SF2524 Matrix Computations for Large-scale Systems Exam

Aids: None Time: Four hours

Grades: E: 16 points, D: 19 points, C: 22 points, B: 25 points, A: 28 points (out of the possible 35 points, including bonus points from homeworks).

Problem 1 (4p)

- (a) How is the Rayleigh quotient iteration for the matrix $A \in \mathbb{R}^{n \times n}$ defined? Answer with formulas and/or algorithm.
- (b) Suppose $Q \in \mathbb{R}^{n \times m}$ is an orthogonal matrix $(Q^T Q = I)$ with n > m. Describe the Gram-Schmidt (GS) procedure.
- (c) Suppose Q is as in (b). Describe the double Gram-Schmidt (DGS) procedure.
- (d) What are the advantages / disadvantages of GS vs DGS?

Problem 2 (4p)

- (a) Let A be a non-singular matrix with eigenvalues in all four quadrants of complex plane. Give a definition of the matrix sign function for this matrix?
- (b) Let $A \in \mathbb{R}^{n \times n}$. Suppose $X_0 = 2A$ and let X_k be defined by

$$X_{k+1} = \frac{1}{2}X_k + X_k^{-1}A, \ k = 1, \dots$$

If the sequence X_0, X_1, \ldots converges, what does it converge to?

(c) Suppose we have very reliable algorithms to compute the matrix functions f and g. Derive a formula that produces the first k derivatives at x = 0 of h(x) = f(g(x)) for scalar-valued x using matrix functions f and g.

Problem 3 (5p) Consider a matrix $A \in \mathbb{R}^{n \times n}$ with $\ell < n$ eigenvalues. Assume A is diagonalizable such that there exists invertible $X \in \mathbb{C}^{n \times n}$ and diagonal $\Lambda \in \mathbb{C}^{n \times n}$ when $A = X^{-1}\Lambda X$.

- (a) How are the iterates of GMRES defined **and** computed? Answer with formulas and/or an algorithm.
- (b) In this course we found that the iterates of GMRES satisfy $||Ax_k-b|| = \min_{p \in P_k^0} ||p(A)b||$. Use this to determine the error of GMRES after $k = \ell$ iterations, under the assumption that no premature breakdown occurs. Note that $\ell < n$ meaning that we have many multiple eigenvalues.
- (c) Suppose $D \in \mathbb{R}^{n \times n}$ is a diagonal matrix with entries d_1, \ldots, d_n and let $b = [b_1, \ldots, b_\ell, 0, \ldots, 0]^T \in \mathbb{R}^n$. What is the structure of the Krylov subspace $\mathcal{K}_k(D, b)$ when $k < \ell$? Use this to show that GMRES for Dx = b is independent of $d_{\ell+1}, \ldots, d_n$.

Problem 4 (3p) Felix the fluid mechanician has to compute f(A)b where $f(z) = \sqrt{z}$ and $A \in \mathbb{R}^{n \times n}$ is a large and sparse matrix. One matrix vector product corresponding to A takes approximately $n^{1.5}/10$ time-units in a particular computing environment, and the orthogonalization of one vector against p (orthogonal) vectors takes 10pn time-units. Clearly state simplifying assumptions, and estimations when analyzing the following situations.

- (a) Felix is an expert on convergence theory for Arnoldi's method for matrix functions and found that we can assume linear convergence for this iteration, and that the convergence factor can be estimated by $\rho = 0.2$. What is the computation time to reach machine precision (as a function n) with Arnoldi's method for matrix functions?
- (b) Newton's method for the matrix square root has quadratic convergence. What is the computation time to reach machine precision for f(A)? Justify assumptions about computation time for matrix-matrix products.

Problem 5 (4p)

- (a) What is the (basic) QR-method? Answer with formulas and/or an algorithm.
- (b) The QR-factorization of a matrix is not unique, unless the sign of the diagonal entries in the diagonal are fixed. Suppose A = QR is a QR-factorization. Find a matrix Psuch that $\tilde{Q} = QP$ and $\tilde{R} = PR$ is a different QR-factorization
- (c) Suppose A_1 is the result of one step of the shifted QR-method. Let A_1 be the result of one step of the shifted QR-method with the other QR-factorization in (b). Derive a formula for \tilde{A}_1 , in terms of A_1 ? How does the non-uniqueness of the QR-factorization influence the QR-method?

Problem 6 (4p) Suppose we have computed an Arnoldi factorization $AQ_k = Q_{k+1}\underline{H}_k$.

- (a) How are the eigenvalue approximations for Arnoldi's method for eigenvalue problems computed from the Arnoldi factorization?
- (b) Suppose $h_{k+1,k} = 0$. Show that an eigenvalue of H_k is an eigenvalue of A.

Problem 7 (5p)

Let v_{k+1} , w_{k+1} , be generated by carrying out k steps of Algorithm X where $A \in \mathbb{R}^{n \times n}$.

- (a) Prove that v_{k+1} and w_{k+1} are elements of certain Krylov subspaces? Which ones?
- (b) Simplify the Algorithm X for the case A is symmetric. Under this symmetry assumption, Algorithm X is equivalent to an algorithm in this course. Which one?
- (c) The iterates of the Algorithm X satisfy

$$AV_k = V_{k+1}\underline{T}_k$$
$$A^T W_k = W_{k+1}\underline{T}_k$$

where $\underline{T}_k \in \mathbb{R}^{(k+1) \times k}$. Express V_k , W_k and \underline{T}_k in terms of quantities in the algorithm.

Algorithm X:

1.
$$\tilde{v}_{1} = b - Ax_{0}, v_{1} = w_{1} = \tilde{v}_{1}/\|\tilde{v}_{1}\|$$

for $k = 1, ...$ until converged
2. $\tilde{v}_{k+1} = Av_{k}$
3. $\tilde{w}_{k+1} = A^{T}w_{k}$
4. $\alpha_{k} = w_{k}^{T}\tilde{v}_{k+1}$
5. $\tilde{v}_{k+1} = \tilde{v}_{k+1} - \alpha_{k}v_{k}$
6. $\tilde{w}_{k+1} = \tilde{w}_{k+1} - \alpha_{k}w_{k}$
7. if $k > 1$
8. $\tilde{v}_{k+1} = \tilde{v}_{k+1} - \beta_{k-1}v_{k}$
9. $\tilde{w}_{k+1} = \tilde{w}_{k+1} - \beta_{k-1}w_{k}$
10. $\gamma_{k} = \|\tilde{v}_{k+1}\|, v_{k+1} = \tilde{v}_{k+1}/\gamma_{k}$
11. $\beta_{k} = \|\tilde{w}_{k+1}\|, w_{k+1} = \tilde{w}_{k+1}/\beta_{k}$
end