

Linear Algebra

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Handling Matrices in C++

The best way to allocate and deallocation of matrices in C++ is using pointers. Recall that a matrix is represented by a double pointer that points to a memory segment holding a sequwncw of double* pointers. So each double* pointer point to a row in the matrix.

When we declare `double** A`, this means that `A[i]` is a pointer to the $i+1$ -th row `A[i]` and `A[i][j]` is matrix entry (i,j) .

This snippet of code shows how we allocate a matrix of $n \times n$

```
int n;  
double ** A;  
  
A = new double*[n];  
  
for (i=0; i<n; i++)  
    A[i] = new double[N];
```

Linear Systems of equations

Gaussian Elimination

The problem is to solve a system of N equations for N unknowns.

$$\begin{aligned}a_{11}x_1 + a_{12}x_2 + \cdots + a_{1N}x_N - b_1 &= 0 \\a_{21}x_1 + a_{22}x_2 + \cdots + a_{2N}x_N - b_2 &= 0 \\&\vdots \\a_{N1}x_1 + a_{N2}x_2 + \cdots + a_{NN}x_N - b_N &= 0\end{aligned}$$

Or in matrix form,

$$\mathbf{Ax} - \mathbf{b} = 0$$

Where,

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & & & \vdots \end{bmatrix}$$

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

$$\mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Gaussian Elimination works on two steps. Forward elimination and back substitution.

Backward substitution is done recursively starting from x_n . This can be mathematically expressed as:

$$x_m = \frac{1}{a_{mm}} \left(b_m - \sum_{k=m+1}^n a_{mk} x_k \right) \quad m = n-1, n-2, \dots, 1 \quad (1)$$

For N equations in N unknowns, the computation time for Gaussian elimination goes as N^3 . For sparse systems (where most coefficients are zero), this calculation time can be greatly reduced.

Pivoting

Sometimes in the matrix \mathbf{A} we encounter very small numbers or even zero in the diagonal entries. This could be fatal as when we do forward elimination.

Consider the forward elimination for these equations.

$$\epsilon x_1 + x_2 + x_3 = 5$$

$$x_1 + x_2 = 3$$

$$x_1 + x_3 = 4$$

$$\epsilon x_1 + x_2 + x_3 = 5$$

$$x_2 \left(1 - \frac{1}{\epsilon} \right) + \frac{x_3}{\epsilon} = 3 - \frac{5}{\epsilon}$$

$$-(1/\epsilon)x_2 + (1 - 1/\epsilon)x_3 = 4 - 5/\epsilon$$

Algorithm for Gaussian Elimination

* Forward Elimination

```
      DO K=1..N-1
DO I = K+1..N
COEFF = A(I,K)/A(K,K)
DO J = K+1,N
A(I,J) = A(I,J) - COEFF * A(K,J)
ENDO
A(I,K) = COEFF
B(I) = B(I)-COEFF*B(K)
ENDDO
ENDDO
```

* Back-substitution

```
      X(N) = B(N)/A(N,N)
DO I = N-1...1
SUM = B(I)
DO J= I+1..N
SUM = SUM - A(I,J)*X(J)
ENDDO
X(I) = SUM/A(I,I)
ENDDO
```