Lecture 03 - Solving systems of linear equations

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Solving Systems of Linear Equations

This lecture aims at solving the following systems of linear equations

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1n}x_n = b_1 \\ a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \cdots + a_{2n}x_n = b_2 \\ a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \cdots + a_{3n}x_n = b_3 \\ \vdots \\ a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nn}x_n = b_n \end{cases}$$

It is written as

$$\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}, \tag{1}$$

where $\boldsymbol{A} \in \mathbb{R}^{n\times n}$, $\boldsymbol{x} \in \mathbb{R}^n$, and $\boldsymbol{b} \in \mathbb{R}^n$.

Matrix Algebra

Given $\boldsymbol{A} = [\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n] \in \mathbb{R}^{n \times n}$

1. $\boldsymbol{a}_i \in \mathbb{R}^n$ a *column vector*.
2. *Transpose* of $\boldsymbol{A}$ is denoted by $\boldsymbol{A}^\top$ with each entry $\left(\boldsymbol{A}^\top\right)_{ij} = a_{ji}$.
3. We say $\boldsymbol{A}$ is *symmetric* if $\boldsymbol{A}^\top = \boldsymbol{A}$.
4. We say $\boldsymbol{I} = \boldsymbol{A}$ is an *identity matrix* $(\boldsymbol{A})_{ij} = 1$ if $i = j$; 0 otherwise.
5. We say $\boldsymbol{A}$ is positive definite if $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} > 0, \forall \boldsymbol{x} \in \mathbb{R}^n \backslash \{0\}$.
6. We say $\boldsymbol{A}$ is diagonally dominant matrix, if $|a_{ii}| > \sum_{j \neq i}^{n} |a_{ij}|, i = 1, 2, \ldots, n$.
7. We say λ is an eigenvalue of $\boldsymbol{A}$ if $\boldsymbol{A}\boldsymbol{x} = \lambda \boldsymbol{x}$ given $\boldsymbol{x} \neq 0$ and we call $\boldsymbol{x}$ is an eigenvector.

Triangle matrix

A matrix of the form

$$\boldsymbol{L} = \begin{bmatrix} \ell_{1,1} & & & & 0 \\ \ell_{2,1} & \ell_{2,2} & & & \\ \ell_{3,1} & \ell_{3,2} & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ \ell_{n,1} & \ell_{n,2} & \dots & \ell_{n,n-1} & \ell_{n,n} \end{bmatrix}$$

is called a **lower triangular matrix**.

$$\boldsymbol{U} = \begin{bmatrix} u_{1,1} & u_{1,2} & u_{1,3} & \dots & u_{1,n} \\ & u_{2,2} & u_{2,3} & \dots & u_{2,n} \\ & & \ddots & \ddots & \vdots \\ & & & \ddots & u_{n-1,n} \\ 0 & & & & u_{n,n} \end{bmatrix}$$

is called an **upper triangular matrix**.

Properties of triangle matrix

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- The transpose of an upper triangular matrix is a lower triangular matrix and vice versa.

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Forward Substitution

The matrix equation $\boldsymbol{L}\mathrm{x} = \mathrm{b}$ can be written as a system of linear equations

$$\begin{aligned} \ell_{1,1}x_1 \quad & = b_1 \\ \ell_{2,1}x_1 + \ell_{2,2}x_2 \quad & = b_2 \\ \vdots \quad \vdots \quad \ddots \quad \vdots \\ \ell_{n,1}x_1 + \ell_{n,2}x_2 + \cdots + \ell_{n,n}x_n & = b_n \end{aligned}$$

The solution can be written as

$$\begin{aligned} x_1 &= \frac{b_1}{\ell_{1,1}}, \\ x_2 &= \frac{b_2 - \ell_{2,1}x_1}{\ell_{2,2}}, \\ &\vdots \\ x_n &= \frac{b_n - \sum_{i=1}^{n-1} \ell_{n,i}x_i}{\ell_{n,n}}. \end{aligned}$$

Inverse of matrix

Idea: The n columns of a nonsingular $n \times n$ matrix $\boldsymbol{A}$ form a basis for the whole space $\mathbb{R}^n$. Therefore, we can uniquely express any vector as a linear combination of them. In particular, the canonical unit vector with 1 in the j th entry and zeros elsewhere, written $\boldsymbol{e}_j$, can be expanded:

$$\boldsymbol{e}_j = \sum_{i=1}^{n} z_{ij} \boldsymbol{a}_i, \qquad j = 1, 2, \ldots, n$$

Let $\boldsymbol{Z}$ be the matrix with entries z_{ij}, and let $\boldsymbol{z}_j$ denote the j th column of $\boldsymbol{Z}$. Then the above can be written $\boldsymbol{e}_j = \boldsymbol{A}\boldsymbol{z}_j$. It can be written concisely as

$$\left[\begin{array}{c|c|c} \boldsymbol{e}_1 & \cdots & \boldsymbol{e}_n \end{array} \right] = \boldsymbol{I} = \boldsymbol{A}\boldsymbol{Z}, \qquad (2)$$

where $\boldsymbol{I}$ is the $n \times n$ matrix known as the identity. The matrix $\boldsymbol{Z}$ is the inverse of $\boldsymbol{A}$. Any square *nonsingular* matrix $\boldsymbol{A}$ has a unique inverse, written $\boldsymbol{A}^{-1}$, that satisfies $\boldsymbol{A}\boldsymbol{A}^{-1} = \boldsymbol{A}^{-1}\boldsymbol{A} = \boldsymbol{I}$.

Inverse of matrix

Theorem 1.1 (Equivalent properties of inverse matrix)

For $\boldsymbol{A} \in \mathbb{R}^{n\times n}$, the following conditions are equivalent:

1. *$\boldsymbol{A}$ has an inverse $\boldsymbol{A}^{-1}$*
2. $\text{rank}(\boldsymbol{A}) = n$
3. *range* $(\boldsymbol{A}) = \mathbb{R}^n$
4. $\text{null}(\boldsymbol{A}) = \{0\}$
5. *0 is not an eigenvalue of $\boldsymbol{A}$*
6. *0 is not a singular value of $\boldsymbol{A}$*
7. $\det(\boldsymbol{A}) \neq 0$
8. *The equation $\boldsymbol{Ax} = 0$ implies $\boldsymbol{x} = 0$*
9. *For each $\boldsymbol{b} \in \mathbb{R}^n$, there is exactly one $\boldsymbol{x} \in \mathbb{R}^n$ such that $\boldsymbol{Ax} = \boldsymbol{b}$*

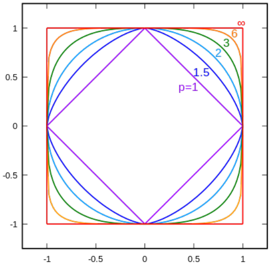
Norms in vector space

To measure vectors, we assign vectors nonnegative numbers.
When $p \geq 1$, we define p-norm of vector $\boldsymbol{x} \in \mathbb{R}^n$ as

$$\|\boldsymbol{x}\|_p \triangleq \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p} \tag{3}$$

Some useful properties:

- $\|\boldsymbol{x}\|_2 \leq \|\boldsymbol{x}\|_1 \leq \sqrt{n}\|\boldsymbol{x}\|_2$
- $\|\boldsymbol{x}\|_\infty \leq \|\boldsymbol{x}\|_2 \leq \sqrt{n}\|\boldsymbol{x}\|_\infty$
- $\|\boldsymbol{x}\|_\infty \leq \|\boldsymbol{x}\|_1 \leq n\|\boldsymbol{x}\|_\infty$
- Cauchy-Schwarz inequality: $|\langle \boldsymbol{x}, \boldsymbol{y} \rangle| \leq \|\boldsymbol{x}\|_2 \cdot \|\boldsymbol{y}\|_2$
- Triangle Inequality $\|\boldsymbol{x}+\boldsymbol{y}\|_p \leq \|\boldsymbol{x}\|_p + \|\boldsymbol{y}\|_p$



The values of coordinates (x_1, x_2), for which the p-norm $\|\boldsymbol{x}\|_p$ takes the value 1, i.e. $\|\boldsymbol{x}\|_p = 1$

Matrix Norm

Definition 1.2 (Matrix Norm)

Consider a vector space of matrices with m rows and n columns. A matrix norm is a function $\|\cdot\| : \mathbb{K}^{m\times n} \to \mathbb{R}$ that must satisfy the following properties: For all scalars $\alpha \in \mathbb{K}$ and matrices $\boldsymbol{A}, \boldsymbol{B} \in \mathbb{K}^{m\times n}$,

- Nonnegativity: $\|\boldsymbol{A}\| \geq 0$, unique zero: $\|\boldsymbol{A}\| = 0 \Leftrightarrow \boldsymbol{A} = 0_{m\times n}$
- Absolutely homogeneous: $\|\alpha \boldsymbol{A}\| = |\alpha| \cdot \|\boldsymbol{A}\|$
- Triangle inequality: $\|\boldsymbol{A} + \boldsymbol{B}\| \leq \|\boldsymbol{A}\| + \|\boldsymbol{B}\|$

- Forbenius norm: $\|\boldsymbol{A}\|_F := \left(\sum_{i,j=1}^{n} |a_{ij}|^2\right)^{1/2}$
- Operator norm: $\|\boldsymbol{A}\|_p = \sup_{\boldsymbol{x}\neq 0} \frac{\|\boldsymbol{A}\boldsymbol{x}\|_p}{\|\boldsymbol{x}\|_p}$, where $1 \leq p \leq \infty$

Matrix properties

Inverse of Simple Matrix

Given an invertible matrix $\boldsymbol{A} \in \mathbb{R}^{2\times 2}$, we have

$$\boldsymbol{A} = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \boldsymbol{A}^{-1} = \frac{1}{\det \boldsymbol{A}} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}.$$

Matrix Condition number

$$\begin{aligned}
\max_{\boldsymbol{e},\boldsymbol{b}\neq 0} \left\{ \frac{\left\|\boldsymbol{A}^{-1}\boldsymbol{e}\right\|}{\|\boldsymbol{e}\|} \frac{\|\boldsymbol{b}\|}{\|\boldsymbol{A}^{-1}\boldsymbol{b}\|} \right\} &= \max_{\boldsymbol{e}\neq 0} \left\{ \frac{\left\|\boldsymbol{A}^{-1}\boldsymbol{e}\right\|}{\|\boldsymbol{e}\|} \right\} \max_{\boldsymbol{b}\neq 0} \left\{ \frac{\|\boldsymbol{b}\|}{\|\boldsymbol{A}^{-1}\boldsymbol{b}\|} \right\} \\
&= \max_{\boldsymbol{e}\neq 0} \left\{ \frac{\left\|\boldsymbol{A}^{-1}\boldsymbol{e}\right\|}{\|\boldsymbol{e}\|} \right\} \max_{\boldsymbol{x}\neq 0} \left\{ \frac{\|\boldsymbol{A}\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \right\} \\
&= \left\|\boldsymbol{A}^{-1}\right\| \cdot \|\boldsymbol{A}\|.
\end{aligned}$$

Eigenvalues of symmetric matrices

Definition 1.3 (Symmetric matrix)

Given any $\boldsymbol{A} \in \mathbb{R}^{n \times n}$, if $\boldsymbol{A}^\top = \boldsymbol{A}$, then we call $\boldsymbol{A}$ is a symmetric matrix.

Definition 1.4 (Orthonormal)

A set of vectors S is orthonormal if the elements of the set are unit vectors that are pairwise orthogonal. Let $S = \{\boldsymbol{u}, \boldsymbol{v}\}$, then $\|\boldsymbol{u}\| = 1, \|\boldsymbol{v}\| = 1$ and $\boldsymbol{u}^\top \boldsymbol{v} = 0$.

Theorem 1.5 (Real eigenvalues of $\boldsymbol{A}$)

Assume that $\boldsymbol{A} \in \mathbb{R}^{n \times n}$ is symmetric with real entries. Then the eigenvalues are real numbers, and the set of unit eigenvectors of $\boldsymbol{A}$ is an orthonormal set $S = \{\boldsymbol{w}_1, \ldots, \boldsymbol{w}_n\}$ that forms a basis of $\mathbb{R}^n$.

Symmetric positive-definite matrices

Definition 1.6 (Symmetric Positive-Definite (SPD))

The matrix $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ if $\boldsymbol{A}^\top = \boldsymbol{A}$. The matrix $\boldsymbol{A}$ is positive-definite if $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} > 0$ for all vectors $\boldsymbol{x} \neq 0$.

Example:

- Show that $\boldsymbol{A} = \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix}$ is SPD: $\boldsymbol{A}$ is symmetric as $\boldsymbol{A}^\top = \boldsymbol{A}$ and applies definition

$$\begin{aligned} \boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} &= \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 2 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \\ &= 2x_1^2 + 4x_1x_2 + 5x_2^2 = 2(x_1 + x_2)^2 + 3x_2^2. \end{aligned}$$

- $\boldsymbol{A} = \begin{bmatrix} 2 & 4 \\ 4 & 5 \end{bmatrix}$ is not SPD. One can show that $\boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} = 2(x_1 + 2x_2)^2 - 3x_2^2$ with $x_1 = -2$ and $x_2 = 1$.

SPD matrices

Theorem 1.7

If $\boldsymbol{A} \in \mathbb{R}^{n\times}$ is a symmetric matrix, then $\boldsymbol{A}$ is positive-definite if and only if all of its eigenvalues are positive.

SPD matrices

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Proof.

Notice that if $\boldsymbol{A}$ is positive-definite and $\boldsymbol{A}\boldsymbol{v} = \lambda \boldsymbol{v}$ for a nonzero vector $\boldsymbol{v}$, then $0 < \boldsymbol{v}^\top \boldsymbol{A}\boldsymbol{v} = \boldsymbol{v}^\top(\lambda \boldsymbol{v}) = \lambda \|\boldsymbol{v}\|_2^2$. Hence, $\lambda > 0$.
On the other hand, if all eigenvalues of $\boldsymbol{A}$ are positive, then write any nonzero $\boldsymbol{x} = c_1 \boldsymbol{v}_1 + \ldots + c_n \boldsymbol{v}_n$ where each $\boldsymbol{v}_i$ are orthonormal unit vectors and not all c_i are zero. Then, we have

$$\begin{aligned} \boldsymbol{x}^\top \boldsymbol{A}\boldsymbol{x} &= (c_1 \boldsymbol{v}_1 + \cdots + c_n \boldsymbol{v}_n)^\top (c_1 \lambda_1 \boldsymbol{v}_1 + \cdots + c_n \lambda_n \boldsymbol{v}_n) \\ &= \lambda_1 \|\boldsymbol{c}_1\|_2^2 + \cdots + \lambda_n \|\boldsymbol{c}_n\|_2^2 > 0. \end{aligned}$$

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Gaussian Elimination

The Naive Gaussian Elimination

- Add or subtract a multiple of one equation from another
- Multiply an equation by a nonzero constant

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \dots & a_{1n} & b_1 \\ a_{21} & a_{22} & \dots & a_{2n} & b_2 \end{array}\right]$$

Subtract $\frac{a_{21}}{a_{11}}$ times row 1 from row 2, we have

$$\left[\begin{array}{cccc|c} a_{11} & a_{12} & \dots & a_{1n} & b_1 \\ 0 & a_{22} - \frac{a_{21}}{a_{11}} a_{12} & \dots & a_{2n} - \frac{a_{21}}{a_{11}} a_{1n} & b_2 - \frac{a_{21}}{a_{11}} b_1 \end{array}\right]$$

Repeat the above procedure until we find $\boldsymbol{U}$

Gaussian Elimination: LU Factorization

The idea of transforming $\boldsymbol{A}$ into an upper triangular $\boldsymbol{U}$ by introducing zeros below the diagonal by subtracting multiples of each row from subsequent rows. This process is equivalent to multiplying $\boldsymbol{A}$ by a sequence of lower triangular $\boldsymbol{L}_k$ on the left:

$$\underbrace{\boldsymbol{L}_{n-1} \cdots \boldsymbol{L}_2 \boldsymbol{L}_1}_{\boldsymbol{L}^{-1}} \boldsymbol{A} = \boldsymbol{U}.$$

Setting $\boldsymbol{L} = \boldsymbol{L}_1^{-1} \boldsymbol{L}_2^{-1} \cdots \boldsymbol{L}_{n-1}^{-1}$ gives $\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}$. Thus we obtain

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

- $\boldsymbol{U}$ is upper triangular
- $\boldsymbol{L}$ is unit lower triangular (diagonals are all ones)

LU Factorization: An example

Let us consider $\boldsymbol{A} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$

First step of Gaussian elimination

$$\boldsymbol{L}_1\boldsymbol{A} = \begin{bmatrix} 1 & & & \\ -2 & 1 & & \\ -4 & & 1 & \\ -3 & & & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & 3 & 5 & 5 \\ & 4 & 6 & 8 \end{bmatrix}$$

The second step

$$\boldsymbol{L}_2\boldsymbol{L}_1\boldsymbol{A} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & -3 & 1 & \\ & -4 & & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & 3 & 5 & 5 \\ & 4 & 6 & 8 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & 2 & 4 \end{bmatrix}$$

LU Factorization: An example (continued)

$$L_3 L_2 L_1 A = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & 2 & 4 \end{bmatrix} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & & 2 \end{bmatrix} = U$$

Compute the product $L = L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1}$.

- L_i^{-1} is just L_i itself, but with each entry below the diagonal negated
- $L_1^{-1} L_2^{-1} \cdots L_{n-1}^{-1}$ is just the unit lower-triangular matrix with the nonzero subdiagonal entries of L_i^{-1} inserted in the appropriate places.

$$\underbrace{\begin{bmatrix} 1 & & & \\ -2 & 1 & & \\ -4 & & 1 & \\ -3 & & & 1 \end{bmatrix}^{-1}}_{L_1^{-1}} = \begin{bmatrix} 1 & & & \\ 2 & 1 & & \\ 4 & & 1 & \\ 3 & & & 1 \end{bmatrix}, \quad \underbrace{\begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} 1 & & & \\ 2 & 1 & & \\ 4 & 3 & 1 & \\ 3 & 4 & 1 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 2 & 1 & 1 & 0 \\ & 1 & 1 & 1 \\ & & 2 & 2 \\ & & & 2 \end{bmatrix}}_{U}$$

Naive Gaussian Elimination

Algorithm 1 Naive Gaussian Elimination

$\boldsymbol{U} = \boldsymbol{A}, \boldsymbol{L} = \boldsymbol{I}$
for $k = 1$ to $n - 1$ **do**
    for $j = k + 1$ to n **do**
        $\ell_{jk} = u_{jk} / u_{kk}$
        $\boldsymbol{u}_{j,k:n} = \boldsymbol{u}_{j,k:n} - \ell_{jk} \boldsymbol{u}_{k,k:n}$
    end for
end for

- **Memory usage**
  To minimize memory use on the computer, both $\boldsymbol{L}$ and $\boldsymbol{U}$ can be written into the same array as $\boldsymbol{A}$.
- **Time complexity**

$$\sum_{k=1}^{n-1} \sum_{j=k+1}^{n} (n - k + 1) \sim \frac{2}{3} n^3 \text{ flops.}$$

Instability of Naive Guassian Elmination

Consider $\boldsymbol{A} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix}$.

- $\boldsymbol{A}$ has full rank with $\kappa(A) = (3+\sqrt{5})/2 \approx 2.618$ in the $\ell_2 - \textit{norm}$.
- We cannot do Gaussian Elimination without swapping.

Consider $\boldsymbol{A} = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 1 \end{bmatrix}$.

- 10^{20} times the first row is subtracted from the second row:

$$\boldsymbol{L} = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix}, \quad \boldsymbol{U} = \begin{bmatrix} 10^{-20} & 1 \\ 0 & 1 - 10^{20} \end{bmatrix}$$

- Suppose $\epsilon_{\text{mach}} \approx 10^{-16}$. The number $1 - 10^{20}$ will not be represented exactly; it will be rounded to the nearest floating point number. Suppose that this is exactly -10^{20}.

Instability of Naive Guassian Elmination

$$\tilde{\boldsymbol{L}} = \begin{bmatrix} 1 & 0 \\ 10^{20} & 1 \end{bmatrix}, \quad \tilde{\boldsymbol{U}} = \begin{bmatrix} 10^{-20} & 1 \\ 0 & -10^{20} \end{bmatrix} \Rightarrow \tilde{\boldsymbol{L}}\tilde{\boldsymbol{U}} = \begin{bmatrix} 10^{-20} & 1 \\ 1 & 0 \end{bmatrix}$$

- The above example gives $\boldsymbol{A} \neq \tilde{\boldsymbol{L}}\tilde{\boldsymbol{U}}$.
- The error could be large when we solve $\boldsymbol{Ax} = \boldsymbol{b}$. For example, with $\boldsymbol{b} = [1, 0]^\top$ we get $\tilde{\boldsymbol{x}} = [0, 1]^\top$, whereas the correct solution is $\boldsymbol{x} \approx [-1, 1]^\top$.

To summarize, we know

- For certain matrices, Naive Gaussian Elimination fails entirely because it attempts division by zero.
- Gaussian elimination, as presented so far, is unstable for solving general linear systems (from backward substitution)
- It is also unstable at forward substitution (image that x_{kk} is too small)

Pivoting

Pivot At step k of Gaussian elimination, multiples of row k are subtracted from rows $k+1, \dots, n$ of the working matrix $\boldsymbol{X}$ in order to introduce zeros in entry k of these rows. In this operation, row k, column k, and especially the entry x_{kk} play special roles. We call x_{kk} the **pivot**. From every entry in the submatrix $\boldsymbol{X}_{k+1:n,k:n}$ is subtracted the product of a number in row k and a number in column k, divided by x_{kk}

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ & x_{kk} & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix} \Longrightarrow \begin{bmatrix} \times & \times & \times & \times & \times \\ & x_{kk} & \times & \times & \times \\ & 0 & \times & \times & \times \\ & 0 & \times & \times & \times \\ & 0 & \times & \times & \times \end{bmatrix}$$

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- Why the kth row and column must be chosen?
- We are free to choose any entry of $\boldsymbol{X}_{k:n,k:n}$ as the pivot, as long as it is nonzero.

Pivoting Strategies

- **Complete pivoting** If every entry of $X_{k:n,k:n}$ is considered as a possible pivot at step k, there are $O\left((n-k)^2\right)$ entries to be examined to determine the largest. Summing over n steps, the total cost of selecting pivots becomes $O\left(n^3\right)$ operations, adding significantly to the cost of Gaussian elimination.

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- **Partial pivoting** Only rows are interchanged. The pivot at each step is chosen as the largest of the $n-k+1$ sub diagonal entries in column k, incurring a total cost of only $O(n-k)$ operations for selecting the pivot at each step, $O\left(n^2\right)$ operations overall.

$$\begin{bmatrix} \times & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & x_{ik} & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix} \xrightarrow{\boldsymbol{P_1}} \begin{bmatrix} \times & \times & \times & \times & \times \\ & x_{ik} & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \\ & \times & \times & \times & \times \end{bmatrix} \xrightarrow{\boldsymbol{L_1}} \begin{bmatrix} \times & \times & \times & \times & \times \\ & x_{ik} & \times & \times & \times \\ & 0 & \times & \times & \times \\ & 0 & \times & \times & \times \\ & 0 & \times & \times & \times \end{bmatrix}$$

After $n-1$ steps, $\boldsymbol{A}$ becomes an upper-triangular matrix $\boldsymbol{U}$:

$$\boldsymbol{L}_{n-1}\boldsymbol{P}_{n-1}\cdots\boldsymbol{L}_2\boldsymbol{P}_2\boldsymbol{L}_1\boldsymbol{P}_1\boldsymbol{A}=\boldsymbol{U}$$

Partial pivoting: Example

Consider $\boldsymbol{A} = \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix}$

Interchange the first and third rows (left-multiplication by $\boldsymbol{P}_1$):

$$\begin{bmatrix} & & 1 & \\ & 1 & & \\ 1 & & & \\ & & & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ 4 & 3 & 3 & 1 \\ 2 & 1 & 1 & 0 \\ 6 & 7 & 9 & 8 \end{bmatrix}$$

The elimination step now looks like this (left-multiplication by $\boldsymbol{L}_1$)

$$\begin{bmatrix} 1 & & & \\ -1/2 & 1 & & \\ -1/4 & & 1 & \\ -3/4 & & & 1 \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ 4 & 3 & 3 & 1 \\ 2 & 1 & 1 & 0 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & -1/2 & -3/2 & -3/2 \\ & -3/4 & -5/4 & -5/4 \\ & 7/4 & 9/4 & 17/4 \end{bmatrix}$$

Partial pivoting: Example (Continued)

The second and fourth rows are interchanged (multiplication by $\boldsymbol{P}_2$)

$$\begin{bmatrix} 1 & & & \\ & & & 1 \\ & & 1 & \\ & 1 & & \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ & -1/2 & -3/2 & -3/2 \\ & -3/4 & -5/4 & -5/4 \\ & 7/4 & 9/4 & 17/4 \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & 7/4 & 9/4 & 17/4 \\ & -3/4 & -5/4 & -5/4 \\ & -1/2 & -3/2 & -3/2 \end{bmatrix}$$

Second elimination step (multiplication by $\boldsymbol{L}_2$)

$$\begin{bmatrix} 1 & & & \\ & 1 & & \\ & \frac{3}{7} & 1 & \\ & \frac{2}{7} & & 1 \end{bmatrix} \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & -\frac{3}{4} & -\frac{5}{4} & -\frac{5}{4} \\ & -\frac{1}{2} & -\frac{3}{2} & -\frac{3}{2} \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{2}{7} & \frac{4}{7} \\ & & -\frac{6}{7} & -\frac{2}{7} \end{bmatrix}$$

Partial pivoting: Example (Continued)

After $\boldsymbol{P}_3$

$$
\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & & 1 \\ & & 1 & \end{bmatrix}
\begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{2}{7} & \frac{4}{7} \\ & & -\frac{6}{7} & -\frac{2}{7} \end{bmatrix}
=
\begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{6}{7} & -\frac{2}{7} \\ & & -\frac{2}{7} & \frac{4}{7} \end{bmatrix}
$$

After $\boldsymbol{L}_3$

$$
\begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & -\frac{1}{3} & 1 \end{bmatrix}
\begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{6}{7} & -\frac{2}{7} \\ & & -\frac{2}{7} & \frac{4}{7} \end{bmatrix}
=
\begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{6}{7} & -\frac{2}{7} \\ & & & \frac{2}{3} \end{bmatrix}
$$

Partial pivoting: Example (Continued)

The final matrix $\boldsymbol{PA} = \boldsymbol{LU}$

$$\begin{bmatrix} & & 1 & \\ & & & 1 \\ & 1 & & \\ 1 & & & \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 & 0 \\ 4 & 3 & 3 & 1 \\ 8 & 7 & 9 & 5 \\ 6 & 7 & 9 & 8 \end{bmatrix} = \begin{bmatrix} 1 & & & \\ \frac{3}{4} & 1 & & \\ \frac{1}{2} & -\frac{2}{7} & 1 & \\ \frac{1}{4} & -\frac{3}{7} & \frac{1}{3} & 1 \end{bmatrix} = \begin{bmatrix} 8 & 7 & 9 & 5 \\ & \frac{7}{4} & \frac{9}{4} & \frac{17}{4} \\ & & -\frac{6}{7} & -\frac{2}{7} \\ & & & \frac{2}{3} \end{bmatrix}$$

- All the subdiagonal entries of $\boldsymbol{L}$ are ≤ 1 in magnitude, a consequence of the property $|x_{kk}| = \max_j |x_{jk}|$ by this partial pivoting.
- $\boldsymbol{L}_3\boldsymbol{P}_3\boldsymbol{L}_2\boldsymbol{P}_2\boldsymbol{L}_1\boldsymbol{P}_1\boldsymbol{A} = \boldsymbol{U}$
- It is equivalent to $\boldsymbol{PA} = \boldsymbol{LU}$, why ?

Gaussian Elimination with Partial Pivoting

Algorithm 2 Gaussian Elimination with Partial Pivoting

$\boldsymbol{U} = \boldsymbol{A}, \boldsymbol{L} = \boldsymbol{I}, \boldsymbol{P} = \boldsymbol{I}$
for $k = 1$ to $n - 1$ **do**
  Select $i \geq k$ to maximize $|u_{ik}|$
  Interchange two rows $u_{k,k:n} \leftrightarrow u_{i,k:n}$
  $\ell_{k,1:k-1} \leftrightarrow \ell_{i,1:k-1}$
  $p_{k,:} \leftrightarrow p_{i,:}$
  for $j = k+1, k+2, \ldots, n$ **do**
    $\ell_{jk} = u_{jk}/u_{kk}$
    $u_{j,k:n} = u_{j,k:n} - \ell_{jk} u_{k,k:n}$
  end for
end for

- **Memory usage** One array as $\boldsymbol{A}$.
- **Time complexity** $\sum_{k=1}^{n-1} \sum_{j=k+1}^{n} (n - k + 1) \sim \frac{2}{3} n^3$ flops.

Cholesky Factorization

Theorem 2.1 (Cholesky Theorem on $\boldsymbol{L}\boldsymbol{L}^\top$-Factorization)

If $\boldsymbol{A}$ is a real, symmetric, and positive definite matrix, then it has a unique factorization, $\mathbf{A} = \mathbf{L}\mathbf{L}^\top$, in which $\mathbf{L}$ is lower triangular with a positive diagonal.

- The complexity of computing $\boldsymbol{L}$ is $\sim n^3/3$ flops
- $\boldsymbol{L}$ is called the *Cholesky factor* of $\boldsymbol{A}$
- It can be interpreted as the "square root" of a p.d. matrix
- It gives a practical method for testing positive definiteness

Intuition of iteration methods

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

where $\boldsymbol{A} \in \mathbb{R}^{n\times n}, \boldsymbol{x} \in \mathbb{R}^n, \boldsymbol{b} \in \mathbb{R}^n$. Suppose $\boldsymbol{x}^0$ be the initial guess of $\boldsymbol{x}^*$. We can measure the estimation error:

$$\boldsymbol{e}^0 \triangleq \boldsymbol{A}^{-1}\boldsymbol{b} - \boldsymbol{x}^0,$$

then the solution can be expressed as

$$\boldsymbol{x}^* = \boldsymbol{x}^0 + \boldsymbol{e}^0.$$

$\boldsymbol{e}^0$ is unknown (hard as the original). Fortunately, we know the residual:

$$\boldsymbol{r}^0 \triangleq \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^0.$$

Notice that $\boldsymbol{A}\boldsymbol{x}^* = \boldsymbol{A}\boldsymbol{x}^0 + \boldsymbol{A}\boldsymbol{e}^0 \Leftrightarrow \boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}^0 + \boldsymbol{A}\boldsymbol{e}^0$. Hence $\boldsymbol{r}^0 = \boldsymbol{A}\boldsymbol{e}^0$.

Intuition of iteration methods

Intuition: We already know that $\boldsymbol{r}^0 = \boldsymbol{A}\boldsymbol{e}^0$. If there is an $\boldsymbol{M}$ such that $\boldsymbol{M}^{-1}\boldsymbol{A}\boldsymbol{e}^0 \approx \boldsymbol{e}^0$, i.e., $\boldsymbol{M}^{-1}\boldsymbol{A} \approx \boldsymbol{I}$, then we can use $\boldsymbol{M}^{-1}\boldsymbol{r}^0$ to approximate $\boldsymbol{e}^0$. Let

$$\boldsymbol{M}\boldsymbol{z}^0 = \boldsymbol{r}^0 \Leftrightarrow \boldsymbol{z}^0 = \boldsymbol{M}^{-1}\boldsymbol{r}^0 \approx \boldsymbol{e}^0. \tag{4}$$

$\boldsymbol{M}^{-1}$ must be cheap!

We hope $\boldsymbol{x}^1 = \boldsymbol{x}^0 + \boldsymbol{z}^0$ is getting closer to $\boldsymbol{x}^*$. To summarize:

1. **Step 1**: Compute residual: $\boldsymbol{r}^0 = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^0$
2. **Step 2**: Solve $\boldsymbol{M}\boldsymbol{z}^0 = \boldsymbol{r}^0$ and use $\boldsymbol{M}^{-1}\boldsymbol{r}^0$ to approximate $\boldsymbol{e}^0$
3. **Step 3**: Get a better solution: $\boldsymbol{x}^1 = \boldsymbol{x}^0 + \boldsymbol{z}^0$

Repeat the above steps until the stop condition is satisfied.

A general idea of iteration methods

We summarize the idea and write it as a linear iteration:

Algorithm 3 Iteration($\boldsymbol{x}^0, \boldsymbol{A}, \boldsymbol{b}, \boldsymbol{M}$)

$\boldsymbol{x}^0, \boldsymbol{A}, \boldsymbol{b}, \boldsymbol{M}$ be initial guesses
for $t = 0, 1, \ldots,$ **do**
    Com. Residual $\boldsymbol{r}^t = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^t$
    Com. Approximate estimation error $\boldsymbol{z}^t = \boldsymbol{M}^{-1}\boldsymbol{r}^t$
    Update $\boldsymbol{x}^{t+1} = \boldsymbol{x}^t + \boldsymbol{z}^t$
end for
Return $\boldsymbol{x}^{t+1}$

- **Q1**: How do we design $\boldsymbol{M}$?
- **Q2**: When will this method converge under what condition?

Jacobi Method

Every i-th equation of $\boldsymbol{Ax} = \boldsymbol{b}$ is

$$\sum_{j=1}^{n} a_{ij} x_j = b_i.$$

To solve the problem, for each x_i at t-th iteration, assume other entries of $\boldsymbol{x}$ remain fixed. This gives

$$x_i^{t+1} = \frac{b_i - \sum_{j \neq i} a_{ij} x_j^t}{a_{ii}}.$$

Notice diagonal elements of $\boldsymbol{A}$ appears in denominator and $\sum_{j \neq i} a_{ij}$ can be decomposed into two parts $\sum_{j<i} a_{ij} + \sum_{j>i} a_{ij}$. Denote

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

Jacobi Method

- In the matrix form, the Jacobi method is:

$$
\begin{aligned}
\boldsymbol{x}_0 &= \text{ initial vector} \\
\boldsymbol{x}_{t+1} &= \boldsymbol{D}^{-1}(\boldsymbol{b} - (\boldsymbol{L} + \boldsymbol{U})\boldsymbol{x}_t) \text{ for } t = 0, 1, 2, \ldots
\end{aligned}
$$

- In the form of Fixed-Point Iteration:

$$
\boldsymbol{x}_{t+1} = g(\boldsymbol{x}_t), \text{ where } g(\boldsymbol{x}_t) = \boldsymbol{D}^{-1}(\boldsymbol{b} - (\boldsymbol{L} + \boldsymbol{U})\boldsymbol{x}_t)
$$

To show that Jacobi is FPI, we have

$$
\begin{aligned}
\boldsymbol{A}\boldsymbol{x} &= \boldsymbol{b} \\
(\boldsymbol{D} + \boldsymbol{L} + \boldsymbol{U})\boldsymbol{x} &= \boldsymbol{b} \\
\boldsymbol{D}\boldsymbol{x} &= \boldsymbol{b} - (\boldsymbol{L} + \boldsymbol{U})\boldsymbol{x}.
\end{aligned}
$$

Jacobi Method

Jacobi method:

$$\boldsymbol{x}_0 = \text{ initial vector}$$
$$\boldsymbol{x}_{t+1} = \boldsymbol{D}^{-1}(\boldsymbol{b} - (\boldsymbol{L} + \boldsymbol{U})\boldsymbol{x}_t) \text{ for } t = 0, 1, 2, \ldots$$

Recall we have an iterative method

Algorithm 4 Iteration($\boldsymbol{x}^0, \boldsymbol{A}, \boldsymbol{b}, \boldsymbol{M}$)

1: $\boldsymbol{x}^0$ be initial guesses
2: **for** $t = 0, 1, \ldots,$ **do**
3: $\quad \boldsymbol{r}^t = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^t$
4: $\quad \boldsymbol{z}^t = \boldsymbol{M}^{-1}\boldsymbol{r}^t$
5: $\quad \boldsymbol{x}^{t+1} = \boldsymbol{x}^t + \boldsymbol{z}^t$
6: **end for**
7: **Return** $\boldsymbol{x}^{t+1}$

Quiz: Find a suitable $\boldsymbol{M}$ and then show that Jacobi method is equivalent to Iteration method. (5 minutes)

Jacobi - An example

An example of the Jacobi method:

$$\begin{bmatrix} 3x_0 + x_1 = 5 \\ x_0 + 2x_1 = 5 \end{bmatrix} \text{ with an initial guess } \begin{bmatrix} x_0 \\ x_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

$$\begin{bmatrix} x_0^0 \\ x_1^0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} x_0^1 \\ x_1^1 \end{bmatrix} = \begin{bmatrix} \frac{5-x_0^0}{3} \\ \frac{5-x_1^0}{2} \end{bmatrix} = \begin{bmatrix} \frac{5}{3} \\ \frac{5}{2} \end{bmatrix}$$

$$\begin{bmatrix} x_0^2 \\ x_1^2 \end{bmatrix} = \begin{bmatrix} \frac{5-x_0^1}{3} \\ \frac{5-x_1^1}{2} \end{bmatrix} = \begin{bmatrix} \frac{5}{6} \\ \frac{5}{3} \end{bmatrix}$$

$$\begin{bmatrix} x_0^3 \\ x_1^3 \end{bmatrix} = \begin{bmatrix} \frac{5-x_0^2}{3} \\ \frac{5-x_1^2}{2} \end{bmatrix} = \begin{bmatrix} \frac{10}{9} \\ \frac{25}{12} \end{bmatrix}$$

Observation: The most recently updated values of the unknowns are not used at each step.

Gauss-Seidel

Gauss-Seidel: the most recently updated values of the unknowns are used at each step. Example:

$$\begin{bmatrix} 3 & 1 & -1 \\ 2 & 4 & 1 \\ -1 & 2 & 5 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} 4 \\ 1 \\ 1 \end{bmatrix}$$

The iteration goes to

$$\begin{aligned} u_{t+1} &= \frac{4 - v_t + w_t}{3} \\ v_{t+1} &= \frac{1 - 2u_{t+1} - w_t}{4} \\ w_{t+1} &= \frac{1 + u_{t+1} - 2v_{t+1}}{5}. \end{aligned}$$

$$x_i^{t+1} = \frac{b_i - \sum_{j<i} a_{ij} x_j^{t+1} - \sum_{j>i} a_{ij} x_j^t}{aii}, \text{ for } i = 1, 2, \ldots, n. \tag{5}$$

Gauss-Seidel

An alternative way: The most recently updated values of the unknowns are used at each step, even if the updating occurs in the current step.
Gauss-Seidel Method:

$$\boldsymbol{x}^0 = \text{ an initial vector}$$
$$\boldsymbol{x}^{t+1} = \boldsymbol{D}^{-1}\left(\boldsymbol{b} - \boldsymbol{U}\boldsymbol{x}^t - \boldsymbol{L}\boldsymbol{x}^{t+1}\right) \text{ for } k = 0, 1, 2, \ldots.$$

Algorithm 5 Iteration($\boldsymbol{x}^0, \boldsymbol{A}, \boldsymbol{b}, \boldsymbol{M}$)

1: $\boldsymbol{x}^0$ be initial guesses
2: **for** $t = 0, 1, \ldots,$ **do**
3: $\quad \boldsymbol{r}^t = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}^t$
4: $\quad \boldsymbol{z}^t = \boldsymbol{M}^{-1}\boldsymbol{r}^t$
5: $\quad \boldsymbol{x}^{t+1} = \boldsymbol{x}^t + \boldsymbol{z}^t$
6: **end for**
7: **Return** $\boldsymbol{x}^{t+1}$

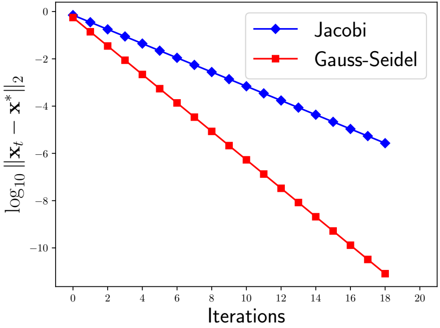
Quiz: Find a suitable $\boldsymbol{M}$ and then show that Gauss-Seidel method is equivalent to Iteration method. (5 minutes)

Comparison between Jacobi and Gauss-Seidel

An example:

$$\begin{bmatrix} 2x_0 - x_1 & = 1 \\ -1x_0 + 2x_1 & = 1 \end{bmatrix}, \text{ where } \boldsymbol{A} = \begin{bmatrix} 2 & -1 \\ -1 & 2 \end{bmatrix}, \boldsymbol{b} = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

We use Jacobi and Gauss-Seidel with $\boldsymbol{x}_0 = [0, 0]^\top$.



Gauss-Seidel converges faster than Jacobi in this example.

Successive Over-Relaxation

Can we do better?
Idea of Successive Over-Relaxation: define each component of the new guess $\boldsymbol{x}^{t+1}$ as a weighted average of ω times the Gauss-Seidel formula and $1-\omega$ times the current guess $\boldsymbol{x}^{t}$.
SOR method:

$$x_i^{(t+1)} = (1-\omega)x_i^{(t)} + \frac{\omega}{a_{ii}}\left(b_i - \sum_{j<i} a_{ij}x_j^{(t+1)} - \sum_{j>i} a_{ij}x_j^{(t)}\right), \qquad (6)$$

where $\quad i = 1, 2, \ldots, n$.

- SOR method is equivalent to Iteration method when $\boldsymbol{M} = \frac{\boldsymbol{D}}{\omega} - \boldsymbol{L}$.