfrac{a_{31}}{a_{11}} a_{11} & a_{32} - \dfrac{a_{31}}{a_{11}} a_{11} & a_{33} - \dfrac{a_{31}}{a_{11}} a_{13} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & \tilde{a}_{22} & \tilde{a}_{23} \\ 0 & \tilde{a}_{32} & \tilde{a}_{33} \end{bmatrix}$$

Gaussian Elimination

And finally the elimination of the a_{32} coefficient

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\dfrac{\tilde{a}_{32}}{\tilde{a}_{22}} & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & \tilde{a}_{22} & \tilde{a}_{23} \\ 0 & \tilde{a}_{32} & \tilde{a}_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & \tilde{a}_{22} & \tilde{a}_{23} \\ 0 & \tilde{a}_{32} - \dfrac{\tilde{a}_{32}}{\tilde{a}_{22}} \tilde{a}_{22} & \tilde{a}_{33} - \dfrac{\tilde{a}_{32}}{\tilde{a}_{22}} \tilde{a}_{23} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & \tilde{a}_{22} & \tilde{a}_{23} \\ 0 & 0 & \tilde{\tilde{a}}_{33} \end{bmatrix}$$

Gaussian Elimination

This result can be generalized. The Gaussian elimination algorithm can always be represented by a product of single lower triangular matrices $T_{ij}(-c)$ with the appropriate coefficients in the lower triangular part of the matrix. These appropriate coefficients are nothing else than the coefficient used in the elimination algorithm.

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -\dfrac{\tilde{a}_{32}}{\tilde{a}_{22}} & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -\dfrac{a_{31}}{a_{11}} & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -\dfrac{a_{21}}{a_{11}} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & \tilde{a}_{22} & \tilde{a}_{23} \\ 0 & 0 & \tilde{\tilde{a}}_{33} \end{bmatrix}$$

$$U = T_{32}\left(-\frac{\tilde{a}_{32}}{\tilde{a}_{22}}\right) T_{31}\left(-\frac{a_{31}}{a_{11}}\right) T_{21}\left(-\frac{a_{21}}{a_{11}}\right) A$$

An example

$$A = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 5 \\ 3 & 5 & 6 \end{bmatrix}$$

$$\underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -3 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\mathbf{T}} \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 5 \\ 3 & 5 & 6 \end{bmatrix} = \begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & 1 \\ 0 & 0 & -2 \end{bmatrix}$$

$$\mathbf{T} \qquad \mathbf{A} \quad = \quad \mathbf{U}$$

What can we do with this ?

- We can represent the Gauss algorithm with a product of matrixes representing the elimination steps.

$$T_1 T_2 T_3 A = U$$

- Using Matrix Algebra, we can easily invert the algorithm.

Inverting the Gauss algorithm

- From $T_1 T_2 T_3 A = U$, we can have :

$$A = \left(T_1 T_2 T_3\right)^{-1} U$$

$$A = T_3^{-1} T_2^{-1} T_1^{-1} U$$

$$A = LU$$

What is the inverse of T_{ij}(-*c*)?

It turns out that the computation of this inverse is very simple. Following theorem applies:

> ***Theorem:***
>
> The inverse of $T_{ij}(-c)$ is $T_{ij}^{-1}(-c) = T_{ij}(c)$

***The proof can be done directly by verification*

What is the inverse of T ?

$$\begin{bmatrix} 1 & 0 & 0 \\ -c & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} - ca_{11} & a_{22} - ca_{12} & a_{23} - ca_{13} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ -c & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ +c & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

For our example

$$\underbrace{\begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & -1 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\\-3 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\-2 & 1 & 0\\0 & 0 & 1\end{bmatrix}}_{\mathbf{T}}\begin{bmatrix}1 & 2 & 3\\2 & 3 & 5\\3 & 5 & 6\end{bmatrix}=\begin{bmatrix}1 & 2 & 3\\0 & -1 & 1\\0 & 0 & -2\end{bmatrix}$$

$$\mathbf{A} \quad \mathbf{=} \quad \mathbf{U}$$

$$\begin{bmatrix}1 & 2 & 3\\2 & 3 & 5\\3 & 5 & 6\end{bmatrix}=\underbrace{\begin{bmatrix}1 & 0 & 0\\+2 & 1 & 0\\0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\\+3 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\0 & 1 & 0\\0 & +1 & 1\end{bmatrix}}_{\mathbf{T}^{-1}}\begin{bmatrix}1 & 2 & 3\\0 & -1 & 1\\0 & 0 & -2\end{bmatrix}$$

$$\mathbf{A} \quad \mathbf{=} \quad \mathbf{T^{-1}} \quad \mathbf{U}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 5 \\ 3 & 5 & 6 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ +2 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ +3 & 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & +1 & 1 \end{bmatrix}}\begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & 1 \\ 0 & 0 & -2 \end{bmatrix}$$

$$\mathbf{A} \quad = \quad \mathbf{T}^{-1} \quad \mathbf{U}$$

$$\begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 5 \\ 3 & 5 & 6 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 3 & 1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 2 & 3 \\ 0 & -1 & 1 \\ 0 & 0 & -2 \end{bmatrix}$$

$$\mathbf{A} \quad = \quad \mathbf{L}\,\mathbf{U}$$

$$T_{21}^{-1}\left(-\frac{a_{21}}{a_{11}}\right)T_{31}^{-1}\left(-\frac{a_{31}}{a_{11}}\right)T_{32}^{-1}\left(-\frac{\tilde{a}_{32}}{\tilde{a}_{22}}\right)=\begin{bmatrix}1 & 0 & 0\\ \frac{a_{21}}{a_{11}} & 1 & 0\\ 0 & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ \frac{a_{31}}{a_{11}} & 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & \frac{\tilde{a}_{32}}{\tilde{a}_{22}} & 1\end{bmatrix}=\begin{bmatrix}1 & 0 & 0\\ \frac{a_{21}}{a_{11}} & 1 & 0\\ \frac{a_{31}}{a_{11}} & \frac{\tilde{a}_{32}}{\tilde{a}_{22}} & 1\end{bmatrix}$$

Therefore:

$$\begin{bmatrix}1 & 0 & 0\\ \frac{a_{21}}{a_{11}} & 1 & 0\\ \frac{a_{31}}{a_{11}} & \frac{\tilde{a}_{32}}{\tilde{a}_{22}} & 1\end{bmatrix}\cdot\begin{bmatrix}a_{11} & a_{12} & a_{13}\\ 0 & \tilde{a}_{22} & \tilde{a}_{23}\\ 0 & 0 & \tilde{\tilde{a}}_{33}\end{bmatrix}=\begin{bmatrix}a_{11} & a_{12} & a_{13}\\ a_{21} & a_{22} & a_{23}\\ a_{31} & a_{32} & a_{33}\end{bmatrix}$$

Note: be careful of the correct choice of the sign used in the coefficient of the matrix T

Example

$$A = \begin{bmatrix} 2 & 5 & 1 \\ 6 & 11 & 1 \\ -4 & -2 & 3 \end{bmatrix}$$

$$\begin{bmatrix} 2 & 5 & 1 \\ 6 & 11 & 1 \\ -4 & -2 & 3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ -2 & -2 & 1 \end{bmatrix} \cdot \begin{bmatrix} 2 & 5 & 1 \\ 0 & -4 & -2 \\ 0 & 0 & 1 \end{bmatrix}$$

Solution

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 5 & 1 \\ 6 & 11 & 1 \\ -4 & -2 & 3 \end{bmatrix}$$

Gauss elimination for column 1

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ -2 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 5 & 1 \\ 0 & -4 & -2 \\ 0 & 8 & 5 \end{bmatrix}$$

Gauss elimination for column 2

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 3 & 1 & 0 \\ -2 & -2 & 1 \end{bmatrix} \begin{bmatrix} 2 & 5 & 1 \\ 0 & -4 & -2 \\ 0 & 0 & 1 \end{bmatrix}$$

Crout's method

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 & 0 \\ l_{21} & l_{22} & 0 \\ l_{31} & l_{32} & l_{33} \end{bmatrix} \begin{bmatrix} 1 & u_{12} & u_{13} \\ 0 & 1 & u_{23} \\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} l_{11} & (l_{11}u_{12}) & (l_{11}u_{13}) \\ l_{21} & (l_{21}u_{12} + l_{22}) & (l_{21}u_{13} + l_{22}u_{23}) \\ l_{31} & (l_{31}u_{12} + l_{32}) & (l_{31}u_{13} + l_{32}u_{23} + l_{33}) \end{bmatrix}$$

Crout's method

We can find, therefore, the elements of the matrices [L] and [U] by equating the two above matrices:

$$
\begin{cases}
l_{11} = a_{11};\ l_{21} = a_{21};\ l_{31} = a_{31} \\
l_{11}u_{12} = a_{12}, \quad \text{hence} \quad u_{12} = \dfrac{a_{12}}{l_{11}} = \dfrac{a_{12}}{a_{11}} \\
l_{21}u_{12} + l_{22} = a_{22}, \quad \text{hence} \quad l_{22} = a_{22} - l_{21}u_{12} \\
l_{31}u_{12} + l_{32} = a_{32}, \quad \text{hence} \quad l_{32} = a_{32} - l_{31}u_{12} \\
l_{11}u_{13} = a_{13}, \quad \text{hence} \quad u_{13} = \dfrac{a_{13}}{l_{11}} = \dfrac{a_{13}}{a_{11}} \\
l_{21}u_{13} + l_{22}u_{23} = a_{23}, \quad \text{hence} \quad u_{23} = \dfrac{a_{23} - l_{21}u_{13}}{l_{22}} \\
l_{31}u_{13} + l_{32}u_{23} + l_{33} = a_{33}, \quad \text{hence} \quad l_{33} = a_{33} - l_{31}u_{13} - l_{32}u_{23}
\end{cases}
$$

Crout's method

For a general n×n matrix, you have to apply the following expressions to find the LU decomposition of a matrix [A]:

$$l_{ij} = \left\{ a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \right\} \quad ; i \geq j;\ i=\mathbf{1},2,\ldots,\mathbf{n}$$

$$u_{ij} = \left\{ \frac{a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}}{l_{ii}} \right\} \quad ; i < j;\ j=\mathbf{2},3,\ldots,\mathbf{n}$$

$$u_{ii} = 1 \quad ; i = 1,2,\ldots,n$$

Solution of equations

Now to solve our system of linear equations, we can express our initial system:

$$[A]\{x\} = \{b\}$$

Under the following form

$$[A]\{x\} = [L][U]\{x\} = \{b\}$$

To find the solution {x} , we define first a vector {z}

$$\{z\} = [U]\{x\}$$

Our initial system becomes, then:

$$[L]\{z\} = \{b\}$$

As [L] is a lower triangular matrix the {z} can be computed starting by $\mathbf{z}_1$ until $\mathbf{z}_n$. Then the value of {z} can be found using the equation

$$[L]\{z\}=\{b\}$$

As [U] is an upper triangular matrix, it is possible to compute {x} using a backward substitution process starting x_n until x_1.

$$\{z\}=[U]\{x\}$$

Solving equations with the LU decomposition

In summary, following method can be applied to solve a system of linear equation

- Step 1: Decompose the matrix A by LU decomposition: $A=LU$
- Step 2: Compute z by forward substitution using $Lz=b$
- Step 3: Compute x by backward substitution using $Ux=z$.

An example

$$x + 2y - z = 3$$

$$2x + y - 2z = 3$$

$$-3x + y + z = -6$$

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ -6 \end{bmatrix}$$

Step 1: A=LU

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

Step 2: Compute z with Lz=b

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ -6 \end{bmatrix}$$

$$\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 3 \\ -3 \\ -4 \end{bmatrix}$$

Step 3: Compute x with Ux=z

$$\begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 3 \\ -3 \\ -4 \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 3 \\ 1 \\ 2 \end{bmatrix}$$

LU decomposition

Recall from last lecture

- We have seen how we can decompose

$$[A]=[L][U]$$

- Useful to solve systems of equations Ax=b:

$$\boxed{\begin{array}{l} Ax=LUx=b \\ \text{Write } z=Ux \Rightarrow Lz=b \end{array}}$$

Step 1: Decompose the matrix A by LU decomposition: $A=LU$

Step 2: Compute z by forward substitution using $Lz=b$

Step 3: Compute x by backward substitution using $Ux=z$.

Problem

- Since LU decomposition is related to Gauss elimination → same pitfalls → ***Division by zero***

$$\begin{bmatrix} 0 & 1 & -1 \\ 1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}$$

How can we obtain the LU decomposition of the above matrix?

Partial pivoting

- Remember that we introduced partial pivoting strategy in the Gauss algorithm to avoid numerical problems
- How can we implement partial pivoting in the A=LU decomposition ?
- This can be done with the help of *permutation* matrices.

Permutation matrix

Definition:

A **permutation matrix** P is a matrix consisting of all zeros, except for a single 1 in every row and column.

Equivalently, a permutation matrix is created by applying arbitrary row exchanges for the identity matrix.

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \quad \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \quad \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Theorem:

Let ***P*** be a permutation matrix formed by a particular set of row exchanges applied to the identity matrix. Then, for any matrix ***A***, ***PA*** is the matrix obtained applying exactly the same set of row exchange to ***A***.

Example:

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} = \begin{bmatrix} a & b & c \\ g & h & i \\ d & e & f \end{bmatrix}$$

PA=LU decomposition

Example: find the PA=LU decomposition of following matrix:

$$A = \begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix}$$

Solution:

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 1 \end{bmatrix}\begin{bmatrix} 4 & 4 & -4 \\ 0 & 2 & 2 \\ 0 & 0 & 8 \end{bmatrix}$$

Solving equations with the PA=LU decomposition

- Step 1: Decompose the matrix A by $PA=LU$ decomposition: $PA=LU$
- Step 2: Compute z by forward substitution using $Lz=Pb$
- Step 3: Compute x by backward substitution using $Ux=z$.

An example

$$2x + 1y + 5z = 5$$

$$4x + 4y - 4z = 0$$

$$x + 3y + z = 6$$

$$\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 5 \\ 0 \\ 6 \end{bmatrix}$$

[A] {x} = {b}

Step 1: PA=LU

$$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}\begin{bmatrix} 2 & 1 & 5 \\ 4 & 4 & -4 \\ 1 & 3 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 1 \end{bmatrix}\begin{bmatrix} 4 & 4 & -4 \\ 0 & 2 & 2 \\ 0 & 0 & 8 \end{bmatrix}$$

Step 2: Compute z with Lz=Pb

$$\begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{4} & 1 & 0 \\ \frac{1}{2} & -\frac{1}{2} & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 5 \\ 0 \\ 6 \end{bmatrix} = \begin{bmatrix} 0 \\ 6 \\ 5 \end{bmatrix}$$

$$\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 6 \\ 8 \end{bmatrix}$$

Step 3: Compute x with Ux=z

$$\begin{bmatrix} 4 & 4 & -4 \\ 0 & 2 & 2 \\ 0 & 0 & 8 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 6 \\ 8 \end{bmatrix}$$

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}$$

Matrix inverse

If a matrix [A] is square, there is another matrix $[A]^{-1}$, called the inverse of [A]; such as:

$[A][A]^{-1}=[A]^{-1}[A]=[I]$; Identity matrix

$$A \cdot A^{-1} = A^{-1} \cdot A = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 \\ \vdots & 0 & \ddots & \vdots \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Matrix inverse

To compute the inverse matrix, the first column of $[A]^{-1}$ is obtained by solving the problem (for 3×3 matrix):

$$[A]\{x\} = \{b\} = \begin{Bmatrix} 1 \\ 0 \\ 0 \end{Bmatrix}$$

; second column: $[A]\{x\} = \{b\} = \begin{Bmatrix} 0 \\ 1 \\ 0 \end{Bmatrix}$

; and third column: $[A]\{x\} = \{b\} = \begin{Bmatrix} 0 \\ 0 \\ 1 \end{Bmatrix}$

The best way to implement such a calculation is to use LU decomposition.

An other way to read the definition

- Each column *j* of A^{-1} is the solution of :

$$Ax = b_j = \left[\begin{array}{c} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{array}\right] \begin{array}{l} \\ \\ \\ \leftarrow j \\ \\ \\ \\ \end{array}$$

Computing A^{-1}

Without Partial Pivoting

- Step 1: Decompose A=LU
- Step 2: Solve all equations $Ax=b_j$
  - Compute *z* by forward substitution using $Lz=b_j$
  - Compute *x* by backward substitution using $Ux=z$
- Step 3: Write A^{-1}

With Partial Pivoting

- Step 1: Decompose PA=LU
- Step 2: Solve all equations $PAx=Pb_j$
  - Compute *z* by forward substitution using $Lz=Pb_j$
  - Compute *x* by backward substitution using $Ux=z$
- Step 3: Write A^{-1}

An example

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}$$

Step 1: A=LU

Without Partial Pivoting

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix}$$

Step 2: Solve all $Ax=b_j$

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Step 2: Solve all $Ax=b_j$

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \\ -\frac{5}{3} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \\ -\frac{5}{3} \end{bmatrix} \qquad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ \frac{2}{3} \\ \frac{5}{6} \end{bmatrix}$$

Step 2: Solve all Ax=b$_j$

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \qquad \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ \frac{7}{3} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix} \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ \frac{7}{3} \end{bmatrix} \qquad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{3} \\ -\frac{7}{6} \end{bmatrix}$$

Step 2: Solve all $Ax=b_j$

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -3 & -\frac{7}{3} & 1 \end{bmatrix}\begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} z_1 \\ z_2 \\ z_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & -1 \\ 0 & -3 & 0 \\ 0 & 0 & -2 \end{bmatrix}\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \qquad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} \\ 0 \\ -\frac{1}{2} \end{bmatrix}$$

Step 3: Write A^{-1}

$$\begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} \frac{1}{2} \\ \frac{2}{3} \\ \frac{5}{6} \end{bmatrix} \qquad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{3} \\ -\frac{7}{6} \end{bmatrix} \qquad \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} \\ 0 \\ -\frac{1}{2} \end{bmatrix}$$

$$\begin{bmatrix} 1 & 2 & -1 \\ 2 & 1 & -2 \\ -3 & 1 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{2}{3} & -\frac{1}{3} & 0 \\ \frac{5}{6} & -\frac{7}{6} & -\frac{1}{2} \end{bmatrix}$$

Gauss-Seidel Method

- An iterative method

Approach

- The system $Ax=b$ is reshaped by solving the first equation for x_1, the second equation for x_2, and the third for x_3, …and nth equation for x_n.

Gauss-Seidel Method

For a 3x3 system

$$x_1 = \frac{b_1 - a_{12}x_2 - a_{13}x_3}{a_{11}}$$

$$x_2 = \frac{b_2 - a_{21}x_1 - a_{23}x_3}{a_{22}}$$

$$x_3 = \frac{b_3 - a_{31}x_1 - a_{32}x_2}{a_{33}}$$

A simple way to obtain initial guesses for all x's to start the solution process is to assume that they are zero.

These zeros can be substituted into x_1 equation to calculate a new $x_1 = b_1/a_{11}$.

Then we substitute this new value of x_1 along with the previous guess of zero for x_3 into the second equation to find x_2. The process is repeated for the third equation to calculate a new estimate for x_3

Gauss-Seidel Method

- New x_1 is obtained by using the new estimates of x_2 and x_3. The procedure is repeated until the convergence criterion is satisfied:

$$\left|\varepsilon_{a,i}\right| = \left|\frac{x_i^j - x_i^{j-1}}{x_i^j}\right| 100\% \prec \varepsilon_s$$

For all i, where j and $j-1$ are the present and previous iterations.

Fig. 11.4

First Iteration

$$x_1 = (c_1 - a_{12}x_2 - a_{13}x_3)/a_{11}$$
$$x_2 = (c_2 - a_{21}x_1 - a_{23}x_3)/a_{22}$$
$$x_3 = (c_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

$$x_1 = (c_1 - a_{12}x_2 - a_{13}x_3)/a_{11}$$
$$x_2 = (c_2 - a_{21}x_1 - a_{23}x_3)/a_{22}$$
$$x_3 = (c_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

Second Interation

$$x_1 = (c_1 - a_{12}x_2 - a_{13}x_3)/a_{11}$$
$$x_2 = (c_2 - a_{21}x_1 - a_{23}x_3)/a_{22}$$
$$x_3 = (c_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

$$x_1 = (c_1 - a_{12}x_2 - a_{13}x_3)/a_{11}$$
$$x_2 = (c_2 - a_{21}x_1 - a_{23}x_3)/a_{22}$$
$$x_3 = (c_3 - a_{31}x_1 - a_{32}x_2)/a_{33}$$

(a) Gauss Seidel

(b) Jacobi method p.291

In Gauss-Seidel method, the values $x_1^{k+1}, x_2^{k+1}, \ldots, x_i^{k+1}$ computed in the current iteration as well as $x_{i+2}^{k}, x_{i+3}^{k}, \ldots, x_n^{k}$ are used in finding the value x_{i+1}^{k+1}

This implies that always **the most recent approximations** are used during the computation. The general expression is:

$$x_i^{k+1} = \frac{1}{a_{ii}}\left[b_i - \sum_{j=1}^{i-1} \underbrace{a_{ij} x_j^{k+1}}_{NEW} - \sum_{j=i+1}^{n} \underbrace{a_{ij} x_i^{k}}_{OLD} \right]$$; i=1,2,...,n; k=1,2,3, ...

In Jacobi iteration method, all the new values are computed using the values at the previous iteration. This implies that both the present and the previous set of values have to be stored.

Gauss-Seidel method will improve the storage requirement as well as the convergence.

Convergence Criterion for Gauss-Seidel Method

- The Gauss-Seidel method has two fundamental problems as many iterative method:
  - It is sometimes nonconvergent, and
  - If it converges, converges very slowly.
- Recalling that sufficient conditions for convergence of two linear equations, *u(x,y)* and *v(x,y)* are

$$\left|\frac{\partial u}{\partial x}\right| + \left|\frac{\partial u}{\partial y}\right| \prec 1$$

$$\left|\frac{\partial v}{\partial x}\right| + \left|\frac{\partial v}{\partial y}\right| \prec 1$$

- Similarly, in case of two simultaneous equations, the Gauss-Seidel algorithm can be expressed as

$$u(x_1, x_2) = \frac{b_1}{a_{11}} - \frac{a_{12}}{a_{11}} x_2$$

$$v(x_1, x_2) = \frac{b_2}{a_{22}} - \frac{a_{21}}{a_{22}} x_1$$

$$\frac{\partial u}{\partial x_1} = 0 \qquad \frac{\partial u}{\partial x_2} = -\frac{a_{12}}{a_{11}}$$

$$\frac{\partial v}{\partial x_1} = -\frac{a_{21}}{a_{22}} \qquad \frac{\partial v}{\partial x_2} = 0$$

- Substitution into convergence criterion of two linear equations yield:

$$\left|\frac{a_{12}}{a_{11}}\right| \prec 1 \qquad \left|\frac{a_{21}}{a_{22}}\right| \prec 1$$

- In other words, the absolute values of the slopes must be less than unity for convergence:

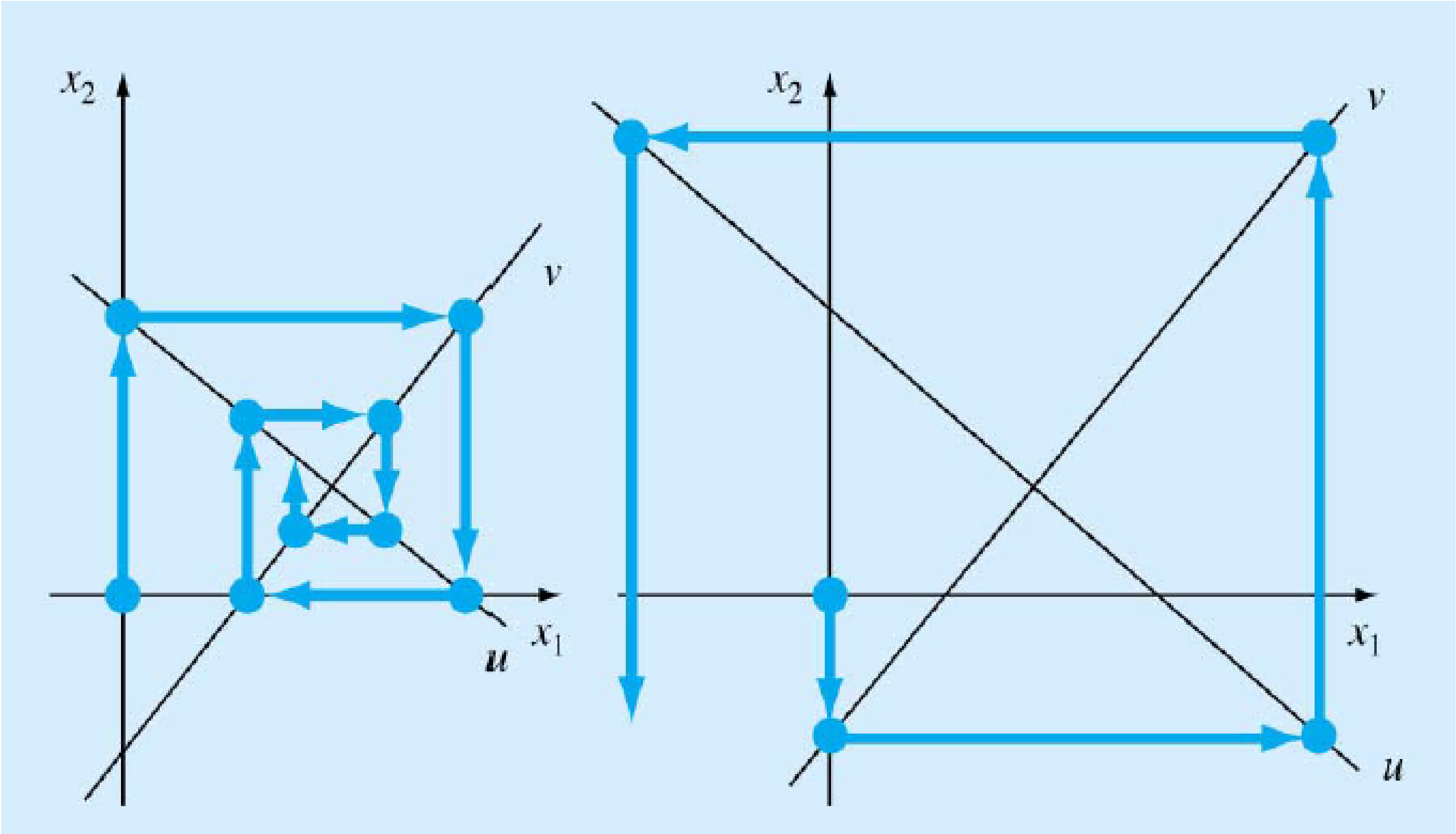
$$|a_{11}| \succ |a_{12}|$$

$$|a_{22}| \succ |a_{21}|$$

For n equations :

$$|aii| \succ \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{i,j}|$$

Figure 11.5



(a) (b)