Advanced Numerical Analysis Homework 7

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Throughout this homework, $\|\cdot\|$ denotes the ℓ_2-norm. We also let $\langle \cdot, \cdot \rangle$ denote the standard Euclidean inner-product on $\mathbb{R}^m$ (thus $\langle v, w \rangle = v^\top w$ for all $v, w \in \mathbb{R}^m$). Finally we set $\varepsilon = \varepsilon_{\text{machine}}$ to be the machine coefficient.

1 Problem 1

Exercise 1. 1. Recall that A is Hermitian if $A^H = A$ and skew-Hermitian if $A^H = -A$. Show that the eigenvalues of a Hermitian matrix (e.g., real symmetric) are real, and those of a skew-Hermitian (e.g., real skew-symmetric) are purely imaginary. In both cases, show that the eigenvectors associated with distinct eigenvalues are orthogonal.

2. For a block upper triangular

$$F = \begin{pmatrix} F_{11} & F_{12} & \cdots & F_{1n} \\ & F_{22} & \cdots & F_{2n} \\ & & \ddots & \vdots \\ & & & F_{nn} \end{pmatrix},$$

show that $\Lambda(F) = \bigcup_{k=1}^{n} \Lambda(F_{kk})$, where $\Lambda(-)$ denotes the spectrum (all eigenvalues) of a matrix.

Solution 1. 1.

2. Characteristic polynomial

2 Problem 2

Exercise 2. 1. Given a complex Schur form $U^H AU = T$, where T is upper triangular, show that the first k columns $u_1, \dots, u_k$ of U span an invariant subspace of A, that is

$$A\text{span}\{u_1, \dots, u_k\} = \text{span}\{Au_1, \dots, Au_k\} \subseteq \text{span}\{u_1, \dots, u_k\}.$$

2. Let $U \in \mathbb{R}^{n \times p}$ (where $n > p$) contains basis vectors of an invariant subspace of A, such that $AU = UM$ for some $M \in \mathbb{R}^{p \times p}$. Show that the eigenvalues of M are also eigenvalues of A. If, in addition, $W \in \mathbb{R}^{n \times m}$ (where $n > m > p$) has orthonormal columns, and $\text{col}(U) \subseteq \text{col}(W)$, show that the eigenvalues of M are eigenvalues of $W^\top AW$.

Solution 2.

3 Problem 3

Exercise 3. 1. Describe a procedure to post-process the Q and R factors of Givens or Householder QR, such that the R factor has all non-negative diagonal entries

2. Verify numerically that the Simultaneous Iteration is equivalent to the unshifted QR iteration. To this end, first construct an upper Hessenberg H_0 as follows rng(default); H0 = triu(randn(7,7),−1); Implement the Simultaneous Iteration and the QR iteration, described in Trefethen's book, Chapter 28. Feel free to use MATLAB's qr, followed by the post-processing in part (1), and the '*' operation directly to form $H^{(k)} = R^{(k)}Q^{(k)}$ (that is, no need to use the Givens rotations to perform the QR iteration as usually supposed

to). Compare the projection matrices $H_{SI}^{(k)}$ in (28.10) for simultaneous iteration and $H_{QR}^{(k)}$ in (28.13) in the QR iteration. Find the relative difference

$$\frac{\|H_{SI}^{(k)} - H_{QR}^{(k)}\|_F}{\|H_{SI}^{(k)}\|}$$

for $k = 3, 30, 300$ and 3000, and the relative difference in the eigenvalues of $H_{SI}^{(k)}$ and $H_{QR}^{(k)}$ at these steps? What if the post-processing is not used, and in this case, do $H_{SI}^{(k)}$ and $H_{QR}^{(k)}$ have numerically the same eigenvalues?

3. Find the eigenvalues of H_0, then use the theory we learned from class to estimate the rate of convergence of $H_{QR}^{(k)}$ toward the quasi-upper triangular T of the real Schur form. About how many iterations are needed to achieve

$$\frac{\|H_{QR}^{(k)} - T\|_F}{\|T\|_F} \approx \varepsilon$$

Solution 3. table

$\|b - A\hat{x}\| / \|A\| \|\hat{x}\|$	BACKSLASH	HOUSE
A_2	$3.1026e - 08$	$3.1026e - 08$
A_3	$5.4432e - 17$	$3.3642e - 17$

4 Problem 4

Exercise 4. (Trefethen's book Prob. 28.2, but for the nonsymmetric case).

1. Explore the nonzero structure of the Q factor of the QR factorization of an upper Hessenberg matrix, and verify that RQ is also upper Hessenberg. For clarity, you may give an illustration for a 5×5 upper Hessenberg.

2. The computation of $H^{(k)} = R^{(k)}Q^{(k)}$, if done naively (by direct evaluation of the matrix-matrix multiplication), would need $O(n^3)$ operations. Fortunately, $H^{(k)}$ can be computed only in $O(n^2)$ operations. Explain, by Givens rotations, how this is achieved. Make sure that you do see the difference in cost.

Solution 4.

Appendix

Classical Gram-Schmidt

```
function [Q,R] = gs(A)

[m,n] = size(A); Q = zeros(m,n); V = zeros(m,n); R = zeros(m,n);

for j = 1:n
   V(:,j) = A(:,j);
   for i = 1:j-1
      R(i,j) = Q(:,i)'*A(:,j);
      V(:,j) = V(:,j) - R(i,j)*Q(:,i);
   end;
   R(j,j) = norm(V(:,j)) ;
   Q(:,j) = V(:,j) / R(j,j) ;
   end;
end;
```

Modified Gram-Schmidt

```
function [Q,R] = mgs(A)

[m,n] = size(A); Q = zeros(m,n); V = A; R = zeros(n,n);

for i = 1:n
   R(i,i) = norm(V(:,i));
   Q(:,i) = V(:,i) / R(i,i);
   for j = (i+1):n
      R(i,j) = Q(:,i)'*V(:,j);
      V(:,j) = V(:,j) - R(i,j)*Q(:,i);
   end;
end;
```

Double Modified Gram-Schmidt

```
function [Q,R] = mgsd(A)

[Q1,R1] = mgs(A);
[Q,R2] = mgs(Q1);
R = R2*R1;
```

Householder Factorization

```
function [V,R] = house(A)

[m,n] = size(A); V = zeros(m,n);

for k = 1:n
   x = A(k:m,k);
   V(k:m,k) = sign(x(1))*norm(x)*eye(m-k+1,1)+x;
   V(k:m,k) = V(k:m,k)/norm(V(k:m,k));
   A(k:m,k:n) = A(k:m,k:n) - 2*V(k:m,k)*(V(k:m,k)'*A(k:m,k:n));
end

R = A(1:n,:);
```

Evaluate Qb or Q^*b

```
function [b] = houseev(V,b,transpose)

[m,n] = size(V);

if transpose
   for k = 1:n
     b(k:m) = b(k:m) - 2*V(k:m,k)*(V(k:m,k)'*b(k:m));
   end;
else
   for k = n:-1:1
      b(k:m) = b(k:m) - 2*V(k:m,k)*(V(k:m,k)'*b(k:m));
   end;
end;
```

Form $\widehat{Q}$ From House

```
function Q = houseformQ(V)

[m,n] = size(V); Q = zeros(m,n);

for j = 1:n
    x = zeros(m,1);
    x(j,1) = 1;
    Q(:,j) = houseev(V,x,0);
end;
```

Least Squares via Householder QR

```
function x = leastsquareshouseQR(A,b)

[V,R] = house(A);
y   = houseev(V,b,1);
y   = y(1:n);
x = R\y;
```