SF2524 Matrix Computations for Large-scale Systems
Solution sketch

Aids: None Time: Four hours

Grades: E: 14 points, D: 16 points, C: 18 points, B: 20 points, A: 22 points (out of the possible 27 points, including bonus points from homeworks).

Problem 1 (4p)

(a) What is an Arnoldi factorization? Describe the properties of the matrices involved in the factorization.

(b) Suppose r_A is the Rayleigh quotient for A and suppose r_H is the Rayleigh quotient for H_m. Find a function f such that $r_H(z) = f(r_A(Q_m z))$ for all z. In other words, express $r_H(z)$ in terms of $r_A(Q_m z)$

(c) Suppose the eigenvector approximation $\tilde{x} = Q_m z$ has accuracy $\mathcal{O}(\alpha^m)$ for some small value α. What is the order of magnitude of the accuracy of the eigenvalue approximation $r_A(Q_m z)$, if A is symmetric?

Solution:

(a) An Arnoldi factorization of a matrix $A \in \mathbb{R}^{n\times n}$ consists of matrices $Q_{m+1} = [Q_m, q_{m+1}] \in \mathbb{R}^{n\times m+1}$ and $\underline{H}_m \in \mathbb{R}^{(m+1)\times m}$ such that

$$AQ_m = Q_{m+1}\underline{H}_m$$

where Q_{m+1} is an orthogonal matrix and $\underline{H}_m$ is a Hessenberg matrix.

(b) We note that we have directly from definition of the Rayleigh quotient that

$$r_A(Q_m z) = \frac{(Q_m z)^T A Q_m z}{z^T Q_m^T A Q_m z} = \frac{(Q_m z)^T A Q_m z}{z^T Q_m^T Q_{m+1}\underline{H}_m z}.$$

Since Q_{m+1} is orthogonal and Q_m are the first columns of Q_{m+1}, we have $Q_{m+1}^T Q_m = [I, 0] \in \mathbb{R}^{(m+1)\times m}$ and $Q_{m+1}^T Q_m \underline{H}_m = [I, 0]\underline{H}_m = H_m \in \mathbb{R}^{m\times m}$, with the standard notation for H_m. Therefore,

$$r_A(Q_m z) = \frac{z^T H_m z}{z^T z} = r_H(z).$$

We have $f(x) = x$.

(c) Since A is symmetric, the Rayleigh quotient is quadratic in the eigenvector error. Hence,

$$r_A(Q_m z) - \lambda = O(\|Q_m z \pm v\|^2) = O(\alpha^{2m}).$$

Problem 2 (4p)

(a) Describe the basic QR-method, in formulas or simple MATLAB-code.

(b) Describe the shifted QR-method, in formulas or simple MATLAB-code.

(c) Suppose $A \in \mathbb{R}^{n\times n}$ satisfies the property $A = \rho A^T$ for some value ρ. Show that this property is preserved by the QR-method. Under what conditions is it preserved for the shifted QR-method?

Solution:

(a) Given a matrix A we set $A_0 = A$ and repeat

- Compute a QR-factorization of A_i such that $Q_i R_i = Q_i$
- Compute the next matrix with $A_{i+1} = R_i Q_i$

(b) The shifted QR-method is (for a given sequence of shifts $\sigma_0, \ldots$)

- Compute a QR-factorization of A_i such that $Q_i R_i = A_i - \sigma_i I$
- Compute the next matrix with $A_{i+1} = R_i Q_i + \sigma_i I$

(c) Suppose $A_0 = \rho A_0^T$ or equivalently $\rho A_0 = A_0$. From the formulas above, we have

$$A_{i+1} = R_i Q_i = Q_i^T A Q_i.$$

Therefore

$$A_1^T = (Q_1 A Q_1)^T = Q_1 A_0^T Q_1 = \rho Q_1^T A_0 Q_1 = \rho A_1$$

Hence, by induction the property is preserved unconditionally. (Strictly speaking, it is only preserved if σ_i is real, but the question did not specify if σ is real or complex.) The unshifted QR-method is a special case of the shifted QR-method, so it is always preserved for the unshifted QR-method.

Problem 3 (3p) Prove the following generalization of the min-max theory for the convergence of GMRES. Suppose $A \in \mathbb{R}^{n\times n}$ is a symmetric matrix and suppose $b = c_1 v_1 + \cdots + c_\ell v_\ell$ with $\ell < n$, and $v_1, \ldots, v_\ell$ are normalized eigenvectors of A. The constants $c_1, \ldots, c_\ell$ are non-zero and satisfy $c_1^2 + \cdots + c_\ell^2 = 1$. Show that

$$\|Ax_k - b\| \leq \min_{p \in P_k^0} \max_{i=1,\ldots,\ell} |p(\lambda_i)|.$$

where x_k is the iterate generated by k steps of GMRES. You may use any theorem in the course.
Hint: You may use that symmetric matrices are diagonalizable and that the eigenvectors are orthogonal.

Solution: Since A is symmetric, we know it is diagonalizable with $A = V\Lambda V^{-1}$ where $V^{-1} = V^T$ and Λ diagonal. By the definition of GMRES we have

$$\|Ax_k - b\| = \min_{x\in\mathcal{K}_k(A,b)} \|Ax - b\| = \min_{p\in P_k^0} \|p(A)b\|,$$

where we used that how a residual $Ax - b$ is parameterized by a polynomial (as in the lecture notes). We now use that $b = c_1v_1 + \cdots + c_\ell v_\ell$, and note that $p(A)v_i = p(\lambda_i)v_i$ since v_i are eigenvectors. Therefore

$$\min_{p\in P_k^0} \|p(A)b\|^2 = \min_{p\in P_k^0} \|p(A)(c_1v_1 + \cdots + c_\ell v_\ell)\|^2 = \min_{p\in P_k^0} \|c_1p(\lambda_1)v_1 + \cdots + c_\ell p(\lambda_\ell)v_\ell\|^2 =$$
$$\min_{p\in P_k^0} \left(\tilde{V}\begin{bmatrix} p(\lambda_1)c_1 \\ \vdots \\ p(\lambda_\ell)c_\ell \end{bmatrix}\right)^T \left(\tilde{V}\begin{bmatrix} p(\lambda_1)c_1 \\ \vdots \\ p(\lambda_\ell)c_\ell \end{bmatrix}\right)$$

where $\tilde{V} = [v_1, \ldots, v_\ell]$. Since $v_1, \ldots, v_\ell$ are orthonormal, $\tilde{V}^T\tilde{V} = I$ and

$$\left(\tilde{V}\begin{bmatrix} p(\lambda_1)c_1 \\ \vdots \\ p(\lambda_\ell)c_\ell \end{bmatrix}\right)^T \left(\tilde{V}\begin{bmatrix} p(\lambda_1)c_1 \\ \vdots \\ p(\lambda_\ell)c_\ell \end{bmatrix}\right) = \begin{bmatrix} p(\lambda_1)c_1 \\ \vdots \\ p(\lambda_\ell)c_\ell \end{bmatrix}^T \begin{bmatrix} p(\lambda_1)c_1 \\ \vdots \\ p(\lambda_\ell)c_\ell \end{bmatrix} = |c_1|^2|p(\lambda_1)|^2 + \cdots + |c_\ell|^2|p(\lambda_\ell)|^2 \leq$$
$$(|c_1|^2 + \cdots + |c_\ell|^2) \max_{i=1,\ldots,\ell} |p(\lambda_i)|^2 = \max_{i=1,\ldots,\ell} |p(\lambda_i)|^2$$

Hence,

$$\|Ax_k - b\| \leq \min_{p\in P_k^0} \max_{i=1,\ldots,\ell} |p(\lambda_i)|.$$

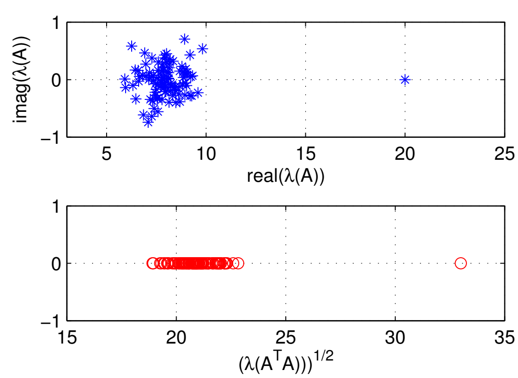
Q.E.D

Problem 4 (5p)

Suppose the eigenvalues and singular values of a matrix A are as in the figure to the right. Give a constant $\beta < 1$ such that after k iterations we have

$$\text{err} \leq \alpha\beta^k.$$

for method ♣. Define also how the error *err* is measured. You may invoke any theorem in the course. Answer this for ...



(a) ♣ = GMRES

(b) ♣ = CGN (sometimes called CGNE)

(c) ♣ = Arnoldi's method for eigenvalues corresponding to the eigenvalue close to $\lambda_0 \approx 20$.

Solution: We read-off properties from the figures to the right.

(a) With the single disk specialization of the GMRES min-max bound we have

$$\frac{\|Ax-b\|}{\|b\|} \le \|V\|\|V^{-1}\| \frac{\rho|^k}{|c|}$$

where $\rho = 7.5$ and $c = 12.5$ which corresponds to a disk of radius ρ centered at c covering the eigenvalues.

(b) The CGN min-max bound can be specialized in a similar way where we instead need to include the eigenvalues

$$\frac{\|Ax-b\|_{A^{-1}}}{\|b\|_{A^{-1}}} \le \frac{\rho|^k}{|c|}$$

We select $\rho = (33-17)/2 = 8$ and $c = (33+17)/2 = 25$ such that we have $\beta = 8/25 = 0.32$.

(c) In the Arnoldi method for eigenvalue problems we measure the error with the quantity $\|(I - QQ^*)x_i\|$ which measures (the sine of) the angle between the Krylov subspace and the eigenvector. The bound states that

$$\|(I - QQ^*)x_i\| \le \xi_i \varepsilon_i^{(k)}$$

where

$$\xi_i = \sum_{j=1, j\neq i}^{n} \frac{|\alpha_j|}{|\alpha_i|}.$$

The coefficient $\varepsilon_i^{(k)}$ can be bounded using a disk including all eigenvalues except the eigenvalue we are considering:

$$\varepsilon_i^{(k)} \le \left(\frac{\rho}{|\lambda_i - c|}\right)^{k-1}$$

where we can select $\rho = 3$ and $c = 7.5$ such that

$$\frac{\rho}{|\lambda_i - c|} \approx \frac{3}{|20-7.5|} \approx 1/4.$$

Problem 5 (4p) Suppose $A \in \mathbb{R}^{n\times n}$ is a lower triangular matrix. (Note: Not upper triangular) Let f be an analytic function and let $F = f(A)$ be the corresponding matrix function.

(a) What is in general the non-zero structure of F?

(b) Provide a derivation of a formula for f_{ij} only involving the ith and jth row and column of A and F.

(c) How can the formula be used to construct an algorithm for the matrix function of a lower triangular matrix?

Solution:

(a) Since A is lower triangular, $f(A) = F$ is also lower triangular. This can be seen from the Taylor definition

$$f(A) = \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!} A^i.$$

Clearly, A^i is lower triangular if A is lower triangular.

(b) The proof is a variation of the derivation of the Schur-Parlett method, but for a lower triangular matrix. Let the i,j element of F be $f_{i,j}$. From the basic properties of matrix functions, we know that F and A commute such that

$$0 = FA - AF$$

We consider row i and column j of this equation, and assume $j > i$:

$$\begin{aligned} 0 &= \sum_{\ell=1}^{n} f_{i,\ell} a_{\ell,j} - \sum_{\ell=1}^{n} a_{i,\ell} f_{\ell,j} \\ &= \sum_{\ell=j}^{i} (f_{i,\ell} a_{\ell,j} - a_{i,\ell} f_{\ell,j}) \\ &= f_{i,j} a_{j,j} - a_{i,j} f_{j,j} + f_{i,i} a_{i,i} - a_{i,j} f_{i,j} + \sum_{\ell=j+1}^{i-1} (f_{i,\ell} a_{\ell,j} - a_{i,\ell} f_{\ell,j}) \end{aligned}$$

By solving this equation for $f_{i,j}$ we obtain

$$f_{i,j} = \frac{a_{i,j}(f_{j,j} - f_{i,,i}) - \sum_{\ell=j+1}^{i-1} (f_{i,\ell} a_{\ell,j} - a_{i,\ell} f_{\ell,j})}{a_{i,i} - a_{j,j}}. \qquad (\star)$$

(c) The diagonal of F are directly given by $f_{i,i} = f(a_{i,i})$. The rest of the matrix can be computed by applying ($\star$) many times. We apply it one subdiagonal at a time, starting with the first sub-diagonal. This is completely analogous to the Schur-Parlett method but working with subdiagonals below the main diagonal. (An illustration is appropriate in answer.)

Problem 6 (4p)

(a) What is a φ-function and how can the matrix function $\varphi(A)$ be used to solve ordinary differential equations?

(b) How is the Krylov approximation f_m of $\varphi(A)b$ constructed from the Arnoldi factorization? If a small matrix function has to be computed, propose a procedure.

(c) In this course a theorem stated that (under appropriate assumptions on the matrix A) the Krylov approximation f_m satisfies

$$\|f_m - f(A)b\| \leq \alpha \min_{p \in P_{m-1}} \max_{i=1,\ldots,n} |f(\lambda_i) - p(\lambda_i)|.$$

Suppose A has eigenvalues λ_i, $i = 1, \ldots, n$ such that $|\lambda_i| < 1/2$. Specialize the formula and bound it with an explicit formula involving m showing that the approximation error goes to zero very fast. Problem (c) can be answered without answering (a)-(b).
Hint: You may find it useful that the remainder term of the Taylor expansion at zero of the φ-function satisfies: $|R_N(x)| \leq c|x|^N/N!$.

Solution:

(a) A φ function is the matrix function associated with the scalar function

$$\varphi(x) = \frac{e^z - 1}{z},$$

which for non-singular A can be written as

$$\varphi(A) = A^{-1}(\exp(A) - I). \qquad (\star\star)$$

(b) The Krylov approximation of the φ function (and any matrix function) is given computed from the Arnoldi factorization:

$$AQ_m = Q_{m+1}\underline{H}_m.$$

We let

$$\varphi(A)b = Q_m\varphi(H_m)e_1\|b\|$$

where $q_1 = b/\|b\|$. The matrix function $\varphi(H_m)$ can for instance be computed with ($\star\star$). If H_m is singular, a general method, such as Taylor approximation approach might is better.

(c) Let T_N be the truncated Taylor series approximation of f. According to the hint

$$|\varphi(x) - T_N(x)| \leq c\frac{|x|^N}{N!}.$$

We also have from the question that

$$\|f_m - \varphi(A)b\| \leq \alpha \min_{p \in P_{m-1}} \max_{i=1,\ldots,n} |\varphi(\lambda_i) - p(\lambda_i)|. \leq \alpha|\varphi(\lambda_i) - q(\lambda_i)|$$

for any polynomial $q \in P_{m-1}$. In particular, the bound holds for the truncated Taylor polynomial $q = T_{m-1}$. Therefore,

$$\|f_m - \varphi(A)b\| \leq \alpha c \max_{i=1,\ldots,n} \frac{|\lambda_i|^{m-1}}{(m-1)!}$$

Let ρ be the largest eigenvalue in modulus, $\rho = \max_{i=1,\ldots,n} |\lambda_i|$, which is also known as the spectral radius of the matrix. Then

$$\|f_m - \varphi(A)b\| \leq \alpha c\frac{\rho^{m-1}}{(m-1)!}$$

For sufficiently large m we have $\rho^{m-1} < (m-1)!$ which shows (exponential) convergence.