DELFT UNIVERSITY OF TECHNOLOGY
Faculty of Electrical Engineering, Mathematics and Computer Science

The final grade of the test: (total number of points)/5

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TEST SCIENTIFIC COMPUTING (wi4201)
Wednesday January 22 2025, 13:30-16:30

1. Below 5 statements are given. If the statement is true give a short proof. If the statement is wrong give a counter example or an explanation.

   (a) $\mathbf{u} \in \mathbb{R}^n \Rightarrow \|\mathbf{u}\|_2 \leq \sqrt{n}\|\mathbf{u}\|_\infty$. (2 pt.)

   (b) $D \in \mathbb{R}^{n\times n}$ is a diagonal matrix, where $d_{i,i} = \frac{i}{n}$. For $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ the operator $(\mathbf{x}, \mathbf{y})_D$ is defined as: $(\mathbf{x}, \mathbf{y})_D = \mathbf{x}^T D\mathbf{y}$. $(\mathbf{x}, \mathbf{y})_D$ is an inner product. (2 pt.)

   (c) $Q \in \mathbb{R}^{n\times n}$ is an orthogonal matrix. The spectrum of A and Q^TAQ are the same. (2 pt.)

   (d) Let $\rho(A)$ be the spectral radius of A.

   $$\rho(A) < 1 \Rightarrow (I - A) \text{ is non-singular, and } \sum_{k=0}^{\infty} A^k = (I - A)^{-1}$$

   (2 pt.)

   (e) The amount of work per iteration of the Bi-CGSTAB method remains constant as a function of the number of iterations; (2 pt.)

2. Consider the following partial differential equation

   $$-\frac{\partial^2 u(x,y)}{\partial x^2} - \frac{\partial^2 u(x,y)}{\partial y^2} + ku(x,y) = k(x,y) \text{ for } (x,y) \in \Omega = [0,1] \times [0,1]$$

   and Dirichlet boundary conditions on the boundary $u(x,y) = 0$ for $(x,y) \in \partial\Omega$. Here, k is a real constant. For the discretization we use m intervals in both coordinate directions.

   (a) Show that the partial differential equation is elliptic. (1 pt.)

   (b) Give a discretization of the equation such that the truncation error is $O(h^2)$.(2 pt.)

(c) Give the stencil of this discretization in an interior node and in the lower left corner. Note that the boundary conditions are eliminated. (2 pt.)

(d) We use lexicographic ordering of the unknowns. Give the structure of the matrix A and its bandwidth. Motivate why A is symmetric. (2 pt.)

(e) Take $k = 2$. Use Gershgorin's theorem to approximate the eigenvalues. (1 pt.)

(f) Take $k = -2$. Use Gershgorin's theorem to approximate the eigenvalues. (1 pt.)

(g) Taking into account your answers for $k = 2$ and $k = -2$, which Krylov subspace method would you recommend? Include a motivation for your answer. (1 pt.)

3. (a) We are given

$$A_1 = \begin{bmatrix} 1 & 1 & 1 \\ 2 & 3 & 5 \\ 4 & 6 & 8 \end{bmatrix},$$

Find the LU decomposition such that $A_1 = LU$. Clearly show your computations and the construction of the Gauss vectors. (4 pt.)

(b) We are now given

$$A_2 = \begin{bmatrix} 1 & 1 & 1 \\ 2 & \mathbf{2+\boldsymbol{\varepsilon}} & 5 \\ 4 & 6 & 8 \end{bmatrix}, b = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

such that $A_2 x = b$ and ε is a small real constant.

The LU decomposition (without pivoting) of A_2 is given by

$$\hat{L} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 4 & \frac{2}{\varepsilon} & 1 \end{bmatrix}, \hat{U} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & \varepsilon & 3 \\ 0 & 0 & 4 - \frac{6}{\varepsilon} \end{bmatrix},$$

such that if we use $\hat{L}$ and $\hat{U}$ to solve $A_2 x = b$, we get

$$x \approx \begin{bmatrix} \frac{7}{3} \\ -\frac{2}{3} \\ -\frac{2}{3} \end{bmatrix}$$

Now suppose ε is of machine precision order, such that $4 - \frac{6}{\varepsilon} \approx -\frac{6}{\varepsilon}$ in $\hat{U}$. In that case, we get

$$\hat{U} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & \varepsilon & 3 \\ 0 & 0 & -\frac{6}{\varepsilon} \end{bmatrix}$$

What happens to the solution x? What can you say about the growth of the error? (2 pt.)

(c) Finally, we are given

$$A_3 = \begin{bmatrix} 1 & 1 & 1 \\ 2 & \mathbf{2} & 5 \\ 4 & 6 & 8 \end{bmatrix}.$$

Use partial pivoting to construct $PA_3 = LU$. In your answer clearly show why the LU decomposition without pivoting breaks down. (4 pt.)

4. Consider the linear system $A\mathbf{u} = \mathbf{f}$, where $A \in \mathbb{R}^{n\times n}$ is an SPD matrix.

(a) If A is SPD show that $||\mathbf{u}||_A = \sqrt{\mathbf{u}^T A\mathbf{u}}$ is a norm.
(Hint: a norm has the following properties: $||\mathbf{u}|| \geq 0$ with equality only for $\mathbf{u} = \mathbf{0}$, $||c\mathbf{u}|| = |c|||\mathbf{u}||$ and $||\mathbf{u}+\mathbf{v}|| \leq ||\mathbf{u}||+||\mathbf{v}||$. In the proofs you can use the inequality $\mathbf{u}^T A\mathbf{v} \leq ||\mathbf{u}||_A||\mathbf{v}||_A$. (2 pt.)

(b) We assume that $\mathbf{u}^1 \in$ span $\{\mathbf{r}^0\}$. Determine $\mathbf{u}^1$ such that $\|\mathbf{u}-\mathbf{u}^1\|_A \leq \|\mathbf{u}-\mathbf{y}\|_A$ for all $\mathbf{y} \in$ span $\{\mathbf{r}^0\}$. (2 pt.)

(c) The matrix A corresponds to a shifted discretized Poisson operator. The eigenvalues are given by

$$\lambda_{k,\ell} = 5 - 2\cos\frac{\pi k}{61} - 2\cos\frac{\pi \ell}{61} \quad , \quad 1 \leq k, \ell \leq 60.$$

Determine the linear rate of convergence for the Conjugate Gradient method. (2 pt.)

(d) If the convergence of the Conjugate Gradient method is too slow a preconditioner M could be used. Give three properties for matrix M in order to be a suitable preconditioner. How can such a preconditioner be combined with Conjugate Gradient in order to obtain the Preconditioned Conjugate Gradient method? (2 pt.)

(e) Consider matrix A given by: $A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 81 & -1 \\ 0 & -1 & 81 \end{pmatrix}$ Give an estimate of the convergence of CG and give an estimate of the number of iterations needed such that

$$\frac{\|\mathbf{u}-\mathbf{u}^k\|_{\tilde{A}}}{\|\mathbf{u}-\mathbf{u}^0\|_{\tilde{A}}} \leq 10^{-12}.$$

Take for the preconditioner the best diagonal matrix and answer the same questions for PCG. (2 pt.)

5. In this exercise we consider variants of the Power method to approximate the eigenvalues of a matrix $A \in \mathbb{R}^{n\times n}$. The Power method is given by:

$\mathbf{q}_0 \in \mathbb{R}^n$ is given
for $k = 1, 2, ...$

$\mathbf{z}_k = A\mathbf{q}_{k-1}$
$\mathbf{q}_k = \mathbf{z}_k / \|\mathbf{z}_k\|_2$
$\lambda^{(k)} = \mathbf{q}_{k-1}^T \mathbf{z}_k$

endfor

The eigenvalues are ordered such that $|\lambda_1| > |\lambda_2| \geq ... \geq |\lambda_n|$. The corresponding eigenvectors are denoted by $\{\mathbf{v}_1, ..., \mathbf{v}_n\}$.

(a) We assume that $\mathbf{q}_{k-1}$ can be written as $\mathbf{q}_{k-1} = \mathbf{v}_1 + \mathbf{w}$ with $\|\mathbf{w}\|_2 = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right)$. Show that

$$|\lambda_1 - \lambda^{(k)}| = O\left(\left|\frac{\lambda_2}{\lambda_1}\right|^k\right) .$$

(2.5 pt.)

(b) Given a matrix $A \in \mathbb{R}^{n \times n}$, where

$$\lambda_1 = 1000 \ , \quad \lambda_2 = 999 \ \text{ and } \ \lambda_n = 900 \ .$$

Explain how the shifted Power method can be used to approximate λ_1 and give an optimal value for the shift. (2.5 pt.)

(c) Note that the Power method is a linearly converging method. Give a good stopping criterion for the Power method. (2.5 pt.)

(d) Given a matrix $A \in \mathbb{R}^{n \times n}$, where

$$\lambda_1 = 1000 \ , \quad \lambda_{n-1} = 1.1 \ \text{ and } \ \lambda_n = 1 \ .$$

Give a fast converging method to approximate λ_n. (2.5 pt.)