Department of Mathematical Sciences

Examination paper for
TMA4205 Numerical Linear Algebra (solution)

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Permitted examination support material: C: Specified, written and handwritten examination support materials are permitted. A specified, simple calculator is permitted (either Citizen SR-270X or Hewlett Packard HP30S). The permitted examination support materials are:

- Y. Saad: Iterative Methods for Sparse Linear Systems. 2nd ed. SIAM, 2003 (book or printout)
- L. N. Trefethen and D. Bau: Numerical Linear Algebra, SIAM, 1997 (book or photocopy)
- G. Golub and C. Van Loan: Matrix Computations. 3rd ed. The Johns Hopkins University Press, 1996 (book or photocopy)
- E. Rønquist: Note on The Poisson problem in $\mathbb{R}^2$: diagonalization methods (printout)
- K. Rottmann: Matematisk formelsamling
- Your own lecture notes from the course (handwritten)

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Note: This solution is more detailed than what was expected at the exam.

Problem 1

a) We see that A is symmetric, so it is Hermitian ($A^{\mathrm{H}} = A$). Then $A^{\mathrm{H}}A = A^2 = AA^{\mathrm{H}}$, which proves that A is normal.

b) Since A is Hermitian, the eigenvalues of A are real. Proof: Let $Ax = \lambda x$, with $\|x\|_2 = 1$. Then

$$\lambda = \lambda x^{\mathrm{H}}x = x^{\mathrm{H}}\lambda x = x^{\mathrm{H}}Ax = x^{\mathrm{H}}A^{\mathrm{H}}x = (Ax)^{\mathrm{H}}x = \bar{\lambda}x^{\mathrm{H}}x = \bar{\lambda},$$

so λ is real.

c) Let us first find a bound for the eigenvalues of A by using Gershgorin's theorem. Each Gershgorin disc has centre in d. All elements of A are real and of the same sign as d, so the radius of each Gershgorin disc is equal to the absolute value of the sum of the elements of each row, where we do not include the element on the diagonal. All these radiuses must be smaller than

$$2|d|\sum_{i=1}^{\infty}\frac{1}{3^i} = 2|d|\left(\frac{1}{1-1/3} - 1\right) = |d|.$$

Thus, all the eigenvalues are contained inside the disc with centre d and radius $r < |d|$.

We will now prove that A does *not* have to be positive definite. Consider the case where $d < 0$. Then all the eigenvalues λ are negative. Let $Ax = \lambda x$, where $\|x\|_2 = 1$. Then

$$x^{\mathrm{T}}Ax = x^{\mathrm{T}}\lambda x = \lambda x^{\mathrm{T}}x = \lambda < 0,$$

so A can not be positive definite.

d) From **c)** we know that the Gershgorin discs do not contain zero, so A has no eigenvalue equal to zero.

Assume now that A is singular. Then $\det A = 0$, and $\lambda = 0$ is an eigenvalue of A since it is a solution of the characteristic equation $\det(A - \lambda\mathrm{I}) = 0$. This contradicts the fact that A has no eigenvalues equal to zero, so A must be nonsingular.

e) The Jacobi iteration matrix is

$$G = \mathrm{I} - D^{-1}A,$$

where $D = d\mathrm{I}$ is the diagonal part of A. Thus,

$$G = -\begin{bmatrix} 0 & 1/3 & 1/9 & \cdots & 1/3^{n-1} \\ 1/3 & 0 & 1/3 & \cdots & 1/3^{n-2} \\ 1/9 & 1/3 & 0 & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & 1/3 \\ 1/3^{n-1} & 1/3^{n-2} & \cdots & 1/3 & 0 \end{bmatrix}.$$

We can use the same type of arguments as in **c)** to show that the eigenvalues of G are located in a disc with centre 0 and radius $r < 1$. This proves that the spectral radius $\rho(G) < 1$, and the Jacobi iteration converges for any initial vector.

f) From the hint, we know that L^{-1} is a lower-triangular Toeplitz matrix, so we must find $a_1, a_2, \dots, a_n$ so that

$$\mathrm{I} = LL^{-1} = d\begin{bmatrix} 1 & & & & \\ 1/3 & 1 & & & \\ 1/9 & 1/3 & 1 & & \\ \vdots & \vdots & \ddots & \ddots & \\ 1/3^{n-1} & 1/3^{n-2} & \cdots & 1/3 & 1 \end{bmatrix}\begin{bmatrix} a_1 & & & & \\ a_2 & a_1 & & & \\ a_3 & a_2 & a_1 & & \\ \vdots & \vdots & \ddots & \ddots & \\ a_n & a_{n-1} & \cdots & a_2 & a_1 \end{bmatrix}$$

We calculate the first column of the product, starting with the topmost element:

$$\begin{aligned} 1 = da_1 &\implies a_1 = 1/d, \\ 0 = d(a_1/3 + a_2) = 1/3 + da_2 &\implies a_2 = -1/(3d), \\ 0 = d(a_1/9 + a_2/3 + a_3) = da_3 &\implies a_3 = 0, \\ 0 = d(a_1/27 + a_2/9 + a_3/3 + a_4) = da_4 &\implies a_4 = 0, \\ &\ \ \vdots \\ 0 = da_n &\implies a_n = 0. \end{aligned}$$

Thus,

$$L^{-1} = d^{-1}\begin{bmatrix} 1 & & & \\ -1/3 & 1 & & \\ & \ddots & \ddots & \\ & & -1/3 & 1 \end{bmatrix}.$$

g) For Gauss–Seidel iteration, the iteration matrix is

$$G = \mathrm{I} - L^{-1}A = \begin{bmatrix} 0 & -1/3 & -1/3^2 & -1/3^3 & \cdots & -1/3^{n-1} \\ 0 & 1/3^2 & -8/3^3 & -8/3^4 & \cdots & -8/3^n \\ 0 & 0 & 1/3^2 & -8/3^3 & \cdots & -8/3^{n-1} \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & 1/3^2 & -8/3^3 \\ 0 & 0 & \cdots & 0 & 0 & 1/3^2 \end{bmatrix}.$$

We see that G is upper-triangular, so the eigenvalues of G are the diagonal elements. Thus, the spectral radius is $\rho(G) = 1/9$.

If we use the alternative L^{-1} mentioned in the problem text, we get $\rho(G) = 19/27$.

Problem 2 Using centred finite differences with step length h, we discretize the 2D Helmholtz equation

$$\begin{aligned} -\nabla^2 u - \alpha u = f \quad &\text{in} \quad \Omega = (0,1)\times(0,1), \\ u = 0 \quad &\text{on} \quad \partial\Omega, \end{aligned}$$

where α is a positive constant, and $f\colon \Omega \to \mathbb{R}$, and obtain

$$-\frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{h^2} - \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} - \alpha u_{i,j} = f_{i,j}. \tag{1}$$

We now follow the note by E. Rønquist to construct a diagonalization method based on (1). Let U be the matrix with elements $u_{i,j}$ and G the matrix with elements $h^2 f_{i,j}$. Let T be the tridiagonal Toeplitz matrix with 2 on the diagonal and -1 on the sub- and super-diagonals. Then (1) can be written as

$$TU + UT - h^2\alpha U = G. \tag{2}$$

The matrix T is symmetric and can be orthogonally diagonalized $T = Q\Lambda Q^{\mathrm{T}}$, where $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. We can then write (2) as

$$Q\Lambda Q^{\mathrm{T}} U + UQ\Lambda Q^{\mathrm{T}} - h^2\alpha U = G,$$

or

$$\Lambda Q^{\mathrm{T}} UQ + Q^{\mathrm{T}} UQ\Lambda - h^2\alpha Q^{\mathrm{T}} UQ = Q^{\mathrm{T}} GQ.$$

Define $\tilde{U} = Q^{\mathrm{T}} UQ$ with elements $\tilde{u}_{i,j}$, and $\tilde{G} = Q^{\mathrm{T}} GQ$ with elements $\tilde{g}_{i,j}$. Then

$$\Lambda\tilde{U} + \tilde{U}\Lambda - h^2\alpha\tilde{U} = \tilde{G}.$$

Consider the element in position (i, j) of this equation:

$$\lambda_i \tilde{u}_{i,j} + \tilde{u}_{i,j}\lambda_j - h^2\alpha\tilde{u}_{i,j} = \tilde{g}_{i,j},$$

or

$$\tilde{u}_{i,j} = \frac{\tilde{g}_{i,j}}{\lambda_i + \lambda_j - h^2\alpha}.$$

Thus, we can write the diagonalization method as:

1. Compute $\tilde{G} = Q^{\mathrm{T}} G Q$.
2. Compute $\tilde{u}_{i,j} = \tilde{g}_{i,j}/(\lambda_i + \lambda_j - h^2\alpha)$.
3. Compute $U = Q\tilde{U}Q^{\mathrm{T}}$.

Note: The method fails if there exists a combination of i and j so that $h^2\alpha = \lambda_i + \lambda_j$.

Problem 3

a) A Krylov subspace is a subspace based on a matrix $A \in \mathbb{R}^{n\times n}$ and a vector $v \in \mathbb{R}^n$. The definition is

$$\mathcal{K}_m(A, v) = \operatorname{span}\{v, Av, A^2v, \dots, A^{m-1}v\} \subseteq \mathbb{R}^n.$$

Any vector in $\mathcal{K}_m(A, v)$ can be written as $q_{m-1}(A)v$, where q_{m-1} is a polynomial of degree not exceeding $m-1$, and $q_{m-1}(0) = \mathrm{I}$.

The Arnoldi process is an algorithm which finds an orthonormal basis of $\mathcal{K}_m(A, v)$ by application of the Gram–Schmidt process. Let these basis vectors be the columns of the matrix V_m. The Arnoldi process also finds a Hessenberg matrix H_m, so that

$$H_m = V_m^{\mathrm{T}} A V_m. \tag{3}$$

b) We insert $A = \mathrm{I} + B$ into (3).

$$H_m = V_m^{\mathrm{T}}(\mathrm{I} + B)V_m = V_m^{\mathrm{T}}V_m + V_m^{\mathrm{T}}BV_m = \mathrm{I} + V_m^{\mathrm{T}}BV_m.$$

Observe that since $B^{\mathrm{T}} = -B$

$$H_m^{\mathrm{T}} = \mathrm{I} - V_m^{\mathrm{T}}BV_m,$$

so $H_m - \mathrm{I}$, must also be skew-symmetric. However, since H_m is Hessenberg, $H_m - \mathrm{I}$ is also Hessenberg, which proves that $H_m - \mathrm{I}$ is tridiagonal. Thus, H_m must be tridiagonal and have the matrix structure

$$H_m = \begin{bmatrix} 1 & -\beta_2 & & \\ \beta_2 & 1 & \ddots & \\ & \ddots & \ddots & -\beta_m \\ & & \beta_m & 1 \end{bmatrix}. \tag{4}$$

c) The Arnoldi MGS process is

1: $r_0 = b - Ax_0$, $\beta_1 = \|r_0\|_2$, $v_1 = r_0/\beta_1$
2: **for** $j = 1, \ldots, m$ **do**
3: $\quad w_j = Av_j$
4: $\quad$ **for** $i = 1, \ldots, j$ **do**
5: $\quad\quad h_{i,j} = (w_j, v_i)$
6: $\quad\quad w_j = w_j - h_{i,j}v_i$
7: $\quad$ **end for**
8: $\quad h_{j+1,j} = \|w_j\|_2$
9: $\quad v_{j+1} = w_j/h_{j+1,j}$
10: **end for**

From (4), we see that

$$h_{j+1,j} = \beta_{j+1}.$$

This takes care of lines 8–9 in the algorithm. We also see that

$$h_{j,j} = 1, \qquad h_{j-1,j} = -\beta_j.$$

This enables us to replace lines 3–7 with

$$w_j = Av_j - h_{j-1,j}v_{j-1} - h_{j,j}v_j = Av_j + \beta_j v_{j-1} - v_j = Bv_j + \beta_j v_{j-1},$$

for $2 \leq j \leq m$. The case $j = 1$ must be handled separately:

$$w_1 = Av_1 - h_{1,1}v_1 = Av_1 - v_1 = Bv_1.$$

We can combine these cases if we define $v_0 = 0$. Thus, the algorithm becomes

$r_0 = b - Ax_0$, $\beta_1 = \|r_0\|_2$, $v_1 = r_0/\beta_1$, $v_0 = 0$
for $j = 1, \ldots, m$ **do**
$\quad w_j = Bv_j + \beta_j v_{j-1}$
$\quad \beta_{j+1} = \|w_j\|_2$
$\quad v_{j+1} = w_j/\beta_{j+1}$
end for

d) To obtain a D-Lanczos-like method, we combine the full orthogonalization method (FOM) with the Arnoldi process from **c)**, and use simplifications as in the derivation of D-Lanczos. The update equations for the FOM are

$$y_m = \beta_1 H_m^{-1} \mathrm{e}_1, \qquad x_m = x_0 + V_m y_m,$$

where $\mathrm{e}_1 = [1, 0, \dots, 0]^{\mathrm{T}}$.

We are given the LU-factorization

$$H_m = L_m U_m = \begin{bmatrix} 1 & & & \\ \lambda_2 & 1 & & \\ & \ddots & \ddots & \\ & & \lambda_m & 1 \end{bmatrix} \begin{bmatrix} \eta_1 & -\beta_2 & & \\ & \ddots & \ddots & \\ & & \eta_{m-1} & -\beta_m \\ & & & \eta_m \end{bmatrix}.$$

By multiplying together L_m and U_m and comparing with H_m, we find

$$\eta_1 = 1, \qquad \lambda_i = \frac{\beta_i}{\eta_{i-1}}, \qquad \eta_i = 1 + \lambda_i \beta_i = 1 + \frac{\beta_i^2}{\eta_{i-1}}, \quad \text{for} \quad 2 \le i \le m.$$

By induction, this shows that all $\eta_i \ge 1$. Since none of the elements on the diagonal (i.e. the eigenvalues) of L_m and H_m are zero, they are both nonsingular. Thus,

$$x_m = x_0 + V_m H_m^{-1} \beta_1 \mathrm{e}_1 = x_0 + V_m U_m^{-1} L_m^{-1} \beta_1 \mathrm{e}_1.$$

Now, define $P_m = V_m U_m^{-1}$ and $z_m = L_m^{-1} \beta_1 \mathrm{e}_1$, so that

$$x_m = x_0 + P_m z_m.$$

Define

$$\begin{aligned} P_m &= [p_1 \mid p_2 \mid \cdots \mid p_m] = [P_{m-1} \mid p_m], \\ V_m &= [v_1 \mid v_2 \mid \cdots \mid v_m] = [V_{m-1} \mid v_m], \\ U_m &= [u_1 \mid u_2 \mid \cdots \mid u_m] = \left[\begin{array}{c|c} U_{m-1} & \begin{matrix} \\ -\beta_m \end{matrix} \\ \hline & \eta_m \end{array}\right]. \end{aligned}$$

Then we can write $P_m U_m = V_m$ as

$$\begin{aligned} P_m U_m &= [P_{m-1} \mid p_m] \left[\begin{array}{c|c} U_{m-1} & \begin{matrix} \\ -\beta_m \end{matrix} \\ \hline & \eta_m \end{array}\right] \\ &= [P_{m-1} U_{m-1} \mid -\beta_m p_{m-1} + \eta_m p_m] \\ &= [V_{m-1} \mid v_m] = V_m, \end{aligned} \tag{5}$$

giving $P_{m-1}U_{m-1} = V_{m-1}$ (which is consistent with $P_m U_m = V_m$), and

$$-\beta_m p_{m-1} + \eta_m p_m = v_m \implies p_m = \frac{1}{\eta_m}(v_m + \beta_m p_{m-1}). \tag{6}$$

Next, define

$$L_m = \left[\begin{array}{c|c} L_{m-1} & \\ \hline \lambda_m & 1 \end{array}\right] \qquad \text{and} \qquad z_m = \left[\begin{array}{c} z_{m-1} \\ \hline \zeta_m \end{array}\right],$$

where $z_{m-1}^{\mathrm{T}} = [z_{m-2}^{\mathrm{T}} \mid \zeta_{m-1}]$, and so on. Then, since $L_m z_m = \beta_1 \mathrm{e}_1$, we get that $L_{m-1} z_{m-1} = \beta_1 \mathrm{e}_1$ (which is consistent with $L_m z_m = \beta_1 \mathrm{e}_1$), and

$$\lambda_m \zeta_{m-1} + \zeta_m = 0 \implies \zeta_m = -\lambda_m \zeta_{m-1}.$$

Define x_{m-1} so that it is consistent with $x_m = x_0 + P_m z_m$, i.e. define

$$x_{m-1} = x_0 + P_{m-1} z_{m-1}.$$

We can now express x_m using x_{m-1} in the following way:

$$\begin{aligned} x_m &= x_0 + P_m z_m \\ &= x_0 + [P_{m-1} \mid p_m] \left[\begin{array}{c} z_{m-1} \\ \hline \zeta_m \end{array}\right] \\ &= x_0 + P_{m-1} z_{m-1} + \zeta_m p_m \\ &= x_{m-1} + \zeta_m p_m. \end{aligned}$$

We now have all the equations we need to step from x_{m-1} to x_m, but we also need starting values for all the variables. Since $U_1 = \eta_1 = 1$, (5) gives us that $p_1 = v_1$. If we define $p_0 = 0$, the update equation (6) gives us exactly this. Furthermore, if we define $\lambda_1 = 0$, we can use the update equation $\eta_m = 1 + \lambda_m \beta_m$ for $m = 1$ as well. We also need a value for ζ_1. Since $L_1 = 1$ and $z_1 = \zeta_1$, the equation $L_1 z_1 = \beta_1 \mathrm{e}_1$ gives us $\zeta_1 = \beta_1$. The starting values for r_0, β_1, v_1 and v_0 are given in the Arnoldi MGS algorithm from **c)**.

Combining all this with the Arnoldi MGS algorithm, we get the D-Lanczos-like algorithm (we suppress the convergence test, and reuse w_m as w in each iteration):

$r_0 = b - Ax_0$, $\beta_1 = \zeta_1 = \|r_0\|_2$, $v_1 = r_0/\beta_1$, $v_0 = p_0 = 0$, $\lambda_1 = 0$
for $m = 1, 2, \dots$ **do**
  if $m > 1$ **then**
    $\lambda_m = \beta_m/\eta_{m-1}$
    $\zeta_m = -\zeta_{m-1}\lambda_m$
  end if
  $\eta_m = 1 + \lambda_m\beta_m$
  $p_m = (v_m + \beta_m p_{m-1})/\eta_m$
  $x_m = x_{m-1} + \zeta_m p_m$
  $w = Bv_m + \beta_m v_{m-1}$
  $\beta_{m+1} = \|w\|_2$
  $v_{m+1} = w/\beta_{m+1}$
end for

Problem 4

a) We want to find $M = U\Sigma V^{\mathrm{H}}$, where U and V are unitary, and Σ is diagonal with non-negative elements. Note that M is symmetric, so it can be orthogonally diagonalized as $M = Q\Lambda Q^{\mathrm{T}}$. Thus, if the eigenvalues of M are non-negative, the diagonalization is an SVD with $U = V = Q$ and $\Sigma = \Lambda$.

We start by calculating the eigenvalues of M by solving the equation $\det(M - \lambda\mathrm{I}) = 0$. This gives us $\lambda_1 = 100$, $\lambda_2 = 50$ and $\lambda_3 = 0$, which are all non-negative. Thus, the singular values are $\sigma_i = \lambda_i$, or

$$\Sigma = \begin{bmatrix} 100 & 0 & 0 \\ 0 & 50 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

The eigenvectors $\hat{v}_i$ associated with the eigenvalues λ_i are solutions of

$$M\hat{v}_i = \lambda_i\hat{v}_i. \tag{7}$$

The unitary matrix $V = [v_1 \mid v_2 \mid v_3]$ is formed by setting $v_i = \hat{v}_i/\|\hat{v}_i\|_2$. From (7), we get

$$\hat{v}_1 = [4, 3, 5]^{\mathrm{T}}, \qquad \hat{v}_2 = [4, 3, -5]^{\mathrm{T}}, \qquad \hat{v}_3 = [3, -4, 0]^{\mathrm{T}},$$

and by normalizing, we get

$$U = V = \begin{bmatrix} 4/\sqrt{50} & 4/\sqrt{50} & 3/5 \\ 3/\sqrt{50} & 3/\sqrt{50} & -4/5 \\ 5/\sqrt{50} & -5/\sqrt{50} & 0 \end{bmatrix}.$$

b) In general we have that $\sigma_i = \sqrt{\lambda_i(M^{\mathrm{H}}M)}$. For our symmetric matrix, $M = M^{\mathrm{H}}$, so $\sigma_i = |\lambda_i(M)|$. We showed in **a)** that all the eigenvalues of M are positive, so we get that the eigenvalues and singular values of M are equal to each other,

$$\sigma_i = \lambda_i.$$

c) The rank of M is equal to the number of nonzero singular values, so we immediately see that $\operatorname{rank} M = 2$.

d) We can get the best low-rank approximation $\tilde{M} \approx M$ through the use of the SVD in the sense that $\|M - \tilde{M}\|$ is minimized in the Euclidean or Frobenius norm. In the course, we showed that we could decompose M as

$$M = \sum_{i=1}^{3} \sigma_i u_i v_i^{\mathrm{H}},$$

and that the best approximation of rank at most equal to k is obtained by truncating the series above after k terms. Thus, the best rank-one approximation is

$$\tilde{M} = \sigma_1 u_1 v_1^{\mathrm{H}} = \sigma_1 v_1 v_1^{\mathrm{T}} = \begin{bmatrix} 32 & 24 & 40 \\ 24 & 18 & 30 \\ 40 & 30 & 50 \end{bmatrix}.$$