Numerical Linear Algebra. QS 1 *(MT 2017)*

Optional question: Qn 4

1. Show that $H(w)^2 = I$ when H is a Householder matrix.

2. Show that $\|x\|_\infty = \max_i |x_i|$ satisfies the axioms for a vector norm.

3. Show that if $\|x\|$ is a vector norm then $\sup_x \frac{\|A\,x\|}{\|x\|}$ satisfies the axioms for a matrix norm. Further show that

$$\|A\,B\| \le \|A\|\,\|B\|.$$

4. From the definition of the vector 1–norm show that

$$\|A\|_1 = \max_j \sum_i |a_{ij}|.$$

5. By considering the individual columns a_j of A and b_j of $B = Q\,A$, show that

$$\|Q\,A\|_{\mathrm{F}} = \|A\|_{\mathrm{F}}$$

if Q is an orthogonal matrix.

6. By using the definition of the vector 2–norm and the SVD show that

$$\|A\|_2 = \sigma_1$$

where σ_1 is the largest singular value.

7. (a) For $A \in \mathbb{R}^{m\times n}$ show that the singular values of A are the square roots of the eigenvalues of $A^{\mathrm{T}}\,A$ if $m \ge n$ or of $A\,A^{\mathrm{T}}$ is $m \le n$. (You might want to consider what A and A^{T} do to the singular vectors.)
(b) Check the above using matlab: e.g. set

$$A = \begin{bmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{bmatrix}$$

$lam = eig(A' * A)$ and $sing = svd(A)$.

8. If $A \in \mathbb{R}^{n\times n}$ is nonsingular, what is the SVD of A^{-1} in terms of that of A?

Numerical Linear Algebra. QS 2 *(MT 2017)*

Optional questions: Qns 5, 8

1. For the linear least squares problem: $\min_x \|A\,x - b\|_2$, show that the solution obtained by QR factorisation of A is the same as the vector y obtained by solving the (square) linear system of equations $A^{\mathrm{T}}\,A\,y = A^{\mathrm{T}}\,b$ (the "normal equations").

Can you devise a way of solving the linear least squares problem by employing the SVD?

2. For given positive data $\{y_i\}$ at times $\{t_i\}$ respectively, formulate a linear least squares problem to determine the best values of the three parameters a, λ, μ in a model of the form

$$y = ae^{\lambda(t-\mu)}.$$

Comment on this least squares problem. If the data is $\{12, 5, 2, 1\}$ at $\{0, 1, 2, 3\}$ use matlab to compute the QR factorization (`[Q,R]=qr(A)`) and thence compute the solution.

3. Show that if "shifts" are incorporated into the QR algorithm so that it becomes

$$\begin{cases} \text{Factor} \quad (A_k - \mu_k\, I) = Q_k\, R_k \\ \text{and} \qquad A_{k+1} = R_k\, Q_k + \mu_k\, I \end{cases}$$

for $k = 1, 2, \cdots$ with $A = A_1$, then all the matrices A_k, $k = 1, 2, \cdots$ are similar and thus have the same eigenvalues.

4. In matlab, by typing

$$\begin{cases} [q, r] = qr(a) \qquad \text{(see help qr)} \\ a = r * q, \end{cases}$$

successively, observe convergence of the QR algorithm for the matrix

$$A = \begin{bmatrix} 9 & 1 & 1 \\ 1 & 5 & 0 \\ 1 & 1 & 2 \end{bmatrix}, \qquad (a = [9, 1, 1; 1, 5, 0; 1, 1, 2]).$$

Use the matlab command **eig** to check.

5. By showing that for distinct $u, v \in \mathbb{R}^n$ with $\|u\|_2 = \|v\|_2$ there exists w such that $u^{\mathrm{T}} H(w) = v^{\mathrm{T}}$ where H is the Householder matrix, constructively prove that for any $A \in \mathbb{R}^{n\times n}$ there exists an orthogonal matrix Q and a lower triangular matrix L such that $A = L\,Q$.

6. If $x = (x_1, x_2, \cdots, x_n)^{\mathrm{T}}$ show that the choice of rotation angle $\theta = \cos^{-1}\left(\frac{x_i}{\sqrt{x_i^2+x_k^2}}\right)$ makes $y_k = 0$ where $y = J(i,k)\,x$. Hence show that a QR factorisation of a tridiagonal (or more generally an upper Hessenberg) matrix $A \in \mathbb{R}^{n\times n}$ can be achieved using Givens rotations as follows:

$$J(n-1,n)\cdots J(2,3)\,J(1,2)\,A = R.$$

What is Q?

7. Perform Gauss Elimination by hand on the linear system $A\,x = [11, 6, 4]^{\mathrm{T}}$ where A is the matrix in Question 4. Check your multipliers and the resulting upper triangular matrix by doing $[L,U] = lu(A)$ in matlab.

8. Note that no row swaps would have occured in the above example even if partial pivoting was employed (as it is in matlab's lu). Change the (3,1) entry in A to 10 so that pivoting (row swapping) occurs at least in the first column: do $[L,U] = lu(A)$ and check that $P\,A = L\,U$.

9. $A \in \mathbb{R}^{n\times n}$ is "Strictly Column Diagonally Dominant", (SCDD) if

$$|a_{jj}| > \sum_{i=1, i\neq j}^{n} |a_{ij}|$$

for each $j = 1, 2, \cdots, n$.

If A is SCDD and a partial pivoting strategy is used with Gauss Elimination, why is there no row swapping at the first stage (i.e. when zeros are introduced into the first column)? If after this stage the matrix is in the form

$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & & & \\ \vdots & & \boxed{\quad B \quad} & \\ 0 & & & \end{pmatrix},$$

by considering the general column of B

$$\left(a_{2j} - \frac{a_{21}}{a_{11}}\,a_{1j},\, a_{3j} - \frac{a_{31}}{a_{11}}\,a_{1j}, \cdots, a_{nj} - \frac{a_{n1}}{a_{11}}\,a_{1j}\right)^{\mathrm{T}}$$

prove that B is SCDD. Hence by induction row swapping is not required at any stage for SCDD matrices.

10. If $A\,x = b$ and $(A + \delta\,A)\,(x + \delta\,x) = b$ show that

$$\frac{\|\delta\,x\|}{\|x + \delta\,x\|} \leq \|A\|\|A^{-1}\|\frac{\|\delta\,A\|}{\|A\|}.$$

11. (Optional: use for revision later if you wish)

(Part C exam question from 2009) What is an orthogonal matrix? Suppose that $Q \in \mathbb{R}^{m\times m}$ and $Z \in \mathbb{R}^{n\times n}$ are orthogonal matrices and define $Q_\ell \in \mathbb{R}^{m\times \ell}$ to be the matrix comprising the first ℓ columns of Q, analogously $Z_h \in \mathbb{R}^{n\times h}$ to be the matrix comprising the first h columns of Z. If $A \in \mathbb{R}^{m\times n}$, $m \geq n$, is an arbitrary matrix, prove that $\|AZ_h\|_2 \leq \|A\|_2$ for any integer h with $1 \leq h \leq n$. For what $\ell, 1 \leq \ell \leq m$ is it necessarily true that $\|Q_\ell^T A\|_2 = \|A\|_2$?

What is a Givens rotation matrix, $J(i, k, \theta), i \neq k$? Show that $J(i, k, \theta)$ is orthogonal and that if $y = J(i, k, \theta)x$ then a particular choice of θ which you should identify will ensure that $y_k = 0$ where y_j is the j^{th} entry of the vector y. What value of θ would ensure that $y_i = 0$?

Using these results, what sequence of Givens rotation matrices will perform a QR factorisation of a tridiagonal matrix $A \in \mathbb{R}^{n\times n}$? What sequence of Givens rotation matrices will perform a QR factorisation of a general full matrix $A \in \mathbb{R}^{n\times n}$?

Numerical Linear Algebra. QS 3 *(MT 2017)*

Optional questions: Qns 1, 4

1. If $A\,x = b$ and $(A + \delta\,A)\,(x + \delta\,x) = b$ show that

$$\frac{\|\delta\,x\|}{\|x + \delta\,x\|} \le \|A\|\|A^{-1}\|\frac{\|\delta\,A\|}{\|A\|}.$$

2. If Q is orthogonal prove that the condition number for linear systems satisfies $\kappa(Q) = 1$ at least when the $\|\cdot\|_2$ is used. What is the relationship between solving a linear least squares problem via QR factorization and via Cholesky factorization of the normal equations $A^T Ax = A^T b$?

3. Consider $A = \{a_{i,j} : i, j = 1, \ldots, n\}, a_{i,j} = 1/(i + j - 1)$. (See `help hilb` in matlab).

Use `matlab` to compute the condition number for $n = 4, 8, 12$ (`help cond`). For $n = 12$ compute `b=A*ones(n,1)` and then try to recover the solution $x = (1, 1, \ldots, 1)^T$ by Gaussian Elimination which in matlab is the result of `x=A\b`.

4. Explicitly show that if $A \in \mathbb{R}^{n\times n}$ is lower triangular then Gauss–Seidel iteration <u>is</u> forward substitution. This might imply that if A is nearly lower triangle (has few, small entries above the diagonal) then G–S might converge well (fast!). What should you do if you want to apply G–S iteration to a nearly upper triangular matrix?

5. For any $A \in \mathbb{R}^{n\times n}$ show that $\rho(A) \le \|A\|$ in any operator norm.

6. If λ is an eigenvalue of $A \in \mathbb{R}^{n\times n}$ then $(A - \lambda I)\,x = 0$ (*) for some $x \neq 0$. Suppose k is such that $|x_k| = \max_i |x_i|$, then the k^{th} equation of (*) is

$$(a_{kk} - \lambda)\,x_k = -\sum_{j=1,j\neq k}^{n} a_{kj}\,x_j.$$

Deduce that

$$|a_{kk} - \lambda| \leq \sum_{j=1,j\neq k}^{n} |a_{kj}| :$$

you have proved the Gershgorin Circle Theorem: that every eigenvalue of a matrix lies in at least one of the discs $\{z \in \mathbb{C} : \quad |a_{kk} - z| \leq \sum_{j=1,j\neq k}^{n} |a_{kj}|\}$.

For the matrix

$$A = \begin{bmatrix} 9 & 1 & 1 \\ 1 & 5 & 0 \\ 1 & 1 & 3 \end{bmatrix}$$

use this theorem to show that the spectral radius of the Jacobi iteration matrix is less or equal to $\frac{2}{3}$.

7. Using matlab on the matrix $A \in \mathbb{R}^{10\times 10}$ which has $a_{ii} = \frac{1}{2}$,

$$a_{ij} = \begin{cases} 0 & \text{if } i > j, \\ 1 & \text{if } i < j \end{cases}$$

(try $tril(ones(10,10)) - \frac{1}{2} * eye(10,10)$).

Calculate $\|A^k\|_\infty$ for $k = 1, \cdots, 50$ $(norm(A^k), inf)$. What is $\rho(A)$ and how does it relate to what you observe? (see `help for` about loops in matlab).

8. Prove that for the linear system $A\,x = b$, the symmetric SOR method

$$(D + \omega\,L)\;x^{(k+\frac{1}{2})} = \omega\,b + ((1-\omega)\,D - \omega\,U)\;x^{(k)}, \tag{1}$$

$$(D + \omega\,U)\;x^{(k+1)} = \omega\,b + ((1-\omega)\,D - \omega\,L)\;x^{(k+\frac{1}{2})} \tag{2}$$

where $A = D + L + U$, (D is a diagonal matrix, L is a strictly lower triangular matrix, U is a strictly upper triangular matrix), corresponds to the splitting $A = M - N$ where M is the symmetric matrix

$$\frac{1}{\omega\,(2-\omega)}\;(D + \omega\,L)\;D^{-1}\;(D + \omega\,U)\,.$$

9. If A is Strictly Row Diagonally Dominant (SRDD) prove that Jacobi iteration converges for any right hand side b and any stating guess $x^{(0)}$.

10. As in question 9 above, but prove that Gauss-Seidel converges under the same conditions.

Numerical Linear Algebra. QS 4 *(MT 2017)*

Optional questions: Qns 5, 8

1. (a) For the 5–point finite difference approximation of the Laplacian on $[0,1]\times[0,1]$ with Dirichlet Boundary Conditions on a regular mesh of size h with $(n+1)\,h=1$, verify that for each $r,\, s \in \{1,\cdots,n\}$, the vector $U^{r\,s}$ with components $u^{rs}_{jk} = \sin r\,j\,\pi\,h\,\sin s\,k\,\pi\,h$ is an eigenvector of the Jacobi iteration matrix with corresponding eigenvalue $\lambda^{rs} = \frac{1}{2}\,(\cos r\,\pi\,h + \cos s\,\pi\,h)$.

(b) Show that μ, v are an eigenvalue and eigenvector of the Gauss–Siedel iteration matrix for $A = D+L+U$, (D is a diagonal matrix, L is a strictly lower triangular matrix, U is a strictly upper triangular matrix), if and only if $(\mu\,D + \mu\,L + U)\,v = 0$. For the 5–point problem above show that v^{rs} with components $v^{rs}_{jk} = \mu^{\frac{j+k}{2}}\,\sin r\,j\,\pi\,h\,\sin s\,k\,\pi\,h$ is an eigenvector of the G–S iteration matrix. What is the corresponding eigenvalue? Which of Jacobi or G–S iteration will converge more rapidly for this problem? Is G–S suitable for use as a smoother in multigrid?

2. Consider using multigrid to solve the 1–dimensional boundary value problem,

$$-u'' = f, \quad x\in[0,1], \quad u(0) = 0 = u(1)$$

approximately by the finite difference

$$-u_{j-1} + 2\,u_j - u_{j+1} = h^2\,f, \quad j = 1,2,\ldots,n$$

on a regular grid $jh, j = 0,1,\ldots,n+1$ with $(n+1)\,h = 1$ and n odd.

If $u^e = (u_2, u_4, \cdots, u_{n-1})^T$ is a vector of the coarse grid unknowns, show that prolongation to fine grid values $(u_1, u_2, \cdots, u_n)^T$ by linear interpolation between adjacent points can be represented by $P\,u^e$ where

$$P = \begin{bmatrix} \frac{1}{2} & & & & \\ 1 & & & & \\ \frac{1}{2} & \frac{1}{2} & & & \\ & 1 & & & \\ & \frac{1}{2} & \frac{1}{2} & & \\ & & 1 & \cdot & \\ & & & \cdot & \\ & & & \cdot & \\ & & & \frac{1}{2} & \frac{1}{2} \\ & & & & 1 \\ & & & & \frac{1}{2} \end{bmatrix} \in \mathbb{R}^{n\times\frac{n-1}{2}}$$

What restriction does $R = \frac{1}{2}\,P^T$ represent?

3. Consider a two-grid iteration for $A\mathbf{u} = \mathbf{f}$ with no post-smoothing. Here P is the prolongation, R the restriction and the smoothing iteration is based on the splitting $A = M - N$. Denote by $\mathbf{u}_s^{(i)}$ the result of k pre-smoothing steps on the i^{th} multigrid iterate $\mathbf{u}^{(i)}$. Show that the next two-grid iterate is

$$\mathbf{u}^{(i+1)} = \mathbf{u}_s^{(i)} + P\overline{A}^{-1}R(\mathbf{f} - A\mathbf{u}_s^{(i)}).$$

By further showing that

$$\mathbf{f} - A\mathbf{u}_s^{(i)} = A(I - M^{-1}A)^k(\mathbf{u} - \mathbf{u}^{(i)}),$$

demonstrate that

$$\mathbf{u} - \mathbf{u}^{(i+1)} = (A^{-1} - P\overline{A}^{-1}R)A(I - M^{-1}A)^k(\mathbf{u} - \mathbf{u}^{(i)}).$$

4. Similarly to problem 3, show that if m post-smoothing iterations are also employed then

$$\mathbf{u} - \mathbf{u}^{(i+1)} = (I - M^{-1}A)^m(A^{-1} - P\overline{A}^{-1}R)A(I - M^{-1}A)^k(\mathbf{u} - \mathbf{u}^{(i)}).$$

5. Show that in two-grid iteration the residual $\mathbf{r}^{(i)} = A\mathbf{e}^{(i)}$ satisfies

$$\mathbf{r}^{(i+1)} = (I - AM^{-1})^m A(A^{-1} - P\overline{A}^{-1}R)(I - AM^{-1})^k\mathbf{r}^{(i)}.$$

6. By writing the two-grid iteration matrix

$$(I - M^{-1}A)^m(A^{-1} - \alpha P\overline{A}^{-1}P^T)A(I - M^{-1}A)^k$$

for a symmetric matrix A, with restriction equal to αP^T for some real positive α, in the form $I - M_{MG}^{-1}A$, show that M_{MG} is symmetric when $k = m$ and M is symmetric. You should assume that $\overline{A}$ is symmetric. It follows that two-grid iteration corresponds to a symmetric splitting $A = M_{MG} - N$ under these conditions.

7. Similarly to problem 6, show that provided $k = m$, then employing M^T in the post-smoother and M in the pre-smoother results in a symmetric two-grid splitting matrix M_{MG} when M is non-symmetric. This is of relevance when for example Gauss-Seidel smoothing is used since M^T then corresponds to reversing the ordering of the variables.

8. In this question the restriction is $R = \alpha P^T$ where P is the prolongation and the Galerkin coarse grid operator $\overline{A} = \alpha P^T AP$ is used. Writing

$$G^{pre} = (A^{-1} - \alpha P\overline{A}^{-1}P^T)A(I - M^{-1}A)^k$$

for the two-grid iteration matrix when only pre-smoothing is used and

$$G^{post} = (I - M^{-1}A)^m(A^{-1} - \alpha P\overline{A}^{-1}P^T)A$$

for the two-grid iteration matrix when only post-smoothing is used, show that

$$G^{post}G^{pre} = (I - M^{-1}A)^m(A^{-1} - \alpha P\overline{A}^{-1}P^T)A(I - M^{-1}A)^k$$

is the standard two-grid iteration matrix with m post-smoothing and k pre-smoothing iterations. It follows that if $\|G^{pre}\| < 1$ and $\|G^{post}\| < 1$ then the standard two-grid iteration is convergent in the same norm.

9. Show that for the 5-point matrix, relaxed Jacobi smoothing with $\theta = 4/5$ ensures that all of the eigenvalues with $r > n/2$ *or* $s > n/2$ (which correspond to eigenvectors with high frequency variation in at least one of the coordinate directions) lie in $(-3/5, 3/5]$.

Numerical Linear Algebra QS 5 *(MT 2017)*

Optional questions: Qns 2, 7

1. If $A \in \mathbb{R}^{n\times n}$ is such that $\mathrm{diag}(A) = I$, what polynomial p_k satisfies

$$x - x^{(k)} = p_k(A)(x - x^{(0)})$$

where x is the exact solution of $Ax = b$ and $\{x^{(j)}, j = 0, 1, \ldots\}$ are the iterate vectors produced by Jacobi iteration?

If $x^{(0)} = 0$ is chosen, for what polynomial is $x^{(k)} = q_k(A)b$?

2. (Section C exam questions 2001) If $A = M - N$ with A, M, $N \in \mathbb{R}^{n\times n}$, A, M nonsingular and $M^{-1}N$ diagonalisable, prove that the iteration

$$Mx^{(k)} = Nx^{(k-1)} + b, \qquad k = 1, 2, \ldots$$

will generate a sequence $\{x^{(k)}\}$ which converges to the solution x of $Ax = b$ for any starting guess $x^{(0)}$ if and only if the eigenvalues λ of $M^{-1}N$ satisfy $|\lambda| < 1$. Further, if $M^{-1}N$ is symmetric so that there is a basis $\{v_i, i = 1, \ldots, n\}$ for $\mathbb{R}^n$ of orthonormal eigenvectors of $M^{-1}N$, show that

$$v_i^T(x - x^{(k)}) = \lambda_i^k\, v_i^T(x - x^{(0)})$$

where λ_i is the eigenvalue corresponding to the eigenvector v_i.

For the remainder of this question you should assume that $|\lambda| < 1$ is a necessary and sufficient condition for convergence regardless of whether $M^{-1}N$ is or is not diagonalisable.

The Successive Overelaxation Method (SOR) is: $x^{(0)}$ arbitrary,

for $\quad k = 1, 2, \ldots$

for $i = 1, \ldots, n$

$$x_i^{(k)} = (1-\omega)x_i^{(k-1)} + \omega\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k)} - \sum_{j=i+1}^{n} a_{ij}x_j^{(k-1)}\right) \Big/ a_{ii}$$

end

end

where $A = \{a_{ij}, i, j = 1, \ldots, n\}$, $b = \{b_i, i = 1, \ldots, n\}$ and $\omega \in \mathbb{R}$. In terms of the diagonal matrix D, the strictly lower triangular matrix L and the strictly upper triangular matrix U such that $A = D + L + U$, write the SOR iteration in matrix form.

Suppose that $D = I$. By considering the determinant of the SOR iteration matrix or otherwise show that if $\omega \notin (0, 2)$ then SOR iteration can not be convergent. If further, $L^2 = 0$, show that the SOR iteration is convergent if and only if the eigenvalues of $(I - \omega L)A$ lie in $B(1/\omega, 1/\omega)$ where $B(a, b)$ is the open disc with centre a and radius b.

3. Suppose that $A = M - N \in \mathbb{R}^{m\times m}$ and it is desired to solve the linear system $Ax = b$. State a theorem which gives necessary and sufficient conditions for convergence of the vector sequence $\{x^{(i)}\}$ generated by the iteration: for initial guess $x^{(0)}$ compute

$$Mx^{(i+1)} = Nx^{(i)} + b, \qquad i = 0, 1, \dots .$$

For Jacobi iteration what is M? Prove that if $A = \{a_{i,j}\}$ and

$$|a_{i,i}| > \sum_{j\neq i} |a_{i,j}|, \qquad i = 1, 2, \dots, m \quad (\star)$$

then Jacobi iteration converges. If $m = n^2$ and $A = D + L + U$ where $D = \mathrm{diag}(D_1, D_2, \dots, D_n)$ and $D_i \in \mathbb{R}^{n\times n}, i = 1, 2, \dots, n$ are the diagonal blocks of A, L is the lower triangular part of $A - D$ and U is the upper triangular part of $A - D$, prove that the iteration based on the splitting $M = D$ will converge provided that the condition $(\star)$ holds. If for each $i = 1, 2, \dots, n$, D_i is the tridiagonal matrix

$$\begin{pmatrix} 4 & -1 & & & \\ -1 & 4 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 4 & -1 \\ & & & -1 & 4 \end{pmatrix}$$

and

$$A = \begin{pmatrix} D_1 & -I & & & \\ -I & D_2 & -I & & \\ & \ddots & \ddots & \ddots & \\ & & -I & D_{n-1} & -I \\ & & & -I & D_n \end{pmatrix}$$

where $I \in \mathbb{R}^{n\times n}$ is the identity matrix, find the eigenvalues of the iteration matrix based on the splitting $M = D$ and show that the spectral radius of the iteration matrix is

$$1 - \pi^2/(n+1)^2 + O(n^{-4})$$

for large n.

4. Show that the (iteration) matrix

$$T = \begin{bmatrix} 0 & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 \end{bmatrix}$$

has eigenvalues $\frac{2}{3}$, $-\frac{1}{3}$ and $-\frac{1}{3}$ and that $\left(T - \frac{2}{3}I\right)\left(T + \frac{1}{3}I\right) = 0$. Convince yourself (by using matlab, maple or otherwise) that no power of T is the zero matrix, but $T^k \to 0$ as $k \to \infty$. Define, however, a polynomial iterative method which will terminate after 2 iterations.

5. Verify that for arguements $|t| \geq 1$ the definition

$$T_k(t) = \frac{1}{2^{k-1}} \cosh k \left(\cosh^{-1} t\right)$$

defines the same (Chebyshev) polynomial as

$$T_k(x) = \frac{1}{2^{k-1}} \cos k \left(\cos^{-1} t\right)$$

for $|t| \leq 1$. Verify that (at least) for $t > \cosh(ln2)$, $T_k(t) \to \infty$ as $k \to \infty$.

6. If the eigenvalues λ of an iteration matrix S satisfy $|\lambda| \leq \rho < 1$ and $y^{(k)}$, $k = 2, 3, \cdots$ are the iterates obtained by using Chebyshev polynomials

$$\hat{T}_k(x) = \frac{T_k\left(\frac{x}{\rho}\right)}{T_k\left(\frac{1}{\rho}\right)} \quad \text{(i.e. shifted onto } [-\rho, \rho] \text{ and scaled so that } \hat{T}_k(1) = 1)$$

in a polynomial iteration based on S, show that

$$T_{k+1}(\frac{1}{\rho})\, e^{(k+1)} = \frac{1}{\rho}\, T_k(\frac{1}{\rho})\, S\, e^{(k)} - \frac{1}{4}\, T_{k-1}(\frac{1}{\rho})\, e^{(k-1)}$$

(at least for $k \geq 3$) where $e^{(k)} = y^{(k)} - x$ and x is the exact solution satisfying $x = S\,x + g$. (You may want first to obtain a 3–term recurrence for the $\hat{T}_k$). From this show that

$$y^{(k+1)} = w_{k+1} \left(S\, y^{(k)} + g - y^{(k-1)}\right) + y^{(k-1)}$$

where

$$w_{k+1} = \frac{1}{\rho} \frac{T_k\left(\frac{1}{\rho}\right)}{T_{k+1}\left(\frac{1}{\rho}\right)} = 1 + \frac{1}{4} \frac{T_{k-1}\left(\frac{1}{\rho}\right)}{T_{k+1}\left(\frac{1}{\rho}\right)}.$$

This shows that it is unnecessary to compute the iterates $x^{(k)}$ of the simple iteration involving S since the w_k can be computed easily using the 3 term recurrence for Chebyshev polynomials.

7. Let $A \in \mathbb{R}^{n^2 \times n^2}$ be the matrix which arises from 5–point finite difference replacement of the Laplacian with Dirichlet boundary conditions on a regular grid on the unit square. (Assume that A is scaled so that it has 4's on the diagonal). It is desired to solve $(\sigma\, I + A)\, x = b$ where $0 < \sigma \in \mathbb{R}$ using polynomial iteration based on the simple Jacobi iteration $(\sigma\, I {+} D)\, x^{(k+1)} = -(L{+}U)\, x^{(k)} {+} b$. By using Geshgorins Theorem (or otherwise) show that the eigenvalues of the iteration matrix satisfy $|\lambda| \leq \frac{4}{4+\sigma}$. Hence estimate convergence of Chebyshev polynomial iteration (as in previous question) if $\sigma = \frac{1}{2}$.

Numerical Linear Algebra QS 6 *(MT 2017)*

Optional questions: Qns 1, 6

1. Show that the Chebyshev Polynomials $T_n(x) = \frac{1}{2^{n-1}} \cos n \left(\cos^{-1} x\right)$ satisfy

$$\int_{-1}^{1} \frac{T_n(x)\, T_m(x)}{\sqrt{1-x^2}}\, dx = 0$$

when $n \neq m$.

This shows that the Chebyshev polynomials are the orthogonal polynomials with respect to the inner product

$$< p, q >= \int_{-1}^{1} \frac{p(x)\, q(x)}{\sqrt{1-x^2}}\, dx$$

ie. $T_n \in \Pi_n, n = 0, 1, \ldots$ and $< T_n, T_m >$ is equal to zero except when $n = m$ (when it is clearly positive.)

2. If $A \in \mathbb{R}^{n\times n}$ is nonsingular, show that GMRES breaks down at the ℓ^{th} iteration (ie. $h_{\ell+1,\ell} = 0$) if and only if $x_\ell = x$ (ie. if and only if the solution of the linear system has been found).

3. Let $Q_k R_k$ be a QR factorization of $\widehat{H}_k$ where $Q_k = J_1, J_2, \ldots, J_k$ with J_j being a single $(j+1)\times(j+1)$ Givens rotation matrix for each j. If $\widehat{H}_{k+1}$ is computed from $\widehat{H}_k$ by appending the one further column computed by the next step of the Arnoldi algorithm, show that only one further Givens rotation J_{k+1} gives the QR factorization of $\widehat{H}_{k+1}$.

4. Continuing from the question above: If $s = \sin\theta$ in the Givens rotation in J_{k+1}, show that

$$\|r_k\|_2 = |s|\|r_{k-1}\|_2.$$

Hence for the sequence of succesive residuals $r_k, k = 0, 1, 2, \ldots$ computed by the GMRES method, $\{\|r_k\|_2, k = 0, 1, 2, \ldots\}$ must reduce monotonically. Are there any circumstances in which the convergence is not strictly monotonic?

5. Show how GMRES will converge on the linear system $Ax = b$ with $x_0 = 0$ when

$$A = \begin{bmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \end{bmatrix}, \qquad b = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}.$$

Hand calculation (it is simple in this example to work out what the residual vectors must be!) is best here if you want to learn something!

6. If

$$A = \begin{bmatrix} I & B_2 & & & & \\ & I & B_3 & & & \\ & & I & \ddots & & \\ & & & I & B_{k-1} & \\ & & & & I & B_k \\ & & & & & I \end{bmatrix}$$

for arbitrary submatrices B_i of appropriate dimension, show that $(I - A)^k = 0$.

What is the maximum number of steps that unrestarted GMRES would take to solve a linear system with matrix A?

7. Use matlab (`[x,flag,relres,iter,resvec]=gmres(A,b,[],1.e-6,size(A,1))`) with suitably chosen matrices A and b as below to investigate the behaviour of GMRES.

Note in the form above matlab will use unrestarted GMRES, `flag=0` will indicate successful convergence (the relative residual norm - `relres` - less than 10^{-6} in less than dimension(A) `=size(A,1)` iterations), `iter` is the number of restarts (should be 1 with no restarting) and iterations taken and `resvec` is the vector of residual norms at each iteration (hence `semilogy(resvec)` will plot the convergence curve). See `help gmres` if you want to read more or change any of the defaults.

(i) `A=randn(n); b=ones(n,1);` for `n=7,47,...` as you choose (and have patience for! (note `ctrl C` will interrupt a computation). These are dense matrices!

(ii) `A=sprandn(100,100,0.1); b=ones(100,1);`. This is a sparse 100×100 matrix with approximately 10 non-zero entries per row (ie. `0.1` of the 10,000 entries non-zero).

(iii) `A=sprandn(100,100,0.1) +2*eye(100,100); b=ones(100,1);`

(iv) `A=sprandn(100,100,0.1) +4*eye(100,100); b=ones(100,1);`

(v) a diagonalisable matrix that has few distinct eigenvalues
eg. `X=randn(9,9); A=X*diag([1,1,-4,3,3,-4,-4,-4,3])/X`
(note `/X` is an more efficient way of computing `*inv(X)` and that it is possible that an X generated with random entries is singular, but is rarely so!)

(vi) any matrix

8. (entirely voluntary)

(I know this to be true (indeed for many matrices), but do not have as elementary a proof of it as I would like: hence I offer a pint of beer/gin&tonic/orange juice to the first person to show me a proof)

Prove that the Gauss-Seidel iteration matrix for the 5-point matrix is not diagonalisable.

Numerical Linear Algebra QS 7 *(MT 2017)*

Optional questions: Qns 5, 8

1. Derive and write down the MINRES algorithm and show that the work per iteration is $O(n)$ for a sparse real symmetric matrix with $O(1)$ entries per row.

2. Consider the recurrence

$$\gamma_{j+1}\mathbf{v}_{j+1} = A\mathbf{v}_j - \delta_j\mathbf{v}_j - \gamma_j\mathbf{v}_{j-1}, \quad 1 \le j \le k-1,$$

where $\mathbf{v}_1$ is an arbitrary vector with $\|\mathbf{v}_1\|_2 = 1$, $\mathbf{v}_0 = 0$, $\delta_j = \mathbf{v}_j^T A\mathbf{v}_j$, and γ_j is chosen so that $\|\mathbf{v}_j\|_2 = 1$. Prove that for a real symmetric matrix A this procedure generates an orthonormal basis for the Krylov subspace $\mathcal{K}_k(A, \mathbf{v}_1)$. (Hint: use induction and note that for a symmetric matrix A

$$\langle A\mathbf{v}_j, \mathbf{v}_{j-1}\rangle = \langle \mathbf{v}_j, A\mathbf{v}_{j-1}\rangle = \mathbf{v}_j^T A\mathbf{v}_{j-1},$$

and also that $A\mathbf{v}_{j-1} = \gamma_j\mathbf{v}_j + \mathbf{w}$, with $\mathbf{w} \in \mathtt{span}\{\mathbf{v}_1, \ldots, \mathbf{v}_{j-1}\}$.)

3. For a chosen $\mathbf{x}_0$, if $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$ and $\mathbf{p}_0 = \mathbf{r}_0$ and for $k = 0, 1, \ldots$

$$\begin{aligned}
&\alpha_k = \langle \mathbf{p}_k, \mathbf{r}_k\rangle / \langle \mathbf{p}_k, A\mathbf{p}_k\rangle \\
(1)\quad &\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k\mathbf{p}_k \\
(2)\quad &\mathbf{r}_{k+1} = \mathbf{b} - A\mathbf{x}_{k+1} \\
&\beta_k = -\langle \mathbf{p}_k, A\mathbf{r}_{k+1}\rangle / \langle \mathbf{p}_k, A\mathbf{p}_k\rangle \\
(3)\quad &\mathbf{p}_{k+1} = \mathbf{r}_{k+1} + \beta_k\mathbf{p}_k
\end{aligned}$$

show that (2) and (1) imply

$$\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k A\mathbf{p}_k.$$

Prove that the definition of α_k implies $\langle \mathbf{r}_{k+1}, \mathbf{p}_j\rangle = 0$ for $j = k$ and that the definition of β_k implies $\langle \mathbf{p}_{k+1}, A\mathbf{p}_j\rangle = 0$ for $j = k$. Prove also that $\langle \mathbf{r}_{k+1}, \mathbf{r}_j\rangle = 0$ for $j = k$. Now by employing induction in k for $k = 1, 2, \ldots$, prove these three assertions for $j = 1, 2, \ldots, k-1$. (The inductive assumption will be that

$$\langle \mathbf{r}_k, \mathbf{p}_j\rangle = 0, \quad \langle \mathbf{r}_k, \mathbf{r}_j\rangle = 0, \quad \langle \mathbf{p}_k, A\mathbf{p}_j\rangle = 0, \quad j = 0, 1, \ldots, k-1$$

and you may wish to tackle the assertions in this order.)

4. By expanding $\|\mathbf{x} - (\mathbf{x}_k + \alpha \mathbf{p}_k)\|_A^2$ and using simple calculus, show that the value $\alpha = \mathbf{p}_k^T \mathbf{r}_k / \mathbf{p}_k^T A \mathbf{p}_k$ is minimising. Use the result of the question above to further show that $\mathbf{p}_k^T \mathbf{r}_k = \mathbf{r}_k^T \mathbf{r}_k$ and that and alternative formula for β_k is

$$\beta_k = \frac{\mathbf{r}_{k+1}^T \mathbf{r}_{k+1}}{\mathbf{r}_k^T \mathbf{r}_k}.$$

These equivalent formulae give the form of the Conjugate Gradient Algorithm usually used for computation:

For a chosen $\mathbf{x}_0$, if $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$ and $\mathbf{p}_0 = \mathbf{r}_0$ and for $k = 0, 1, \ldots$

$$\begin{aligned}
&\alpha_k = \langle \mathbf{r}_k, \mathbf{r}_k \rangle / \langle \mathbf{p}_k, A\mathbf{p}_k \rangle \\
(1) \quad &\mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k \\
(2) \quad &\mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k A\mathbf{p}_k \\
&\beta_k = \langle \mathbf{r}_{k+1}, \mathbf{r}_{k+1} \rangle / \langle \mathbf{r}_k, \mathbf{r}_k \rangle \\
(3) \quad &\mathbf{p}_{k+1} = \mathbf{r}_{k+1} + \beta_k \mathbf{p}_k
\end{aligned}$$

5. Based on the form of the Conjugate Gradient algorithm given in the question above, write an efficient implementation (in pseudocode or matlab notation) which requires only one matrix×vector product at each iteration and minimises the number of vector operations.

6. Use matlab (`[x,flag,relres,iter,resvec]=pcg(A,b,1.e-6,size(A,1))`) with suitably chosen matrices A and b as below to investigate the behaviour of Conjugate Gradients.

Note in the form above matlab will use unpreconditioned Conjugate Gradients, `flag=0` will indicate successful convergence (the relative residual norm - `relres` - less than 10^{-6} in less than dimension(A) `=size(A,1)` iterations), `iter` is the number of iterations taken and `resvec` is the vector of residual norms at each iteration (hence `semilogy(resvec)` will plot the convergence curve). See `help pcg` if you want to read more or change any of the defaults.

(i) `A=randn(n); A=A*A'; b=ones(n,1);` for `n=7,47,...` as you choose (and have patience for! (note `ctrl C` will interrupt a computation). These are dense matrices!

(ii) `A=sprandsym(100,0.1,invkappa,1); b=ones(100,1);`. This is a sparse 100×100 symmetric and positive definite matrix with approximately 10 non-zero entries per row (ie. `0.1` of the 10,000 entries non-zero) and with $\|\cdot\|_2$-norm condition number `1/invkappa`. Try `pcg` with well-conditioned matrices (small κ or `invkappa` just less than 1) and badly conditioned matrices (large κ or `invkappa` nearly zero).

(iii) a symmetric and positive definite matrix that has few distinct eigenvalues
eg. `X=randn(9,9); X=orth(X); A=X*diag([1,1,4,3,3,4,4,4,3])*X'`
(note that it is possible that an X generated with random entries is singular, but is rarely so!)

(iv) any of the above with a preconditioner of your choice.

The remaining questions are really on the work of week 8: please leave them to attempt after the last lectures on this course,

7. Derive the preconditioned Congugate Gradient Algorithm with preconditioner P:

For a chosen $\mathbf{x}_0$, if $\mathbf{r}_0 = \mathbf{b} - A\mathbf{x}_0$ and $\mathbf{z}_0$ solves $P\mathbf{z}_0 = \mathbf{r}_0$ with $\mathbf{p}_0 = \mathbf{z}_0$ and for $k = 0, 1, \ldots$

$$
\begin{aligned}
& \alpha_k = \langle \mathbf{z}_k, \mathbf{r}_k \rangle / \langle \mathbf{p}_k, A\mathbf{p}_k \rangle \\
(1) \quad & \mathbf{x}_{k+1} = \mathbf{x}_k + \alpha_k \mathbf{p}_k \\
(2) \quad & \mathbf{r}_{k+1} = \mathbf{r}_k - \alpha_k A\mathbf{p}_k \\
(3) \quad & \text{Solve } P\mathbf{z}_{k+1} = \mathbf{r}_{k+1} \\
& \beta_k = \langle \mathbf{z}_{k+1}, \mathbf{r}_{k+1} \rangle / \langle \mathbf{z}_k, \mathbf{r}_k \rangle \\
(4) \quad & \mathbf{p}_{k+1} = \mathbf{z}_{k+1} + \beta_k \mathbf{p}_k
\end{aligned}
$$

by considering the unpreconditioned Conjugate Gradient Algorithm as in Question 4 above applied to

$$H^{-1}AH^{-T}\mathbf{v} = H^{-1}\mathbf{b}, \quad \mathbf{v} = H^T\mathbf{x}$$

where $P = HH^T$.

(Hint you may wish to write $\widehat{A} = H^{-1}AH^{-T}$, $\widehat{\mathbf{x}} = H^T\mathbf{x}$, $\widehat{\mathbf{b}} = H^{-1}\mathbf{b}$ and write down the Conjugate Gradient algorithm for $\widehat{A}\widehat{\mathbf{x}} = \widehat{\mathbf{b}}$ to generate $\{\widehat{\mathbf{x}}_k\}$, $\{\widehat{\mathbf{p}}_k = H^T\mathbf{p}_k\}$ etc.)

8. Consider a symmetric coefficient matrix A, show that if the splitting matrix M is also symmetric, then the iteration matrix $S = I - M^{-1}A$ is symmetric with respect to the A inner product; that is

$$\langle S\mathbf{x}, \mathbf{y} \rangle_A = \langle \mathbf{x}, S\mathbf{y} \rangle_A.$$

This means that S (and indeed S^k, where k is the number of iteration steps) may be used as a preconditioner with Conjugate Gradients.