Mathematical Preliminaries

CENG6202: Advanced Computational Methods in Geotechnical Engineering

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Vectors

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

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

The *transpose* of vector $\boldsymbol{a}$:

$$\boldsymbol{a}^{\mathsf{T}} = \{a_1 \; a_2 \; \cdots \; a_n\}$$

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

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

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

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

The dot product can also be written as

$$\boldsymbol{a} \cdot \boldsymbol{b} = \boldsymbol{a}^{\intercal} \boldsymbol{b} = \{a_1 \; a_2 \; \cdots \; a_n\} \left\{ \begin{array}{c} b_1 \\ b_2 \\ \vdots \\ b_n \end{array} \right\} = \sum_{i=1}^{n} a_i b_i$$

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The dot product can also be written as

$$\boldsymbol{a} \cdot \boldsymbol{b} = \boldsymbol{a}^{\mathsf{T}} \boldsymbol{b} = \{a_1 \ a_2 \ \cdots \ a_n\} \left\{ \begin{array}{c} b_1 \\ b_2 \\ \vdots \\ b_n \end{array} \right\} = \sum_{i=1}^{n} a_i b_i$$

The product $\boldsymbol{a}\boldsymbol{b}^{\mathsf{T}}$, however, results in a matrix, i.e.

$$\boldsymbol{a}\boldsymbol{b}^{\mathsf{T}} = \left\{ \begin{matrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{matrix} \right\} \{b_1 \; b_2 \; \cdots \; b_n\} = \begin{bmatrix} a_1 b_1 & a_1 b_2 & \cdots & a_1 b_n \\ a_2 b_1 & a_2 b_2 & \cdots & a_2 b_n \\ \vdots & \vdots & & \vdots \\ a_n b_1 & a_n b_2 & \cdots & a_n b_n \end{bmatrix}$$

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

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

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

The elements of vector $\boldsymbol{c}$ are

$$\boldsymbol{c} = \left\{ \begin{array}{c} a_2 b_3 - a_3 b_2 \\ a_3 b_1 - a_1 b_3 \\ a_1 b_2 - a_2 b_1 \end{array} \right\}$$

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Matrices

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

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

The *transpose* of matrix $\boldsymbol{A}$:

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

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 $\boldsymbol{A}$:

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

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

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

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Addition, subtraction, scalar multiplication and transposition:

1. $\boldsymbol{A} \pm \boldsymbol{B} = \boldsymbol{B} \pm \boldsymbol{A}$
2. $(\boldsymbol{A} \pm \boldsymbol{B})^\mathsf{T} = \boldsymbol{A}^\mathsf{T} \pm \boldsymbol{B}^\mathsf{T}$
3. $(\boldsymbol{A}^\mathsf{T})^\mathsf{T} = \boldsymbol{A}$
4. $(s\boldsymbol{A})^\mathsf{T} = s(\boldsymbol{A}^\mathsf{T})$

Addition, subtraction, scalar multiplication and transposition:

1. $\boldsymbol{A} \pm \boldsymbol{B} = \boldsymbol{B} \pm \boldsymbol{A}$
2. $(\boldsymbol{A} \pm \boldsymbol{B})^{\intercal} = \boldsymbol{A}^{\intercal} \pm \boldsymbol{B}^{\intercal}$
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1. $\boldsymbol{A} \pm \boldsymbol{B} = \boldsymbol{B} \pm \boldsymbol{A}$
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Matrix-Vector multiplication:

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

Vector-Matrix multiplication:

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

$$= \{y_1 a_{11} + \cdots + y_n a_{n1} \quad \cdots \quad y_1 a_{1m} + \cdots + y_n a_{nm}\}$$

Matrix-Vector multiplication:

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

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$$= \{y_1a_{11} + \cdots + y_na_{n1} \quad \cdots \quad y_1a_{1m} + \cdots + y_na_{nm}\}$$

Matrix-Vector multiplication:

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

Vector-Matrix multiplication:

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

$$= \{y_1 a_{11} + \cdots + y_n a_{n1} \quad \cdots \quad y_1 a_{1m} + \cdots + y_n a_{nm}\}$$

Matrix-Vector multiplication:

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

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Vector-Matrix multiplication:

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

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$$= \{y_1 a_{11} + \cdots + y_n a_{n1} \quad \cdots \quad y_1 a_{1m} + \cdots + y_n a_{nm}\}$$

Bilinear form:

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

Quadratic form:

$$\boldsymbol{x}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{x} \rightarrow \text{Scalar}$$

A matrix $\boldsymbol{A}$ is called positive-definite if

$$\boldsymbol{z}^{\mathsf{T}}\boldsymbol{A}\boldsymbol{z} > 0 \qquad \forall \boldsymbol{z} \neq 0$$

Matrix-Matrix multiplication:

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

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

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

Some properties of inverse:

1. $(A^{-1})^{-1} = A$
2. $(A^{\mathsf{T}})^{-1} = (A^{-1})^{\mathsf{T}}$
3. $(AB)^{-1} = B^{-1}A^{-1}$

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

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

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

Equivalent linear system:

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

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

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

Remaining unknowns by back substitution:

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

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

$$\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}$$

such that

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

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

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

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$

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

$$\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}$$

such that

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

Elements of L and U can be calculated from:

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

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$

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

$$\boldsymbol{A} = \boldsymbol{LU}$$

such that

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

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

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

$$u_{ij} = a_{ij} - \sum_{k=1}^{i-1} l_{ik} u_{kj}$$

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

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

Two simpler systems to solve:

$$\boldsymbol{Ly} = \boldsymbol{b}$$
$$\boldsymbol{Ux} = \boldsymbol{y}$$

Solutions:

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

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

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Two simpler systems to solve:

$$\begin{aligned} \boldsymbol{Ly} &= \boldsymbol{b} \\ \boldsymbol{Ux} &= \boldsymbol{y} \end{aligned}$$

Solutions:

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

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Coefficient matrix $\boldsymbol{A}$ is decomposed such that

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

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

$$\left(\boldsymbol{D} + \boldsymbol{L}'\right)\boldsymbol{x} = \boldsymbol{b} - \boldsymbol{U}'\boldsymbol{x}$$

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

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

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:

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

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$$\left(\boldsymbol{D} + \boldsymbol{L}'\right)\boldsymbol{x} = \boldsymbol{b} - \boldsymbol{U}'\boldsymbol{x}$$

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

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

Forward substitution expression of iteration procedure

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

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Scalar factor ω is introduced to the linear system

$$\omega \left(\boldsymbol{L}' + \boldsymbol{D} + \boldsymbol{U}' \right) \boldsymbol{x} = \omega \boldsymbol{b}$$

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

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

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

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