The physical basis of the asymptotic growth arises from the process of advective-diffusive exchange that takes place in a heterogeneous medium consisting of lenses having higher and lower values of hydraulic conductivity. In such a medium, a solute will advance advectively faster in a high-conductive zone and the resulting concentration gradient between high- and low-conductive zones will give rise to transverse diffusive transport. Mass is thus removed from the front of the plume and stored temporarily in the low-conductive layers. When the plume has passed the low-conductive zone, the concentration gradient reverses and the mass moves back into the high-conductive zone to be added to the tail end of the plume. In an aquifer containing many of these zones of differing conductivity, the aggregate of these mass exchanges, seen over the system as a whole, results in an apparent growth of the overall dispersivity. Eventually, the process stabilizes at the level of the asymptotic dispersivity. The study also confirmed that the transverse vertical dispersivity remains at its local value.

The dispersivity reaches its asymptotic value at a travel distance of about 40-50 correlation lengths from the source (Frind *et al.*, 1987). For pre-asymptotic conditions, unfortunately, rigorously valid scale-dependent dispersivity relationships that are easy to implement in numerical models have not yet been developed. Although the microscale approach is valid, its cost renders it impractical in normal situations. A dilemma therefore arises in the modelling of advective-dispersive transport in the pre-asymptotic range. One possible option may be to select an empirical dispersivity function that takes on a local value at the source and grows to the required asymptotic value. Fortunately, field problems may not be overly sensitive to the precise value of the dispersivity as long as it is in the correct range (Frind and Molson, 1989).

3. SOLUTION OF SIMULTANEOUS EQUATIONS

Numerical solutions of problems in groundwater studies create systems of simultaneous equations which could be very large. The number of unknown parameters in these equations are often between 100 and 1000, sometimes up to one million. The equations are also generally banded. Efficient techniques are required to solve these equations. The equations

are usually represented using matrix notations.

Consider the following set of linear equations:

$$\begin{aligned} 2x_1 - 5x_2 + x_3 &= 6 \\ -x_1 + 7x_2 - 2x_3 &= -2 \\ 4x_2 + 9x_3 &= 1 \end{aligned}$$

In matrix notation, this set of equations is written as:

$$\begin{bmatrix} 2 & -5 & 1 \\ -1 & 7 & -2 \\ 0 & 4 & 9 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \end{Bmatrix} = \begin{Bmatrix} 6 \\ -2 \\ 1 \end{Bmatrix}$$

or in the general form:

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ a_{31} & a_{32} & \cdots & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ x_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ \cdot \\ \cdot \\ b_n \end{Bmatrix}$$

The *coefficients* are contained in [A], the vector of *knowns* is {b} while {x} is the vector of *unknowns*. The matrix equation can be written in a more simplified notation as [A] {x} = {b}, where [A] may have *n* rows and *m* columns. When *n* is equal to *m*, the matrix is described as a SQUARE matrix. Other special forms of matrices include the following:

- SYMMETRIC MATRIX - The elements in the matrix are symmetric with respect to the diagonal, (i.e., $a_{ij} = a_{ji}$)

- SKEW SYMMETRIC MATRIX - A square matrix with a negative symmetrY with respect to the diagonal (i.e. $a_{ij} = a_{ji}$ for $i \neq j$)

- DIAGONAL MATRIX - A square matrix in which all elements are zero except at the diagonal (i.e., $a_{ij} = 0$ for $i \neq j$)

- IDENTITY (or UNIT) MATRIX - A diagonal matrix with diagonal elements equal to unity (i.e., $a_{ij} = 0$ for $i \neq j$; $a_{ij} = 1$ for i=j). It is denoted as [I].

- TRIANGULAR MATRIX - A square matrix with all - zero elements either above or below the diagonal elements.

- NULL MATRIX - A matrix in which all elements are zero (i.e., $a_{ij} = 0$).

3.1 Matrix Operations

3.1.1 Addition and Subtraction

Two matrices, [A] and [B] can be added (or subtracted) to obtain [C] only if their dimensions are the same. The procedure requires that corresponding elements of [A] and [B] are added (or subtracted) to obtain [C] such that $c_{ij} = a_{ij} \pm b_{ij}$ for all values of i and j.

3.1.2 Multiplication

A matrix [A] can be multiplied by [B] only if the column size of [A] is identical to the row size of [B]. The product formed, [C] = [A] [B] will have the column size of [A] and the row size of [B]. The elements in the product are obtained as:

$$c_{ij} = \sum_{k=1}^{m} a_{ik}\, b_{kj} \; (i=1, \ldots, n;\; j=1, \ldots, r)$$

Note that matrix multiplication is not commutative (i.e. [A] [B] ≠ [B] [A]). In many cases, [A] [B] may be defined while [B] [A] is undefined.

3.1.3 Transpose of a Matrix

The transpose of a matrix, denoted as $[A]^T$ can be obtained from [A] by interchanging the column and row elements such that:

$$a^T_{ij} = a_{ji}$$

The transpose of a product is obtained by:

$([A]\,[B])^T = [B]^T\,[A]^T$

3.2 Definitions

3.2.1 Determinant of a Matrix

The determinant of a matrix [A] (denoted as det A or $|A|$), and defined only for a square matrix) is obtained as:

$$|A| = \sum_{i=1}^{n} a_{ij} \cdot [cof(a_{ij})] = \sum_{j=1}^{n} a_{ij} \cdot [cof(a_{ij})]$$

where the cofactor (cof) is defined by:
and the minor is the determinant of the submatrix obtained by deleting the *i*th row and the *j*th

$$cof\ (a_{ij}) = (-1)^{i+j} \cdot [minor\ (a_{ij})]$$

column of the original matrix. Using the definition above, the determinant of a 2 x 2 matrix can be obtained as:

$$|A| = \begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix} = a_{11}\ a_{22} - a_{21}\ a_{12}$$

Similarly, the determinant of a 3 x 3 matrix can be obtained as:

$$|A| = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} = a_{11}(+1) \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} + a_{12}(-1) \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13}(+1) \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$

3.2.2 Inverse of a Matrix

The inverse of a matrix (denoted as $[A]^{-1}$) is defined by:

$$[A]^{-1} = \frac{1}{|A|}\ adj\ [A] \qquad\qquad |A| \neq 0$$

where the adjoint (adj [A]) is obtained as:

$$\text{adj } [A] = [\text{cof } A]^T$$

For example,

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

The inverse satisfies the equalities:

$$[A]^{-1}[A] = [A][A]^{-1} = [I] \qquad \text{(Identity matrix)}$$

3.3 Matrix Solution by Inversion

Given a set of simultaneous equations:

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

The vector of unknown parameters can be obtained by pre-multiplying each side of the matrix equation by the inverse of [A], thus:

$$[A]^{-1}[A]\{X\} = [A]^{-1}\{B\}$$

i.e. $[I]\{X\} = [A]^{-1}\{B\}$

or $\{X\} = [A]^{-1}\{B\}$

Exercise:

Solve by Inversion

$$\begin{bmatrix} 2 & 0 & 1 \\ 4 & 6 & -5 \\ 0 & 1 & 5 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{Bmatrix} 7 \\ 1 \\ 4 \end{Bmatrix}$$

3.4 Cramer's Rule

This is a convenient method for hand calculations of small (2x2 or 3x3) system of equations:

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

The k^{th} term in the unknown vector {x} is:

$$x_k = \frac{\det A_k}{\det A} = \frac{| A_k |}{| A |} \qquad | A | \neq 0$$

$|A_k|$ is obtained by replacing the k^{th} column in |A| with the vector {B}:

$$| A_k | = \begin{vmatrix} a_{11} & a_{12} & a_{13} \cdots & a_{1,k-1} & b_1 & a_{1,k+1} & \cdots & a_{1n} \\ a_{21} & & & a_{2,k-1} & b_2 & a_{2,k+1} & \cdots & a_{2n} \\ | & & & & | & & & | \\ | & & & & | & & & | \\ a_{n1} & & & & b_n & & & a_{nn} \end{vmatrix}$$

The number of operations (multiplication and division) is On^4 (of the order of n^4) where n is the band width.

Exercise

Solve by Cramer's rule:

$$\begin{bmatrix} 2 & 1 & 2 \\ 3 & 1 & -1 \\ 1 & 4 & 1 \end{bmatrix} \begin{Bmatrix} x \\ y \\ z \end{Bmatrix} = \begin{Bmatrix} 10 \\ 2 \\ 12 \end{Bmatrix}$$

3.5 Gaussian Elimination

This is the most widely used method of solving simultaneous equations.

3.5.1 Elementary Row Operations

Consider the system:

$$\begin{matrix} 1) \\ 2) \\ 3) \\ 4) \end{matrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \\ a_{41} & a_{42} & a_{43} & a_{44} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{Bmatrix}$$

From (2), subtract (1) x a_{21}/a_{11} to obtain (2′).

For example:

$$a_{21} - \frac{a_{21}}{a_{11}} a_{11} = 0$$

$$a_{22} - \frac{a_{21}}{a_{11}} a_{12} = a_{22}'$$

$$\vdots \qquad\qquad \vdots$$

$$b_2 - \frac{a_{21}}{a_{11}} b_1 = b_2'$$

In a similar manner, subtract (1) x a_{31}/a_{11} from (3) and (1) x a_{41}/a_{11} from (4).
(a_{11} is the pivot). This results in:

Next, subtract (2′) x a_{32}'/a_{22}' from (3′) and (2′) x a_{42}'/a_{22}' from (4′) to obtain:
Note that the new pivot is a_{22}'. Then subtract (3″) x a_{43}''/a_{33}'' from (4″) to obtain:

$$
\begin{matrix} 1\,) \\ 2')\\ 3')\\ 4') \end{matrix}
\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22}' & a_{23}' & a_{24}' \\ 0 & a_{32}' & a_{33}' & a_{34}' \\ 0 & a_{42}' & a_{43}' & a_{44}' \end{bmatrix}
\begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix}
\begin{Bmatrix} b_1 \\ b_2' \\ b_3' \\ b_4' \end{Bmatrix}
$$

$$
\begin{matrix} 1 \\ 2' \\ 3'' \\ 4'' \end{matrix}
\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22'} & a_{23'} & a_{24'} \\ 0 & 0 & a_{33''} & a_{34''} \\ 0 & 0 & a_{43''} & a_{44''} \end{bmatrix}
\begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix}
=
\begin{Bmatrix} b_1 \\ b_2' \\ b_3'' \\ b_4'' \end{Bmatrix}
$$

$$
\begin{bmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ 0 & a_{22}' & a_{23}' & a_{24}' \\ 0 & 0 & a_{33}'' & a_{34}'' \\ 0 & 0 & 0 & a_{44}''' \end{bmatrix}
\begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix}
=
\begin{Bmatrix} b_1 \\ b_2' \\ b_3'' \\ b_4''' \end{Bmatrix}
$$

We can now solve for x, starting at the bottom, thus:

$$x_k = \frac{b_4'''}{a_{44}'''}$$

$$x_3 = \frac{1}{a_{33}''} (b_3'' - a_{34}'' x_4)$$

$$x_2 = \frac{1}{a_{22}'} (b_2' - a_{23}' x_3 - a_{24}' x_4)$$

$$x_1 = \frac{1}{a_{11}} (b_1 - a_{12} x_2 - a_{13} x_3 - a_{14} x_4)$$

3.5.2 Gauss-Jordan Elimination

The elimination is also done on the upper part of the matrix above the diagonal. Each row is divided by the appropriate pivot, resulting in:

$$\begin{bmatrix} 1 & & & 0 \\ & 1 & & \\ & & 1 & \\ 0 & & & 1 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{Bmatrix} = \begin{Bmatrix} b_1' \\ b_2'' \\ b_3''' \\ b_4'''' \end{Bmatrix}$$

The reader is referred to section 6.4 in Hornbeck (1975) for details. Because we always divide by the pivot, it is numerically important that the pivot is non-zero.

3.5.3 Matrix Inversion by Gauss-Jordan Elimination

For a square matrix [A], an inverse $[A]^{-1}$) is defined such that the product gives a unit matrix, thus:

$$[A]\ [A]^{-1} = [I]$$

i.e. [A] is transformed to [I]:

$$[A]\ [A^{-1}] = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}$$

The same transformation is performed on the right-hand side to obtain $[A]^{-1}$:

$$[I]\ [A]^{-1} = [A]^{-1}$$

3.5.4 Generalized Gauss Elimination Procedure (L - U Decomposition)

This procedure is useful in problems with repeated right-hand sides such as in time marching schemes or multiple loading conditions. Consider:

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

If this corresponds to a real physical system ([A] is positive-definite), then [A] can be decomposed or factored into unique upper and lower triangular matrices:

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

so:

$$[L]\ [U]\ \{ X \} = \{ B \}$$

let:

$$[U]\ \{ X \} = \{ Y \}$$

then:

$$[L]\ \{ Y \} = \{ B \}$$

Solve for y:

$$\begin{bmatrix} l_{11} & & 0 \\ l_{21} & l_{22} & \\ l_{31} & l_{32} & l_{33} \\ | & & \\ | & & \\ l_{n1} & & \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ y_3 \\ | \\ | \\ y_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \\ | \\ | \\ b_n \end{Bmatrix}$$

$$y_1 = \frac{b_1}{l_{11}}$$

$$y_2 = \frac{b_2 - l_{21}\, y_1}{l_{22}}$$

etc.

Solve for x from:

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

$$\begin{bmatrix} u_{11} & u_{12} & & u_{1n} \\ & & & u_{2n} \\ & & & | \\ & & & | \\ 0 & & u_{n-1\,,\,n-1} & u_{n-1\,,\,n} \\ & & & u_{nn} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ | \\ | \\ x_{n-1} \\ x_n \end{Bmatrix} = \begin{Bmatrix} y_1 \\ y_2 \\ | \\ | \\ y_{n-1} \\ y_n \end{Bmatrix}$$

$$X_{n-1} = \frac{y_{n-1} - u_{n-1,n}\, x_n}{u_{n-1,n-1}}$$

The sequence of elementary row operations can be expressed as (for 4 x 4)

$$[L_3][L_2][L_1][A]\{ x \} = [L_3][L_2][L_1]\{ B \}$$

$$x_n = \frac{y_n}{u_{nn}}$$

where:

$$[L_1] = \begin{bmatrix} 1 & & & \\ \frac{a_{21}}{a_{11}} & 1 & & \\ \frac{-a_{31}}{a_{11}} & 0 & 1 & \\ \frac{-a_{41}}{a_{11}} & 0 & 0 & 1 \end{bmatrix}$$

let:

$$[L_3][L_2][L_1] = [L^*]$$

$$[L_2] = \begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & \frac{-a_{32}'}{a_{22}'} & 1 & \\ 0 & \frac{a_{42}'}{a_{22}'} & 0 & 1 \end{bmatrix}$$

$$[L_3] = \begin{bmatrix} 1 & & & \\ 0 & | & & \\ 0 & 0 & | & \\ 0 & 0 & \frac{a_{43}''}{a_{33}''} & 1 \end{bmatrix}$$

then:

$$[L^*][A]\{ x \} = [L^*]\{ B \}$$

but the result of the elementary row operations is an upper triangular matrix. Since the decomposition must be unique, this means that:

$$[L^*][A] \equiv [U]$$

likewise:

$$[L^*]\{ B \} \equiv \{ Y \}$$

since:

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

Premultiply above equation by $[L^*]^{-1}$:

$$[L^*]^{-1}[L^*][A] = [L^*]^{-1}[U]$$

therefore:

$$[A] = [L^*]^{-1}[U]$$

$$= [L]\ [U]$$

$$[L^*]^{-1}[L^*]\{B\} = [L^*]^{-1}\ \{Y\}$$

$$\{\ B\ \} = [L]\ \{\ Y\ \}$$

Thus, after obtaining [L] and [U], the right hand side {B} can be handled independently. So:

$$[L] = [L^*]^{-1}$$

$$= ([L_3][L_2][L_1])^{-1}$$

$$= [L_1]^{-1}[L_2]^{-1}[L_3]^{-1}$$

$$= \left(\begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & 0 & 1 & \\ 0 & 0 & \frac{a_{43}''}{a_{33}''} & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & \frac{a_{32}'}{a_{22}'} & 1 & \\ 0 & \frac{-a_{42}'}{a_{22}'} & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ \frac{a_{21}}{a_{11}} & 1 & & \\ \frac{a_{31}}{a_{11}} & 0 & 1 & \\ \frac{-a_{41}}{a_{11}} & 0 & 0 & 1 \end{bmatrix} \right)^{-1}$$

$$= \begin{bmatrix} 1 & & & \\ \frac{a_{21}}{a_{11}} & 1 & & \\ \frac{a_{31}}{a_{11}} & 0 & 1 & \\ \frac{a_{41}}{a_{11}} & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & \frac{a_{32}'}{a_{22}'} & 1 & \\ 0 & \frac{a_{42}'}{a_{22}'} & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & 0 & 1 & \\ 0 & 0 & \frac{a_{43}''}{a_{33}''} & 1 \end{bmatrix}$$

multiply out:

$$L = \begin{bmatrix} 1 & & & \\ \frac{a_{21}}{a_{11}} & 1 & & \\ \frac{a_{31}}{a_{11}} & \frac{a_{32}'}{a_{22}'} & 1 & \\ \frac{a_{41}}{a_{11}} & \frac{a_{42}'}{a_{22}'} & \frac{a_{43}''}{a_{33}''} & 1 \end{bmatrix}$$

[L] contains the pivots used in the elementary row operations to obtain [U].

The general procedure to solve [A] {x} = {B} is as follows:

1. Decompose [A] to obtain [L] and [U]

   - obtain [U] from elementary row operations
   - store pivot elements in [L]

2. Solve [L] {Y} = {B}

3. Solve [U] {x} = {y}

Repeat steps 2 and 3 only for repeated right-hand sides.

3.5.5 Ill-Conditioning

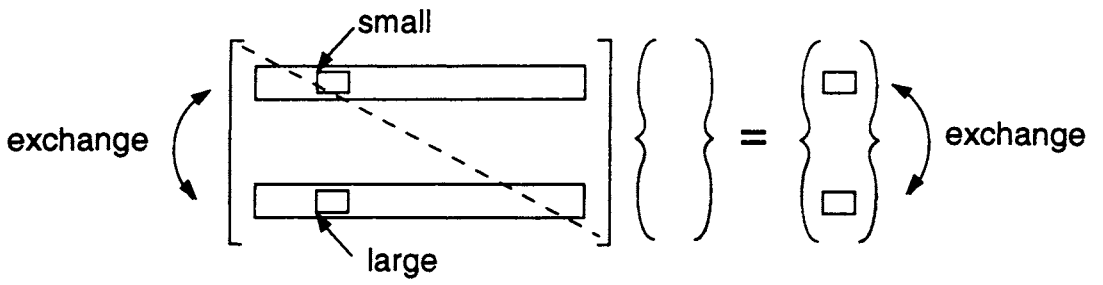
If *det* A is small in relation to the norm (magnitude) of the matrix, it may be ill-conditioned.

$$norm\ A = \sqrt{\sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}^2}$$

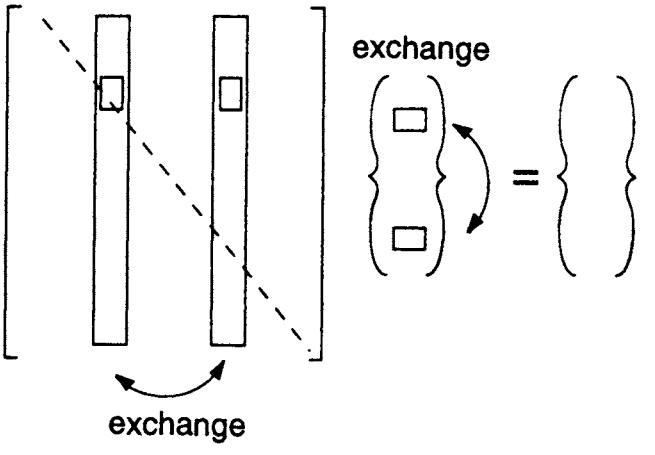
However, if the matrix represents a real, well-posed physical problem that is known to have a unique solution, ill-conditioning does not generally occur.

3.5.6 Row and Column Interchange

If a pivot is small, it may cause problems due to roundoff errors (note that a zero pivot will cause a solution failure). This can often be avoided by re-arranging rows or columns to place the largest element in the pivot position, thus:



Row interchange



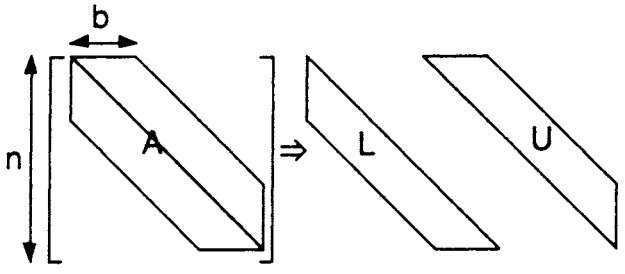
Column interchange

Note: Column interchanges must be kept track of in order to replace the unknowns to their

original positions after solving the equations.

3.5.7 Banded Matrices

Most physical problems lead to banded matrices.



Banded matrices

Operations Count

To solve [A] {x} = [B] with A banded, requires the following number of operations (multiplication and division):

- about nb^2 operations are required to decompose, and
- 2nb operations are required to solve

To solve by inversion and back multiplication $\{x\} = [A]^{-1}\{B\}$ requires:

- inversion - about n^3 (Gauss-Jordan method)
- multiply - about n^3

Note that the advantage of the band is lost when solving by inversion.

3.6 Cholesky Method

This method is applicable to symmetric positive-definite matrices only. Being symmetric the lower and upper triangular matrices obtained after decomposition will be the transpose of each other.

$$[A] = [L]\,[U]$$

$$= [L]\,[L]^T = [U]^T[U]$$

$$\begin{bmatrix} u_{11} & & & & & \\ u_{12} & u_{22} & & & & \\ u_{13} & u_{23} & u_{33} & & & \\ | & & & | & & \\ | & & & & | & \\ u_{1n} & & & & & u_{nn} \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & u_{13} & & & u_{1n} \\ & u_{22} & u_{23} & & & \\ & & u_{33} & & & \\ & & & | & & \\ & & & & | & \\ & & & & & u_{nn} \end{bmatrix}$$

$$= \begin{bmatrix} a_{11} & a_{12} & a_{13} & - & - & a_{1n} \\ a_{21} & a_{22} & & & & \\ a_{31} & & & & & \\ | & & & & & \\ | & & & & & \\ a_{n1} & & & & & a_{nn} \end{bmatrix}$$

Multiply out:

Row 1:

$$u_{11}^2 = a_{11} \qquad \rightarrow u_{11} = \sqrt{a_{11}}$$

$$u_{11}\, u_{12} = a_{12} \qquad \rightarrow \qquad u_{12} = \frac{a_{12}}{u_{11}}$$

$$u_{11}\, u_{13} = a_{13} \qquad \rightarrow u_{13} = \frac{a_{13}}{u_{11}}$$

Row 2:

$$u_{12}^2 + u_{22}^2 = a_{22} \rightarrow \sqrt{a_{22} - u_{12}^2}$$

$$u_{12}u_{13} + u_{22}u_{23} = a_{23} \rightarrow u_{23} = \frac{a_{23} - u_{12}u_{13}}{u_{22}}$$

etc.

In general, the decomposition is:

$$u_{ii} = \sqrt{a_{ii} - \sum_{k=1}^{i-1} u_{ki}^2}$$

$$u_{ij} = \frac{a_{ij} - \sum_{k=1}^{i-1} u_{ki}u_{kj}}{u_{ii}}$$

This is done independently of the right-hand side. The solution is completed by forward and backward substitution.

Equation with multiple right-hand sides:

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

Forward substitution:

$$\begin{bmatrix} u_{11} & & & \\ u_{12} & u_{22} & & 0 \\ u_{13} & u_{23} & u_{33} & \\ | & & & \\ | & & & \\ u_{1n} & - & - & u_{nn} \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ | \\ | \\ y_n \end{Bmatrix}_l = \begin{Bmatrix} b_1 \\ b_2 \\ | \\ | \\ b_n \end{Bmatrix}_l$$

$$y_i = \frac{1}{u_{ii}} \left[b_i - \sum_{k=1}^{i-1} (u_{ki}\, y_k) \right]$$

Backward Substitution:

$$\begin{bmatrix} u_{11} & u_{12} & & & u_{1n} \\ & u_{22} & | & & \\ & & & | & \\ & & & | & \\ & & & | & \\ & & u_{n-1,n-1} & u_{n-1,n} & \\ & & & & u_{nn} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ | \\ | \\ x_n \end{Bmatrix}_l = \begin{Bmatrix} y_1 \\ y_2 \\ | \\ | \\ y_n \end{Bmatrix}_l$$

$$x_i = \frac{1}{u_{ii}} \left[y_i - \sum_{k=i-1}^{n} (u_{ik}\, x_k) \right]$$

3.7 Thomas Algorithm

This method is applicable to tridiagonal matrices.

$$A = \begin{bmatrix} d_1 & f_1 & & & \\ e_2 & d_2 & f_2 & & \\ & & & f_{n-1} & \\ & & & d_{n-1} & \\ & & e_n & d_n & \end{bmatrix}$$

It can be shown that if [A] is banded, [L] and [U] will also be banded and have the same band width as [A].

Let [L] [U] = [A]

$$\begin{bmatrix} 1 & & \\ l_2 & 1 & 0 \\ & l_3 & \\ & & \\ 0 & & l_n \quad 1 \end{bmatrix} \begin{bmatrix} u_1 & g_1 & & 0 \\ & u_2 & g_2 & \\ & & & \\ & 0 & & g_{n-1} \\ & & & u_n \end{bmatrix} = \begin{bmatrix} u_1 & g_1 & & \\ l_2u_1 & (l_2g_1+u_2) & g_2 & \\ & l_3u_2 & (l_3g_2+u_3) & g_3 \\ & & | & | \quad | \\ & & & | \quad | \end{bmatrix}$$

Equating the product with [A] above, it can be deduced that:

$$g_i = f_i$$

$$u_i = d_1$$

$$l_i = \frac{e_i}{u_{i-1}} \qquad i=2, \cdots, n$$

$$u_i = d_i - l_i f_{i-1} \qquad i=2, \cdots, n$$

Solve: [A] {X} = {B}

Forward Substitution:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ l_2 & 1 & 0 & 0 & 0 \\ 0 & l_3 & 1 & 0 & 0 \\ & & & l_n & 1 \end{bmatrix} \begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{Bmatrix} = \begin{Bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{Bmatrix}$$

$y_1 = b_1$

$y_i = b_i - l_i y_{i-1} \qquad i=2, \ldots, n$

Backward Substitution:

$$\begin{bmatrix} u_1 & f_1 & & & \\ & u_2 & f_2 & & \\ & & u_3 & f_3 & \\ & & & u_4 & f_{n-1} \\ & & & & u_n \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix} = \begin{Bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{Bmatrix}$$

$$x_i = \frac{y_i - f_i x_{i+1}}{u_i} \qquad i = n-1,--,1$$

$$x_n = \frac{y_n}{u_n} \quad \frac{y_n}{u_n}$$

Exercise

Solve by Thomas Method:

$$\begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & 0 \\ & -1 & 2 & -1 & \\ 0 & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{Bmatrix} = \begin{Bmatrix} 8 \\ 0 \\ 0 \\ 0 \\ 2 \end{Bmatrix}$$

3.8 Gauss-Seidel Iterative Method

This method is generally used for sparse, diagonally-dominant matrices.

Consider:

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

Make an initial guess for x_2 and x_3 (in the absence of better information, set them to 0). Solve 1 for x_1:

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

Using the calculated value for x_1 and the initial guess for x_3, solve 2 for x_2, thus:

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

Then solve 3 for x_3, thus:

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

Repeat the procedure until successive results agree. The general Gauss-Seidel formula is:

$$x_i = \frac{1}{a_{ii}} \left[b_i - \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} x_j \right] \quad i=1,2, \cdots ,n$$

where x_j on the right-hand side is always the most recent value. In this method, convergence is guaranteed if:

$$| a_{ii} | > \sum_{\substack{j=1 \\ i \neq 1}}^{n} | a_{ij} |$$

However, convergence may also be obtained if this condition is not satisfied, as long as the diagonal term is the largest number in the row:

$$| a_{ii} | > \left| \sum_{j \neq i} a_{ij} \right|$$

3.8.1 Convergence Criteria

Convergence criteria can either be *absolute* or *relative.*

Absolute:

$$| x_i^{k+1} - x_i^{(k)} | \leq \varepsilon \qquad (a \text{ specified limit})$$

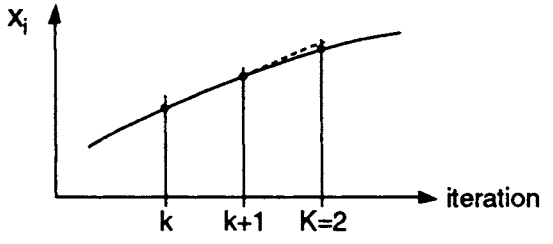
This criterion is often used when the magnitude of the results and the desired accuracy (number of decimals) are known. Note that results may continue to change after the convergence criterion have been satisfied.

$$\left| \frac{x_i^{(k+1)} - x_i^{(k)}}{x_i^{(k+1)}} \right| \leq \varepsilon$$

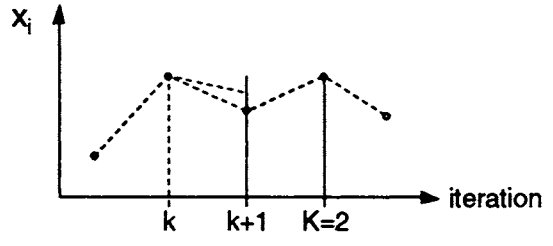
This criterion tests the percentage change in each unknown. It may be used when the magnitude of results is unknown but may cause problems if some numbers are close to zero.

3.8.2 Point Relaxation

If convergence is monotonic, it could be accelerated by extrapolation. If it is oscillatory, convergence can be improved by damping the oscillations.



(a) Point relaxation



(b) Point relaxation

Convergence can be accelerated by extrapolation from $x_i^{(k+1)}$ or in the case of (b), convergence could be improved by damping the oscillations. This is done by modifying calculated values obtained by the iteration formula according to:

$$x_i^{(k+1)} - x_i^{(k)} + \lambda\ (x_i^{(k+1)} - x_i^{(k)})$$

The value of $x_i^{(k+1)}$ is understood to be that calculated by the iteration formula. This can also be written as:

$$x_i^{(k+1)} = \lambda\, x_i^{(k+1)} + (1 - \lambda)\, x_i^{(k)}$$

Thus the value used is the weighted average between the calculated value and the previous value, such that:

$0 < \lambda < 1$ underrelaxation (damping)
$\lambda = 1$ standard Gauss-Seidel iteration
$1 < \lambda < 2$ overrelaxation (acceleration)

3.8.3 Advantages and Disadvantages of Iterative Methods

Some of the advantages of iterative methods include the following:

- it is self-correcting
- round-off error does not accumulate
- it can be programmed to operate only on non-zero terms
- there is no matrix fill-in
- it is suitable for calculators and small computers

The major disadvantage of iterative methods is that they need fast convergence and good initial guess to be competitive with direct methods.

4. FINITE DIFFERENCES

4.1 Basic Principles

The basic objective of finite difference methods is to approximate the differential terms in the governing differential equations by corresponding different terms. The resulting difference