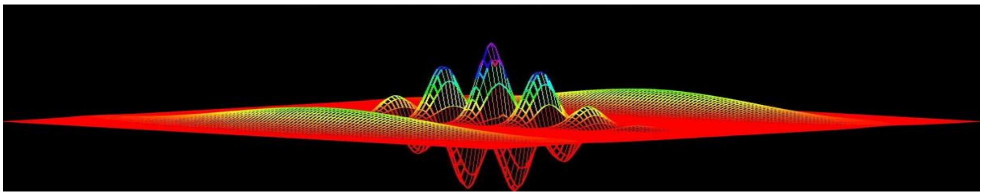
Computational Physics

numerical methods with C++ (and UNIX)



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Computational Physics
Numerical methods

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Systems of linear equations

A system of algebraic equations has the form :

$$\begin{aligned}
A_{11}x_1 + A_{12}x_2 + \cdots + A_{1n}x_n &= b_1\\
A_{21}x_1 + A_{22}x_2 + \cdots + A_{2n}x_n &= b_2\\
&\vdots\\
A_{n1}x_1 + A_{n2}x_2 + \cdots + A_{nn}x_n &= b_n
\end{aligned}$$

where both the coefficients $\mathbf{A_{ij}}$ and the constants $\mathbf{b_j}$ are known and $\mathbf{x_i}$ represent the unknowns

$$\begin{pmatrix} A_{11} & A_{12} & \cdots & A_{1n}\\ A_{11} & A_{12} & \cdots & A_{1n}\\ \vdots & \vdots & \vdots & \vdots\\ A_{n1} & A_{n2} & \cdots & A_{nn} \end{pmatrix} \begin{pmatrix} x_1\\ x_2\\ \vdots\\ x_n \end{pmatrix} = \begin{pmatrix} b_1\\ b_2\\ \vdots\\ b_n \end{pmatrix}$$

Uniqueness of solution and conditioning

- ✔ A system of $\mathbf{n}$ linear equations with $\mathbf{n}$ unknowns has a unique solution if the determinant is *nonsingular* : $|\mathbf{A}| \neq \mathbf{0}$
  a nonsingular matrix has all rows and columns independent (not linear combination)
  - ☞ the magnitude of the determinant of $\mathbf{A}$ can be...compared to the norm of the matrix $||\mathbf{A}|| \neq \mathbf{0}$

$$|\mathbf{A}| << ||\mathbf{A}||$$

  - ☞ norm of the matrix

$$||\mathbf{A}|| = \sqrt{\sum_{i=1}^{n}\sum_{j=1}^{n} A_{ij}^2} \qquad ||\mathbf{A}|| = \max_{1\le i\le n} \sum_{i=1}^{n} |A_{ij}|$$

- ✔ In most cases it is sufficient compare the determinant with the magnitudes of the matrix elements

Uniqueness and conditioning (cont.)

✔ The condition number associated with the linear equation $\mathbf{Ax} = \mathbf{b}$ gives a bound on how inaccurate the solution $\mathbf{x}$ will be.
one can think of the condition number as being (very roughly) the rate at which the solution, $\mathbf{x}$, will change with respect to a change in $\mathbf{b}$

- ☞ conditioning is a property of the matrix and shall be around 1
- ☞ A problem with a low condition number is said to be **well-conditioned**, while a problem with a high condition number is said to be **ill-conditioned**

Ill-conditioned system

Suppose the system :

$$\begin{cases} 2x + y & = 3 \\ 2x + 1.001y & = 0 \end{cases}$$

Solution :

$$\begin{cases} x & = 1501.5 \\ y & = -3000 \end{cases}$$

Determinant :

$$|\mathbf{A}| = \mathbf{0.002}$$

The system is ill-conditioned since $|\mathbf{A}|$ is much smaller than the norm of the coefficients matrix $\mathbf{A}$ or more simple, than the coefficients of the matrix
To verify the ill-conditioning of the system just change by 0.1% the value 1.001 and check the new result :

$$\begin{cases} 2x + y & = 3 \\ 2x + \mathbf{1.002}y & = 0 \end{cases} \Rightarrow \quad ?$$

The solutions of ill-conditioned cannor be trusted because round-off errors during computation can change completely the solution !

System of linear eqs : solving

- ✔ Systems of linear algebraic equations can be solved with **direct** and **iterative** methods
- ✔ Direct methods transform original eqs into equivalent eqs
  - ☞ equivalent eqs have the same solution
  - ☞ matrix determinant may change
- ✔ Elementary operations that leave the solution unchanged are :
  - ☞ exchanging equations (changes sign of determinant $\left|\mathbf{A}'\right| = -|\mathbf{A}|$)
  - ☞ multiply equation by nonzero constant λ ($\left|\mathbf{A}'\right| = \lambda\,|\mathbf{A}|$)
  - ☞ multiply equation by nonzero constant and subtract it from another equation ($|\mathbf{A}'| = |\mathbf{A}|$)

Solving (cont.)

Method	Initial form	Final form
Gauss elimination	$\mathbf{A}\ \mathbf{x} = \mathbf{b}$	$\mathbf{U}\ \mathbf{x} = \mathbf{c}$
LU decomposition	$\mathbf{A}\ \mathbf{x} = \mathbf{b}$	$\mathbf{LU}\ \mathbf{x} = \mathbf{b}$
Gauss-Jordan elimination	$\mathbf{A}\ \mathbf{x} = \mathbf{b}$	$\mathbf{I}\ \mathbf{x} = \mathbf{c}$

$|\mathbf{A}|$ ≡ matrix of coefficients

$|\mathbf{U}|$ ≡ upper triangular matrix

$|\mathbf{L}|$ ≡ lower triangular matrix

$|\mathbf{I}|$ ≡ identity matrix

$$\mathbf{U} = \begin{pmatrix} U_{11} & U_{12} & U_{13} & \cdots & U_{1n} \\ 0 & U_{22} & U_{23} & \cdots & U_{2n} \\ 0 & 0 & U_{33} & \cdots & U_{3n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \vdots & U_{nn} \end{pmatrix}$$

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \vdots & 1 \end{pmatrix} \qquad \mathbf{L} = \begin{pmatrix} L_{11} & 0 & 0 & \cdots & 0 \\ L_{21} & L_{22} & 0 & \cdots & 0 \\ L_{31} & L_{32} & L_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ L_{n1} & L_{32} & L_{n3} & \vdots & L_{nn} \end{pmatrix}$$

Gauss elimination

- Solves the system in two steps : elimination phase and solution phase
- The elimination phase transforms the equation $\mathbf{A}\mathbf{x} = \mathbf{b}$ into $\mathbf{U}\mathbf{x} = \mathbf{c}$
  - a *pivot* equation (i) is multiplied by a constant λ and subtracted to another one (j)

    $\boxed{\text{Row}_j - \lambda_{ij} \times \text{Row}_i}$
- The equations are then solved by back substitution
- *Note : the determinant of a triangular matrix (U or L) is easy to compute :* $|\mathbf{A}| = |\mathbf{U}| = U_{11} \times U_{22} \times \cdots \times U_{nn}$

The augmented coefficient matrix is very convenient for making the computations

$$\left(\begin{array}{ccccc|c} A_{11} & A_{12} & A_{13} & \cdots & A_{1n} & b_1 \\ A_{21} & A_{22} & A_{23} & \cdots & A_{2n} & b_2 \\ A_{31} & A_{32} & A_{33} & \cdots & A_{3n} & b_3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{n1} & A_{n2} & A_{n3} & \vdots & A_{nn} & b_n \end{array}\right)$$

As example, to transform Row_2 we have to multiply the *pivot* line (here Row_1 by hypothesis...you can interchange rows !) by :

$$\lambda_{12} = \frac{A_{21}}{A_{11}}$$

Gauss elimination algorithm : example

$$\begin{cases} 4x_1 - 2x_2 + x_3 = 11 & (1) \\ -2x_1 + 4x_2 - 2x_3 = -16 & (2) \\ x_1 - 2x_2 + 4x_3 = 17 & (3) \end{cases}$$

Gauss elimination algorithm

Let's suppose we already transformed our matrix up to row $k = 3$

It means, $\text{Row}_{k=3}$ is now the *pivot* line and all equations below ($\text{Row} > 3$) are still to be transformed

$$\left(\begin{array}{cccccc|c} A_{11} & A_{12} & A_{13} & \cdots & A_{1n} & b_1 \\ 0 & A_{22} & A_{23} & \cdots & A_{2n} & b_2 \\ 0 & 0 & A_{33} & \cdots & A_{3n} & b_3 \\ \hline 0 & 0 & A_{i3} & \vdots & A_{in} & b_i \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & A_{n3} & \vdots & A_{nn} & b_n \end{array}\right)$$

To eliminate the element A_{i3} of the row below the *pivot* we do :

$$\boxed{\text{Row}_i - \lambda \times \text{Row}_{pivot} \rightarrow \text{Row}_i}$$

$$\boxed{\lambda = A_{i3}/A_{k3}}$$

```
// matrix n x n
loop on pivot row (k): k = 0, n-2
  loop on rows below pivot: i = k+1, n-1
     - for every row:
       compute lambda A(i,k)/A(k,k)
     - transform row i:
       only elements (i, k+1:n)
       need to be stored
     - transform also constant value
```


Back substitution phase

✔ After Gauss elimination we got an equation involving a upper triangular matrix $\mathbf{U}$: $\mathbf{Ux} = \mathbf{c}$

$$\left(\begin{array}{ccccc|c} A_{11} & A_{12} & A_{13} & \cdots & A_{1n} & c_1 \\ 0 & A_{22} & A_{23} & \cdots & A_{2n} & c_2 \\ 0 & 0 & A_{33} & \cdots & A_{3n} & c_3 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \vdots & A_{nn} & c_n \end{array}\right)$$

✔ Now, we need to solve equations by starting on the simplest one (the last row) and going back

The solutions :

1) $$A_{nn}x_n = c_n \quad \Rightarrow x_n = c_n/A_{nn}$$

k) $$A_{kk}x_k + A_{k,k+1}x_{k+1} + \cdots + A_{kn}x_n = c_k \quad \Rightarrow x_k = \frac{1}{A_{kk}}\left(c_k - \sum_{j=k+1}^{n} A_{kj}x_j\right)$$

Pivoting

- ✔ If the element of the *pivot* row and column being used to transform subsequent rows is zero, just reorder the equations by moving the pivot row to the end of the matrix
- ✔ Reordering of the equations may also be needed if the pivot element, although different from zero, is very small

$$[\mathbf{A}|\mathbf{b}] = \left(\begin{array}{ccc|c} \delta & -1 & 1 & 0 \\ -1 & 2 & -1 & 0 \\ 2 & -1 & 0 & 1 \end{array}\right)$$

$$[\mathbf{A}'|\mathbf{b}'] = \left(\begin{array}{ccc|c} \delta & -1 & 1 & 0 \\ 0 & 2-1/\delta & -1+1/\delta & 0 \\ 0 & -1+2/\delta & 2/\delta & 1 \end{array}\right)$$

$$[\mathbf{A}'|\mathbf{b}'] \simeq \left(\begin{array}{ccc|c} \delta & -1 & 1 & 0 \\ 0 & -1/\delta & +1/\delta & 0 \\ 0 & +2/\delta & 2/\delta & 1 \end{array}\right)$$

Two last equations contradict each other !

Pivoting with reordering

The augmented coeff matrix

$$[\mathbf{A}|\mathbf{b}] = \left(\begin{array}{ccc|c} \delta & \mathbf{-1} & \mathbf{1} & \mathbf{0} \\ -1 & 2 & -1 & 0 \\ 2 & -1 & 0 & 1 \end{array}\right)$$

$\text{Row}_1 \leftrightarrow \text{Row}_2$

$$[\mathbf{A}|\mathbf{b}] = \left(\begin{array}{ccc|c} -1 & 2 & -1 & 0 \\ \delta & \mathbf{-1} & \mathbf{1} & \mathbf{0} \\ 2 & -1 & 0 & 1 \end{array}\right)$$

$\text{Row}_2 - (-\delta) \times \text{Row}_1 \rightarrow \text{Row}_2$

$\text{Row}_3 - (-2) \times \text{Row}_1 \rightarrow \text{Row}_3$

$$[\mathbf{A}'|\mathbf{b}'] = \left(\begin{array}{ccc|c} -1 & 2 & -1 & 0 \\ 0 & -1+2\delta & +1-\delta & 0 \\ 0 & 3 & -2 & 1 \end{array}\right)$$

$\text{Row}_3 - 3/(-1+2\delta) \times \text{Row}_2 \rightarrow \text{Row}_3$

$$[\mathbf{A}'|\mathbf{b}'] = \left(\begin{array}{ccc|c} -1 & 2 & -1 & 0 \\ 0 & -1+2\delta & +1-\delta & 0 \\ 0 & 0 & -\frac{1+\delta}{2\delta-1} & 1 \end{array}\right)$$

$$[\mathbf{A}'|\mathbf{b}'] \simeq \left(\begin{array}{ccc|c} -1 & 2 & -1 & 0 \\ 0 & -1 & +1 & 0 \\ 0 & 0 & 1 & 1 \end{array}\right)$$

Back substitution gives :

$$x_3 = 1$$
$$x_2 = x_3 = 1$$
$$x_1 = 2x_2 - x_3 = 1$$

Diagonal dominance

- A matrix $\mathbf{A}$ $n \times n$ is said to be **diagonally dominant** if each diagonal element is larger in absolute than the sum of the other elements on the same row

$$\boxed{|\mathbf{A_{ii}}| > \sum_{\substack{j=1 \\ i \neq j}}^{n} |A_{ij}| \qquad i = 1, 2, ..., n}$$

- If the coefficient matrix of the equation system $\mathbf{Ax} = \mathbf{b}$ is diagonally dominant, it means the equations are already arranged in a optimal order
  - the strategy shall be to reorder the coefficient matrix in order to get diagonal dominance approach
  - the pivot element is as large as possible when compared to other elements in the pivot row

The **relative size** of an element A_{ij} in the row **i** of the matrix $\mathbf{A}$:

$$r_{ij} = \frac{|A_{ij}|}{s_i}$$

where s_i is the **scale factor** of row **i** correponding to the absolute value of the largest element in ith row

Gauss elimination with pivoting

algorithm

```
1) store the maximum absolute value of every row on array s(i)

2) loop on rows i = 0, n-1

   - check if pivot element A(i,i) is the best one
     by looking to all elements from the same column
     below the pivot candidate, and choosing the one
     with the largest relative size

   - identify the row with largest relative size element

   - if different from the pivot row candidate swap it
     void SwapRows(int i, int j, double *s);

   - if largest relative size element is very small (<tol)
     the matrix i singular

   - proceed with elimination phase
```

Gauss elimination with pivoting

Example

The coeff matrix

$$[\mathbf{A}] = \begin{pmatrix} 2 & -2 & 6 \\ -2 & 4 & 3 \\ -1 & 8 & 4 \end{pmatrix}$$

The vector of constants

$$[\mathbf{b}] = \begin{pmatrix} 16 \\ 0 \\ -1 \end{pmatrix}$$

The augmented coeff matrix and the vector of max row values

$$[\mathbf{A}] = \left(\begin{array}{ccc|c} 2 & -2 & 6 & 16 \\ -2 & 4 & 3 & 0 \\ -1 & 8 & 4 & -1 \end{array}\right) \qquad [\mathbf{s}] = \begin{pmatrix} 6 \\ 4 \\ 8 \end{pmatrix}$$