Lab Session 13

MA-581 : Numerical Computations Lab | R. Alam | November 08, 2021

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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 $\|E\|_2 = \texttt{norm(H - Q*R)}$. 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. The Householder QR factorization is backward stable., that is, if $\hat{Q}$ and $\hat{R}$ are computed QR factors of A using reflectors then $\|\hat{Q}^T\hat{Q} - I\|_2 = \mathcal{O}(\mathbf{u})$ and $A + E = \hat{Q}\hat{R}$ for some matrix E such that $\|E\|_2/\|A\|_2 = \mathcal{O}(\mathbf{u})$. This, however, does not necessarily mean that $\hat{Q}$ and $\hat{R}$ will be close to the exact Q and R. This can be test as follows:

```
>>R = triu(randn(50)); % compute a 50-by-50 random upper triangular matrix.
>>[Q, X] = qr(randn(50)); % compute a 50-by-50 random unitary matrix Q.
>>A = Q*R; % A is a matrix with known QR factors.
>>[S, T] = qr(A); % Computes Householder QR factorization of A.
```

Setting `E = S*T - A`, we have `A+E = S*T`. Compute `norm(E)` and `norm(S'*S-eye(50))`. What is your conclusion?

Now compute `[norm( Q-S ), norm( R-T )]`
to conclude that `S` and `T` are very far from the known QR factors Q and R of A. This illustrates that the Householder QR factorization is not **forward stable**.

*** End ***