Department of molecular science and nanosystems 2022/23
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Exercise Class Numerical Methods

Direct and Iterative Methods for Linear Systems

Direct Methods

Exercise 1: Write a script that takes as input a symmetric and positive matrix A and solves a linear system $Ax = b$ using the Cholesky factorization. At the end print the solution $\bar{x}$ and the residual $r = Ax - b$.

Exercise 2: Write a script that takes as input a tridiagonal matrix A and solve a linear system $Ax = b$ using Thomas's algorithm. At the end print the solution $\bar{x}$ and the residual $r = Ax - b$.

- You can test your script with any tridiagonal matrix.
- Solve numerically

$$-u(x) = \pi^2 \sin(\pi x) \quad x \in [0,1]$$
$$u(0) = 0 = u(1)$$

What is the exact solution?

Iterative Methods

Exercise 3: Write a script that checks if a matrix $A \in \mathbb{R}^{n\times n}$ is diagonally dominant.

Exercise 4: Write a script which reads a square matrix $A \in \mathbb{R}^{n\times n}$ and a vector $b \in \mathbb{R}^n$ and solves the linear system $Ax = b$ with Jacobi's method. Plot the history of the the residual $\|r\|$.

Exercise 5: Write a script which reads a square matrix $A \in \mathbb{R}^{n\times n}$ and a vector $b \in \mathbb{R}^n$ and solves the linear system $Ax = b$ with Gauss-Seidel's method. Plot the history of the the residual $\|r\|$

Test your iterative methods with the following matrices in such way the solution is given by a vector of ones of the right dimension. Study the convergence of Jacobi and Gauss-Seidel methods: compute the spectral radius of the iteration matrix for each matrix.

- Build a matrix A_h such that $h = \{2, 4, 6, 8, 10\}$ using the following script
```
A = rand(10):
A = A - diag(diag(A));
s = sum(abs(A),2);
A = A+h*diag(s);
```
In this situation we change the diagonal dominance of the matrix A_h .
- $A = \begin{pmatrix} 3 & 0 & 4 \\ 7 & 4 & 2 \\ -1 & 1 & 2 \end{pmatrix}, \qquad A = \begin{pmatrix} -3 & 3 & -6 \\ -4 & 7 & -8 \\ 5 & 7 & -9 \end{pmatrix},$
- $A = \begin{pmatrix} 4 & 1 & 1 \\ 2 & -9 & 0 \\ 0 & -8 & -6 \end{pmatrix}, \qquad A = \begin{pmatrix} 7 & 6 & 9 \\ 4 & 5 & -4 \\ -7 & -3 & 8 \end{pmatrix}.$