Simulation in Materials Engineering

BLOCK 2: Fundamentals of numerical analysis

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Outline

1. Introduction to programming
2. Linear systems of equations
   - Introduction
   - Direct methods
   - Iterative methods and sparse matrices
3. Non linear equations and systems
4. Ordinary differential equations (ODEs)

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1 Introduction to programming

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3 Non linear equations and systems

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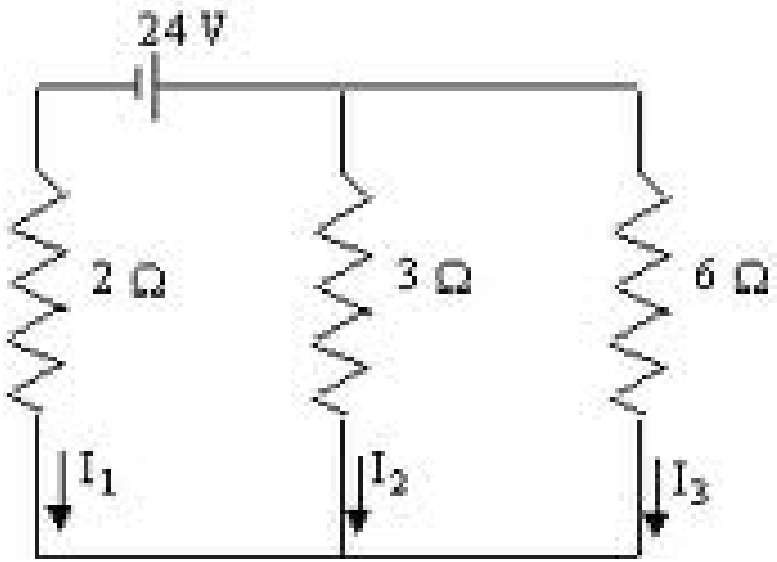
Introduction:Why linear equations are important?

They appear everytime in solving many engineering problems:

- The resolution of an electric network using Kirchoff laws leads to a system of equations of the intensities.
- The resolution of a hydraulic network, where the presures of each node are the unknowns



Introduction:Why linear equations are important?

- The numerical solution of any Partial Differential Equation, generally leads to a system of linear equations: i.e. heat equation in 1D solved by finite differences

$$U_t = U_{xx}$$
$$U(0,t) = U(1,t) = 0$$
$$U(x,0) = U_0(x)$$

The domain in space is discretized using a mesh $x_0, ..., x_J$ and in time using a mesh $t_0, ..., t_N$. The solution at each point/time is $u(x_j, t_n) = u_j^n$.
The unknowns here are the nodal temperatures at $n+1$ and the linear equation that result is

$$(1+2r)u_j^{n+1} - ru_{j-1}^{n+1} - ru_{j+1}^{n+1} = u_j^n$$

, r depending on a relation between spatial and time increment

Introduction

A linear system of equations is a set of m equations, each of them consisting on a linear combination of n unknowns, $x_i, i = 1...n$ and an indpendent term $b_i, i = 1...m$

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ &\vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= b_m \end{aligned}$$

1. If the system has a solution and this solution is unique. This in known as a compatible determined system
2. If the system has solution, but there exist infinite solutions, the system is called compatible indetermined system
3. If the system does not have a solution, the system is incompatible

Introduction

The linear system can be rewritten using matrices,

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

where

$$\mathbf{A}_{mn} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ & \vdots & & \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}; \quad \mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}; \quad \mathbf{b} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{bmatrix}$$

In this case, the type of system can be obtained using the *Rouchee-Fröbenius* theorem

1. if $\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{A}|\mathbf{b}) = n$ the system is compatible determined
2. if $\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{A}|\mathbf{b}) < n$ the system is compatible undetermined
3. if $\text{rank}(\mathbf{A}) \neq \text{rank}(\mathbf{A}|\mathbf{b})$ the system is uncompatible

Introduction

Examples,

$$\begin{aligned} 3x + 2y + z &= 1 \\ 2x + z &= 2 \\ x + y &= 1 \end{aligned}$$

is compatible and determined: has a unique solution
$x = 3, y = -2, z = -4$

$$\begin{aligned} 3x + 2y + z &= 1 \\ 2x + z &= 2 \\ x + 2y &= -1 \end{aligned}$$

is compatible and undetermined, solutions can be parametrized and correspond to $x = 1 - \lambda/2, y = -1 + \lambda/4, z = \lambda$

Introduction

$$\begin{aligned} 3x + 2y + z &= 1 \\ 2x + z &= 2 \\ x + 2y &= 1 \end{aligned}$$

is incompatible and no values of x, y, z can fulfill the 3 equations

Direct solution of determined linear systems

- The classic method (secondary school) to solve the system, Cramers rule

$$x_i = \frac{\det(\mathbf{A}_i)}{\det(\mathbf{A})}$$

  being $\mathbf{A}_i$ the matrix formed substituting the i-th column of $\mathbf{A}$ by $\mathbf{b}$

- The Cramers rule computes n+1 determinants, using Laplace $O(n) = 2(n+1)!$, what means that if $n = 20$, a computer with 10Gflops will take more than 324 years to solve the system!!

Classification of algorithms

In order to obtain the solution of a linear system, different methods can be used. They can be classified in two groups

- *direct methods* s if they yield the solution of the system in a finite number of steps, i.e. Cramer rule, LU decompostion
- *iterative methods* if they require (in principle) an infinite number of steps. In this case, the solution is approached by truncating the method and obtaining an approximate but accurate approach

For a *dense* matrix, no algorithm could provide a solution with less than $\approx n^2$ operations, but the use of one or other type of method will give better performance depending on the structure of the matrix.

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Direct methods: LU decomposition

Assuming a compatible and determined system of the type

$$\mathbf{Ax} = \mathbf{b} \tag{1}$$

Being **A** non-singular, and if its leading principal minors are non-zero, then it can be proved that the matrix admit a decomposition such that

$$\mathbf{A} = \mathbf{LU}$$

with **L** a lower diagonal matrix and **U** an upper diagonal matrix:

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

Direct methods: LU decomposition

In this case the equation 1 can be solved by two triangular systems

$$\mathbf{Ly} = \mathbf{b} \tag{2}$$

$$\mathbf{Ux} = \mathbf{y} \tag{3}$$

This systems are much easier to solve, the first system (2) can be solved by a *forward substitution*

$$y_1 = \frac{b_1}{l_{11}}$$

$$y_2 = \frac{b_2}{l_{22}} - \frac{l_{21}}{l_{22}} y_1$$

$$\vdots$$

$$y_i = \frac{1}{l_{ii}}(b_i - \sum_{j=1}^{j=i-1} l_{ij} y_j), \text{ for } i = 2, ..., n$$

Direct methods: LU decomposition

and after that, the second system (3) can also be solved recursively by a *backward substitution* provinding the final solution of the initial problem 1

$$x_n = \frac{y_{nn}}{u_{nn}}$$

$$\vdots$$

$$x_i = \frac{1}{u_{ii}}(b_i - \sum_{j=i+1}^{n} u_{ij}x_j), \text{ for } i = n-1, ..., 1$$

The number of operations for solving by forward substitution the system (2) is n^2 and the same number is necessary for the system (3), giving an order of $O(n^2)$ for the substitution step (yet the decomposition has not been solved and evaluated).

Gaussian elimination

The equation $\mathbf{A} = \mathbf{LU}$ does not have a unique solution, for example in a $3x3$ matrix only 9 equations are available for 12 unknows. In general there exist n^2 equations and $n^2 + n$ unknowns.
If $l_{ii} = 1, i = 1, ..., n$ then the solution is unique and can be computed using *Gaussian elimination*

```
[n m]=size(A);
if n==m
l=eye(n);
for k=1:n-1
   for i=k+1:n
      l(i,k)=A(i,k)/A(k,k);
      for j=k+1:n
         A(i,j)=A(i,j)-l(i,k)*A(k,j);
      endfor
   endfor
endfor
for i=1:n
   for j=i:n
      u(i,j)=A(i,j);
   endfor
endfor
disp(l);
disp(u);
else disp('Non square matrix')
endif
```

Gaussian elimination

The term $A(k,k)$ that appears during the k-th eliminations of the matrix is called *pivot*.The total number is $n-1$ pivots

OCTAVE/MATLAB exercise

- Write as a function the Gaussian elimination algorithm being **A** the input and **L** and **U** the outputs
- Define the matrix `A=[1 2 3 4;2 8 5 -2;3 5 3 0;4 -2 0 1]` and obtain **L** and **U**
- Obtain the value of **A** as the product of **L** and **U**
- Define the matrix `A=[ 1 2 3; 2 4 5; 3 5 6]` and obtain **L** and **U**. What happens? Why?
- Add to the function of **LU** decomposition the to obtention of the determinant
- Obtain the order of magnitude $O(n)$ of the method to decompose a general *nxn* matrix

Gaussian elimination summary

- The **LU** decomposition works only if **A** is non-singular ($\det(\mathbf{A}) \neq 0$) , and if its leading principal minors are non-zero
- Gaussian elimination provides the decomposition and the algorithm is of order $O(n) = 2n^3/3$ (non demonstrated here). In addition, two substitutions, each $O(n^2)$, have to be done for solving the system
- The method serves to obtain the determinant with $O(n^3)$ just by multiplying the diagonal elements of **U**

LU decomposition with pivoting

The **LU** decomposition works only if **A** non-singular ($\det(\mathbf{A}) \neq 0$) , and if its leading principal minors are non-zero. This condition is directly fulfilled for

1. A symmetric and positive definite* matrix **A**, this means that

$$^{*}\text{for all } \mathbf{x} \neq 0,\ \mathbf{x} \in \mathbb{R}^n, \mathbf{x}^T\mathbf{A}\mathbf{x} > 0$$

2. A diagonally dominated matrix>

$$|a_{ii}| \geq \sum_{j \neq i} |a_{ij}| \quad \text{for all } i$$

example, the matrix $\mathbf{A} = \begin{bmatrix} 3 & -2 & 1 \\ 1 & -3 & 2 \\ -1 & 2 & 4 \end{bmatrix}$

If **A** is non-singular but does the condition of the principal minors Gauss elimination does not work but a special type of factorization can be applied. This happens if some pivot becomes 0 during decomposition!

The pivoting technique

Example $\mathbf{A} = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 3 & 4 \\ 2 & 4 & 1 \end{bmatrix}$ does not admit a **LU** decomposition, but the new matrix $\mathbf{A} = \begin{bmatrix} 1 & 3 & 4 \\ 0 & 1 & 2 \\ 2 & 4 & 1 \end{bmatrix}$ consisting of permuting rows 1 and 2 does work.

OCTAVE/MATLAB exercise

Run the Gaussian elimination program with the two matrices of the example
The original matrix **A** is invertible, then, which condition is not fulfilling to admit a **LU** decomposition?
For the matrix $\mathbf{A} = \begin{bmatrix} 1 & 1 + .5E-15 & 3 \\ 2 & 2 & 20 \\ 3 & 6 & 4 \end{bmatrix}$, obtain **L**, **U** using *LU*.
Now compute $\mathbf{A} - \mathbf{LU}$. What happens?

The pivoting technique

- For a general invertible **A** matrix, the rows can be permuted in order to avoid the divisions by zero that the Gaussian elimination algorithm produces (when *pivots* are 0 or very small).
- Moreover, a general algorithm will search for each row during the decomposition the row in which pivot is maximum as absolute value, and interchange both.

```
for k = 1:n
   find r such that |a(r,k)|=max|a(r,k)|, r=k,..,n
   exchange row k with row r
  for i = k+1:n
    l(i,k) = a(i,k)/a(k,k)
    for j = k+1:n
      a(i,j) = a(i,j)-l(i,k)*a(k,j)
    endfor
  endfor
endfor
```

The pivoting technique

- The row permutations of the original **A** are made as soon as this becomes necessary, without carrying out any a priori transformation on A.This technique is given the name of pivoting by row.
- The factorization returns then the original matrix up to a row permutation

$$\mathbf{PA} = \mathbf{LU}$$

, being **P** the permutation matrix.

- In this case $\mathbf{Ax} = \mathbf{b} \rightarrow \mathbf{P}^{-1}\mathbf{LUx} = \mathbf{b} \rightarrow \mathbf{LUx} = \mathbf{Pb}$, and the systems to be solved are

$$\mathbf{Ly} = \mathbf{Pb}$$

$$\mathbf{Ux} = \mathbf{y}$$

The pivoting technique

MATLAB and OCTAVE provides a built in algorithm for general LU-decomposition, it can be called by

```
[L U]=lu(A)
[L U P]=lu(A)
```

OCTAVE/MATLAB exercise

- For the matrix of the last example, $\mathbf{A} = \begin{bmatrix} 0 & 1 & 2 \\ 1 & 3 & 4 \\ 2 & 4 & 1 \end{bmatrix}$, obtain $\mathbf{L}, \mathbf{U}, \mathbf{P}$
- Obtain $\mathbf{A}$ back from $\mathbf{L}, \mathbf{U}, \mathbf{P}$
- Write `[L U]=lu(A)`, What is now the value of $\mathbf{L}$?

The pivoting technique

OCTAVE/MATLAB exercise

Write a MATLAB function that solves a linear system using *LU*-decomposition. Built-in function `lu()` can be used, so only the substitution must be programmed.

- Inputs: **A**, **b**
- Output: **x**, cpu time consumed

Check the behavior of the program generating matrices of different indexes using `A=rand(n,n)`, `B=tril(a,0)`, `C=triu(a,0)`

Accuracy of LU-methods

- Although a matrix satisfies the conditions for a *LU* decomposition, big errors might appear if pivot elements are near to zero. This errors are alleviated with the pivoting technique, but results might be yet rather unsatisfactory.
- Let be the system $\mathbf{Ax} = \mathbf{b}$ and let $\hat{\mathbf{x}}$ be the exact solution. Then, if the system is numerically solved, the relative error in the solution $\mathbf{x}$ can be defined as

$$\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|}$$

- If the independent term is slightly modified (a rounding error when constructing $\delta\mathbf{b}$) then the new system becomes ($\mathbf{Ax} = \mathbf{b} + \delta\mathbf{b}$). It can be demonstrated that the relative error (difference between exact solution using $\delta\mathbf{b}$ or $\mathbf{b} + \delta\mathbf{b}$) is bounded by

$$\frac{\|\mathbf{x} - \hat{\mathbf{x}}\|}{\|\mathbf{x}\|} \leq K(\mathbf{A}) \frac{\|\delta\mathbf{b}\|}{\|\mathbf{b}\|}$$

Accuracy of LU-methods

- The value $K(\mathbf{A})$ is called *spectral condition number of the matrix* $\mathbf{A}$ and in the particular case of symmetric positive definite $K(\mathbf{A}) = \frac{|\lambda|_{max}}{|\lambda|_{min}}$ being $|\lambda|_{max}$ and $|\lambda|_{min}$ the maximum and minimum modulus of the eigenvalues of $\mathbf{A}$.
- $K(\mathbf{A}) \geq 1$, and the bigger its value, the faster the error amplification.
- When $K(\mathbf{A})$ is large, the matrix is $ill - conditioned$: the error in the solution might be large even with small errors in the system coefficients.
- The MATLAB/OCTAVE expression to obtain the *spectral condition number of the matrix* $\mathbf{A}$, is `cond(A)`.

Accuracy of LU-methods

Let be the systems (a) and (b)

$$(a)\begin{cases} x+y=2 \\ x+1.001y=2 \end{cases} \qquad (b)\begin{cases} x+y=2 \\ x+1.001y=2.001 \end{cases}$$

The solution of (a) is $x=2, y=0$, while the solution of (b) is $x=1, y=1$, so the coefficient matrix **A** is ill-condition ed

OCTAVE/MATLAB exercise

Obtain L and U using gauss substitution and solve the system
Obtain the condition number of the matrix of coefficients
Obtain the eigenvalues of the matrix by using `eig(A)`, which is the relation between condition number and the eigenvalues?

The MATLAB/OCTAVE command for solving linear systems

In order to solve directly a linear system $\mathbf{Ax} = \mathbf{b}$ in the better way in MATLAB/OCTAVE a new command can be used:

```
x=A\b
```

It will call different algorithms to solve the system depending on the type of matrix:

- If **A** is upper or lowe triangular, it will just use the substitution algorithm
- In case **A** is symmetric and with real positive diagonal elements will use Cholesky decomposition (a less general but faster method than LU)
- Otherwise, pivoting LU decomposition will be used

OCTAVE/MATLAB exercise

Solve again the different examples of previous exercises for random value of **b**

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Iterative methods

- An iterative method for the solution of the linear system $\mathbf{Ax} = \mathbf{b}$ consists in setting up a sequence of $\{\mathbf{x}^{(k)}, k \geq 0\}$ that converges to the exact solution

$$\lim_{k \to \infty} \mathbf{x}^{(k)} = \mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$$

, for any initial vector $\mathbf{x}^{(0)}$.

- A possible solution is the succession

$$\mathbf{x}^{(k+1)} = \mathbf{B}\mathbf{x}^{(k)} + \mathbf{g}$$

, where $\mathbf{B}$ is a suitable matrix and $\mathbf{g}$ is a vector depending on $\mathbf{b}$ and $\mathbf{A}$ (operating $\mathbf{g} = (\mathbf{I} - \mathbf{B})\mathbf{A}^{-1}\mathbf{b}$)

- A valid $\mathbf{B}$ should ensure convergency for any $\mathbf{x}^{(0)}$, and that is fulfilled in the case of symmetric, definite positive $\mathbf{B}$ with maximum absolute value of eigenvalues (spectral ratio)$\rho(\mathbf{B}) \leq 1$.

Iterative methods: Jacobi

If the diagonal entries of A are nonzero, let **D** be the diagonal matrix $\mathbf{D} = \mathrm{diag}(a_{11}, a_{22}, \cdots, a_{nn})$, the Jacobi iterative method consist on this series

$$\mathbf{x}^{(k+1)} = \mathbf{D}^{-1}(\mathbf{D} - \mathbf{A})\mathbf{x}^{(k)} + \mathbf{D}^{-1}\mathbf{b}$$

where $\mathbf{D}^{-1}$ is just the inverse of the diagonal terms.
If the matrix **A** is strictly diagonally dominant by row, then the Jacobi method converges.

OCTAVE/MATLAB exercise

Write a MATLAB function that provides the Jacobi iterative solution for a given n term. Apply the method to $\mathbf{A} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 2 & 8 & 5 & -2 \\ 3 & 5 & 3 & 0 \\ 4 & -2 & 0 & 1 \end{bmatrix}$ and

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

Iterative methods: Other methods and when to stop

- The error of a given iterative solution $\mathbf{x}^{(k)}$ can be measured by the *residual*, $r = \|\mathbf{b} - \mathbf{A}\mathbf{x}^{(k)}\|$.
- Once fixed the desired precision, a given method needs a certain number of iterations to reach that error (converge).
- The convergence rate depends on the method and on the matrix!
- Several methods can be found on the literature: *Gauss-Seidel, Richardson, Gradient* and *Conjugate Gradient*
- In general, iterative methods are faster than direct methods to obtain a solution when the matrix $\mathbf{A}$ is dense.
- For *sparse banded* linear system with small band-with, direct methods are faster

Sparse matrices

- In Engineering and Physic, large systems of linear equations (thousands of unknowns) usually appear as a result of the discretization of a partial derivative equation as the heat conduction, elasticity equations, etc.
- Fortunately, the coefficient matrices of the systems are full of zero terms, what is known as sparse matrices
- The memory needed to save a sparse system in a clever way may be of $O(n)$ instead of the $O(n^2)$ needed when all the matrix terms are saved.
- In addition, direct methods as LU can be adapted for sparse matrices resulting in computational costs much smaller than $O(n^2)$

Sparse matrices

A sparse matrix can be defined in several ways. MATLAB uses a system consisting on saving 3 vectors instead a full *nxn* matrix. The *nz* non-zero terms are saved in a vector of dimension *m*, and the positions of that terms are saved in the original matrix by other 2 vectors.

- In order to store a full $\mathbf{A}_{nxn}$ matrix as a sparse matrix, the function `AA=sparse(A)`
- In order to define directly the sparse matrix, declare it first with the maximum numbers of *nz* non-zero terms `AA=spalloc(n,n,nz)`, and then add each non-zero term using $A(i,j) = a_{ij}$
- Any matrix function of MATLAB (i.e. `inv(A)`, `det(A)`, `...` can be made with a sparse stored matrix, and the algorithms used in that case will be addapted for sparse matrices

Sparse matrices

OCTAVE/MATLAB exercise

Create a matrix 100x100 with diagonal terms equal to 1. and with 1000 terms of random position i, j and value
Inverse the matrix using `inv(A)`, and check the time
Create a sparse matrix from the original one, invert it and check the time
Compare the time for both cases