

Mathematical Preliminaries

CENG6202: Advanced Computational Methods in
Geotechnical Engineering

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Fall Semester 2019

- 1 Vectors
- 2 Matrices
- 3 Linear System of Equations

1 Vectors

2 Matrices

3 Linear System of Equations

Vectors

A vector is a column of numbers. For example, vector \mathbf{a} of size n is written as

$$\mathbf{a} = \begin{Bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{Bmatrix}$$

The *transpose* of vector \mathbf{a} :

$$\mathbf{a}^T = \{a_1 \ a_2 \ \cdots \ a_n\}$$

The *magnitude* or *norm* of vector \mathbf{a} is defined as

$$\|\mathbf{a}\| = \sqrt{a_1^2 + a_2^2 + \cdots + a_n^2}$$

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The *dot product* (also called *scalar product*) of two vectors \mathbf{a} and \mathbf{b} , each of size n , is defined as:

$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^n a_i b_i = a_1 b_1 + a_2 b_2 + \cdots + a_n b_n$$

The dot product can also be written as

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{a}^T \mathbf{b} = \{a_1 \ a_2 \ \cdots \ a_n\} \begin{Bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{Bmatrix} = \sum_{i=1}^n a_i b_i$$

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The product $\mathbf{a}\mathbf{b}^\top$, however, results in a matrix, i.e.

$$\mathbf{a}\mathbf{b}^\top = \begin{Bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{Bmatrix} \{b_1 \ b_2 \ \cdots \ b_n\} = \begin{bmatrix} a_1b_1 & a_1b_2 & \cdots & a_1b_n \\ a_2b_1 & a_2b_2 & \cdots & a_2b_n \\ \vdots & \vdots & & \vdots \\ a_nb_1 & a_nb_2 & \cdots & a_nb_n \end{bmatrix}$$

The *cross product* of three-dimensional vectors $\mathbf{a}^T = \{a_1 \ a_2 \ a_3\}$ and $\mathbf{b}^T = \{b_1 \ b_2 \ b_3\}$ is a vector (say \mathbf{c}) and is defined as

$$\mathbf{c} = \mathbf{a} \times \mathbf{b} = \|\mathbf{a}\| \|\mathbf{b}\| \sin \theta \mathbf{n}$$

where θ is the angle between \mathbf{a} and \mathbf{b} and \mathbf{n} is a unit normal vector ($\|\mathbf{n}\| = 1$) to the plane of \mathbf{a} and \mathbf{b} .

The elements of vector \mathbf{c} are

$$\mathbf{c} = \begin{Bmatrix} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{Bmatrix}$$

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Matrices

A matrix \mathbf{A} with n rows and m columns is written as:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix}$$

The *transpose* of matrix \mathbf{A} :

$$\mathbf{A}^T = \begin{bmatrix} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{12} & a_{22} & \cdots & a_{n2} \\ \vdots & \vdots & & \vdots \\ a_{1m} & a_{2m} & \cdots & a_{nm} \end{bmatrix}$$

Square matrix: $n = m$

Symmetric matrix: Square and $a_{ij} = a_{ji}$

Skew matrix: Square and $a_{ij} = -a_{ji}$

Skew-symmetric matrix: Square, $a_{ii} = 0$ and $a_{ij} = -a_{ji}$

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Upper and Lower triangular decompositions of \mathbf{A} :

$$\mathbf{U} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix} \quad \text{and} \quad \mathbf{L} = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix}$$

Strictly upper and strictly lower triangular decompositions of \mathbf{A} :

$$\mathbf{U}' = \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ 0 & 0 & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix} \quad \text{and} \quad \mathbf{L}' = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ a_{21} & & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & 0 \end{bmatrix}$$

Upper and Lower triangular decompositions of A :

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Addition, subtraction, scalar multiplication and transposition:

① $\mathbf{A} \pm \mathbf{B} = \mathbf{B} \pm \mathbf{A}$

② $(\mathbf{A} \pm \mathbf{B})^T = \mathbf{A}^T \pm \mathbf{B}^T$

③ $(\mathbf{A}^T)^T = \mathbf{A}$

④ $(s\mathbf{A})^T = s(\mathbf{A}^T)$

Addition, subtraction, scalar multiplication and transposition:

① $A \pm B = B \pm A$

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Matrix-Vector multiplication:

$$\mathbf{A}\mathbf{x} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix} \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{Bmatrix} = \begin{Bmatrix} a_{11}x_1 + a_{12}x_2 + \cdots a_{1m}x_m \\ a_{21}x_1 + a_{22}x_2 + \cdots a_{2m}x_m \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + \cdots a_{nm}x_m \end{Bmatrix}$$

Vector-Matrix multiplication:

$$\mathbf{y}^\top \mathbf{A} = \{y_1 \quad y_2 \quad \cdots \quad y_n\} \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix}$$

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Bilinear form:

$$\mathbf{y}^T \mathbf{A} \mathbf{x} \rightarrow \text{Scalar}$$

Quadratic form:

$$\mathbf{x}^T \mathbf{A} \mathbf{x} \rightarrow \text{Scalar}$$

A matrix \mathbf{A} is called **positive-definite** if

$$\mathbf{z}^T \mathbf{A} \mathbf{z} > 0 \quad \forall \mathbf{z} \neq 0$$

Matrix-Matrix multiplication:

$$\begin{aligned}
 \mathbf{AB} &= \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & a_{22} & \cdots & a_{2m} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nm} \end{bmatrix} \begin{bmatrix} b_{11} & b_{12} & \cdots & b_{1p} \\ b_{21} & b_{22} & \cdots & b_{2p} \\ \vdots & \vdots & & \vdots \\ b_{m1} & b_{m2} & \cdots & b_{mp} \end{bmatrix} \\
 &= \begin{bmatrix} a_{11}b_{11} + \cdots + a_{1m}b_{m1} & \cdots & a_{11}b_{1p} + \cdots + a_{1m}b_{mp} \\ a_{21}b_{11} + \cdots + a_{2m}b_{m1} & \cdots & a_{21}b_{1p} + \cdots + a_{2m}b_{mp} \\ \vdots & & \vdots \\ a_{n1}b_{11} + \cdots + a_{nm}b_{m1} & \cdots & a_{n1}b_{1p} + \cdots + a_{nm}b_{mp} \end{bmatrix}
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Matrices

↪ Inverse

The *inverse* of a matrix A is denoted by A^{-1} and

$$AA^{-1} = A^{-1}A = I$$

where

$$I = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

Some properties of inverse:

- $(A^{-1})^{-1} = A$
- $(A^T)^{-1} = (A^{-1})^T$
- $(AB)^{-1} = B^{-1}A^{-1}$

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The *inverse* of a matrix \mathbf{A} is denoted by \mathbf{A}^{-1} and

$$\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = \mathbf{I}$$

where

$$\mathbf{I} = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix}$$

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$$|A| = \sum_{k=1}^n a_{ik} (-1)^{i+k} |A_{ik}|, \quad k = 1, \dots, n$$

Some properties of determinants:

- $|AB| = |A| |B|$ for square matrices A and B of the same size.
- $|A^T| = |A|$
- $|A^{-1}| = 1/|A|$
- $|sA| = s^n |A|$ for an $n \times n$ matrix A .
- $|I| = 1$ for an identity matrix of any size.

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A **block matrix** or **partitioned matrix** is a matrix that is composed of submatrices:

$$P = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

A **block diagonal matrix** is a square diagonal matrix in which the diagonal elements are square matrices of any size and the off-diagonal elements are zero or zero matrices of any size:

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1 Vectors

2 Matrices

3 Linear System of Equations

Linear System of Equations

The final problem to be solved in computational science and engineering usually takes the form:

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

Homogeneous system of equations ($\mathbf{b} = \mathbf{0}$):

$$\mathbf{A}\mathbf{x} = \mathbf{0}$$

Given a matrix \mathbf{A} of size $m \times n$ and a vector \mathbf{b} of size m :

- If $n < m$, the system is called **over-determined** and there is no solution.
- If $n > m$, the system is **under-determined** and the equations may be solved as far as possible.
- If $m = n$ and \mathbf{A} is non-singular, a direct solution can be obtained.

Linear System of Equations

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Linear System of Equations

↪ Solution Methods

Direct Methods: Examples

- Gaussian Elimination
- LU Factorization

Iterative Methods: Examples

- Jacobi Iteration
- Gauss-Seidel Iteration
- Successive Over-Relaxation (SOR)

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Linear System of Equations

↪ Direct Methods: Gaussian Elimination

Elementary row operations on **augmented matrix** $A|\mathbf{b}$ to get a simpler system $A'|\mathbf{b}'$:

$$A|\mathbf{b} = \left[\begin{array}{cccc|c} a_{11} & a_{12} & \cdots & a_{1n} & b_1 \\ a_{21} & a_{22} & \cdots & a_{2n} & b_2 \\ \vdots & \vdots & & \vdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} & b_n \end{array} \right] \implies A'|\mathbf{b}' = \left[\begin{array}{cccc|c} a'_{11} & a'_{12} & \cdots & a'_{1n} & b'_1 \\ 0 & a'_{22} & \cdots & a'_{2n} & b'_2 \\ \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & \cdots & a'_{nn} & b'_n \end{array} \right]$$

Equivalent linear system:

$$\left[\begin{array}{cccc} a'_{11} & a'_{12} & \cdots & a'_{1n} \\ 0 & a'_{22} & \cdots & a'_{2n} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & a'_{nn} \end{array} \right] \begin{Bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{Bmatrix} = \begin{Bmatrix} b'_1 \\ b'_2 \\ \vdots \\ b'_n \end{Bmatrix}$$

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Linear System of Equations

↪ Direct Methods: Gaussian Elimination

Solution for x_n from the n^{th} row as

$$x_n = \frac{b'_n}{a'_{nn}}$$

Remaining unknowns by back substitution:

$$x_i = \frac{1}{a'_{ii}} \left(b'_i - \sum_{j=i+1}^n a'_{ij} x_j \right)$$

Linear System of Equations

↪ Direct Methods: Gaussian Elimination

Solution for x_n from the n^{th} row as

$$x_n = \frac{b'_n}{a'_{nn}}$$

Remaining unknowns by back substitution:

$$x_i = \frac{1}{a'_{ii}} \left(b'_i - \sum_{j=i+1}^n a'_{ij} x_j \right)$$

Linear System of Equations

↪ Direct Methods: *LU* Factorization

Coefficient matrix *A* first decomposed into lower and upper triangular matrices:

$$A = LU$$

such that

$$L = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix} \quad U = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

Elements of *L* and *U* can be calculated from:

$$l_{ij} = \frac{1}{u_{ii}} \left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \right)$$
$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$

Linear System of Equations

↪ Direct Methods: LU Factorization

Coefficient matrix A first decomposed into lower and upper triangular matrices:

$$A = LU$$

such that

$$L = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix} \quad U = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

Elements of L and U can be calculated from:

$$l_{ij} = \frac{1}{u_{ii}} \left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \right)$$
$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$

Linear System of Equations

↪ Direct Methods: *LU* Factorization

Coefficient matrix \mathbf{A} first decomposed into lower and upper triangular matrices:

$$\mathbf{A} = \mathbf{LU}$$

such that

$$\mathbf{L} = \begin{bmatrix} l_{11} & 0 & \cdots & 0 \\ l_{21} & l_{22} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ l_{n1} & l_{n2} & \cdots & l_{nn} \end{bmatrix} \quad \mathbf{U} = \begin{bmatrix} u_{11} & u_{12} & \cdots & u_{1n} \\ 0 & u_{22} & \cdots & u_{2n} \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & u_{nn} \end{bmatrix}$$

Elements of \mathbf{L} and \mathbf{U} can be calculated from:

$$l_{ij} = \frac{1}{u_{ii}} \left(a_{ij} - \sum_{k=1}^{j-1} l_{ik} u_{kj} \right)$$
$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$

Linear System of Equations

↪ Direct Methods: *LU* Factorization

The linear system $\mathbf{Ax} = \mathbf{b}$ may now be written as

$$(\mathbf{LU})\mathbf{x} = \mathbf{b} \Rightarrow \mathbf{L}(\mathbf{Ux}) = \mathbf{b}$$

Two simpler systems to solve:

$$\mathbf{Ly} = \mathbf{b}$$

$$\mathbf{Ux} = \mathbf{y}$$

Solutions:

$$y_1 = \frac{b_1}{l_{11}} \quad y_i = \frac{1}{l_{ii}} \left(b_i - \sum_{j=1}^{i-1} l_{ij}y_j \right) \quad i = 2, \dots, n$$

$$x_n = \frac{y_n}{u_{nn}} \quad x_i = \frac{1}{u_{ii}} \left(y_i - \sum_{j=i+1}^n u_{ij}x_j \right) \quad i = n-1, \dots, 1$$

Linear System of Equations

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Linear System of Equations

↪ Iterative Methods: Gauss-Seidel Iteration

Coefficient matrix A is decomposed such that

$$A = L' + D + U'$$

Linear system $Ax = b$ now written as

$$(D + L')x = b - U'x$$

Solve for x on the LHS based on assumed/previous x on the RHS:

$$x^{(k+1)} = (D + L')^{-1} (b - U'x^{(k)})$$

Forward substitution expression of iteration procedure

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i+1}^n a_{ij}x_j^{(k)} \right)$$

Perform iteration until an error criterion is satisfied:

$$\|x^{(k+1)} - x^{(k)}\| \leq e$$

Linear System of Equations

↪ Iterative Methods: Gauss-Seidel Iteration

Coefficient matrix \mathbf{A} is decomposed such that

$$\mathbf{A} = \mathbf{L}' + \mathbf{D} + \mathbf{U}'$$

Linear system $\mathbf{A}\mathbf{x} = \mathbf{b}$ now written as

$$(\mathbf{D} + \mathbf{L}')\mathbf{x} = \mathbf{b} - \mathbf{U}'\mathbf{x}$$

Solve for \mathbf{x} on the LHS based on assumed/previous \mathbf{x} on the RHS:

$$\mathbf{x}^{(k+1)} = (\mathbf{D} + \mathbf{L}')^{-1} (\mathbf{b} - \mathbf{U}'\mathbf{x}^{(k)})$$

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Linear System of Equations

↪ Iterative Methods: Successive Over-Relaxation (SOR)

Coefficient matrix A is decomposed such that

$$A = L' + D + U'$$

Scalar factor ω is introduced to the linear system

$$\begin{aligned}\omega (L' + D + U') x &= \omega b \\ \Rightarrow (D + \omega L') x &= \omega b - [\omega U' + (\omega - 1)D] x\end{aligned}$$

Solve for x on the LHS based on assumed/previous x on the RHS:

$$x^{(k+1)} = (D + \omega L')^{-1} \left(\omega b - [\omega U' + (\omega - 1)D] x^{(k)} \right)$$

Forward substitution expression of iteration procedure

$$x_i^{(k+1)} = (1 - \omega)x_i^{(k)} + \frac{\omega}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i+1}^n a_{ij}x_j^{(k)} \right)$$

Perform iteration until an error criterion is satisfied:

$$\|x^{(k+1)} - x^{(k)}\| \leq e$$

Linear System of Equations

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Coefficient matrix \mathbf{A} is decomposed such that

$$\mathbf{A} = \mathbf{L}' + \mathbf{D} + \mathbf{U}'$$

Scalar factor ω is introduced to the linear system

$$\omega (\mathbf{L}' + \mathbf{D} + \mathbf{U}') \mathbf{x} = \omega \mathbf{b}$$

$$\Rightarrow (\mathbf{D} + \omega \mathbf{L}') \mathbf{x} = \omega \mathbf{b} - [\omega \mathbf{U}' + (\omega - 1) \mathbf{D}] \mathbf{x}$$

Solve for \mathbf{x} on the LHS based on assumed/previous \mathbf{x} on the RHS:

$$\mathbf{x}^{(k+1)} = (\mathbf{D} + \omega \mathbf{L}')^{-1} \left(\omega \mathbf{b} - [\omega \mathbf{U}' + (\omega - 1) \mathbf{D}] \mathbf{x}^{(k)} \right)$$

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