Lab Session 8

MA 423 : Matrix Computations Lab 2023 R. Alam

1. The purpose of this experiment is to illustrate that QR factorization by Householder reflector (MATLAB command `[Q, R] = qr(A)`) is better than modified Gram-Schmidt scheme (MGS) and classical Gram-Schmidt scheme (CGS).

   Consider the n-by-n Hilbert matrix H (use MATLAB command `H = hilb(n)` to generate H). Your task is to use different methods listed below to orthonormalize the columns of H for $n = 7$ and $n = 12$.

   (a) Write a MATLAB function implementing classical Gram-Schmidt method (CGS).

   ```
   function [Q, R] = cgsqr(A)
   % [Q, R] = cgsqr(A) employs classical Gram-Schmidt scheme to compute
   % an isometry Q, an upper triangular matrix R such that A=QR.

   [m, n] = size(A); %  Assume that m >= n
   Q = A; R = zeros(n);
   for k = 1:n
    R(1:k-1,k) = Q(:,1:k-1)' * A(:,k);
    Q(:,k) = A(:,k)- Q(:,1:k-1) * R(1:k-1,k);
    R(k,k) = norm(Q(:,k));
    Q(:,k) = Q(:,k)/R(k,k);
   end
   ```

   (b) Write a MATLAB function implementing modified Gram-Schmidt method (MGS).

   ```
   function [Q, R] = mgsqr(A)
   % [Q, R] = mgsqr(A) employs modified Gram-Schmidt scheme to compute
   % an isometry Q, an upper triangular matrix R such that A=QR.

   [m,n] = size(A);  % Assume that m >=n
   Q = A; R = zeros(n);
   for k = 1:n
   R(k,k) = norm(Q(:,k));
   Q(:,k) = Q(:,k)/R(k,k);
   R(k,k+1:n) = Q(:,k)' * Q(:,k+1:n);
   Q(:,k+1:n) = Q(:,k+1:n) - Q(:,k) * R(k,k+1:n);
   end
   ```

   (c) QR decomposition with reflectors. Use MATLAB command `[Q,R] = qr(H, 0)`, which produces an 'economy size' QR decomposition of H with Q being an isometry.

   Examine the deviation from orthonormality by computing $\|Q' * Q - \texttt{eye(n)}\|_2$ in each case (MATLAB command `norm(eye(n)-Q'*Q)`). Setting $E := QR - H$, we have $H + E = QR$. Check the residual norm $\|E\|_2 =$ `norm(H - Q*R)`. The small residual error of order $\mathcal{O}(\mathbf{u})$ as well as small deviation from orthonormality of order $\mathcal{O}(\mathbf{u})$ imply that the algorithm is backward stable. In other words, the algorithm computes QR factroization of a slightly perturbed matrix which is indistinguishable from A. Test the backward stability of CGS, MGS and Householder QR factorization.

   Find the condition number of H and check whether or not the matrix Q obtained from the MGS program satisfies $\|Q' * Q - \texttt{eye(n)}\|_2 \approx u * \texttt{cond(H)}$.

   Did you get what you would expect in light of the values of unit roundoff $\mathbf{u}$ and $\text{cond}(H)$? Which among all the above methods produces the smallest deviation from orthonormality?

2. This experiment is about detecting nearly rank deficiency of a matrix A via QR factorization $A = QR$ by monitoring the size of diagonal entries of R. Generate the test matrix A as follows.

```
[U, X] = qr(randn(80));
[V, X] = qr(randn(80));
S = diag( 2 .^ (-1:-1:-80));
A = U*S*V; % Note A has small singular values and is nearly rank deficient.
```

Now compute QR factorization of A using `cgsqr`, `mgsqr` and the matlab function `qr`:

```
[QC, RC] = cgsqr(A);
[QM, RM] = mgsqr(A);
[Q, R] = qr(A);
```

To test how close these matrices are to being unitary, compute
`norm( QC'*QC-eye(80)), norm( QM'*QM-eye(80)), norm(( Q'*Q-eye(80))`.
Which method is worse? Which method gives better result?

To explain your results, plot the absolute values of the diagonal entries of `RC, RM, R`. Use commands

```
x= (1:80)';
hold off
semilogy(x, abs(diag( RC ) ), 'bo')
hold on
semilogy(x, abs(diag( RM ) ), 'rx')
semilogy(x, abs(diag( R ) ), 'k+')
title('abs(diag(R)) for cgs, mgs and qr')
gtext('cgs=o, mgs = x, qr=+')
```

Do the diagonal entries of R show near rank deficiency of A. Which method is better?

3. **Assignment.** Your task is to find polynomials $p_5(t)$ and $p_{18}(t)$ of degree 5 and 18, respectively, that best fit the function $f(t) = \sin(\pi t/5) + \dfrac{t}{5}$ for $t_1 = -5, t_2 = -4.5, \ldots, t_{23} = 6$, that is, `t = (-5:.5:6)'`. For $k = 5, 18$, determine the polynomial p_k whose coefficients are given by x (that is, $p_k(t) := \sum_{j=1}^{k+1} x_j t^{j-1}$) by solving LSP $Ax = b$ in two different ways: solve LSP $Ax = b$ using QR factorization of A and QR factorization of the augmented matrix $\begin{bmatrix} A & b \end{bmatrix}$. Here are the details.

   Let `[Q, R] = cgsqr(A)` and `[Q, R] = mgsqr(A)` be MATLAB functions implementing classical Gram-Schmidt and modified Gram-Schmidt methods. For $k = 5$ and $k = 18$, perform the following computations.

   (a) Compute `[Q, R] = cgsqr([A b])` and use `R` to solve the LSP $Ax = b$. Compute the residual `res1` $:= \|Ax - b\|_2$ from the matrix `R`. Call the polynomial $p_1(t)$.

   Next compute `[QC, RC] = cgsqr(A)` and use `QC` and `RC` to solve the LSP $Ax = b$. Compute the residual `res2` $:= \|Ax - b\|_2$. Call the polynomial $p_2(t)$. Which method gives a better fit (small residual error)? Plot $p_1(t), p_2(t)$ and $f(t)$ in a single plot and comment on the result.

   (b) Compute `[Q, R] = mgsqr([A b])` and use `R` to solve the LSP $Ax = b$. Compute the residual `res3` $:= \|Ax - b\|_2$ from the matrix `R`. Call the polynomial $p_3(t)$.

   Next compute `[QM, RM] = mgsqr(A)` and use `QM` and `RM` to solve the LSP $Ax = b$. Compute the residual `res4` $:= \|Ax - b\|_2$. Call the polynomial $p_4(t)$. Which method gives a better fit (small residual error)? Plot $p_3(t), p_4(t)$ and $f(t)$ in a single plot and comment on the result.

   (c) Compute `[Q, R] = qr([A b])` and use `R` to solve the LSP $Ax = b$. Compute the residual `res5` $:= \|Ax - b\|_2$ from the matrix `R`. Call the polynomial $p_5(t)$.

   Next solve the LSP $Ax = b$ using MATLAB command `x = A\b` and compute the residual `res6` $:= \|Ax - b\|_2$. Call the polynomial $p_6(t)$. Which method gives a better fit (small residual error)? Plot $p_5(t), p_6(t)$ and $f(t)$ in a single plot and comment on the result.

(d) Plot the data points (t_i, f_i), $f(t)$, and the best fit polynomials of degree 5 and 18 obtained from (c) in a single plot. Use the command `axis([-10 10 -3 3])` to set the axes. Which polynomial gives a better fit?

Among the six methods, which method provides the best fit? What is the impact of the condition number of A on these methods? **12 marks**

*** End ***