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FACULTY OF ELECTRICAL ENGINEERING, MATHEMATICS AND COMPUTER SCIENCE

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TEST SCIENTIFIC COMPUTING (wi4201)
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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) $A \in \mathbb{R}^{n \times n}$, $\Rightarrow \|A\|_1 = \|A\|_\infty$. (2 pt.)

   (b) assume A to be the 3-by-3 matrix

   $$A = \begin{pmatrix} 2 & 1 & -1 \\ 4 & 3 & 0 \\ -1 & -2 & 4 \end{pmatrix}.$$

   Give the three Gershgorin disks that contain the eigenvalues of the matrix A; (2 pt.)

   (c) $A \in \mathbb{R}^{n \times n}$ and assume $\mathbf{u}$ to be an eigenvector of A with eigenvalue λ. The Krylov subspace $K^k(A, \mathbf{u})$ is a subspace in $\mathbb{R}^n$. Give the dimension of this space, and explain your answer. (2 pt.)

   (d) $A \in \mathbb{R}^{n \times n}$ $\rho(A) \leq \|A\|$ for any multiplicative norm $\|.\|$. (2 pt.)

   (e) $A \in \mathbb{R}^{n \times n}$ is a lower triangular matrix with zero elements on the main diagonal $\Rightarrow A^n = 0$. (2 pt.)

2. For a given function f we consider the following boundary value problem:

   $$-\frac{d^2u(x)}{dx^2} + \lambda u(x) = f(x) \text{ for } 0 < x < 1, \quad (1)$$

   where λ is a positive real number, with boundary conditions

   $$u(0) = 0 \text{ and } u(1) = 0. \quad (2)$$

   A finite difference method is used on a uniform mesh with N intervals and mesh width $h = 1/N$.

   (a) Give the finite difference stencil for internal grid points and show that it is $O(h^2)$. (1 pt.)

(b) The eigenvectors $\mathbf{v}^k$ of the resulting coefficient matrix A are given and have components:

$$v_i^k = \sin(k\pi\, x_i) = \sin(k\pi\,(i-1)\,h) \text{ for } 1 \le i \le N+1 \tag{3}$$

derive an expression for the corresponding eigenvalues λ_k as a function of the meshwidth h by computing the action of A^h on these eigenvectors. It suffices here to consider the matrix rows corresponding to the grid nodes not having any connections to the boundary nodes. (Hint: $\sin(\alpha+\beta)+\sin(\alpha-\beta) = 2\sin(\alpha)\cos(\beta)$). (3 pt.)

(c) Show that the matrix A is SPD. (2 pt.)

(d) The perturbed solution $\mathbf{u}+\Delta\mathbf{u}$ solves the system $A(\mathbf{u}+\Delta\mathbf{u}) = \mathbf{f}+\Delta\mathbf{f}$. Show that $\|\frac{\Delta\mathbf{u}\|}{\|\mathbf{u}\|} \le \kappa(A)\frac{\|\Delta\mathbf{f}\|}{\|\mathbf{f}\|}$ where $\kappa(A)$ denotes the condition number of A measured in the norm $\|\cdot\|$. Give an upperbound for $\kappa_2(A)$ as a function of the meshwidth h. (2 pt.)

(e) To solve the linear system, one can use a direct or an iterative method. Which method is preferred (motivate your answer)? (2 pt.)

3. (a) Show that if $A \in \mathbb{R}^{n\times n}$ has an LU decomposition and is nonsingular, then L and U are unique, where we assume that $l_{i,i} = 1$. (2 pt.)

(b) The k-th Gauss-vector $\alpha^{(k)} \in \mathbb{R}^n$ is defined as

$$\alpha^{(k)} = (\underbrace{0,\ldots,0}_{k},\underbrace{\mathbf{b}_k/a_{k,k}^{(k-1)}}_{n-k})^T . \tag{4}$$

Give an expression for $(M_{n-1}...M_1)^{-1}$, where $M_k^{-1} = I + \alpha^{(k)}\mathbf{e}_k^T$. (2 pt.)

(c) Suppose we have a penta-diagonal matrix $A \in \mathbb{R}^{n\times n}$. For a given m, where $1 < m < n$, we know that the elements $a(i-m,i)$, $a(i-1,i)$, $a(i,i)$, $a(i,i+1)$, and $a(i,i+m)$, are nonzero. Give the non-zero pattern of the L and U matrix after the LU-decomposition without pivotting. (2 pt.)

(d) Give the outline of the LU-decomposition method (without pivotting) to solve $A\mathbf{u} = \mathbf{f}$, where $A \in \mathbb{R}^{n\times n}$ is a non-singular penta-diagonal matrix and give the amount of flops. (2 pt.)

4. In this exercise we have to solve a linear system $A\mathbf{u} = \mathbf{f}$, where A is an $n \times n$ non-singular matrix.

(a) Take $\mathbf{u}_1 = \alpha\mathbf{f}$. Derive an expression for α such that $\|\mathbf{u}-\mathbf{u}_1\|_{A^TA}$ is minimal. (2 pt.)

(b) The CGNR method is the CG method applied to $A^TA\mathbf{u} = A^T\mathbf{f}$. Show that the 2-norm of the residuals is monotone decreasing. (2 pt.)

(c) Give a 3×3 non-diagonal matrix such that CGNR converges in one iteration for every right-hand side vector $\mathbf{f}$. (2 pt.)

(d) Given the algorithm

Bi-CGSTAB method

$\mathbf{u}^0$ is an initial guess; $\mathbf{r}^0 = \mathbf{f} - A\mathbf{u}^0$;
$\bar{\mathbf{r}}^0$ is an arbitrary vector, such that $(\bar{\mathbf{r}}^0)^T\mathbf{r}^0 \neq 0$, e.g., $\bar{\mathbf{r}}^0 = \mathbf{r}^0$;
$\rho_{-1} = \alpha_{-1} = \omega_{-1} = 1$;
$\mathbf{v}^{-1} = \mathbf{p}^{-1} = 0$;
for $i = 0, 1, 2, ...$ do
  $\rho_i = (\bar{\mathbf{r}}^0)^T\mathbf{r}^i$; $\beta_{i-1} = (\rho_i/\rho_{i-1})(\alpha_{i-1}/\omega_{i-1})$;
  $\mathbf{p}^i = \mathbf{r}^i + \beta_{i-1}(\mathbf{p}^{i-1} - \omega_{i-1}\mathbf{v}^{i-1})$;
  $\hat{\mathbf{p}} = M^{-1}\mathbf{p}^i$;
  $\mathbf{v}^i = A\hat{\mathbf{p}}$;
  $\alpha_i = \rho_i/(\bar{\mathbf{r}}^0)^T\mathbf{v}^i$;
  $\mathbf{s} = \mathbf{r}^i - \alpha_i\mathbf{v}^i$;
  if $\|\mathbf{s}\|$ small enough then
    $\mathbf{u}^{i+1} = \mathbf{u}^i + \alpha_i\hat{\mathbf{p}}$; quit;
  $\mathbf{z} = M^{-1}\mathbf{s}$;
  $\mathbf{t} = A\mathbf{z}$;
  $\omega_i = \mathbf{t}^T\mathbf{s}/\mathbf{t}^T\mathbf{t}$;
  $\mathbf{u}^{i+1} = \mathbf{u}^i + \alpha_i\hat{\mathbf{p}} + \omega_i\mathbf{z}$;
  if $\mathbf{u}^{i+1}$ is accurate enough then quit;
  $\mathbf{r}^{i+1} = \mathbf{s} - \omega_i\mathbf{t}$;
end for

The matrix M in this scheme represents the preconditioning matrix. Determine the minimal amount of memory and flops per iteration. (2 pt.)

(e) Give a comparison of the mathematical properties of the CGNR and Bi-CGSTAB method (both without preconditioning). (2 pt.)

5. In this exercise we consider variants of the Power method to approximate the eigenvalues of a matrix A. The Power method is given by:

$\mathbf{q}_0 \in \mathbb{R}^n$ is given
for $k = 1, 2, ...$
  $\mathbf{z}_k = A\mathbf{q}_{k-1}$
  $\mathbf{q}_k = \mathbf{z}_k/\|\mathbf{z}_k\|_2$
  $\lambda^{(k)} = \bar{\mathbf{q}}_{k-1}^T\mathbf{z}_k$
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 $\mathbf{q}_k$ can be written as $\mathbf{q}_k = \mathbf{v}_1 + \mathbf{w}$ 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.)