Al-Ayen University
College of Petroleum Engineering

Numerical Methods and Reservoir Simulation

Lecturer: Dr. Mohammed Idrees Al-Mossawy

L8: Methods of Solving Systems of Linear Equations (Part 1)

Outlines

- Definition of a System of Linear Equations
- General Methods for Solving Linear Equations
  - Direct Methods for Solving Linear Equations
    - Gaussian Elimination Method
    - Thomas Algorithm
      - **Example**

Definition of a System of Linear Equations

A system of equations of the form

$$
\begin{aligned}
a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n &= b_1 \\
a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n &= b_2 \\
\vdots \qquad\qquad & \vdots \quad \vdots \\
a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n &= b_m
\end{aligned}
$$

is called a linear system of m equations with n unknowns (x1, x2, . . . , xn). *Discretization of PDEs of flow in porous media by the implicit finite difference approximation leads to linear system of equations with same number of equations and unknowns.*

General Methods for Solving Linear Equations

Basically, there are two main approaches for solving sets of linear equations involving ***direct methods*** and ***iterative methods*** as follows**:**

Direct Methods for Solving Linear Equations

Suppose that we have a system of n equations in n unknown $x_1, x_2, \ldots, x_n$.

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n &= b_2 \\ \vdots \qquad\qquad & \vdots \quad \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n &= b_n \end{aligned}$$

This can be represented in matrix form as

$$\mathbf{A}\,\mathbf{x} = \mathbf{b}$$

where

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \ldots & a_{1n} \\ a_{21} & a_{22} & \ldots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \ldots & a_{nn} \end{pmatrix} \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

- Remember that any mathematical operation we perform on one of the linear equations (e.g. multiplying through by $x2$) must be performed on both sides of the equation i.e. on the a_{ij} and the b_i.
- Therefore, we can transform the above matrix equation into the following form:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ 0 & a_{22} & a_{23} & \dots & a_{2n} \\ 0 & 0 & a_{33} & \dots & a_{3n} \\ \vdots & \vdots & \ddots & \dots & \dots \\ 0 & 0 & \dots & 0 & a_{nn} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{pmatrix}$$

$$\underline{A}.\underline{x} = \underline{b}$$

- This process is called the ***Forward Elimination.*** The coefficient matrix ***A*** is ***upper triangular*** with zero elements below the main diagonal. The solution can be found by the ***Back Substitution*** process:

$$\begin{aligned} x_n &= \frac{1}{a_{nn}} b_n, \\ x_{n-1} &= \frac{1}{a_{n-1,n-1}} \left(b_{n-1} - a_{n-1,n} x_n \right), \\ \vdots &= \vdots \\ x_1 &= \frac{1}{a_{11}} \left(b_1 - \sum_{j=2}^{n} a_{1j} x_j \right), \end{aligned}$$

Direct Methods for Solving Linear Equations

Gaussian Elimination Method

Carl Friedrich Gauss (1777 – 1855) – a German mathematician and scientist.

Example

We start with the system of equations

$$\begin{aligned} x_1 + 2x_2 + 3x_3 &= 6 \\ 2x_1 + 2x_2 + 2x_3 &= 6 \\ x_1 + 8x_2 + x_3 &= 10 \end{aligned} \quad \Longrightarrow \quad \begin{pmatrix} 1 & 2 & 3 \\ 2 & 2 & 2 \\ 1 & 8 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 6 \\ 6 \\ 10 \end{pmatrix}$$

It is useful to rewrite it in the ***augmented*** form

$$\left(\begin{array}{ccc|c} 1 & 2 & 3 & 6 \\ 2 & 2 & 2 & 6 \\ 1 & 8 & 1 & 10 \end{array}\right) \Longrightarrow \begin{matrix} \\ R2 - 2R1 \\ R3 - R1 \end{matrix} \left(\begin{array}{ccc|c} 1 & 2 & 3 & 6 \\ 0 & -2 & -4 & -6 \\ 0 & 6 & -2 & 4 \end{array}\right) \Longrightarrow \begin{matrix} \\ \\ R3 + 3R2 \end{matrix} \left(\begin{array}{ccc|c} 1 & 2 & 3 & 6 \\ 0 & -2 & -4 & -6 \\ 0 & 0 & -14 & -14 \end{array}\right)$$

The linear system of equations is now in upper ***triangular*** form and we can easily recover the solution:

$$\begin{aligned} x_3 &= 1 \\ x_2 &= 1 \\ x_1 &= 1 \end{aligned}$$

Pitfalls of Gaussian Elimination Method

- There are two potential pitfalls:

1. Division by zero: May occur in the forward elimination steps. Consider the set of equations:

$$\begin{aligned} 10x_2 \quad - 7x_3 &= 7 \\ 6x_1 + 2.099x_2 + 3x_3 &= 3.901 \\ 5x_1 - \quad x_2 \quad + 5x_3 &= 6 \end{aligned}$$

2. Round-off error: Prone to round-off errors. This is true when there are large numbers of equations as errors propagate.

- To avoid division by zero as well as reduce (not eliminate) round-off error, ***Gaussian elimination with partial pivoting*** is the method of choice.

Gaussian Elimination with Partial Pivoting

- ***Gaussian Elimination with Partial Pivoting*** ensures that each step of ***Forward Elimination*** is performed with the pivoting element $|a_{kk}|$ having the largest absolute value.

- At the beginning of any step (k_{th}) of ***forward elimination***, find the ***maximum absolute value*** of:

$$|a_{kk}|, |a_{k+1,k}|, \ldots\ldots\ldots\ldots\ldots, |a_{nk}|$$

If In the p[th] row, the maximum of the values is $|a_{pk}|$ then switch rows p and k.

$$k \le p \le n,$$

Example:

Changing the rows according to $|a_{kk}|$ at the second step of ***Forward Elimination.***

$$\begin{bmatrix} 10 & -7 & 0 \\ 0 & -0.001 & 6 \\ 0 & 2.5 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 6.001 \\ 2.5 \end{bmatrix} \Rightarrow \begin{bmatrix} 10 & -7 & 0 \\ 0 & 2.5 & 5 \\ 0 & -0.001 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 7 \\ 2.5 \\ 6.001 \end{bmatrix}$$

Thomas Algorithm

- Thomas algorithm is a simplified form of Gaussian elimination that can be used to solve ***tridiagonal*** systems of equations.

- Consider a system of N algebraic equations having a tridiagonal coefficient matrix given as follows:

$$\begin{bmatrix} b_1 & c_1 & 0 & 0 & & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & & 0 & 0 \\ . & & & & & & \\ . & & & & & & \\ . & & & & & & \\ 0 & & & & a_{N-1} & b_{N-1} & c_{N-1} \\ 0 & 0 & 0 & & & a_N & b_N \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ . \\ . \\ \\ P_{N-1} \\ P_N \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ . \\ . \\ \\ d_{N-1} \\ d_N \end{bmatrix}$$

Thomas Algorithm

Given

$$\left[\begin{array}{ccccc:c} b_1 & c_1 & 0 & 0 & & d_1 \\ a_1 & b_2 & c_2 & 0 & & d_2 \\ 0 & \ddots & \ddots & \ddots & 0 & \\ 0 & 0 & a_{n-2} & b_{n-1} & c_{n-1} & d_{n-1} \\ & & & a_{n-1} & b_n & d_n \end{array}\right]$$

STEP 1: ***Eliminate lower diagonal elements***

for j=2:n

$$\left[\begin{array}{ccccc:c} b_1 & c_1 & 0 & 0 & & d_1 \\ 0 & \boxed{\overline{b}_2} & c_2 & 0 & & \boxed{\overline{d}_2} \\ 0 & \ddots & \ddots & \ddots & 0 & \\ 0 & 0 & 0 & \overline{b}_{n-1} & c_{n-1} & \overline{d}_{n-1} \\ & & & 0 & \overline{b}_n & \overline{d}_n \end{array}\right]$$

$\overline{\mathrm{b}}(j) = b(j) - \{a(j-1)/\overline{\mathrm{b}}(j-1)\}*c(j-1)$

$\overline{\mathrm{d}}(j) = d(j) - \{a(j-1)/\overline{\mathrm{b}}(j-1)\}*\overline{\mathrm{d}}(j-1)$

end

STEP 2: ***Back substitution***

$$\left[\begin{array}{ccccc:c} b_1 & c_1 & 0 & 0 & & d_1 \\ 0 & \overline{b}_2 & c_2 & 0 & & \overline{d}_2 \\ 0 & \ddots & \ddots & \ddots & 0 & \\ 0 & 0 & 0 & \overline{b}_{n-1} & c_{n-1} & \overline{d}_{n-1} \\ & & & 0 & \overline{b}_n & \overline{d}_n \end{array}\right]$$

for i=n-1:-1:1

$P(i) = \{\overline{\mathrm{d}}(i) - c(i)*P(i+1)\}/\overline{\mathrm{b}}(i);$

end

$P(n) = \overline{\mathrm{d}}(n)/\overline{\mathrm{b}}(n)$

Example

Solve the following set of linear equations using *Thomas algorithm.*

$$2.04\,P_1 - P_2 = 40.8$$

$$-P_1 + 2.04\,P_2 - P_3 = 0.8$$

$$-P_2 + 2.04\,P_3 - P_4 = 0.8$$

$$-P_3 + 2.04\,P_4 = 200.8$$

Solution:

1. The set of linear equations can be written in matrix form as follows:

$$\begin{bmatrix} 2.04 & -1 & 0 & 0 \\ -1 & 2.04 & -1 & 0 \\ 0 & -1 & 2.04 & -1 \\ 0 & 0 & -1 & 2.04 \end{bmatrix} \begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \end{bmatrix} = \begin{bmatrix} 40.8 \\ 0.8 \\ 0.8 \\ 200.8 \end{bmatrix}$$

$$
\begin{bmatrix}
b_1 & c_1 & 0 & 0 & & 0 & 0 \\
a_2 & b_2 & c_2 & 0 & & 0 & 0 \\
0 & a_3 & b_3 & c_3 & & 0 & 0 \\
. & & & & & & \\
. & & & & & & \\
. & & & & & & \\
0 & & & & a_{N-1} & b_{N-1} & c_{N-1} \\
0 & 0 & 0 & & & a_N & b_N
\end{bmatrix}
\begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ . \\ . \\ \\ P_{N-1} \\ P_N \end{bmatrix}
=
\begin{bmatrix} d_1 \\ d_2 \\ d_3 \\ . \\ . \\ \\ d_{N-1} \\ d_N \end{bmatrix}
\qquad
\begin{bmatrix}
2.04 & -1 & 0 & 0 \\
-1 & 2.04 & -1 & 0 \\
0 & -1 & 2.04 & -1 \\
0 & 0 & -1 & 2.04
\end{bmatrix}
\begin{bmatrix} P_1 \\ P_2 \\ P_3 \\ P_4 \end{bmatrix}
=
\begin{bmatrix} 40.8 \\ 0.8 \\ 0.8 \\ 200.8 \end{bmatrix}
$$

2. Find $\overline{b}_1 = b_1$

$$\overline{b}_i = \left(b_i - \frac{a_i\, c_{i-1}}{\overline{b}_{i-1}}\right) \quad \text{for } \mathbf{i}=2,3,\ldots,N$$

$$\overline{b}_1 = 2.04$$
$$\overline{b}_2 = 2.04 - (-1/2.04)(-1) = 1.550$$
$$\overline{b}_3 = 2.04 - (-1/1.550)(-1) = 1.395$$
$$\overline{b}_4 = 2.04 - (-1/1.395)(-1) = 1.323$$

3. Find $\bar{d}_1 = d_1$

$$\bar{d}_i = \left(d_i - \frac{a_i \bar{d}_{i-1}}{\bar{b}_{i-1}}\right) \quad \text{for } \mathbf{i}=2,3,\dots,N$$

$$\bar{d}_1 = 40.8$$

$$\bar{d}_2 = 0.8 - (-1/2.04)\,40.8 = 20.8$$

$$\bar{d}_3 = 0.8 - (-1/1.550)\,20.8 = 14.221$$

$$\bar{d}_4 = 200.8 - (-1/1.395)\,14.221 = 210.996$$

4. The back substitution gives;

$$P_N = \frac{\bar{d}_N}{\bar{b}_N} \qquad P_i = \frac{\bar{d}_i - c_i P_{i+1}}{\bar{b}_i}, \quad i = N-1, N-2, \dots, 1$$

$$P_4 = 210.996/1.323 = 159.480$$

$$P_3 = [14.221 - (-1)159.48]/1.395 = 124.538$$

$$P_2 = [20.800 - (-1)124.538]/1.550 = 93.778$$

$$P_1 = [40.800 - (-1)93.778]/2.040 = 65.970$$

THANK YOU