

Lab Session 9

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 $\|Q' * Q - \text{eye}(n)\|_2$ in each case (MATLAB command `norm(eye(n)-Q'*Q)`). Setting $E := QR - H$, we have $H + E = QR$. Check the residual norm $\|E\|_2 = \text{norm}(H - Q * R)$. The small residual error of order $\mathcal{O}(u)$ as well as small deviation from orthonormality of order $\mathcal{O}(u)$ imply that the algorithm is backward stable. In other words, the algorithm computes QR factorization 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 $\|Q' * Q - \text{eye}(n)\|_2 \approx u * \text{cond}(H)$.

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

2. Your task is to find the polynomial $p(t)$ of degree 18 that best fits the function $f(t) = \sin(2\pi t) + \frac{t}{5}$ for $t_1 = -5, t_2 = -4.5, \dots, t_{23} = 6$. Determine the polynomial p whose coefficients are given by x (that is, $p(t) := \sum_{j=1}^{19} x_j t^{j-1}$) 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 $[A \ b]$. Here are the details.

Let $[Q, R] = \text{cgsqr}(A)$ and $[Q, R] = \text{mgsqr}(A)$ be MATLAB functions implementing classical Gram-Schmidt and modified Gram-Schmidt methods.

- (a) Compute $[Q, R] = \text{cgsqr}([A \ b])$ and use R to solve the LSP $Ax = b$. Compute the residual $\text{res1} := \|Ax - b\|_2$ from the matrix R . Call the polynomial $p_1(t)$.
Next compute $[QC, RC] = \text{cgsqr}(A)$ and use QC and RC to solve the LSP $Ax = b$. Compute the residual $\text{res2} := \|Ax - b\|_2$. 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 $[Q, R] = \text{mgsqr}([A \ b])$ and use R to solve the LSP $Ax = b$. Compute the residual $\text{res3} := \|Ax - b\|_2$ from the matrix R . Call the polynomial $p_3(t)$.
Next compute $[QM, RM] = \text{mgsqr}(A)$ and use QM and RM to solve the LSP $Ax = b$. Compute the residual $\text{res4} := \|Ax - b\|_2$. 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 $[Q, R] = \text{qr}([A \ b])$ and use R to solve the LSP $Ax = b$. Compute the residual $\text{res5} := \|Ax - b\|_2$ from the matrix R . Call the polynomial $p_5(t)$.
Next solve the LSP $Ax = b$ using MATLAB command $x = A \setminus b$ and compute the residual $\text{res6} := \|Ax - b\|_2$. 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.

Among the six methods, which methods provide the best fit? What is the impact of the condition number of A on these methods?

*** End ***