

# Linear Algebra : Matrices

In linear algebra, a commonly encountered situation is where we need to solve matrix equation of the form

$$A \cdot x = b$$

where  $A$  is an  $n \times n$  matrix,  $x$ ,  $b$  can either be  $n \times 1$  vectors (as in solving system of linear equations) or  $n \times n$  matrices (as in inverse).

The solution implies determining the vector  $x$

$$x = A^{-1} b \quad \text{where} \quad A^{-1} = A_c^T / |A|$$

where  $|A|$  is the determinant and  $A_c$  are the cofactors. Although numerically doable, far more efficient methods exist to calculate inverse.

- ▶ **Direct elimination** : Gauss-Jordan, LU decomposition, Cholesky decomposition which are used for small, dense matrices and are memory intensive, possibly slower and difficult to parallelize.
- ▶ **Iterative methods** : Gauss-Jacobi, Gauss-Seidel, Conjugate gradient, GMRES which are useful for large, particularly sparse matrices and lend themselves to parallelization.

# Linear equations: Gauss-Jordan method

Consider solving a linear system of equations, say with 3 variables

$$A \cdot X = B \Rightarrow \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

To solve  $(x_1, x_2, x_3)$ , the Gauss-Jordan method suggests to write the above equation in an *augmented matrix* form,

$$\left[ A | B \right] \equiv \left[ \begin{array}{ccc|c} a_{11} & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \end{array} \right]$$

Using Gauss-Jordan elimination, convert the *augmented matrix* in *reduced row echelon form* (RREF) eventually yielding

$$\left[ \begin{array}{ccc|c} 1 & 0 & 0 & \tilde{b}_1 \\ 0 & 1 & 0 & \tilde{b}_2 \\ 0 & 0 & 1 & \tilde{b}_3 \end{array} \right]$$

thus solving the linear equations :  $x_1 = \tilde{b}_1$ ,  $x_2 = \tilde{b}_2$ ,  $x_3 = \tilde{b}_3$ .

# RREF

In *reduced row echelon form*,

1. all rows with only zero entries are at the bottom of the matrix
2. the first nonzero entry in a row (called **pivot**) of each nonzero row is to the right of the leading entry of the row above it
3. leading entry *i.e.* pivot in any nonzero row is 1
4. all other entries in row or column containing a leading 1 are zeros.

Illustration : 
$$\begin{pmatrix} 1 & -2 & 3 \\ 0 & 1 & -4 \\ 0 & 0 & 1 \end{pmatrix}$$

The way to achieve RREF by Gauss-Jordan involves any one or a combination of three elementary row operations

- ▶ swapping two rows
- ▶ multiplying a row by a nonzero number
- ▶ adding or subtracting a multiple of one row to another row

Operation involving rows is called *partial pivoting*.

*Full pivoting* (recommended by Numerical Recipes) : both row and column operations.

# Partial pivoting

Say the augmented matrix we want to reduce to **RREF** be

$$\left[ \begin{array}{ccc|c} 0 & a_{12} & a_{13} & b_1 \\ a_{21} & a_{22} & a_{23} & b_2 \\ a_{31} & a_{32} & a_{33} & b_3 \end{array} \right]$$

$a_{11}$  is either 0 or order(s) of magnitude small compared to  $a_{21}$ ,  $a_{31}$   
 $\rightarrow a_{31}, a_{21} \gg a_{11}$  and let  $a_{31} > a_{21}$ . To get leftmost nonzero entry at the top, swap  $R_3 \leftrightarrow R_1$

$$\left[ \begin{array}{ccc|c} a_{31} & a_{32} & a_{33} & b_3 \\ a_{21} & a_{22} & a_{23} & b_2 \\ 0 & a_{12} & a_{13} & b_1 \end{array} \right] \equiv \left[ \begin{array}{ccc|c} a_{11}^0 & a_{12}^0 & a_{13}^0 & b_1^0 \\ a_{21}^0 & a_{22}^0 & a_{23}^0 & b_2^0 \\ a_{31}^0 & a_{32}^0 & a_{33}^0 & b_3^0 \end{array} \right]$$

where  $a_{11}^0$  is the *pivot element*, new row  $R_1^0$  is the *pivot row* and new column  $C_1^0$  is the *pivot column*. Reduce  $R_1^0/a_{11}^0 \rightarrow R_1^1$ ,

$$\left[ \begin{array}{ccc|c} 1 & a_{12}^1 & a_{13}^1 & b_1^1 \\ a_{21}^0 & a_{22}^0 & a_{23}^0 & b_2^0 \\ a_{31}^0 & a_{32}^0 & a_{33}^0 & b_3^0 \end{array} \right], \quad a_{1,2,3}^1 = a_{1,2,3}^0/a_{11}^0, \quad b_1^1 = b_1^0/a_{11}^0$$

# Partial pivoting

Reduce the **pivot column**  $C_1$  by adding / subtracting multiples of pivot row from the following rows

$$a_{2(1,2,3)}^1 = a_{2(1,2,3)}^0 - a_{21}^0 * R_1^1, \quad b_2^1 = b_2^0 - a_{21}^0 * b_1^1$$

$$a_{3(1,2,3)}^1 = a_{3(1,2,3)}^0 - a_{31}^0 * R_1^1, \quad b_3^1 = b_3^0 - a_{31}^0 * b_1^1$$

$$\Rightarrow \left[ \begin{array}{ccc|c} 1 & a_{12}^1 & a_{13}^1 & b_1^1 \\ 0 & \boxed{a_{22}^1} & a_{23}^1 & b_2^1 \\ 0 & a_{32}^1 & a_{33}^1 & b_3^1 \end{array} \right]$$

$a_{22}^1$  is new *pivot element* and undergoes the same test of smallness. If needed, **partial pivoting** done; eventually yielding

$$\text{RREF} \Rightarrow \left[ \begin{array}{ccc|c} 1 & 0 & 0 & b_1^3 \\ 0 & 1 & 0 & b_2^3 \\ 0 & 0 & 1 & b_3^3 \end{array} \right]$$

This method is **Gauss-Jordan elimination** using *partial pivoting*. No matter what steps and in which order they are applied, the final augmented matrix is unique.

## Pivoting tryout

Consider the following set of linear equations :

$$\begin{array}{rcl} y + z - 2w & = & -3 \\ x + 2y - z & = & 2 \\ 2x + 4y + z - 3w & = & -2 \\ x - 4y - 7z - w & = & -19 \end{array}$$

Write down the relevant matrices in a file. Construct the augmented matrix and perform partial pivoting of the first row only. Do necessary operations to convert the first column of the augmented matrix in the form  $(1, 0, 0, 0)$  and write down the augmented matrix.

**N.B.** – Remember, while pivoting, swap rows that are below the new pivot row.

## An example :

Consider the equations and its corresponding augmented matrix

$$\left. \begin{array}{rrc} 2y + 5z & = & 1 \\ 3x - y + 2z & = & -2 \\ x - y + 3z & = & 3 \end{array} \right\} \Rightarrow \left[ \begin{array}{ccc|c} 0 & 2 & 5 & 1 \\ 3 & -1 & 2 & -2 \\ 1 & -1 & 3 & 3 \end{array} \right]$$

Since  $a_{11} = 0$  and  $a_{21} > a_{31}$ , we begin by swapping  $R_1 \leftrightarrow R_2$ ,

$$\left[ \begin{array}{ccc|c} 3 & -1 & 2 & -2 \\ 0 & 2 & 5 & 1 \\ 1 & -1 & 3 & 3 \end{array} \right] \xrightarrow{R_1^0/3 \rightarrow R_1^1} \left[ \begin{array}{ccc|c} 1 & -1/3 & 2/3 & -2/3 \\ 0 & 2 & 5 & 1 \\ 1 & -1 & 3 & 3 \end{array} \right]$$

$$\xrightarrow{R_3^0 - R_1^1 \rightarrow R_3^1} \left[ \begin{array}{ccc|c} 1 & -1/3 & 2/3 & -2/3 \\ 0 & 2 & 5 & 1 \\ 0 & -2/3 & 7/3 & 11/3 \end{array} \right]$$

$$\xrightarrow{R_2^1/2 \rightarrow R_2^2} \left[ \begin{array}{ccc|c} 1 & -1/3 & 2/3 & -2/3 \\ 0 & 1 & 5/2 & 1/2 \\ 0 & -2/3 & 7/3 & 11/3 \end{array} \right]$$

$$\xrightarrow{R_1^1 + R_2^2/3 \rightarrow R_1^2} \left[ \begin{array}{ccc|c} 1 & 0 & 9/6 & -3/6 \\ 0 & 1 & 5/2 & 1/2 \\ 0 & -2/3 & 7/3 & 11/3 \end{array} \right]$$

$$\begin{aligned}
 & R_3^1 + 2R_2^2/3 \rightarrow R_3^2 \quad \left[ \begin{array}{ccc|c} 1 & 0 & 9/6 & -3/6 \\ 0 & 1 & 5/2 & 1/2 \\ 0 & 0 & 12/3 & 24/6 \end{array} \right] \\
 & 3R_3^2/12 \rightarrow R_3^3 \quad \left[ \begin{array}{ccc|c} 1 & 0 & 9/6 & -3/6 \\ 0 & 1 & 5/2 & 1/2 \\ 0 & 0 & 1 & 1 \end{array} \right] \quad R_2^2 - 5R_3^3/2 \rightarrow R_2^3 \quad \left[ \begin{array}{ccc|c} 1 & 0 & 9/6 & -3/6 \\ 0 & 1 & 0 & -2 \\ 0 & 0 & 1 & 1 \end{array} \right] \\
 & R_1^2 - 9R_3^3/6 \rightarrow R_1^3 \quad \left[ \begin{array}{ccc|c} 1 & 0 & 0 & -2 \\ 0 & 1 & 0 & -2 \\ 0 & 0 & 1 & 1 \end{array} \right]
 \end{aligned}$$

Therefore, the solution is  $x = -2, y = -2, z = 1$ .

**Gauss-Jordan** can be trivially extend to obtain **inverse** of an invertible matrix. First to test invertibility, determine the **determinant**.

$$\det \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \det \begin{pmatrix} a'_{11} & a'_{12} & a'_{13} \\ 0 & a'_{22} & a'_{23} \\ 0 & 0 & a'_{33} \end{pmatrix} = (-1)^n a'_{11} a'_{22} a'_{33}$$

where  $n$  is the number of times the rows are interchanged,  $a'_{ii} \neq 0$  and none of  $a'_{ii}$  has to be 1.



## Matrix inversion with Gauss-Jordan

Matrix inversion follows similar system of linear equations as before

$$\mathbf{A} \cdot \mathbf{B} = \mathbf{1} \rightarrow \text{augmented matrix : } \left[ \mathbf{A} \mid \mathbf{1} \right] \xrightarrow{G-J} \left[ \mathbf{1} \mid \mathbf{A}^{-1} \right]$$

**Memory requirement :**  $N \times (N + 1)$  for solving linear system of equations and  $N \times (N + N)$  for inverse, ignoring swapping operation (involving sorting).

**Mathematical operations :**  $(N - 1) \times 2$  (multiplication / division and addition / subtraction) for each row reduction.

**Accuracy :** Rounding errors, proportional to  $N$ , quickly built up in solution

For large  $N$  not very suitable – memory requirement  $\propto N^2$  and slow. Typically restricted to  $\sim N = 10$