TMA4205 - Autumn 2012
Exam - Suggested solutions

17.12.2012

Problem 1

The matrix

$$A = \begin{bmatrix} 2 & 0 & 0 & 1 \\ 0 & 3 & -1 & 1 \\ 0 & -1 & 2 & 0 \\ 1 & 1 & 0 & 2 \end{bmatrix} \tag{1}$$

is unitarily similar to an upper Hessenberg matrix H.
This means

$$A = QHQ^T,$$

where Q is a unitary matrix (i.e. $Q^TQ = QQ^T = I$).

a) We observe that A is symmetric. Therefore, since $H = Q^TAQ$, we have that

$$H^T = Q^TA^TQ = Q^TAQ = H.$$

This implies that H is both symmetric and upper Hessenberg.
Thus, H must be tridiagonal.

b) The matrices A and H have the same eigenvalues (by similarity). Also we note the the eigenvalues of A are all real since $A = A^T$. The matrix is diagonally dominant, but not strictly so. By Gerschgorin's theorem, all the eigenvalues lie in the union of the intervals $[1, 3]$, $[1, 5]$, $[0, 4]$. This shows that the eigenvalues of A are all nonnegative. Since A is suppose to be nonsingular, no eigenvalue can be zero. Therefore all the eigenvalues of A are positive. This means all the eigenvalues of H are positive (by similarity). Hence H is SPD.

c) Suppose we were to compute H, we will need to apply two Householder reflectors $Q_1 = I - 2v_1v_1^T$ and $Q_2 = I - 2v_2v_2^T$ from the left and right of the matrix A. This is done in the following order:

$$A \quad \overset{AQ_1}{\longrightarrow} \quad A_1 \quad \overset{A_1Q_1}{\longrightarrow} \quad H_1 \quad \overset{Q_2H_1}{\longrightarrow} \quad A_2 \quad \overset{A_2Q_2}{\longrightarrow} \quad H.$$

We can choose

$$v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \qquad \text{from the first column of } A.$$

We have

$$H_1 = Q_1 A Q_1 = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & 0 & 1 \\ 0 & 0 & 2 & 1 \\ 0 & 1 & 1 & 3 \end{bmatrix}.$$

We now choose

$$v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \qquad \text{from the second column of } H_1.$$

The result is

$$H = Q_2 H_1 Q2 = Q_2 Q_1 A Q_1 Q_2 = Q^T A Q$$

giving

$$Q = Q_1 Q_2.$$

To compute Q we only need to compute the columns:

$$Q = [Qe_1|Qe_2|Qe_3|Qe_4],$$

where e_k, $k = 1, 2, 3, 4$ are the standard Euclidean unit vectors in $\mathbb{R}^4$. Since in the matrix-vector product $Q_j x$ only entries of x from row $j+1$ downwards are altered, we must have that

$$Q_j e_k = e_k, \quad \forall j \geq k.$$

So

$$\begin{aligned} Qe_1 &= Q_1 Q_2 e_1 = e_1, \\ Qe_2 &= Q_1 Q_2 e_2 = Q_1 e_2, \\ Qe_3 &= Q_1 Q_2 e_3, \\ Qe_4 &= Q_1 Q_2 e_4. \end{aligned}$$

The computations are done as follows:

- <u>Compute $Qe_2 = Q_1 e_2$:</u>

$$\begin{aligned} Q_1 e_2 &= e_2 - 2v_1(v_1^T e_2) \\ &= \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix}. \end{aligned}$$

- Compute $Qe_3 = Q_1Q_2e_3$:

$$\begin{aligned} Q_2e_3 &= e_3 - 2v_2(v_2^Te_3) \\ &= \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix} =: w. \\ Qe_3 &= Q_1w = w - 2v_1(v_1^Tw) \\ &= \begin{pmatrix} 0 \\ 0 \\ 0 \\ -1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}. \end{aligned}$$

- Compute $Qe_4 = Q_1Q_2e_4$:

$$\begin{aligned} Q_2e_4 &= e_4 - 2v_2(v_2^Te_4) \\ &= \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} - \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix} =: w. \\ Qe_4 &= Q_1w = w - 2v_1(v_1^Tw) \\ &= \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix} + 0 = \begin{pmatrix} 0 \\ 0 \\ -1 \\ 0 \end{pmatrix}. \end{aligned}$$

Observe that no matrix-vector product is involved in the calculations!

Hence

$$Q = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & -1 & 0 & 0 \end{bmatrix}.$$

Problem 2

a) We consider a matrix of the form

$$A = I + \mu S,$$

where μ is a scalar and S is skew-symmetric.

i) For any vector $x \neq 0$ of compatible dimension we have that

$$x^TAx = x^Tx + \mu x^TSx.$$

Since $S^T = -S$,

$$x^TSx = (x^TSx)^T = -x^TSx \Longrightarrow x^TSx = 0.$$

This implies that $x^TAx > 0$ for any scalar μ. Thus A is SPD.

ii) The Anoldi process with this matrix yields the upper Hessenberg matrix

$$\begin{aligned} H_m &= V_m^T A V_m \\ &= V_m^T V_m + \mu V_m^T S V_m \\ &= I_m + \mu V_m^T S V_m. \end{aligned} \tag{2}$$

The second term in (2) is skew-symmetric, since

$$= (V_m^T S V_m)^T = V_m^T S^T V_m = -V_m^T S V_m. \tag{3}$$

Since both terms in (2) are also upper Hessenberg, and the diagonal entries of a skew-symmmetric matrix are all zeros, H_m must have the tridiagonal form

$$H_m = \begin{bmatrix} 1 & -\eta_2 & & & \\ \eta_2 & 1 & -\eta_3 & & \\ & & \cdots & & \\ & & \eta_{m-1} & 1 & -\eta_m \\ & & & \eta_m & 1 \end{bmatrix}.$$

b) We have the linear system $Ax = b$ where A is SPD, and we consider an orthogonal projection method for which the search and constraint spaces are given by $\mathcal{L} = \mathcal{K} = \operatorname{span}\{r_0, Ar_0\}$ where $r_0 = b - Ax_0$ is the current residual. The solution update $\tilde{x}$ would satisfy that $\tilde{x} - x_0 \in \mathcal{K}$. That means,

$$\tilde{x} = x_0 + \alpha r_0 + \beta A r_0.$$

The corresponding residual vector is given by

$$\tilde{r} = b - A\tilde{x} = r_0 - \alpha A r_0 - \beta A^2 r_0.$$

Also

$$\tilde{e} = x - \tilde{x} = e_0 - \alpha r_0 - \beta A r_0.$$

In the A norm we have that

$$\begin{aligned} \|\tilde{e}\|_A^2 &= (\tilde{e}, \tilde{e})_A \\ &= (\tilde{e}, e_0 - \alpha r_0 - \beta A r_0)_A \\ &= (\tilde{e}, e_0)_A - (\tilde{r}, \alpha r_0 + \beta A r_0), && \text{since } A\tilde{e} = \tilde{r} \\ &= (\tilde{e}, e_0)_A, && \text{since } \tilde{r} \perp \mathcal{L} \\ &= (\tilde{e}, r_0), && \text{since } A e_0 = r_0 \\ &= (e_0 - \alpha r_0 - \beta A r_0, r_0) \\ &= (A^{-1} r_0, r_0) - \alpha (r_0, r_0) - \beta (A r_0, r_0) \\ &= (A^{-1} r_0, r_0) \left[1 - \alpha \frac{(r_0, r_0)}{(A^{-1} r_0, r_0)} - \beta \frac{(A r_0, r_0)}{(A^{-1} r_0, r_0)} \right]. \end{aligned}$$

The result follows, since $(A^{-1} r_0, r_0) = \|e_0\|_A^2$.

To determine the values of the constants $\alpha,\ \beta$ we use the orthogonality condition:

$$\tilde{r} \perp \mathcal{L} = \operatorname{span}\{r_0, Ar_0\}$$

$\Longrightarrow$

$$\begin{cases} \left(r_0 - \alpha A r_0 - \beta A^2 r_0, r_0\right) = 0, \\ \left(r_0 - \alpha A r_0 - \beta A^2 r_0, A r_0\right) = 0 \end{cases}$$

$\Longrightarrow$

$$\begin{cases} \alpha(Ar_0, r_0) + \beta(A^2 r_0, r_0) = (r_0, r_0), \\ \alpha(Ar_0, Ar_0) + \beta(A^2 r_0, Ar_0) = (Ar_0, r_0). \end{cases}$$

Solving this 2×2 system we get

$$\alpha = \frac{1}{\sigma}\left[(A^2 r_0, Ar_0)(r_0, r_0) - (Ar_0, Ar_0)(Ar_0, r_0)\right],$$
$$\beta = \frac{1}{\sigma}\left[(Ar_0, r_0)^2 - (Ar_0, Ar_0)(r_0, r_0)\right],$$

where

$$\sigma = (A^2 r_0, Ar_0)(Ar_0, r_0) - (Ar_0, Ar_0)^2.$$

Now we can determine a lower bound for the term $\beta \dfrac{(Ar_0, r_0)}{(A^{-1} r_0, r_0)}$.

We write

$$\beta \frac{(Ar_0, r_0)}{(A^{-1} r_0, r_0)} = \frac{(Ar_0, r_0)}{(A^{-1} r_0, r_0)} \cdot \frac{(Ar_0, r_0)^2 - (Ar_0, Ar_0)(r_0, r_0)}{(A^2 r_0, Ar_0)(Ar_0, r_0) - (Ar_0, Ar_0)^2}$$
$$= \frac{(r_0, r_0)}{(A^{-1} r_0, r_0)} \cdot \frac{(r_0, r_0)}{(Ar_0, r_0)} \cdot \left(\frac{R_0^2 - R_1}{R_2 - R_1^2}\right),$$

where

$$R_0 = \frac{(Ar_0, r_0)}{(r_0, r_0)}$$
$$R_1 = \frac{(Ar_0, Ar_0)}{(r_0, r_0)} = \frac{(A^2 r_0, r_0)}{(r_0, r_0)}$$
$$R_2 = \frac{(A^2 r_0, Ar_0)}{(Ar_0, r_0)} = \frac{(A^2 r_0, Ar_0)}{(Ar_0, Ar_0)} \cdot \frac{(Ar_0, r_0)}{(r_0, r_0)} \cdot \frac{(r_0, r_0)}{(Ar_0, r_0)}.$$

The following inequalities (based on Rayleigh quotients of A and A^2 can be easily verified:

$$\lambda_{\min} \le R_0 \le \lambda_{\max},$$
$$\lambda_{\min}^2 \le R_1 \le \lambda_{\max}^2,$$
$$\frac{\lambda_{\min}^3}{\lambda_{\max}} \le R_2 \le \frac{\lambda_{\max}^3}{\lambda_{\min}}.$$

Combining these inequalities together with Kantorovich inequality, we get that

$$\beta \frac{(Ar_0, r_0)}{(A^{-1} r_0, r_0)} \ge \frac{4\lambda_{\max}\lambda_{\min}}{(\lambda_{\max} + \lambda_{\min})^2} \cdot \frac{\lambda_{\min}^2 - \lambda_{\max}^2}{\frac{\lambda_{\max}^3}{\lambda_{\min}} - \lambda_{\min}^4} \ge \frac{4\lambda_{\max}\lambda_{\min}^2}{\lambda_{\max}^3 - \lambda_{\min}^5} \left(\frac{\lambda_{\min} - \lambda_{\max}}{\lambda_{\min} + \lambda_{\max}}\right).$$

Problem 3

From the discretization of the Poisson problem we have $Ax = b$ where $A = \text{tridiag}(-1, 2, -1)$. The SSOR method can be re-written compactly as

$$x_{k+1} = (D - \omega F)^{-1} [\omega E + (1 - \omega D)] (D - \omega E)^{-1} [\omega F + (1 - \omega D)] x_k + R_\omega b,$$

where R_ω controls remaining terms. This gives the iteration matrix as

$$G_\omega = (D - \omega F)^{-1} \underbrace{[\omega E + (1 - \omega D)]}_{I} (D - \omega E)^{-1} \underbrace{[\omega F + (1 - \omega D)]}_{II}.$$

a) We use the splitting $A = D - E - F$ to eliminate F from (I), and E from (II). We obtain

$$\begin{aligned} G_\omega &= (D - \omega F)^{-1} [(D - \omega F) - \omega A] (D - \omega E)^{-1} [(D - \omega E) - \omega A] \\ &= \left[I - \omega(D - \omega F)^{-1} A\right] \left[I - \omega(D - \omega E)^{-1} A\right] \\ &= I - \omega(D - \omega F)^{-1} A - \omega(D - \omega E)^{-1} A + \omega^2 (D - \omega F)^{-1} A (D - \omega E)^{-1} A \\ &= I - \omega(D - \omega F)^{-1} [(D - \omega E) + (D - \omega F) - \omega A] (D - \omega E)^{-1} A \\ &= I - \omega(2 - \omega)(D - \omega F)^{-1} D (D - \omega E)^{-1} A. \end{aligned}$$

b) Given $x_{k+1} = M^{-1} N x_k + M^{-1} r_k$, with $A = M - N$ the iteration matrix is given by

$$G = M^{-1} N = I - M^{-1} A.$$

So from the expression for G_ω, it follows that the preconditioner is given by

$$\begin{aligned} M_\omega &= \left(\omega(2 - \omega)(D - \omega F)^{-1} D (D - \omega E)^{-1}\right)^{-1} \\ &= \frac{1}{\omega(2 - \omega)} (D - \omega E) D^{-1} (D - \omega F). \end{aligned}$$

For the given matrix, we observe that $F = E^T$. This implies that M_ω is symmetric. Also $1/(\omega(2 - \omega)) > 0$ since $\omega \in (0, 2)$. Moreover

$$((D - \omega E) D^{-1} (D - \omega F) x, x) = (D^{-1}(D - \omega E^T) x, (D - \omega E^T) x) > 0, \qquad \text{for all } x \neq 0,$$

since both D^{-1} and $(D - \omega E^T)$ are nonsingular (as triangular matrices with determinants given by $\det(D^{-1}) \neq 0$).

This proves that M_ω as well as M_ω^{-1} are SPD.

c) Let

$$f(\omega) = \kappa(M_\omega^{-1} A) = \frac{2an^2 + \lambda_{\min}}{(2 - \omega)\lambda_{\min}} = \gamma \left(\frac{1}{\omega} - \frac{1}{2}\right) + \frac{1}{2 - \omega},$$

where $\gamma = \frac{n^2}{\lambda_{\min}}$, $a = \frac{(2-\omega)^2}{4\omega}$. Then the condition number is minimized when $f'(\omega) = 0$.

$$\begin{aligned} f'(\omega) &= 0 \\ &\Downarrow \\ -\frac{1}{\omega^2} + \frac{1}{(2 - \omega)^2} &= 0, \\ -\gamma(2 - \omega)^2 + \omega^2 &= 0, \\ [\omega - \sqrt{\gamma}(2 - \omega)][\omega + \sqrt{\gamma}(2 - \omega)] &= 0 \end{aligned}$$

For $\omega \in (0, 2)$ we must have

$$\omega - \sqrt{\gamma}(2 - \omega) = 0.$$

Thus

$$\omega_{\text{opt}} = \frac{2\sqrt{\gamma}}{1 + \sqrt{\gamma}}$$

For this value of ω the condition number is given by

$$f(\omega_{\text{opt}}) = \frac{1}{2} + \sqrt{\gamma} = \frac{1}{2} + \frac{n}{2 \sin \frac{\pi}{2n}} \simeq \frac{n^2}{\pi}, \qquad \text{for } n \gg 1.$$

Problem 4

Let

$$A = \begin{bmatrix} -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \\ 1 & 0 & 1 \end{bmatrix}. \tag{4}$$

a) For the convergence of conjugate gradient iterations for the normal equation $A^T Ax = A^T b$ we only require that $A^T A$ be SPD. The normal matrix is clearly symmetric. This means its eigenvalues are real. Also

$$x^T A^T Ax = (Ax)^T (Ax) > 0, \quad \forall x \neq 0,$$

since A is full-rank (by inspection we observe that the columns of A are linearly independent.

b) First we compute

$$A^T A = \begin{bmatrix} -1 & 1 & 0 & 1 \\ 0 & -1 & 1 & 0 \\ 1 & 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 & 1 \\ 1 & -1 & 0 \\ 0 & 1 & -1 \\ 1 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 3 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 3 \end{bmatrix}.$$

The condition number of $A^T A$ can be obtained by

$$\kappa_2(A) = \frac{\lambda_{\max}}{\lambda_{\min}}.$$

To compute the eigenvalues of $A^T A$ we can use the characteristic equation (since this is a small matrix dim < 5).

$$\begin{vmatrix} 3-\lambda & -1 & 0 \\ -1 & 2-\lambda & -1 \\ 0 & -1 & 3-\lambda \end{vmatrix} = 0,$$

$$\Downarrow$$

$$(3-\lambda)[(2-\lambda)(3-\lambda) - 1] + 1[-(3-\lambda)] = 0,$$
$$(3-\lambda)(4-\lambda)(1-\lambda) = 0.$$

The eigenvalues are $\lambda = 1,\ 3,\ 4$. This also shows that A^TA is SPD, since all its eigenvalues are positive. We obtain

$$\kappa_2(A) = \frac{\lambda_{\max}}{\lambda_{\min}} = \frac{4}{1} = 4.$$

Applying a diagonal preconditioner to the normal matrix, yields

$$\begin{bmatrix} 1 & -\frac{1}{3} & 0 \\ -\frac{1}{2} & 1 & -\frac{1}{2} \\ 0 & -\frac{1}{3} & 1 \end{bmatrix}.$$

This contracts the Gerschgorin's discs (intervals in this case) into $[1/2, 3/2]$, $[2/3, 4/3]$, which shows condition now has an upper bound given by

$$\frac{\lambda_{\max}^{\text{prec}}}{\lambda_{\min}^{\text{prec}}} \leq \frac{3/2}{1/2} = 3.$$

This smaller than $\kappa(A^TA) = 4$. Thus the diagonal precondition gives some improvement.

c) If the SVD for A is given by $A = U\Sigma V^T$, then

$$A^TA = V\Sigma^2V^T.$$

This shows that A^TA and Σ^2 are similar. So the singular values of A must satisfy

$$\sigma_1^2 = 4, \quad \sigma_2^2 = 3 \quad \sigma_3^2 = 1,$$

giving

$$\sigma_1 = 2, \quad \sigma_2 = \sqrt{3}, \quad \sigma_3 = 1.$$

d) We compute the 1-, 2-, ∞- and Frobenius-norms of A as follows:

$$\begin{aligned}
\|A\|_1 &\stackrel{\text{def}}{=} \max_{1\leq j\leq 3} \sum_{i=1}^{4} |a_{ij}| = \max\{3, 2, 3\} = 3. \\
\|A\|_\infty &\stackrel{\text{def}}{=} \max_{1\leq i\leq 4} \sum_{j=1}^{3} |a_{ij}| = \max\{2, 2, 2, 2\} = 2. \\
\|A\|_2 &= \sigma_{\max} = \sigma_1 = 2. \\
\|A\|_F &= \sqrt{\sigma_1^2 + \sigma_2^2 + \sigma_3^2} = \sqrt{8} = 2\sqrt{2}.
\end{aligned}$$