

# Introduction to Computational Physics – Exercise 5

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## Numerical linear algebra methods: Tridiagonal matrices

We consider the following tridiagonal  $N \times N$  matrix equation:

$$\underbrace{\begin{pmatrix} b_1 & c_1 & 0 & \cdots & 0 \\ a_2 & b_2 & c_2 & \ddots & \vdots \\ 0 & a_3 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & c_{N-1} \\ 0 & \cdots & 0 & a_N & b_N \end{pmatrix}}_{=: M = (m_{ij})} \underbrace{\begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{N-1} \\ x_N \end{pmatrix}}_{=: \vec{x} = (x_j)} = \underbrace{\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{N-1} \\ y_N \end{pmatrix}}_{=: \vec{y} = (y_i)} \quad (1)$$

**Gauß elimination** is the method of choice when one is interested in the solution  $\vec{x}$  of the linear set of equations  $M\vec{x} = \vec{y}$ , but does not need the information about the inverse matrix  $M^{-1}$  (which we would get using the Gauß-Jordan method). In this case, it is sufficient to convert the matrix  $M$  into an upper (or lower) triangular matrix  $M'$ :

$$M\vec{x} = \vec{y} \quad \xrightarrow{\text{Gauß elimination}} \quad M'\vec{x} = \vec{y}' \quad (2)$$

If we have obtained such a system  $M'\vec{x} = \vec{y}'$  with  $M'$  being in upper triangular form, i.e.  $m'_{ij} = 0$  for  $i > j$ , then we can compute the solution vector  $\vec{x}$  by **back substitution**:

$$x_N = \frac{y'_N}{m'_{N,N}} \quad x_{N-1} = \frac{1}{m'_{N-1,N-1}} (y'_{N-1} - m'_{N-1,N} x_N) \quad \cdots \quad (3)$$

Or in general:

$$x_i = \frac{1}{m'_{ii}} \left( y'_i - \sum_{j>i} m'_{ij} x_j \right) \quad (4)$$

The **Thomas algorithm** is a simplified form of Gauß elimination that can be used to solve tridiagonal systems of equation by creating an upper triangular form  $M'$  of the matrix  $M = (m_{ij})$ :

$$\left. \begin{aligned} m_{i+1,i} &\longrightarrow m_{i+1,i} - m_{ii} \frac{m_{i+1,i}}{m_{ii}} \\ m_{i+1,i+1} &\longrightarrow m_{i+1,i+1} - m_{i,i+1} \frac{m_{i+1,i}}{m_{ii}} \\ y_{i+1} &\longrightarrow y_{i+1} - y_i \frac{m_{i+1,i}}{m_{ii}} \end{aligned} \right\} \quad \text{for } i = 1, \dots, N \quad (5)$$

Python-Code 1: Numerical solution of a tridiagonal system of equations

```

1  # -*- coding: utf-8 -*-
2  """
3  Introduction to Computational Physics
4  - Exercise 05: Numerical Linear Algebra Methods
5                Tridiagonal Matrices and Gaussian Elimination
6  - Group: Simon Groß-Bölting, Lorenz Vogel, Sebastian Willenberg
7  """
8
9  import numpy as np; import matplotlib.pyplot as plt
10 from scipy.sparse import diags; from copy import deepcopy
11
12
13 def Gaussian_elimination(A,y):
14     ''' Numerical subroutine for the iterative expression for
15         Gaussian elimination without pivoting '''
16     a, b = deepcopy(A), deepcopy(y)
17     N = np.shape(a)[0]
18     for i in range(N):
19         for k in range(i+1,N):
20             factor = a[k,i]/a[i,i]
21             b[k] -= b[i]*factor
22             for j in range(i,N):
23                 a[k,j] -= a[i,j]*factor
24     return (a,b)
25
26 def Thomas_algorithm(A,y):
27     ''' Numerical subroutine for the Thomas algorithm (a simplified form
28         of Gaussian elimination that can be used to solve tridiagonal
29         systems of equations) '''
30     a, b = deepcopy(A), deepcopy(y)
31     N = np.shape(a)[0]
32     for i in range(N-1):
33         print(i)
34         factor = a[i+1,i]/a[i,i]
35         a[i+1,i] -= factor*a[i,i]
36         a[i+1,i+1] -= factor*a[i,i+1]
37         b[i+1] -= factor*b[i]
38     return (a,b)
39
40 def backward_substitution(A,y):
41     ''' Numerical subroutine for the iterative expression for
42         backward substitution '''
43     N = np.shape(A)[0]
44     x = np.zeros(N)
45
46     x[N-1] = y[N-1]/A[N-1,N-1]
47     for i in range(N-2,-1,-1):
48         x[i] = (y[i]-A[i,i+1]*x[i+1])/A[i,i]
49     return x
50
51 def solve_tridiagonal_system(a,b,c,y,method):
52     ''' Numerical subroutine that finds the solution vector x for a
53         tridiagonal equation system  $Ax=y$  '''
54     tridiag = diags([a,b,c], [-1,0,1]).toarray() # create tridiagonal matrix
55     if (method=='Gauss'):
56         out = Gaussian_elimination(tridiag,y)
57     elif (method=='Thomas'):
58         out = Thomas_algorithm(tridiag,y)
59     return (tridiag, backward_substitution(out[0],out[1]))
60
61 def relative_error(A,x,y):
62     ''' Function that puts the numerical solution x back into the original
63         matrix equation  $Ax=y$  and finds how much the result deviates from the
64         original right-hand-side y '''
65     return abs(np.dot(A,x)-y)/abs(y)
66
67
68 N = 10 # size of the tridiagonal matrix
69 a = -1.*np.ones(N-1) # values for the diagonal entries a
70 b = 3.*np.ones(N) # values for the diagonal entries b
71 c = -1.*np.ones(N-1) # values for the diagonal entries c
72 y = 0.2*np.ones(N) # values for the right-hand-side vector y

```

```

73 |
74 | tridiag, solution = solve_tridiagonal_system(a,b,c,y,method='Gauss')
75 | rel_error = relative_error(tridiag,solution,y)
76 | print('\nGaussian Elimination:\n')
77 | print('Solution vector:\n{}'.format(solution))
78 | print('Relative Error:\n{}'.format(rel_error))
79 |
80 | tridiag, solution = solve_tridiagonal_system(a,b,c,y,method='Thomas')
81 | rel_error = relative_error(tridiag,solution,y)
82 | print('\nThomas Algorithm:\n')
83 | print('Solution vector:\n{}'.format(solution))
84 | print('Relative Error:\n{}'.format(rel_error))

```