1 Sparse matrices from discrete elliptic PDEs

First I will describe the matrices you will need to work with on this assignment. We will look at three different ways to discretize the following elliptic problem:

\[-u_{xx} = f, \; x \in (0, 1)\]
\[u(0) = a\]
\[u_x(1) = b\]

(1)

You can discretize these over the uniform grid \(x_i = i\Delta x, \; i = 0, 1, ..., N - 1\) (with \(\Delta x = \frac{1}{N-1}\)) in a number of different ways (e.g. finite difference or finite element methods) each yielding different linear algebra problems:

\[Au = b\]

(2)

with \(A \in \mathbb{R}^{m \times m}\) and \(u, b \in \mathbb{R}^m\) and usually \(m = N - 1, N\) or \(N + 1\) (depending on the method of choice) where \(u_i = u(x_i)\). More importantly, the discretization method of choice can lead to a symmetric positive definite \(A\), a symmetric indefinite \(A\) or even a non-symmetric \(A\). We will consider the following three cases in this assignment:

1. Symmetric positive definite:

\[A_1 = \frac{1}{\Delta x} \begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 0 & 1 \end{pmatrix} \in \mathbb{R}^{(N-1) \times (N-1)}, \quad b = \begin{pmatrix} \frac{f_0 + f_1}{2} \Delta x + \frac{a}{\Delta x} \\ \frac{f_1 + f_2}{2} \Delta x \\ \vdots \\ \frac{f_{N-2}}{2} \Delta x + b \end{pmatrix}\]

2. Symmetric indefinite:

\[A_2 = \frac{1}{\Delta x} \begin{pmatrix} 1 & -1 & 0 & 0 & \cdots & 0 & \Delta x \\ -1 & 2 & -1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & -1 & 0 & 1 & 0 \\ \Delta x & 0 & \cdots & 0 & 0 & 0 \\ 0 & \cdots & 0 & -1 & 1 & 0 & \Delta x \end{pmatrix} \in \mathbb{R}^{(N+1) \times (N+1)}, \quad b = \begin{pmatrix} \frac{f_0}{2} \Delta x \\ \frac{f_0 + f_1}{2} \Delta x \\ \frac{f_1 + f_2}{2} \Delta x \\ \vdots \\ \frac{f_{N-2}}{2} \Delta x + b \end{pmatrix}\]

3. Non-symmetric:

\[A_3 = \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & 0 & 0 & \cdots & 0 \\ -1 & 2 & -1 & 0 & \cdots & 0 \\ 0 & -1 & 2 & -1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 2 & -1 \\ 0 & \cdots & 0 & -\Delta x & \Delta x \end{pmatrix} \in \mathbb{R}^{(N-1) \times (N-1)}, \quad b = \begin{pmatrix} f_1 + \frac{a}{\Delta x} \\ f_2 \\ \vdots \\ f_N-2 \\ b \end{pmatrix}\]
Here, \( f_i = f(x_i) \) and \( \bar{f}_i = \frac{\int_{x_{i-1}}^{x_{i+1}} f(x) dx}{\Delta x} \). Use \( u(x) = \sin(2\pi x) \) as the exact solution and generate \( f, a \) and \( b \) accordingly.

2 Programming problems

In the problems that follow, you will need to implement and test GMRES, CG and MINRES on the appropriate matrices above. For each case, you should solve the discrete PDE with \( N = 65,129,257,513 \) (and for all cases, use 64 iterations of the given method). Submit two plots with each problem. The first plot will show me that you have implemented the discrete elliptic PDE correctly. Plot \( \log(||e_N||_{\infty}) \) vs. \( \log(N) \) (where \( e_N \in \mathbb{R}^N \) is the error of the discretization of the PDE: \( e_i^N = \sin(2\pi x_i) - u_i^N \) and \( u_i^N \) is from the discrete problem with resolution \( N \)). Also include a plot of the best-fit line to this data and report the slope. The second plot should be \( \log(||r_k||_2) \) vs. \( k \) and should contain this data for each of the choices of grid resolution \( N = 64,128,256,512 \) (use color coding and a legend to distinguish which is which). In general, the condition number of the discrete PDE will be expected to get worse with \( N \) so you should expect to see slower convergence (in terms of number of iterations required) for the higher resolution problems. In all cases, use an initial guess of \( u_0 = 0 \).

1. Implement the GMRES algorithm and test it on the non-symmetric discrete problems.
2. Implement the CG algorithm and test it on the symmetric positive definite discrete problems.
3. Implement the Jacobi algorithm and test it on the symmetric positive definite discrete problems.
4. Implement the Gauss-Seidel algorithm and test it on the symmetric positive definite discrete problems.

3 Pen and paper

1. Show that you can evaluate the residual for the GMRES algorithm without assembling \( x^k = Q^k \lambda^k \) explicitly.
2. Prove that \( \lambda_k \neq \begin{pmatrix} \lambda_{k-1} \\ \lambda_k \end{pmatrix} \) for the Lanczos CG algorithm (using the notation from the course notes).
3. Prove that Gauss-Seidel converges whenever \( A \) is symmetric positive definite by showing that all the eigenvalues of \( (M^G)^{-1}N^G \) are less than 1 in magnitude and that this then implies convergence of the iterative method.