数值算法 Homework 08

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Problem 1

Let $A \in \mathbb{C}^{n\times n}, x \in \mathbb{C}^n$
Suppose that $X = [x, Ax, \dots, A^{n-1}x] \in \mathbb{C}^{n\times n}$ is nonsingular.
Show that $X^{-1}AX$ is upper Hessenberg.

Proof:
给定 $A \in \mathbb{C}^{n\times n}$ 和 $x \in \mathbb{C}^n$，我们便可以计算序列:

$$\begin{aligned} x_1 &= x \\ x_2 &= Ax_1 = Ax \\ x_3 &= Ax_2 = A^2x \\ &\cdots \\ x_n &= Ax_{n-1} = A^{n-1}x \end{aligned}$$

我们只需计算至 $x_n = A^{n-1}x$ 即可
这是因为 Cayley-Hamilton 定理保证了 $A^k \ (k \geq n)$ 可以表示为 $I_n, A, \dots, A^{n-1}$ 的线性组合.

> **(Cayley-Hamilton 定理, Matrix Analysis 定理 $2.4.3.2$)**
> 设 $p_A(t) := \det(tI_n - A)$ 是 $A \in \mathbb{C}^{n\times n}$ 的特征多项式，则我们有 $p_A(A) = 0_{n\times n}$ 成立.
> 换言之，任意复方阵都满足其特征方程.

我们记:

$$\begin{aligned} X &:= [x_1, x_2, \dots, x_{n-1}, x_n] = [x, Ax, \dots, A^{n-1}x] \\ c &:= -X^{-1}A^n x_1 = [c_1, \dots, c_n]^T \\ H &:= [e_2, e_3, \dots, e_n, -c] = \begin{bmatrix} 0 & & & & -c_1 \\ 1 & 0 & & & -c_2 \\ & 1 & \ddots & & \vdots \\ & & \ddots & 0 & -c_{n-1} \\ & & & 1 & -c_n \end{bmatrix} \end{aligned}$$

(其中我们假设 X 非奇异)
则我们有:

$$\begin{aligned} AX &= [Ax_1, Ax_2, \dots, Ax_{n-1}, Ax_n] \\ &= [x_2, x_3, \dots, x_n, A^n x_1] \\ &= [Xe_2, Xe_3, \dots, Xe_n, X(-X^{-1}A^n x_1)] \quad (\text{note that } c := X^{-1}A^n x_1) \\ &= X[e_2, e_3, \dots, e_n, -c] \\ &= XH \end{aligned}$$

于是我们有 $X^{-1}AX = H$，而 H 是一个上 Hessenberg 矩阵 (具体来说是一个 Frobenius 西型)

Problem 2

Let $A \in \mathbb{C}^{n\times n}$ be an unreduced upper Hessenberg matrix.
(By "unreduced", we mean $A_{i+1,i} \neq 0 \ (\forall \ 1 \leq i \leq n-1)$)
Suppose that A is singular.
Show that the zero eigenvalue appears at the bottom right corner after one QR sweep.
What happens if A is a singular upper Hessenberg matrix with some $A_{i+1,i} = 0$?

Solution:
首先我们注意到奇异的不可约上 Hessenberg 矩阵 $A \in \mathbb{C}^{n\times n}$ 的秩 $\text{rank}(A)$ 一定为 $n-1$
因此 A 的 QR 分解形如:

$$A = QR$$
$$\begin{cases} Q = G_{n-1,n} \cdots G_{1,2} \in \mathbb{C}^{n\times n} \text{ where } G_{1,2}, \dots, G_{n-1,n} \text{ are Givens matrices} \\ R = \begin{bmatrix} R_1 & r \\ & 0 \end{bmatrix} \in \mathbb{C}^{n\times n} \text{ where } R_1 \in \mathbb{C}^{(n-1)\times(n-1)} \text{ is a non-singular upper triangle matrix} \end{cases}$$

于是我们在计算 $\tilde{A} = RQ = RG_{1,2}^H \cdots G_{n-1,n}^H$ 时，其第 n 行的所有元素必然全为零.
这是因为 R 的第 n 行的所有元素全为零，所以无论怎么做列线性组合，第 n 行的所有元素必然全为零.
因此一次 QR 迭代得到的 $\tilde{A} = RQ = Q^H AQ$ 的零特征值将位于 (n,n) 位置.

以 $n=4$ 的情况为例，A 的 Givens QR 分解过程如下:

$$A = \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ & * & * & * \\ & & * & * \end{bmatrix}$$

$$G_{1,2}A = \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ & * & * & * \\ & & * & * \end{bmatrix}$$

$$G_{2,3}(G_{1,2}A) = \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ & 0 & * & * \\ & & * & * \end{bmatrix}$$

$$G_{3,4}(G_{2,3}G_{1,2}A) = \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ & 0 & * & * \\ & & 0 & 0 \end{bmatrix}$$

下面我们计算 $\tilde{A} = RQ$:

$$R = \begin{bmatrix} * & * & * & * \\ 0 & * & * & * \\ & 0 & * & * \\ & & 0 & 0 \end{bmatrix}$$

$$RG_{1,2}^H = \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ & 0 & * & * \\ & & 0 & 0 \end{bmatrix}$$

$$(RG_{1,2}^H)G_{2,3}^H = \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ & * & * & * \\ & & 0 & 0 \end{bmatrix}$$

$$(RG_{1,2}^H G_{2,3}^H)G_{3,4}^H = \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ & * & * & * \\ & & 0 & 0 \end{bmatrix}$$

What happens if A is a singular upper Hessenberg matrix with some $A_{i+1,i} = 0$?
那么一步 QR 后，零特征值会落到第一个不可约 Hessenberg 矩阵的底部.
(如果上三角阵 R 可以是阶梯形式的话，那么也可以把零特征值落到整个 Hessenberg 矩阵的底部)

Problem 3

Let:

$$A = \begin{bmatrix} 0 & & & & 1 \\ 1 & 0 & & & \\ & \ddots & \ddots & & \\ & & 1 & 0 & \\ & & & 1 & 0 \end{bmatrix}$$

What can you say about the convergence of:

- ① the naive QR algorithm
- ② Francis' double-shift QR algorithm

(0) Helper Funtions

计算 Givens 变换的算法为:

$$
\begin{aligned}
&\text{function: } [c, s] = \text{Givens}(a, b)\\
&\quad \text{if } b = 0\\
&\qquad c = 1;\ s = 0\\
&\quad \text{else}\\
&\qquad \text{if } |b| > |a|\\
&\qquad\quad t = \frac{a}{b};\ \ s = \frac{1}{\sqrt{1+t^2}};\ \ c = st\\
&\qquad \text{else}\\
&\qquad\quad t = \frac{b}{a};\ \ c = \frac{1}{\sqrt{1+t^2}};\ \ s = ct\\
&\qquad \text{end}\\
&\quad \text{end}
\end{aligned}
$$

其 Matlab 代码如下:

```
function [c, s] = Givens(a, b)
    % Givens 旋转，计算 cos 和 sin
    if b == 0
        c = 1;
        s = 0;
    else
        if abs(b) > abs(a)
            t = a / b;
            s = 1 / sqrt(1 + t^2);
            c = s * t;
        else
            t = b / a;
            c = 1 / sqrt(1 + t^2);
            s = c * t;
        end
    end
end
```

复数域上的 Householder 变换已于 Homework 02 Problem 02 给出:

```
function [v, beta] = Complex_Householder(x)
    % This function computes the Householder vector 'v' and scalar 'beta' for
    % a given complex vector 'x'. This transformation is used to create zeros
    % below the first element of 'x' by reflecting 'x' along a specific direction.

    n = length(x);
    x = x / norm(x, inf); % Normalize x by its infinity norm to avoid numerical issues

    % Copy all elements of 'x' except the first into 'v'
    v = zeros(n, 1);
    v(2:n) = x(2:n);

    % Compute sigma as the squared 2-norm of the elements of x starting from the second element
    sigma = norm(x(2:n), 2)^2;

    % Check if sigma is near zero, which would mean 'x' is already close to a scalar multiple of e_1
    if sigma < 1e-10
        beta = 0; % If sigma is close to zero, set beta to zero (no transformation needed)
    else
        % Determine gamma to account for the argument of complex number x(1)
        if abs(x(1)) < 1e-10
            gamma = 1; % If x(1) is close to zero, set gamma to 1
        else
            gamma = x(1) / abs(x(1)); % Otherwise, set gamma to x(1) divided by its magnitude
        end

        % Compute alpha as the Euclidean norm of x, including x(1) and sigma
        alpha = sqrt(abs(x(1))^2 + sigma);

        % Compute the first element of 'v' to avoid numerical cancellation
        v(1) = -gamma * sigma / (abs(x(1)) + alpha);

        % Calculate 'beta', the scaling factor of the Householder transformation
        beta = 2 * abs(v(1))^2 / (abs(v(1))^2 + sigma);

        % Normalize the vector 'v' by v(1) to ensure that the first element is 1,
        % allowing for simplified storage and computation of the transformation
        v = v / v(1);
    end
end
```

(1) Algorithm 1

上 Hessenberg 矩阵的显式 QR 迭代:

$$
\begin{array}{l}
\text{Given Hessenberg matrix } H \in \mathbb{R}^{n\times n} \\
\hline
Q = I_n \\
G = \text{Zeros}(n-1, 2) \\
\text{for } k = 1 : n-1 \\
\qquad [c, s] = \text{Givens}(H(k,k), H(k+1,k)) \\
\qquad G(k, 1:2) = [c, s] \\
\qquad H(k:k+1, k:n) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} H(k:k+1, k:n) \\
\qquad Q(1:n, k:k+1) = Q(1:n, k:k+1) \begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T \\
\text{end} \\
R = H \\
\hline
\text{for } k = 1 : n-1 \\
\qquad [c, s] = G(k, 1:2) \\
\qquad H(1:k+1, k:k+1) = H(1:k+1, k:k+1) \begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T \\
\text{end} \\
\tilde{H} = H
\end{array}
$$

Matlab 代码为:

```
function [Q, R, H_tilde] = Hessenberg_Givens_Reduction(H)
    % Given Hessenberg matrix H, apply Givens rotations to reduce it.
    % Outputs:
    %   Q       : Orthogonal matrix obtained from applying Givens rotations.
    %   R       : Resulting Hessenberg matrix after reduction.
    %   H_tilde : Modified Hessenberg matrix after applying additional Givens rotations.

    % Initialize the size of the matrix
    n = size(H, 1);

    % Step 1: Initialize Q as the identity matrix, and G to store Givens rotations
    Q = eye(n);
    G = zeros(n-1, 2); % Each row will store [c, s] values for each rotation

    % Step 2: Apply Givens rotations to H
    for k = 1:n-1
        % Compute Givens rotation parameters [c, s] for H(k, k) and H(k, k+1)
        [c, s] = Givens(H(k, k), H(k+1, k));

        % Store the Givens rotation parameters in G
        G(k, :) = [c, s];

        % Apply Givens rotation to H in rows k and k+1 from column k to end
        H(k:k+1, k:n) = [c, s; -s, c] * H(k:k+1, k:n);

        % Apply the transpose of the Givens rotation to Q in columns k and k+1
        Q(:, k:k+1) = Q(:, k:k+1) * [c, s; -s, c]';
    end

    % Store the result of H as R after the first Givens reduction phase
    R = H;

    % Step 3: Apply stored Givens rotations to update H
    for k = 1:n-1
        % Retrieve the Givens rotation parameters [c, s] from G
        c = G(k, 1);
        s = G(k, 2);

        % Apply the transpose of the Givens rotation to H in rows 1:k+1 and columns k:k+1
        H(1:k+1, k:k+1) = H(1:k+1, k:k+1) * [c, s; -s, c]';
    end

    % Store the modified Hessenberg matrix after the second phase as H_tilde
    H_tilde = H;
end
```

应用上述算法我们发现每步得到的正交矩阵 Q_k 均为:

$$Q_k \equiv Q := \begin{bmatrix} 0 & & & & -1 \\ 1 & 0 & & & \\ & \ddots & \ddots & & \\ & & 1 & 0 & \\ & & & 1 & 0 \end{bmatrix} \quad (\forall\, k \in \mathbb{Z}_+)$$

可以验证 $A_n = (Q^n)^T A (Q^n) = A$，因此对上 Hessenberg 矩阵 A 的显式 QR 迭代不收敛.
以 $n = 4$ 为例:

```
n = 4;
% Set the subdiagonal to 1
A = diag(ones(n-1, 1), -1);

% Set the top right element to 1
A(1, n) = 1;

[Q1, R1, A1] = Hessenberg_Givens_Reduction(A);
[Q2, R2, A2] = Hessenberg_Givens_Reduction(A1);
[Q3, R3, A3] = Hessenberg_Givens_Reduction(A2);
[Q4, R4, A4] = Hessenberg_Givens_Reduction(A3);

% Display results in a formatted way
disp("Results of Hessenberg_Givens_Reduction:")

% Display Q1, R1, A1 side by side
disp("Round 1: [Q1, R1, A1]")
disp([Q1, R1, A1])

% Display Q2, R2, A2 side by side
disp("Round 2: [Q2, R2, A2]")
disp([Q2, R2, A2])

% Display Q3, R3, A3 side by side
disp("Round 3: [Q3, R3, A3]")
disp([Q3, R3, A3])

% Display Q4, R4, A4 side by side
disp("Round 4: [Q4, R4, A4]")
disp([Q4, R4, A4])
```

运行结果:

```
Results of Hessenberg_Givens_Reduction:
Round 1: [Q1, R1, A1]
     0     0     0    -1     1     0     0     0     0     0     0    -1
     1     0     0     0     0     1     0     0     1     0     0     0
     0     1     0     0     0     0     1     0     0     1     0     0
     0     0     1     0     0     0     0    -1     0     0    -1     0

Round 2: [Q2, R2, A2]
     0     0     0    -1     1     0     0     0     0     0     0    -1
     1     0     0     0     0     1     0     0     1     0     0     0
     0     1     0     0     0     0    -1     0     0    -1     0     0
     0     0     1     0     0     0     0     1     0     0     1     0

Round 3: [Q3, R3, A3]
     0     0     0    -1     1     0     0     0     0     0     0    -1
     1     0     0     0     0    -1     0     0    -1     0     0     0
     0     1     0     0     0     0     1     0     0     1     0     0
     0     0     1     0     0     0     0     1     0     0     1     0

Round 4: [Q4, R4, A4]
     0     0     0    -1    -1     0     0     0     0     0     0     1
     1     0     0     0     0     1     0     0     1     0     0     0
     0     1     0     0     0     0     1     0     0     1     0     0
     0     0     1     0     0     0     0     1     0     0     1     0
```

(2) Algorithm 2

(Francis 双位移的 QR 迭代算法, 数值线性代数, 算法 $6.4.2$)

Given Hessenberg matrix $H \in \mathbb{R}^{n\times n}$

$$t = \operatorname{tr}\left(\begin{bmatrix} h_{n-1,n-1} & h_{n-1,n} \\ h_{n,n-1} & h_{n,n} \end{bmatrix}\right) = h_{n-1,n-1} + h_{n,n}$$
$$s = \det\left(\begin{bmatrix} h_{n-1,n-1} & h_{n-1,n} \\ h_{n,n-1} & h_{n,n} \end{bmatrix}\right) = h_{n-1,n-1}h_{n,n} - h_{n-1,n}h_{n,n-1}$$

$$\begin{cases} m_{11} = h_{11}^2 + h_{12}h_{21} - th_{11} + s \\ m_{21} = h_{21}(h_{11}+h_{22}-t) \\ m_{31} = h_{21}h_{32} \end{cases} \quad (\text{note that } Me_1 = \begin{bmatrix} m_{11} \\ m_{21} \\ m_{31} \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} h_{11}^2 + h_{12}h_{21} - th_{11} + s \\ h_{21}(h_{11}+h_{22}-t) \\ h_{21}h_{32} \\ 0 \\ \vdots \\ 0 \end{bmatrix} \text{ where } M = H^2 - tH + sI)$$

$$[v,\beta] = \text{Householder}\left(\begin{bmatrix} m_{11} \\ m_{21} \\ m_{31} \end{bmatrix}\right) \quad (\text{case of } k = 0)$$
$$H(1:3,1:n) = (I_3 - \beta vv^T)H(1:3,1:n) = H(1:3,1:n) - (\beta v)(v^T H(1:3,1:n))$$
$$H(1:4,1:3) = H(1:4,1:3)(I_3 - \beta vv^T) = H(1:4,1:3) - (H(1:4,1:3)v)(\beta v)^T$$

for $k = 1 : n-4$

$\quad [v,\beta] = \text{Householder}(H(k+1:k+3,k))$

$\quad H(k+1:k+3,k:n) = (I_3 - \beta vv^T)H(k+1:k+3,k:n) = H(k+1:k+3,k:n) - (\beta v)(v^T H(k+1:k+3,k:n))$

$\quad H(1:k+4,k+1:k+3) = H(1:k+4,k+1:k+3)(I_3 - \beta vv^T) = H(1:k+4,k+1:k+3) - (H(1:k+4,k+1:k+3)v)($

end

$$[v,\beta] = \text{Householder}(H(n-2:n,n-3)) \quad (\text{case of } k = n-3)$$
$$H(n-2:n,n-3:n) = (I_3 - \beta vv^T)H(n-2:n,n-3:n) = H(n-2:n,n-3:n) - (\beta v)(v^T H(n-2:n,n-3:n))$$
$$H(1:n,n-2:n) = H(1:n,n-2:n)(I_3 - \beta vv^T) = H(1:n,n-2:n) - (H(1:n,n-2:n)v)(\beta v)^T$$

$$[v,\beta] = \text{Householder}(H(n-1:n,n-2)) \quad (\text{case of } k = n-2)$$
$$H(n-1:n,n-2:n) = (I_2 - \beta vv^T)H(n-1:n,n-2:n) = H(n-1:n,n-2:n) - (\beta v)(v^T H(n-1:n,n-2:n))$$
$$H(1:n,n-1:n) = H(1:n,n-1:n)(I_2 - \beta vv^T) = H(1:n,n-1:n) - (H(1:n,n-1:n)v)(\beta v)^T$$

其 Matlab 代码为: (加入了调试信息)

```
function H_tilde = Francis_Double_Shift_QR_Iteration(H)
    % Given a Hessenberg matrix H, apply Francis Double Shift QR Iteration
    % and return the modified Hessenberg matrix H_tilde.

    n = size(H, 1); % Dimension of H
    disp("Original H:")
    disp(H);

    % Step 1: Compute the trace and determinant for the 2x2 bottom right submatrix
    t = H(n-1, n-1) + H(n, n); % Trace of bottom-right 2x2 block
    s = H(n-1, n-1) * H(n, n) - H(n-1, n) * H(n, n-1); % Determinant

    % Step 2: Define the components of Me_1 vector
    m11 = H(1, 1)^2 + H(1, 2) * H(2, 1) - t * H(1, 1) + s;
    m21 = H(2, 1) * (H(1, 1) + H(2, 2) - t);
    m31 = H(2, 1) * H(3, 2);
    Me1 = [m11; m21; m31];

    % Step 3: Apply Householder transformation to Me1 (initial case k=0)
    [v, beta] = Complex_Householder(Me1); % Compute Householder vector and scalar
    % Apply transformation to H
    H(1:3, 1:n) = H(1:3, 1:n) - beta * (v * (v' * H(1:3, 1:n)));
    H(1:4, 1:3) = H(1:4, 1:3) - (H(1:4, 1:3) * v) * (beta * v)';
    disp("After applying Householder of Me1:")
    disp(H);

    % Step 4: Iterate for k = 1 to n-4
    for k = 1:n-4
        [v, beta] = Complex_Householder(H(k+1:k+3, k)); % Compute Householder for each block
        H(k+1:k+3, k:n) = H(k+1:k+3, k:n) - beta * (v * (v' * H(k+1:k+3, k:n)));
        H(1:k+4, k+1:k+3) = H(1:k+4, k+1:k+3) - (H(1:k+4, k+1:k+3) * v) * (beta * v)';
        fprintf("After applying the %d-th Householder:\n", k);
        disp(H);
    end

    % Step 5: Handle case for k = n-3
    [v, beta] = Complex_Householder(H(n-2:n, n-3));
    H(n-2:n, n-3:n) = H(n-2:n, n-3:n) - beta * (v * (v' * H(n-2:n, n-3:n)));
    H(1:n, n-2:n) = H(1:n, n-2:n) - (H(1:n, n-2:n) * v) * (beta * v)';
    fprintf("After applying the %d-th Householder:\n", n-3);
    disp(H);

    % Step 6: Handle case for k = n-2
```

```
    [v, beta] = Complex_Householder(H(n-1:n, n-2));
    H(n-1:n, n-2:n) = H(n-1:n, n-2:n) - beta * (v * (v' * H(n-1:n, n-2:n)));
    H(1:n, n-1:n) = H(1:n, n-1:n) - (H(1:n, n-1:n) * v) * (beta * v)';
    fprintf("After applying the %d-th Householder: (Final matrix)\n", n-2);
    disp(H);

    % Output the modified Hessenberg matrix
    H_tilde = H;
end
```

函数调用:

```
n = 5;
% Set the subdiagonal to 1
A = diag(ones(n-1, 1), -1);

% Set the top right element to 1
A(1, n) = 1;

A1 = Francis_Double_Shift_QR_Iteration(A);
```

运行结果:

```
Original H:
     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

After applying Householder of Me1:
     0     1     0     0     0
     0     0     1     0     0
     0     0     0     0     1
     1     0     0     0     0
     0     0     0     1     0

After applying the 1-th Householder:
     0     0     0     1     0
     1     0     0     0     0
     0     0     0     0     1
     0     0     1     0     0
     0     1     0     0     0

After applying the 2-th Householder:
     0     0     0     1     0
     1     0     0     0     0
     0     1     0     0     0
     0     0     0     0     1
     0     0     1     0     0

After applying the 3-th Householder: (Final matrix)
     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
```

我们发现经过一轮 Francis 双步位移隐式 QR 迭代，矩阵 A 并无变化，因此算法不收敛.

Problem 4

Let $A = \begin{bmatrix} a & d \\ & b \end{bmatrix} \in \mathbb{R}^{2\times 2}$

Design an algorithm to compute an orthogonal matrix $Q \in \mathbb{R}^{2\times 2}$ such that $Q^TAQ = \begin{bmatrix} b & d \\ & a \end{bmatrix}$

(optional) What happens if the matrix A is complex?
(optional) Write a subprogram to perform diagonal swapping of the real Schur form:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix}$$

where A_{11} and A_{22} are either 1×1 or 2×2

Part (1)

Let $A = \begin{bmatrix} a & d \\ & b \end{bmatrix} \in \mathbb{R}^{2\times 2}$

Design an algorithm to compute an orthogonal matrix $Q \in \mathbb{R}^{2\times 2}$ such that $Q^T A Q = \begin{bmatrix} b & d \\ & a \end{bmatrix}$

Solution:

记 $Q = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \in \mathbb{R}^{2\times 2}$ (满足 $c^2+s^2=1$)

于是我们有:

$$
\begin{aligned}
Q^T A Q &= \begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T \begin{bmatrix} a & d \\ & b \end{bmatrix} \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \\
&= \begin{bmatrix} c & -s \\ s & c \end{bmatrix} \begin{bmatrix} ac-ds & as+dc \\ -bs & bc \end{bmatrix} \\
&= \begin{bmatrix} ac^2-dsc+bs^2 & asc+dc^2-bsc \\ asc-ds^2-bsc & as^2+dsc+bc^2 \end{bmatrix} \\
&= \begin{bmatrix} b & d \\ 0 & a \end{bmatrix}
\end{aligned}
$$

问题归结为求解方程组:

$$
\begin{cases} ac^2-dsc+bs^2=b \\ asc+dc^2-bsc=d \\ asc-ds^2-bsc=0 \\ as^2+dsc+bc^2=a \\ c^2+s^2=1 \end{cases}
$$

根据第三个等式我们有 $s[(a-b)c-ds]=0$

- 若 $s=0$，则 $c=\pm1$，根据第四个等式我们有 $a=b$ (因此这种取法可以应对 $a=b$ 的情况)
- 若 $s\neq 0$ (此情况默认 $a\neq b$)，则我们有 $(a-b)c-ds=0$
  - 若 $d=0$，则我们可取 $\begin{cases} c=0 \\ s=1 \end{cases}$ (这个情况可以合并入下面的情况)
  - 若 $d\neq 0$，则我们有 $t=\frac{s}{c}=\frac{a-b}{d}$，可取 $\begin{cases} c=\frac{d}{\sqrt{(a-b)^2+d^2}} \\ s=\frac{a-b}{\sqrt{(a-b)^2+d^2}} \end{cases}$

综上所述，我们得到如下算法:

```
function [c, s] = swap_diagnal(A)
    % Extract elements from matrix A
    a = A(1,1);
    d = A(1,2);
    b = A(2,2);

    % Initialize values of c and s based on conditions
    if abs(a-b) / (abs(a) + abs(b)) < 1e-10
        % Case of a = b
        c = 1;
        s = 0;
    else
        % General case: a ≠ b
        % Calculate c and s based on derived t value
        c = d / sqrt((a - b)^2 + d^2);
        s = (a - b) / sqrt((a - b)^2 + d^2);
    end
end
```

函数调用:

```
rng(51);
A = triu(rand(2, 2));
disp("Original A:");
disp(A);

[c, s] = swap_diagnal(A);
Q = [c, s; -s, c];
A_tilde = Q' * A * Q;
disp("Swapped A:");
disp(A_tilde);
```

运行结果:

```
Original A:
    0.6757    0.3433
         0    0.6440

Swapped A:
    0.6440    0.3433
         0    0.6757
```

Part (2)

What happens if the matrix A is complex?

Let $A = \begin{bmatrix} a & d \\ & b \end{bmatrix} \in \mathbb{C}^{2\times 2}$

Design an algorithm to compute an unitary matrix $Q \in \mathbb{C}^{2\times 2}$ such that $Q^H A Q = \begin{bmatrix} b & d \\ & a \end{bmatrix}$

Solution:

记 $Q = \begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \in \mathbb{C}^{2\times 2}$ (满足 $\begin{cases} c^2 + |s|^2 = 1 \\ c \in \mathbb{R} \\ s \in \mathbb{C} \end{cases}$)

于是我们有:

$$\begin{aligned} Q^H A Q &= \begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix}^H \begin{bmatrix} a & d \\ & b \end{bmatrix} \begin{bmatrix} c & s \\ -\bar{s} & c \end{bmatrix} \\ &= \begin{bmatrix} c & -s \\ \bar{s} & c \end{bmatrix} \begin{bmatrix} ac - d\bar{s} & as + dc \\ -b\bar{s} & bc \end{bmatrix} \\ &= \begin{bmatrix} ac^2 - d\bar{s}c + b|s|^2 & asc + dc^2 - bsc \\ a\bar{s}c - d\bar{s}^2 - b\bar{s}c & a|s|^2 + d\bar{s}c + bc^2 \end{bmatrix} \\ &= \begin{bmatrix} b & d \\ 0 & a \end{bmatrix} \end{aligned}$$

问题归结为求解方程组:

$$\begin{cases} ac^2 - d\bar{s}c + b|s|^2 = b \\ asc + dc^2 - bsc = d \\ a\bar{s}c - d\bar{s}^2 - b\bar{s}c = 0 \\ a|s|^2 + d\bar{s}c + bc^2 = a \\ c^2 + s^2 = 1 \end{cases}$$

根据第三个等式我们有 $\bar{s}[(a-b)c - d\bar{s}] = 0$

- 若 $\bar{s} = 0$，则 $c = \pm 1$，根据第四个等式我们有 $a = b$ (因此这种取法可以应对 $a = b$ 的情况)
- 若 $\bar{s} \neq 0$ (此情况默认 $a \neq b$)，则我们有 $(a-b)c - d\bar{s} = 0$
  - 若 $d = 0$，则我们可取 $\begin{cases} c = 0 \\ s = 1 \end{cases}$ (这个情况可以合并入下面的情况)
  - 若 $d \neq 0$，则我们有 $t = \frac{\bar{s}}{c} = \frac{a-b}{d} = \frac{(a-b)\bar{d}}{|d|^2}$，可取 $\begin{cases} c = \frac{|d|^2}{\sqrt{|a-b|^2|d|^2 + |d|^4}} = \frac{|d|}{\sqrt{|a-b| + |d|^2}} \\ \bar{s} = \frac{(a-b)\bar{d}}{|d|\sqrt{(a-b)^2 + d^2}} \\ s = \frac{(\bar{a}-\bar{b})d}{|d|\sqrt{(a-b)^2 + d^2}} \end{cases}$

    (可以放心，Wilkinson 模型保证两个浮点数 $a - b$ 的运算不会相消)

综上所述，我们得到如下算法:

```
function [c, s] = swap_complex(A)
    % Extract elements from the Hermitian matrix A
    a = A(1,1);
    d = A(1,2);
    b = A(2,2);

    % Initialize values of c and s based on conditions
    if abs(a - b) < 1e-10 * (abs(a) + abs(b))
        % Case of a = b (small difference, considering floating point precision)
        c = 1;    % c = 1 for identity-like rotation
        s = 0;    % s = 0 implies no rotation needed
    else
        % General case: a ≠ b
        % Calculate the magnitude of d and the rotation terms
        norm_factor = sqrt(abs(a - b)^2 + abs(d)^2);

        % Compute c and s
        c = abs(d) / norm_factor;
        s = (conj(a) - conj(b)) * d / (abs(d) * norm_factor); % s is a complex number
    end
```

```
end
```

函数调用:

```
rng(51);
A = triu(rand(2, 2) + 1i * rand(2, 2));
disp("Original A:");
disp(A);

[c, s] = swap_complex(A);
Q = [c, s; -conj(s), c];
A_tilde = Q' * A * Q;
disp("Swapped A:");
disp(A_tilde);
```

运行结果:

```
Original A:
   0.6757 + 0.2842i   0.3433 + 0.1577i
   0.0000 + 0.0000i   0.6440 + 0.3880i

Swapped A:
   0.6440 + 0.3880i   0.3433 + 0.1577i
   0.0000 + 0.0000i   0.6757 + 0.2842i
```

Part (3)

Write a subprogram to perform diagonal swapping of the real Schur form:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ & A_{22} \end{bmatrix}$$

where A_{11} and A_{22} are either 1×1 or 2×2
(参考论文: On Swapping Diagonal Blocks in Real Schur Form (Z. Bai & J. Demmel))

Solution:
设 $A_{11} \in \mathbb{R}^{p\times p}$, $A_{22} \in \mathbb{R}^{q\times q}$

- ① 使用全选主元 Gauss 消去法求解:

$$A_{11}X - XA_{22} = \gamma A_{12}$$
$$\Leftrightarrow$$
$$(I_q \otimes A_{11} - A_{22}^T \otimes I_p)\text{vec}(X) = \gamma\text{vec}(A_{12})$$

  其中我们假设 A_{11} 和 A_{22} 没有公共特征值 (这样 Sylvester 定理保证了上述方程组有唯一解)
  而 $\gamma \leq 1$ 是一个预设的防止上溢的缩放因子.
  全选主元 Gauss 消去法过程中，若有对角元非常小，则设置其为 $\text{eps} \cdot \|I_q \otimes A_{11} - A_{22}^T \otimes I_p\|_F$

- ② 使用 Householder 变换计算 $\begin{bmatrix} -X \\ \gamma I_q \end{bmatrix}$ 的 QR 分解

- ③ 计算 Q^TAQ:

$$Q^TAQ = \begin{bmatrix} \tilde{A}_{22} & \tilde{A}_{12} \\ \tilde{A}_{21} & \tilde{A}_{11} \end{bmatrix}$$

  可以证明 $\tilde{A}_{11}$ 和 A_{11} 具有相同的特征值，而 $\tilde{A}_{22}$ 和 A_{22} 具有相同的特征值.

- ④ 若 $\|\tilde{A}_{21}\|_F \leq \text{eps} \cdot \|A\|_F$，则我们记录 $\tilde{A} = Q^TAQ$ (并将 $\tilde{A}_{21}$ 设为 $0_{p\times q}$)
  否则报错并退出 (这表明向后不稳定，结果不被接受)

- ⑤ 标准化 2×2 对角块 (如果有的话)

粗略的 Matlab 实现:

```
function A_swapped = diagonal_swap(A, gamma)
    % This function performs the diagonal swapping of the real Schur form
    % A is the matrix in real Schur form (block diagonal matrix)
    % gamma is a scaling factor to prevent overflow

    % Step 1: Determine p and q based on the size of A
    n = size(A, 1);
    if n == 2
        p = 1;
        q = 1;
    elseif n == 4
        p = 2;
```

```
        q = 2;
    elseif n == 3
        % If n = 3, check the off-diagonal elements to determine p and q
        if A(2,1) == 0  % If A12 is zero, then p = 1, q = 2
            p = 1;
            q = 2;
        else  % Otherwise, p = 2, q = 1
            p = 2;
            q = 1;
        end
    else
        error('Matrix size n should be 2, 3, or 4.');
    end

    % Step 2: Extract the block components A11, A12, and A22
    A11 = A(1:p, 1:p);  % Top-left block
    A12 = A(1:p, p+1:end);  % Top-right block
    A22 = A(p+1:end, p+1:end);  % Bottom-right block

    % Step 3: Solve the system of equations: A11*X - X*A22 = gamma*A12
    % Construct the system (I_q ⊗ A11 - A22^T ⊗ I_p) * vec(X) = gamma * vec(A12)
    X_vec = solve_system(A11, A22, A12, gamma);

    % Reshape X_vec back to matrix form
    X = reshape(X_vec, [p, q]);

    % Step 4: Apply Householder transformation
    % Form the vector [-X; gamma*I_q]
    [Q, ~] = qr([-X; gamma * eye(q)]);

    % Step 5: Compute Q^T * A * Q
    A_swapped = Q' * A * Q;

    % Extract the (2, 1) blocks from A_swapped
    A21_tilde = A_swapped(q+1:end, 1:q);

    % Step 6: Check if the off-diagonal block A12_tilde is small enough
    if norm(A21_tilde, 'fro') <= eps * norm(A_swapped, 'fro')
        % Set the off-diagonal block to zero
        A_swapped(q+1:end, 1:q) = zeros(p, q);
    else
        error('fatal: the (2,1) block of A_swapped is non-zero!')
    end
end

function X_vec = solve_system(A11, A22, A12, gamma)
    % Solve the system (I_q ⊗ A11 - A22^T ⊗ I_p) * vec(X) = gamma * vec(A12)
    % Use a direct solution or an iterative solver depending on the structure
    % of the system (simplified here as a dense solver for illustrative purposes)

    [p, q] = size(A12);

    % Construct the Kronecker product matrix (I_q ⊗ A11 - A22^T ⊗ I_p)
    K = kron(eye(q), A11) - kron(A22', eye(p));

    % Vectorize the right-hand side (gamma * A12)
    rhs = gamma * A12(:);

    % Solve the linear system
    X_vec = K \ rhs;  % This uses the backslash operator, which is efficient in MATLAB
end
```

函数调用:

```
A = [1, 1, 1;
     0, 2, 3;
     0,-3, 2];
gamma = 1;
A_swapped = diagonal_swap(A, gamma);

disp("Original A:")
disp(A);
disp(eig(A));

disp("A_swapped:");
disp(A_swapped);
disp(eig(A_swapped));
```

运行结果:

```
Original A:
     1     1     1
     0     2     3
     0    -3     2

   1.0000 + 0.0000i
   2.0000 + 3.0000i
   2.0000 - 3.0000i

A_swapped:
    2.2069    3.1919   -0.1017
   -2.8330    1.7931   -1.2999
         0         0    1.0000

   2.0000 + 3.0000i
   2.0000 - 3.0000i
   1.0000 + 0.0000i
```

Problem 5

Implement the following algorithms for Hessenberg reduction:
(a) using Householder reflections;
(b) using Arnoldi process based on modified Gram-Schmidt orthogonalization.

Randomly generate a few matrices and compute the corresponding Hessenberg decomposition $A = QHQ^H$
Check the accuracy in terms of $\|Q^HAQ - H\|_F$ and $\|Q^HQ - I\|_F$ for your Hessenberg reduction implementations.
What do you observe?
(optional) Perturb the matrix A a little bit. How do Q and H change accordingly?

Part (1)

Implement Hessenberg reduction for $A \in \mathbb{C}^{n\times n}$ by Householder reflections.
Check the accuracy in terms of $\|Q^HAQ - H\|_F$ and $\|Q^HQ - I\|_F$ for your Hessenberg reduction implementations.
Perturb the matrix A a little bit.
How do Q and H change accordingly?

Solution:
使用 Householder 变换进行上 Hessenberg 化的算法:

$$
\begin{array}{l}
\text{Given } A \in \mathbb{C}^{n\times n} \\
\hline
W = 0_{n-1,n-2} \\
Y = 0_{n-1,n-2} \\
b = 0_{n-2} \\
\text{for } k = 1 : n-2 \\
\qquad [v, \beta] = \text{Householder}(A(k+1:n, k)) \\
\qquad A(k+1:n, k:n) = (I_{n-k} - \beta vv^H)A(k+1:n, k:n) = A(k+1:n, k:n) - (\beta v)(v^H A(k+1:n, k:n)) \\
\qquad A(1:n, k+1:n) = A(1:n, k+1:n)(I_{n-k} - \beta vv^H) = A(1:n, k+1:n) - (A(1:n, k+1:n)v)(\beta v)^H \\
\qquad Y(k:n-1, k) = v \\
\qquad b(k) = \beta \\
\text{end} \\
\text{for } k = 1 : n-2 \\
\qquad v = Y(k:n-1, k) \\
\qquad \beta = b(k) \\
\qquad \text{if } k = 1 \\
\qquad\qquad W(1:n-1, 1) = -\beta v \\
\qquad \text{else} \\
\qquad\qquad W(1:n-1, k) = W(1:n-1, 1:k-1)[Y(k:n-1, 1:k-1)^H v] \\
\qquad\qquad W(k:n-1, k) = W(k:n-1, k) + v \\
\qquad\qquad W(1:n-1, k) = -\beta W(1:n-1, k) \\
\qquad \text{end} \\
\text{end} \\
H = A \\
Q = \begin{bmatrix} 1 & \\ & I_{n-1} + WY^H \end{bmatrix}
\end{array}
$$

其中使用 WY 迭代来累积 Householder 变换的思想来源于以下算法:

> **(Matrix Computation 算法 5.1.2)**
> 设有 $r \le n$ 个 Householder 变换 $H_1, \ldots, H_r$，其中:

$$H_j = I_n - \beta_j v^{(j)} (v^{(j)})^H$$
$$v^{(j)} = [\underbrace{0, \ldots, 0}_{j-1}, 1, v_{j+1}^{(j)}, \ldots, v_n^{(j)}]^T$$

我们可以计算得到 $W, Y \in \mathbb{C}^{n \times r}$ 满足 $H_1 \cdots H_r = I_n + WY^H$:

$$\begin{aligned}
&Y = v^{(1)} \\
&W = -\beta_1 v^{(1)} \\
&\text{for } j = 2 : r \\
&\qquad z = -\beta_j (I_n + WY^H) v^{(j)} = -\beta_j [v^{(j)} + W(Y^H v^{(j)})] \\
&\qquad W = [W, z] \\
&\qquad Y = [Y, v^{(j)}] \\
&\text{end}
\end{aligned}$$

WY 迭代累积 $n-2$ 个 Householder 变换相比直接累积 $n-2$ 个 Householder 变换并不会减少计算复杂度.
但是可以增加 BLAS3 运算的比例，降低通讯开销，从而减少运行时间.

Matlab 代码为:

```matlab
function [H, Q] = Hessenberg_Reduction_Householder_WY(A)
    % Hessenberg form using WY accumulation of Householder transformations
    % Input:
    % - A: Complex matrix of size n x n
    % Output:
    % - H: Upper Hessenberg form of A
    % - Q: Orthogonal matrix such that A = Q * H * Q'

    % Initialize matrices W and Y for WY accumulation, and vector b for storing betas
    [n, ~] = size(A);
    W = zeros(n-1, n-2);  % Matrix to accumulate transformations for Q
    Y = zeros(n-1, n-2);  % Matrix to store Householder vectors
    b = zeros(1, n-2);    % Vector to store betas

    % Loop through each column (except the last two) for Householder reduction
    for k = 1:n-2
        % Step 1: Compute the Householder vector 'v' and scalar 'beta' for the current column
        [v, beta] = Complex_Householder(A(k+1:n, k));

        % Step 2: Apply the Householder transformation to zero out entries below the subdiagonal
        A(k+1:n, k:n) = A(k+1:n, k:n) - beta * v * (v' * A(k+1:n, k:n));
        A(1:n, k+1:n) = A(1:n, k+1:n) - (A(1:n, k+1:n) * v) * (beta * v)';

        % Step 3: Store the Householder vector in Y and the scalar beta in b
        Y(k:n-1, k) = v;  % Store the Householder vector for later use
        b(k) = beta;      % Store the scalar beta for the Householder transformation
    end

    % Loop to compute the W matrix, which accumulates the Householder transformations
    for k = 1:n-2
        % Step 4: Compute the W matrix for WY transformation
        if k == 1
            % For the first iteration, directly compute W
            W(1:n-1, 1) = -b(1) * Y(1:n-1, 1);
        else
            W(1:n-1, k) = W(1:n-1, 1:k-1) * (Y(k:n-1, 1:k-1)' * Y(k:n-1, k));
            W(k:n-1, k) = W(k:n-1, k) + Y(k:n-1, k);
            W(1:n-1, k) = -b(k) * W(1:n-1, k);
        end
    end

    % Step 5: Extract the upper Hessenberg matrix H from the modified matrix A
    H = A;  % The matrix A is now in upper Hessenberg form after applying Householder

    % Step 6: Compute the orthogonal matrix Q as per WY transformation
    Q = eye(n, n);
    Q(2:n, 2:n) = Q(2:n, 2:n) + W * Y';
end
```

复数域上的 Householder 变换已于 Homework 02 Problem 02 给出:

```matlab
function [v, beta] = Complex_Householder(x)
    % This function computes the Householder vector 'v' and scalar 'beta' for
    % a given complex vector 'x'. This transformation is used to create zeros
    % below the first element of 'x' by reflecting 'x' along a specific direction.

    n = length(x);
    x = x / norm(x, inf); % Normalize x by its infinity norm to avoid numerical issues
```

```
    % Copy all elements of 'x' except the first into 'v'
    v = zeros(n, 1);
    v(2:n) = x(2:n);

    % Compute sigma as the squared 2-norm of the elements of x starting from the second element
    sigma = norm(x(2:n), 2)^2;

    % Check if sigma is near zero, which would mean 'x' is already close to a scalar multiple of e_1
    if sigma < 1e-10
        beta = 0; % If sigma is close to zero, set beta to zero (no transformation needed)
    else
        % Determine gamma to account for the argument of complex number x(1)
        if abs(x(1)) < 1e-10
            gamma = 1; % If x(1) is close to zero, set gamma to 1
        else
            gamma = x(1) / abs(x(1)); % Otherwise, set gamma to x(1) divided by its magnitude
        end

        % Compute alpha as the Euclidean norm of x, including x(1) and sigma
        alpha = sqrt(abs(x(1))^2 + sigma);

        % Compute the first element of 'v' to avoid numerical cancellation
        v(1) = -gamma * sigma / (abs(x(1)) + alpha);

        % Calculate 'beta', the scaling factor of the Householder transformation
        beta = 2 * abs(v(1))^2 / (abs(v(1))^2 + sigma);

        % Normalize the vector 'v' by v(1) to ensure that the first element is 1,
        % allowing for simplified storage and computation of the transformation
        v = v / v(1);
    end
end
```

可视化正交性损失的函数:

```
function visualize_orthogonality_loss(Q, titleStr)
    % Visualizes the componentwise loss of orthogonality |Q^H Q - I_n|
    loss = Q' * Q - eye(size(Q, 2)); % Compute the loss
    figure; % Create a new figure window
    imagesc(log10(abs(loss))); % Display the absolute value of the loss
    colorbar; % Add colorbar to indicate scale
    title(titleStr);
    xlabel('Column Index');
    ylabel('Row Index');
    axis square; % Make the axes square for better visualization
end
```

函数调用:

```
rng(51);
n = 100;
A = rand(n, n) + 1i* rand(n, n);

% Apply the Hessenberg reduction
[H, Q] = Hessenberg_Reduction_Householder_WY(A);

% Display the Frobenius norm of Q' * A * Q - H
disp("Frobenius norm of Q' * A * Q - H:");
disp(norm(Q' * A * Q - H, 'fro'));  % Compute Frobenius norm for forward error

% Display the Frobenius norm of Q' * Q - In
disp("Frobenius norm of Q' * Q - In:");
disp(norm(Q' * Q - eye(n), 'fro'));

% Visualize the loss of orthogonality for Q
visualize_orthogonality_loss(Q, 'Log10 Loss of Orthogonality (Householder Hessenberg Reduction)');

% Perturb the matrix A slightly and repeat the check
% A_perturbed is a slightly perturbed version of A, with a small random perturbation added to each element.
A_perturbed = A + 1e-5 * (randn(n, n) + 1i * randn(n, n));  % Perturb A by a small amount

% Apply the Hessenberg reduction to the perturbed matrix
[H_perturbed, Q_perturbed] = Hessenberg_Reduction_Householder_WY(A_perturbed);

% Check the accuracy for the perturbed case
% Compute and display the forward error between the perturbed and original Hessenberg matrices.
% This tells us how much the Hessenberg matrix changes due to the perturbation in A.
```

```
disp("Frobenius norm of H_perturbed - H: (Forward Error)");
disp(norm(H_perturbed - H, 'fro') / norm(A_perturbed - A, 'fro'));  % Forward error for Hessenberg matrix

% Compute and display the forward error for the orthogonal matrix Q
% This tells us how much the orthogonal matrix Q changes due to the perturbation in A.
disp("Frobenius norm of Q_perturbed - Q: (Forward Error)");
disp(norm(Q_perturbed - Q, 'fro') / norm(A_perturbed - A, 'fro'));  % Forward error for Q

% Compute and display the backward error
% This checks how well the perturbed matrix Q_perturbed and H_perturbed approximate the original matrix A.
% It is a backward error computation that checks the closeness of Q_perturbed * H_perturbed * Q_perturbed' to
A.
disp("Frobenius norm of Q' * A * Q - H: (Backward Error)");
disp(norm(Q_perturbed * H_perturbed * Q_perturbed' - A, 'fro') / norm(A_perturbed - A, 'fro'));  % Backward
error for Hessenberg matrix approximation
```

运行结果:

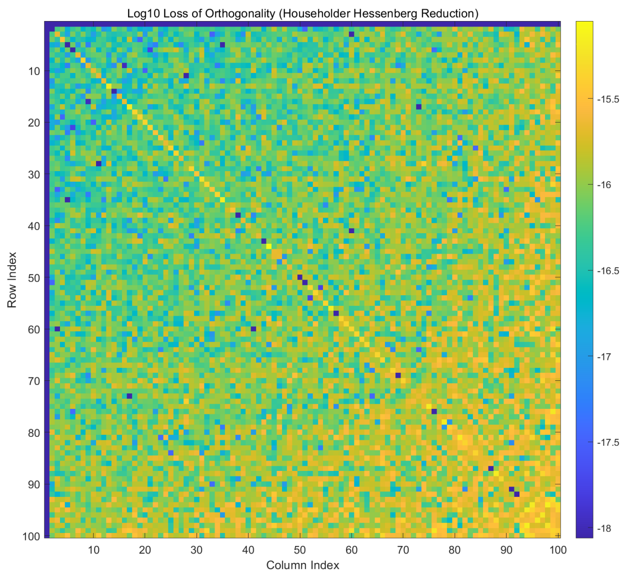
```
Frobenius norm of Q' * A * Q - H:
   1.0942e-13

Frobenius norm of Q' * Q - In:
   1.3307e-14

Frobenius norm of H_perturbed - H: (Forward Error)
   1.0585e+03

Frobenius norm of Q_perturbed - Q: (Forward Error)
  248.1138

Frobenius norm of Q' * A * Q - H: (Backward Error)
    1.0000
```



Part (2)

基于 Gram-Schmidt 正交化实现 Arnoldi 过程的函数已于 Homework 6 Problem 4 给出:
(我们只需将 r 设为 n 即可对 A 进行上 Hessenberg 化)

```
function [Q, H] = Gram_Schmidt_Arnoldi(A, b, r, tolerance, modified, reorthogonalized)
    % Gram_Schmidt_Arnoldi computes an orthonormal basis Q and a Hessenberg matrix H
    % using the Arnoldi process with either Classical or Modified Gram-Schmidt.
    %
    % Inputs:
    %   A - Square matrix of size n x n.
    %   b - Initial vector of size n x 1.
    %   r - Desired rank of the output.
    %   tolerance - Threshold for detecting linear dependence (default: 1e-10).
    %   modified - Flag for using Modified Gram-Schmidt (default: false).
    %   reorthogonalized - Flag for reorthogonalization (default: false).
    %
    % Outputs:
```

```
%   Q - Orthonormal basis of size n x r.
%   H - Upper Hessenberg matrix of size r x r.

% Validate inputs and set default values if not provided
if nargin < 6
    reorthogonalized = false; % Default to not reorthogonalizing
end
if nargin < 5
    modified = false; % Default to Classical Gram-Schmidt
end
if nargin < 4
    tolerance = 1e-10; % Default tolerance for linear dependence
end

% Get the size of the matrix A
n = size(A, 1);

% Check if the desired rank is valid
if r < 1 || r > n
    error("r should be an integer in [1, n]");
end

% Initialize matrices Q and H
Q = zeros(n, n);
Q(:, 1) = b / norm(b); % Normalize the initial vector b
H = zeros(r, r); % Initialize H to zeros
delta = zeros(n, 1); % Temporary variable for inner products

% Set max iterations based on reorthogonalization flag
if reorthogonalized
    max_iter = 2; % More iterations for reorthogonalization
else
    max_iter = 1; % Standard iteration count
end

% Loop to build the orthonormal basis up to r-1 or n-1
for k = 1:r-1
    % Apply the matrix A to the last basis vector
    Q(:, k + 1) = A * Q(:, k);

    if modified
        % Modified Gram-Schmidt process
        for iter = 1:max_iter
            for i = 1:k
                % Compute inner product
                delta(i) = Q(:, i)' * Q(:, k + 1);
                % Update H matrix
                H(i, k) = H(i, k) + delta(i);
                % Orthogonalize the k+1 vector
                Q(:, k + 1) = Q(:, k + 1) - delta(i) * Q(:, i);
            end
        end
    else
        % Classical Gram-Schmidt process
        for iter = 1:max_iter
            % Compute inner products for all previous basis vectors
            delta(1:k) = Q(:, 1:k)' * Q(:, k + 1);
            % Update H matrix
            H(1:k, k) = H(1:k, k) + delta(1:k);
            % Orthogonalize the k+1 vector
            Q(:, k + 1) = Q(:, k + 1) - Q(:, 1:k) * delta(1:k);
        end
    end

    % Compute the norm for the current basis vector
    H(k + 1, k) = norm(Q(:, k + 1));

    % Check for linear dependence by comparing the norm with the tolerance
    if H(k + 1, k) < tolerance
        fprintf("The rank %d is lesser than %d\n", k, r);
        r = k; % Update the rank if linear dependence is detected
        break; % Exit the loop early
    else
        % Normalize the current basis vector
        Q(:, k + 1) = Q(:, k + 1) / H(k + 1, k);
    end
end

% Fill the last column of H
```

```
    H(1:r, r) = Q(:, 1:r)' * (A * Q(:, r));

    % Trim Q and H to the computed effective rank
    Q = Q(:, 1:r);
    H = H(1:r, 1:r);
end
```

函数调用:

```
rng(51);
n = 100;
A = rand(n, n) + 1i* rand(n, n);
b = rand(n, 1) + 1i* rand(n, 1);

% Apply the Hessenberg reduction
% [Q, H] = Gram_Schmidt_Arnoldi(A, b, r, tolerance, modified, reorthogonalized)
[Q, H] = Gram_Schmidt_Arnoldi(A, b, n, 1e-10, true, true);

% Display the Frobenius norm of Q' * A * Q - H
disp("Frobenius norm of Q' * A * Q - H:");
disp(norm(Q' * A * Q - H, 'fro'));  % Compute Frobenius norm for forward error

% Display the Frobenius norm of Q' * Q - In
disp("Frobenius norm of Q' * Q - In:");
disp(norm(Q' * Q - eye(n), 'fro'));

% Visualize the loss of orthogonality for Q
visualize_orthogonality_loss(Q, 'Log10 Loss of Orthogonality (Householder Hessenberg Reduction)');

% Perturb the matrix A slightly and repeat the check
% A_perturbed is a slightly perturbed version of A, with a small random perturbation added to each element.
A_perturbed = A + 1e-5 * (randn(n, n) + 1i * randn(n, n));  % Perturb A by a small amount

% Apply the Hessenberg reduction to the perturbed matrix
% [Q, H] = Gram_Schmidt_Arnoldi(A, b, r, tolerance, modified, reorthogonalized)
[Q_perturbed, H_perturbed] = Gram_Schmidt_Arnoldi(A_perturbed, b, n, 1e-10, true, true);

% Check the accuracy for the perturbed case
% Compute and display the forward error between the perturbed and original Hessenberg matrices.
% This tells us how much the Hessenberg matrix changes due to the perturbation in A.
disp("Frobenius norm of H_perturbed - H: (Forward Error)");
disp(norm(H_perturbed - H, 'fro') / norm(A_perturbed - A, 'fro'));  % Forward error for Hessenberg matrix

% Compute and display the forward error for the orthogonal matrix Q
% This tells us how much the orthogonal matrix Q changes due to the perturbation in A.
disp("Frobenius norm of Q_perturbed - Q: (Forward Error)");
disp(norm(Q_perturbed - Q, 'fro') / norm(A_perturbed - A, 'fro'));  % Forward error for Q

% Compute and display the backward error
% This checks how well the perturbed matrix Q_perturbed and H_perturbed approximate the original matrix A.
% It is a backward error computation that checks the closeness of Q_perturbed * H_perturbed * Q_perturbed' to
A.
disp("Frobenius norm of Q' * A * Q - H: (Backward Error)");
disp(norm(Q_perturbed * H_perturbed * Q_perturbed' - A, 'fro') / norm(A_perturbed - A, 'fro'));  % Backward
error for Hessenberg matrix approximation
```

运行结果:

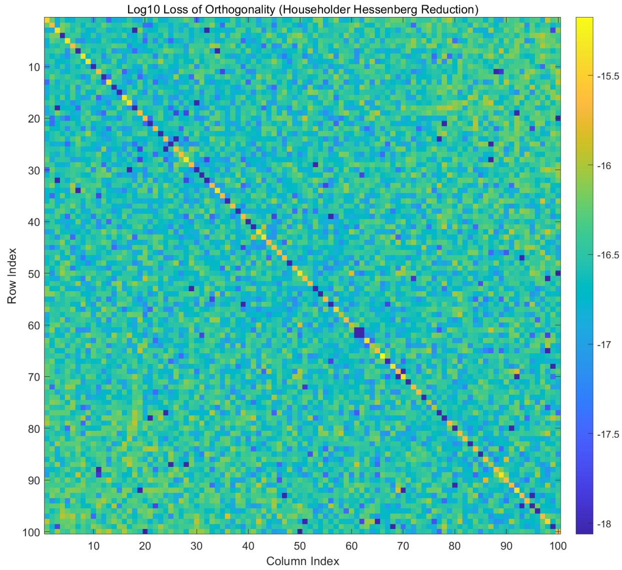
```
Frobenius norm of Q' * A * Q - H:
   5.3483e-14

Frobenius norm of Q' * Q - In:
   4.5518e-15

Frobenius norm of H_perturbed - H: (Forward Error)
   34.0533

Frobenius norm of Q_perturbed - Q: (Forward Error)
    8.0111

Frobenius norm of Q' * A * Q - H: (Backward Error)
    1.0000
```



Log10 Loss of Orthogonality (Householder Hessenberg Reduction)
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