FDU 数值算法 Homework 04

Due: Oct. 15, 2024
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Problem 1

We have mentioned in the lecture that for complex vectors $x,y\in\mathbb{C}^n$,
$\|x\|_2=\|y\|_2>0$ does not guarantee that there exists a Householder reflection H such that $y=Hx$
Please propose a sufficient and necessary condition for the existence of a Householder reflection H such that $y=Hx$
Prove your claim.

Solution:
当且仅当非零向量 $x,y\in\mathbb{C}^n$ 满足 $\begin{cases}\|x\|_2=\|y\|_2\\ x^Hy\in\mathbb{R}\end{cases}$ 时存在 Householder 矩阵 $H:=I_n-2ww^H$ 使得 $y=Hx$

- **充分性:**
  若非零向量 $x,y\in\mathbb{C}^n$ 满足 $\begin{cases}\|x\|_2=\|y\|_2\\ x^Hy\in\mathbb{R}\end{cases}$
  取 $w:=\frac{x-y}{\|x-y\|_2}$，则我们有:

$$\begin{aligned}Hx&=(I_n-2ww^H)x\\&=\left\{I_n-2\frac{(x-y)(x-y)^H}{(x-y)^H(x-y)}\right\}x\\&=x-2\frac{(x-y)^Hx}{x^Hy-y^Hx-x^Hy-y^Hy}(x-y)\quad(\text{note that }\begin{cases}\|y\|_2=\|x\|_2&\Rightarrow y^Hy=x^Hx\\x^Hy\in\mathbb{R}&\Rightarrow y^Hx=\overline{x^Hy}=x^Hy\end{cases})\\&=x-2\frac{x^Hx-x^Hy}{2(x^Hx-x^Hy)}(x-y)\\&=x-(x-y)\\&=y\end{aligned}$$

- **必要性:**
  若存在 Householder 矩阵 $H:=I_n-2ww^H$ 使得 $y=Hx$ (其中 $x,y\in\mathbb{C}^n$ 为给定的非零向量)
  注意到 H 是一个酉矩阵，则根据 l_2 范数的酉不变性我们有:

$$\|y\|_2=\|Hx\|_2=\|x\|_2$$

  此外，注意到 H 是一个 Hermite 阵，
  因此 $x^Hy=x^HHx$ 作为 Hermite 二次型一定是一个实数.

综上所述，命题得证.

实际上我们可以推出更深刻的结论: (Matrix Analysis 定理 $2.1.13$)
给定非零向量 $x,y\in\mathbb{C}^n$ 满足 $\|x\|_2=\|y\|_2$，则我们有如下命题成立:
① 若 x,y 线性相关，即存在 $\theta\in\mathbb{R}$ 使得 $y=e^{i\theta}x$ 成立，则酉矩阵 $U:=e^{i\theta}I_n$ 可使 $y=Ux$
② 当 x,y 线性无关时，设 $\phi\in\mathbb{R}$ 使得 $x^Hy=e^{i\phi}|x^Hy|$ (若 $x^Hy=0$，则取 $\phi=0$)
定义 $w:=\frac{e^{i\phi}x-y}{\|e^{i\phi}x-y\|_2}$ 和 Householder 矩阵 $H:=I_n-2ww^H$
则酉矩阵 $U:=e^{i\phi}H$ 可使 $y=Ux$
显然 U 是**本性 Hermite 的** (essentially Hermitian) (即存在某个 $\varphi\in\mathbb{R}$ 使得 $e^{i\varphi}U$ 是 Hermite 的，具体来说可取 $\varphi=-\phi$)
且对于任意 $z\perp x$，我们都有 $Uz\perp y$

特殊地，若非零向量 $x,y\in\mathbb{R}^n$，则上述结论变为:
① 若 $x=y$，则实正交阵 $U:=I_n$ 可使得 $y=Ux$
② 当 $x\neq y$ 时，定义 $w:=\frac{x-y}{\|x-y\|_2}$ 和 Householder 矩阵 $H:=I_n-2ww^T$，
则实正交阵 $U:=H$ 可使 $y=Ux$

我们只需证明非零向量 $x,y\in\mathbb{C}^n$ 情况下的命题 ②: (其余结论都是平凡的)
回忆起 Cauchy-Schwarz 不等式:

$$|x^Hy|\le\|x\|_2\|y\|_2\ (\forall\ x,y\in\mathbb{C}^n)$$

当且仅当 x,y 线性相关时取等.
当 x,y 线性无关且 $\|x\|_2=\|y\|_2$ 时，我们有:

$$|x^Hy|<\|x\|_2\|y\|_2=\|x\|_2^2=x^Hx$$

设 $\phi\in\mathbb{R}$ 使得 $x^Hy=e^{i\phi}|x^Hy|$ (若 $x^Hy=0$，则取 $\phi=0$)
我们定义:

$$\begin{aligned}w&:=\frac{e^{i\phi}x-y}{\|e^{i\phi}x-y\|_2}\\H&:=I_n-2ww^H\\U&:=e^{i\phi}H\end{aligned}$$

则我们有:

$$\begin{aligned}Ux&=e^{i\phi}Hx\\&=e^{i\phi}(I_n-2ww^H)x\\&=e^{i\phi}\{I_n-2\frac{(e^{i\phi}x-y)(e^{i\phi}x-y)^H}{(e^{i\phi}x-y)^H(e^{i\phi}x-y)}\}x\\&=e^{i\phi}\{x-2\frac{(e^{i\phi}x-y)^Hx}{x^Hx-e^{-i\phi}x^Hy-e^{i\phi}y^Hx+y^Hy}(e^{i\phi}x-y)\}\quad(\text{note that }y^Hy=x^Hx\text{ and }x^Hy=e^{i\phi}|x^Hy|)\\&=e^{i\phi}\{x-2\frac{e^{-i\phi}(x^Hx-e^{i\phi}y^Hx)}{2(x^Hx-|x^Hy|)}(e^{i\phi}x-y)\}\\&=e^{i\phi}x-\frac{(x^Hx-|x^Hy|)}{(x^Hx-|x^Hy|)}(e^{i\phi}x-y)\\&=e^{i\phi}x-(e^{i\phi}x-y)\\&=y\end{aligned}$$

且对于任意 $z\perp x$，我们都有:

$$\begin{aligned}(Uz)^Hy&=z^HU^HUx\\&=z^Hx\qquad\Rightarrow Uz\perp y\\&=0\end{aligned}$$

命题得证.

Problem 2

Describe how to avoid cancellation when constructing Householder reflections in the Householder triangularization algorithm for complex matrices.
(Matrix Computation $5.2.10$)

Solution:
Householder QR 算法中我们要实现的关键步骤是:
给定一个向量 $x\in\mathbb{R}^n$，如何寻找一个 Householder 矩阵 $H:=I_n-2ww^H$ 使得 $Hx=\alpha e_1$，其中 $\alpha\in\mathbb{C}$ 满足 $|\alpha|=\|x\|_2$

Matrix Analysis 定理 $2.1.13$ (证明参见 Problem 1) 为我们提供了指引:

- 首先，为保证该 Householder 矩阵存在，$x^H(\alpha e_1)=\bar{x}_1\alpha$ 应当是一个实数，因此 α 与 x_1 拥有相同的辐角.
  设 $x_1=e^{i\theta}|x_1|$ (其中 $\theta\in\mathbb{R}$)，则 $\alpha=e^{i\theta}\|x\|_2$
- 其次，该 Householder 矩阵的构造如下:

$$\begin{aligned}\alpha&:=e^{i\theta}\|x\|_2\\w&:=\frac{x-\alpha e_1}{\|x-\alpha e_1\|_2}\\H&:=I_n-2ww^H\end{aligned}$$

为避免在 $|x_1| \approx \|x\|_2$ 的情况下计算 $x-\alpha e_1$ 的第一个分量时会出现相消，我们可通过等价变形来进行规避:

$$\begin{aligned} x_1-\alpha &= e^{i\theta}|x_1| - e^{i\theta}\|x\|_2 \\ &= e^{i\theta}(|x_1| - \|x\|_2) \\ &= e^{i\theta}\frac{|x_1|^2 - \|x\|_2^2}{|x_1| + \|x\|_2} \\ &= -e^{i\theta}\frac{|x_2|^2 + \cdots + |x_n|^2}{|x_1| + \|x\|_2} \end{aligned}$$

- 再次，为简化存储，记 $\begin{cases} v = x - \alpha e_1 \\ w = \frac{v}{\|v\|_2} \\ \beta = \frac{2}{v^H v} \end{cases}$ 则我们有:

$$H = I - 2ww^H = I - \frac{2}{v^H v}vv^H = I - \beta vv^H$$

因此我们没必要求出 w，只需求出 v 和 β 即可.
在实际运算中，我们可以将 v 的第一个分量规格化为 1 (这样就无需储存了)
然后将 v 的后 $n-1$ 个分量保存在 x 的后 $n-1$ 个置为 0 的分量上.

- 最后，$v^T v$ 的上溢和下溢也是计算中需要考虑的问题.
为避免溢出，我们可用 $\frac{x}{\|x\|_\infty}$ 代替 x 来构造 v
因为理论上，正数乘是不影响向量单位化结果的，
即对于任意 $\gamma > 0$，向量 γv 和 v 的单位化结果是相同的.

基于上述讨论，我们得到如下算法:

$$\begin{aligned}
&\text{function: } [v,\beta] = \text{Complex_Householder}(x) \\
&\quad n = \text{length}(x) \\
&\quad x = \frac{x}{\|x\|_\infty} \\
&\quad v(2:n) = x(2:n) \\
&\quad \sigma = \|x(2:n)\|_2^2 \quad (\text{This is a real value}) \\
&\quad \text{if } \sigma = 0 \\
&\quad\quad \beta = 0 \\
&\quad \text{else} \\
&\quad\quad \text{if } x_1 = 0 \\
&\quad\quad\quad \gamma = 1 \\
&\quad\quad \text{else} \\
&\quad\quad\quad \gamma = \frac{x_1}{|x_1|} \quad (\text{Let } x_1 = e^{i\theta}|x_1|, \text{ then we have } \gamma = \frac{x_1}{|x_1|} = e^{i\theta}) \\
&\quad\quad \text{end} \\
&\quad\quad \alpha = \sqrt{|x(1)|^2 + \sigma} \quad (\text{This is a real value, which is the } l_2 \text{ norm of vector } x) \\
&\quad\quad v(1) = -\gamma \cdot \frac{\sigma}{|x(1)| + \alpha} \quad (\text{Avoiding cancellation when calculating } v(1)) \\
&\quad\quad \beta = \frac{2|v(1)|^2}{|v(1)|^2 + \sigma} \quad (\text{This is a real value}) \\
&\quad\quad v = \frac{v}{v(1)} \quad (\text{Normalize } v(1) \text{ so that we don't have to store it}) \\
&\quad \text{end}
\end{aligned}$$

其 Matlab 代码为:

```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
```

函数调用:

```
% Define a complex vector x
x = [3 + 4i; 1 + 2i; -1 + 0i; 2 - 3i];

% Call the Complex_Householder function
[v, beta] = Complex_Householder(x);

% Display the results
disp('Vector x:');
disp(x);
disp('Vector v:');
disp(v);
disp('Beta:');
disp(beta);

% Verify the Householder transformation
% Form the Householder matrix
H = eye(length(x)) - beta * (v * v');
disp('Householder Matrix H:');
disp(H);

% Apply the Householder transformation to x
y = H * x;

% Display the transformed vector y
disp('Transformed vector y = H * x (should have 0s below the first element):');
disp(y);
```

输出结果:

```
Vector x:
   3.0000 + 4.0000i
```

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

Vector v:
   1.0000 + 0.0000i
  -1.3470 - 0.2449i
   0.3674 - 0.4898i
   0.7347 + 2.0817i

Beta:
    0.2462

Householder Matrix H:
   0.7538 + 0.0000i   0.3317 - 0.0603i  -0.0905 - 0.1206i  -0.1809 + 0.5126i
   0.3317 + 0.0603i   0.5385 + 0.0000i   0.0923 + 0.1846i   0.3692 - 0.6461i
  -0.0905 + 0.1206i   0.0923 - 0.1846i   0.9077 + 0.0000i   0.1846 + 0.2769i
  -0.1809 - 0.5126i   0.3692 + 0.6461i   0.1846 - 0.2769i  -0.2000 + 0.0000i

Transformed vector y = H * x (should have 0s below the first element):
   3.9799 + 5.3066i
  -0.0000 + 0.0000i
   0.0000 - 0.0000i
  -0.0000 + 0.0000i
```

Problem 3

Write a program to compute the QR factorization of a complex matrix $A \in \mathbb{C}^{n\times n}$ with:

- ① Cholesky QR (i.e. through the Cholesky factorization of $A^H A$)
- ② Householder triangularization

Visualize the (componentwise) loss of orthogonality $|Q^H Q - I_n|$ using well-conditioned and ill-conditioned examples.
(If you use MATLAB/Octave, you may find `imagesc()` helpful)

(0) Preperation

构建良态复方阵的 Matlab 函数:

```
function A = generate_well_conditioned_matrix(n)
    % Generates a well-conditioned random complex matrix of size n x n
    real_part = rand(n) + 1; % Ensure diagonal dominance
    imag_part = rand(n) * 1i;
    A = real_part + imag_part; % Combine to form a complex matrix
    A = (A + A') / 2; % Make it Hermitian (symmetric in real case)

    % Check the condition number
    cond_num = cond(A);
    disp(['Condition number of the well-conditioned matrix: ', num2str(cond_num)]);
end
```

构建病态复方阵的 Matlab 函数:

```
function A = generate_ill_conditioned_matrix(n)
    % Generates an ill-conditioned random complex matrix of size n x n
    % Step 1: Generate specific eigenvalues
    lambda = randn(n); % Example eigenvalues
    lambda(1:2) = [1e-10, 1];

    % Step 2: Generate a random unitary matrix U
    [Q, ~] = qr(randn(n) + 1i * randn(n)); % QR decomposition to get a unitary matrix
```

```
    % Step 3: Construct the diagonal matrix of eigenvalues
    D = diag(lambda(1:n));

    % Step 4: Construct the ill-conditioned matrix A
    A = Q * D * Q'; % Ensure A is Hermitian

    % Check the condition number
    cond_num = cond(A);
    disp(['Condition number of the ill-conditioned matrix: ', num2str(cond_num)]);
end
```

使用 `imagesc()` 检查并可视化 Q 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
```

(1) Cholesky QR

关于 Hermite 阵 $A \in \mathbb{C}^{n\times n}$ 的 Cholesky 分解，一种简单实用的方法是逐元素比较 $A = LL^H$ 来计算 L.

设 $L = \begin{bmatrix} l_{11} & & & \\ l_{21} & l_{22} & & \\ \vdots & \vdots & \ddots & \\ l_{n1} & l_{n2} & \dots & l_{nn} \end{bmatrix} \in \mathbb{C}^{n\times n}$ (可以证明其主对角元都是非负实数)

比较 $A = LL^H$ 两边对应元素，得到 $a_{ij} = \sum\limits_{p=1}^{\min(i,j)} l_{ip}\bar{l}_{jp}\ (1 \le i, j \le n)$

- 首先由 $a_{11} = l_{11}^2$ 得到 $l_{11} = \sqrt{a_{11}}$
  再由 $a_{i1} = l_{11} l_{i1}\ (1 \le i \le n)$ 得到 $l_{i1} = \frac{1}{l_{11}} a_{i1}\ (1 \le i \le n)$
  这样便得到矩阵 L 的第 1 列元素.
- 假设已经计算出 L 的前 $k-1$ 列元素.
  由 $a_{kk} = \sum\limits_{p=1}^{k} l_{kp}\bar{l}_{kp} = \sum\limits_{p=1}^{k} |l_{kp}|^2$ 得到 $l_{kk} = (a_{kk} - \sum\limits_{p=1}^{k-1} |l_{kp}|^2)^{\frac{1}{2}}$
  再由 $a_{ik} = \sum\limits_{p=1}^{k} l_{ip}\bar{l}_{kp} = \sum\limits_{p=1}^{k-1} l_{ip}\bar{l}_{kp} + l_{ik} l_{kk}\ \ (i = k+1, \dots, n)$
  得到 $l_{ik} = \frac{1}{l_{kk}}(a_{ik} - \sum\limits_{p=1}^{k-1} l_{ip}\bar{l}_{kp})\ \ (i = k+1, \dots, n)$
  这样便得到矩阵 L 的第 k 列元素.

上述次序可以调整为按行计算.
由于 A 的元素 a_{ij} 被用来计算 l_{ij} 后就不再使用，故我们可将 L 的元素存储在 A 的对应位置上.
综上所述我们得到如下算法:

Given Hermitian matrix $A \in \mathbb{C}^{n\times n}$

function: $[L] = \text{Complex\_Cholesky}(A)$
    for $k = 1:n$
        $A(k,k) = \sqrt{A(k,k)}$
        $A(k+1:n,k) = A(k+1:n,k)/A(k,k)$
        for $j = k+1:n$
            $A(j:n,j) = A(j:n,j) - A(j:n,k)\overline{A(j,k)}$
        end
    end
    $L = A \odot$ (lower triangular matrix with all ones)   ($\odot$ stands for Hadamand product)
end

其 Matlab 代码如下:

```
function L = Complex_Cholesky(A)
    n = size(A, 1);  % Get the size of matrix A
    for k = 1:n
        % Compute the diagonal element (ensure it's real and positive)
        A(k,k) = sqrt(A(k,k));  % For Hermitian, take the square root of the diagonal

        % Update the subdiagonal using the conjugate of the diagonal element
        A(k+1:n,k) = A(k+1:n,k) / A(k,k);

        for j = k+1:n
            % Update the remaining elements, using conjugate for complex entries
            A(j:n,j) = A(j:n,j) - A(j:n,k) * conj(A(j,k));
        end
    end

    % Return the lower triangular matrix with the Hadamard product
    L = A .* tril(ones(n));  % Hadamard product with a lower triangular matrix
end
```

使用上述算法得到 A^HA 的 Cholesky 分解 $A^HA = LL^H$ 后,
可取 $R = L^H$，并求解上三角方程组 $QR = A$ 得到 Q:

$$QR = [q_1, q_2, \dots, q_n] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & \cdots & r_{2n} \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix} = [a_1, a_2, \dots, a_n] = A$$

显然我们有 $a_k = \sum_{i=1}^{k} r_{ik}q_i \ (k = 1, \dots, n)$ 成立，从而有:

$$q_1 = \frac{1}{r_{11}} a_1$$

$$q_k = \frac{1}{r_{kk}} (a_k - \sum_{i=1}^{k-1} r_{ik} q_i) \ (k = 2, \dots, n)$$

在实际计算中，我们将 Q 存放在 A 所用的存储单元中，并调整运算次序.
于是我们得到如下算法:

$$
\begin{array}{l}
\text{Given matrix } A \in \mathbb{C}^{m\times n} \text{ and upper triangular matrix } R \in \mathbb{C}^{n\times n} \text{ whose diagonal entries are non-negative} \\
\hline
\text{function: } Q = \text{Forward\_Sweep}(A, R) \\
\quad \text{for } k = 1 : n-1 \\
\quad\quad A(1:m,k) = \dfrac{1}{R(1,1)} A(1:m,k) \\
\quad\quad A(1:m,k+1:n) = A(1:m,k+1:n) - A(1:m,k)R(k,k+1:n) \\
\quad \text{end} \\
\quad A(1:m,n) = \dfrac{1}{R(n,n)} A(1:m,n) \\
\quad Q = A \\
\text{end}
\end{array}
$$

其 Matlab 代码如下:

```
function Q = Forward_Sweep(A, R)
    [m, n] = size(A);

    for i = 1:n-1
        % Normalize the current column
        A(1:m, i) = A(1:m, i) / R(i, i);

        % Update the remaining columns
        A(1:m, i+1:n) = A(1:m, i+1:n) - A(1:m, i) * R(i, i+1:n);
    end

    % Normalize the last column
    A(1:m, n) = A(1:m, n) / R(n, n);

    % Set Q
    Q = A;
end
```

合并上述算法我们便得到 Cholesky QR 算法:

$$
\begin{array}{l}
\text{Given matrix } A \in \mathbb{C}^{m\times n} \\
\hline
\text{function: } [Q, R] = \text{Complex\_Cholesky\_QR}(A) \\
\quad L = \text{Complex\_Cholesky}(A) \\
\quad R = L^H \\
\quad Q = \text{Forward\_Sweep}(A, R) \\
\text{end}
\end{array}
$$

其 Matlab 代码为:

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

    % Step 1: Compute the Cholesky decomposition of the product A' * A.
    % This yields a lower triangular matrix L.
    L = Complex_Cholesky(A' * A);

    % Step 2: Obtain R as the conjugate transpose of L.
    % R is an upper triangular matrix needed for the QR factorization.
    R = L';

    % Step 3: Use the Forward Sweep method to compute the orthogonal
    % matrix Q based on the original matrix A and the matrix R.
    Q = Forward_Sweep(A, R);
end
```

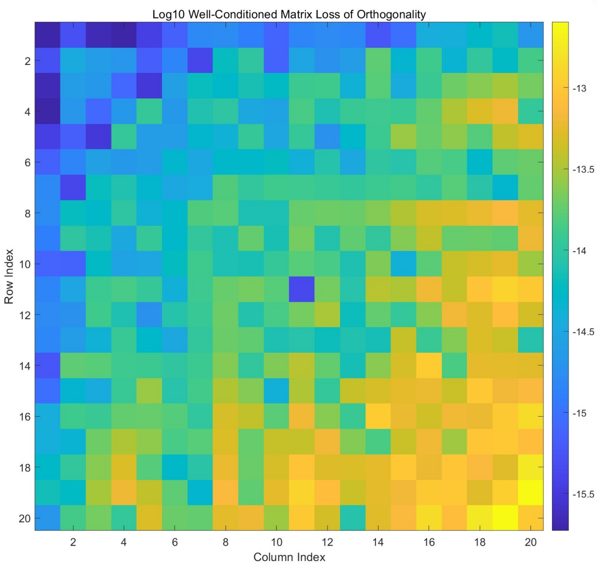
函数调用:

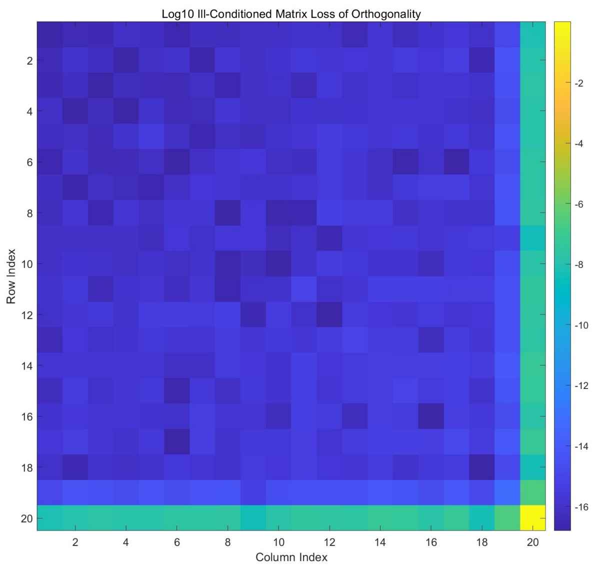
```
% Set the random seed for reproducibility
rng(51);
n = 20;
```

```
% Generate a well-conditioned complex matrix
A_well = generate_well_conditioned_matrix(n); % 5x5 matrix
% Perform Cholesky QR
[Q_well, R_well] = Complex_Cholesky_QR(A_well);

% Check if Q * R is close to A
disp('Frobenius norm of A - Q * R for well-conditioned example:');
disp(norm(Q_well * R_well - A_well, 'fro'))

% Visualize loss of orthogonality for well-conditioned matrix
visualize_orthogonality_loss(Q_well, 'Well-Conditioned Matrix Loss of Orthogonality');

% Generate an ill-conditioned complex matrix
A_ill = generate_ill_conditioned_matrix(n); % 5x5 matrix
% Perform Cholesky QR
[Q_ill, R_ill] = Complex_Cholesky_QR(A_ill);

% Check if Q * R is close to A
disp('Frobenius norm of A - Q * R for ill-conditioned example:');
disp(norm(Q_ill * R_ill - A_ill, 'fro'))

% Visualize loss of orthogonality for ill-conditioned matrix
visualize_orthogonality_loss(Q_ill, 'Ill-Conditioned Matrix Loss of Orthogonality');
```

输出结果:

```
Condition number of the well-conditioned matrix: 279.2377
Frobenius norm of A - Q * R for well-conditioned example:
   4.3332e-15

Condition number of the ill-conditioned matrix: 20693749868.9697
Frobenius norm of A - Q * R for ill-conditioned example:
   7.1736e-16
```





(2) Householder QR

复数域上的 Householder 变换的计算算法已在 Problem 2 中给出.
复数域上的 Householder QR 算法即为:

$$
\begin{aligned}
&\text{function: } [Q,R] = \text{Complex\_Householder\_QR}(A)\\
&\quad [m,n] = \text{size}(A)\\
&\quad Q = I_m\\
&\quad \text{for } k = 1:\min(m-1,n)\\
&\quad\quad [v,\beta] = \text{Complex\_Householder}(A(k:m,k))\\
&\quad\quad A(k:m,k:n) = (I_{m-k+1} - \beta vv^H)A(k:m,k:n) = A(k:m,k:n) - (\beta v)(v^H A(k:m,k:n))\\
&\quad\quad Q(1:m,k:m) = Q(1:m,k:m)(I_{m-k+1} - \beta vv^H) = Q(1:m,k:m) - (Q(1:m,k:m)v)(\beta v)^H\\
&\quad \text{end}\\
&\text{end}
\end{aligned}
$$

其 Matlab 代码为:

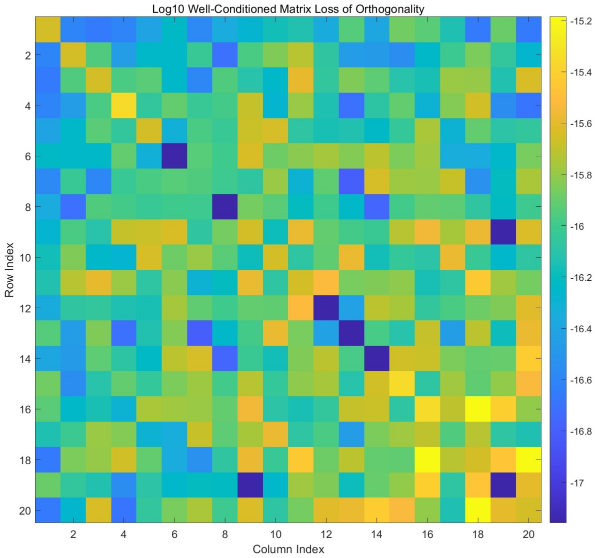
```matlab
function [Q, R] = Complex_Householder_QR(A)
    [m, n] = size(A);
    Q = eye(m); % Initialize Q as the identity matrix
    R = A; % Initialize R as A

    for k = 1:min(m-1, n)
        [v, beta] = Complex_Householder(R(k:m, k)); % Apply Complex Householder

        % Update R
        R(k:m, k:n) = R(k:m, k:n) - (beta * v) * (v' * R(k:m, k:n));

        % Update Q
        Q(1:m, k:m) = Q(1:m, k:m) - (Q(1:m, k:m) * v) * (beta * v');
    end
end
```

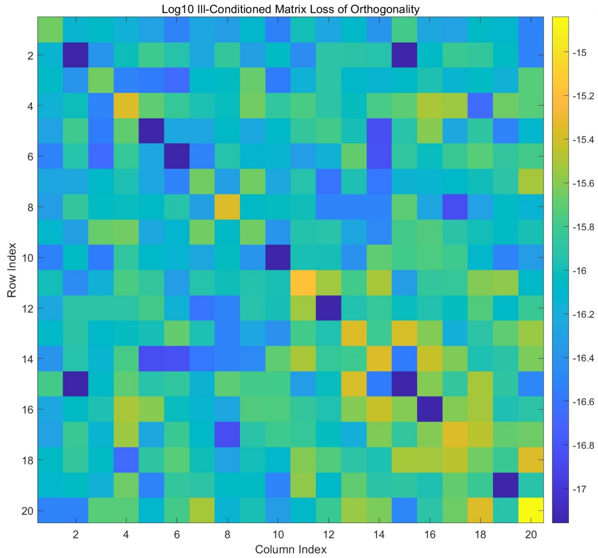
函数调用:

```matlab
% Set the random seed for reproducibility
rng(51);
n = 20;

% Generate a well-conditioned complex matrix
A_well = generate_well_conditioned_matrix(n); % 5x5 matrix
% Perform Householder QR
[Q_well, R_well] = Complex_Householder_QR(A_well);

% Check if Q * R is close to A
disp('Frobenius norm of A - Q * R for well-conditioned example:');
disp(norm(Q_well * R_well - A_well, 'fro'))

% Visualize loss of orthogonality for well-conditioned matrix
visualize_orthogonality_loss(Q_well, 'Log10 Well-Conditioned Matrix Loss of Orthogonality');

% Generate an ill-conditioned complex matrix
A_ill = generate_ill_conditioned_matrix(n); % 5x5 matrix
% Perform Householder QR
[Q_ill, R_ill] = Complex_Householder_QR(A_ill);

% Check if Q * R is close to A
disp('Frobenius norm of A - Q * R for ill-conditioned example:');
disp(norm(Q_ill * R_ill - A_ill, 'fro'))

% Visualize loss of orthogonality for ill-conditioned matrix
visualize_orthogonality_loss(Q_ill, 'Log10 Ill-Conditioned Matrix Loss of Orthogonality');
```

输出结果:

```
Condition number of the well-conditioned matrix: 279.2377
Frobenius norm of A - Q * R for well-conditioned example:
   8.7266e-15

Condition number of the ill-conditioned matrix: 20693749868.9697
Frobenius norm of A - Q * R for ill-conditioned example:
   2.3290e-15
```





对比 Cholesky QR 的结果我们发现 Householder QR 无论是数值稳定性还是正交性损失都是更优的.

Problem 4

Design an efficient algorithm to compute the QR factorization of A:

$$A = \begin{bmatrix} \alpha_1 & \gamma_2 & \gamma_3 & \cdots & \gamma_{n-1} & \gamma_n \\ \beta_2 & \alpha_2 & & & & \\ \beta_3 & & \alpha_3 & & & \\ \vdots & & & \ddots & & \\ \beta_{n-1} & & & & \alpha_{n-1} & \\ \beta_n & & & & & \alpha_n \end{bmatrix} \in \mathbb{R}^{n \times n}$$

Solution:
(计算 Givens 变换, 数值线性代数, 算法 $3.2.2$)

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

- ① 首先使用 Givens 变换将稀疏矩阵 A 化为上 Hessenberg 矩阵 H，得到 $A = Q_1 H$
为让讨论更加直观，考虑 $n = 5$ 的情形:

$$A = \begin{bmatrix} \ast & \ast & \ast & \ast & \ast \\ \ast & \ast & & & \\ \ast & & \ast & & \\ \underline{\ast} & & & \ast & \\ \underline{\ast} & & & & \ast \end{bmatrix}$$

$$G_{4,5}A = \begin{bmatrix} \ast & \ast & \ast & \ast & \ast \\ \ast & \ast & & & \\ \underline{\ast} & & \ast & & \\ \underline{\ast} & & & \ast & \ast \\ & & & \ast & \ast \end{bmatrix}$$

$$G_{3,4}(G_{4,5}A) = \begin{bmatrix} \ast & \ast & \ast & \ast & \ast \\ \underline{\ast} & \ast & & & \\ \underline{\ast} & & \ast & \ast & \ast \\ & & \ast & \ast & \ast \\ & & & \ast & \ast \end{bmatrix}$$

$$G_{2,3}(G_{3,4}G_{4,5}A) = \begin{bmatrix} \ast & \ast & \ast & \ast & \ast \\ \ast & \ast & \ast & \ast & \ast \\ & \ast & \ast & \ast & \ast \\ & & \ast & \ast & \ast \\ & & & \ast & \ast \end{bmatrix}$$

对于一般的 n 阶稀疏矩阵 A,
我们可以确定 $n-2$ 个 Givens 变换 $G_{n-1,n},\dots,G_{2,3}$ 使得 $G_{2,3}\cdots G_{n-1,n}A = H$
令正交阵 $Q_1 = (G_{2,3}\cdots G_{n-1,n})^{-1} = (G_{2,3}\cdots G_{n-1,n})^T = G_{n-1,n}^T\cdots G_{2,3}^T$
即得到 $A = Q_1 H$
具体算法如下:

Given Sparse matrix $A \in \mathbb{R}^{n\times n}$

$Q = I_n$
for $k = n-1 : -1 : 2$
$\quad [c,s] = \text{Givens}(H(k,1), H(k+1,1))$
$$H(k:k+1,1:n) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} H(k:k+1,1:n) \quad \left(\begin{cases} H(k,1:n) = cH(k,1:n) + sH(k+1,1:n) \\ H(k+1,1:n) = -sH(k,1:n) + cH(k+1,1:n) \end{cases}\right)$$
$$Q(1:n,k:k+1) = Q(1:n,k:k+1)\begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T \quad \left(\begin{cases} Q(1:n,k) = cQ(1:n,k) + sQ(1:n,k+1) \\ Q(1:n,k+1) = -sQ(1:n,k) + cQ(1:n,k+1) \end{cases}\right)$$
end
$H = A$

Matlab 代码如下:

```
function [Q, H] = Upper_Hessenberg(A)
    % 将稀疏矩阵 A 上 Hessenberg 化
    [n, ~] = size(A);
    Q = eye(n);  % 初始化为单位矩阵
    for k = n-1:-1:2
        [c, s] = Givens(A(k, 1), A(k+1, 1));

        % 对 A 进行 Givens 变换
        G = [c s; -s c];  % 2x2 Givens 旋转矩阵
        A(k:k+1, :) = G * A(k:k+1, :);

        % 累积 Givens 变换到 Q
        Q(:, k:k+1) = Q(:, k:k+1) * G';
    end
    H = A;
end
```

- ② 然后使用 Givens 变换对上 Hessenberg 矩阵 H 进行上三角化，得到 $H = Q_2 R$
为让讨论更加直观，考虑 $n=5$ 的情形:

$$H=\begin{bmatrix}\underline{*}&*&*&*&*\\ \underline{*}&*&*&*&*\\ 0&*&*&*&*\\ 0&0&*&*&*\\ 0&0&0&*&*\end{bmatrix}$$

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

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

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

$$G_{4,5}(G_{3,4}G_{2,3}G_{1,2}H)=\begin{bmatrix}*&*&*&*&*\\ 0&*&*&*&*\\ 0&0&*&*&*\\ 0&0&0&\underline{*}&*\\ 0&0&0&\underline{0}&*\end{bmatrix}\overset{\Delta}{=}R$$

对于一般的 n 阶上 Hessenberg 矩阵 H,
我们可以确定 $n-1$ 个 Givens 变换 $G_{1,2},\ldots,G_{n-1,n}$ 使得 $G_{n-1,n}\cdots G_{1,2}H=R$
令正交阵 $Q_2=(G_{n-1,n}\cdots G_{1,2})^{-1}=(G_{n-1,n}\cdots G_{1,2})^T=G_{1,2}^T\cdots G_{n-1,n}^T$
即得到 H 的 QR 分解 $H=Q_2R$
具体算法如下:

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

$Q=I_n$
for $k=1:n-1$
$\quad [c,s]=\text{Givens}(H(k,k),H(k+1,k))$
$\quad H(k:k+1,k:n)=\begin{bmatrix}c&s\\-s&c\end{bmatrix}H(k:k+1,k:n)\quad \left(\begin{cases}H(k,k:n)=cH(k,k:n)+sH(k+1,k:n)\\H(k+1:k:n)=-sH(k,k:n)+cH(k+1,k:n)\end{cases}\right)$
$\quad Q(1:n,k:k+1)=Q(1:n,k:k+1)\begin{bmatrix}c&s\\-s&c\end{bmatrix}^T\quad \left(\begin{cases}Q(1:n,k)=cQ(1:n,k)+sQ(1:n,k+1)\\Q(1:n,k+1)=-sQ(1:n,k)+cQ(1:n,k+1)\end{cases}\right)$
end
$R=H$

Matlab 代码如下:

```
function [Q, R] = Hessenberg_QR(Q, H)
    % 对上 Hessenberg 矩阵 H 进行 QR 分解
    [n, ~] = size(H);
    for k = 1:n-1
        % 计算 Givens 旋转参数
        [c, s] = Givens(H(k, k), H(k+1, k));

        % 对 H 进行 Givens 变换
        G = [c s; -s c];  % 2x2 Givens 旋转矩阵
        H(k:k+1, k:n) = G * H(k:k+1, k:n);
        H(k+1, k) = 0;

        % 累积 Givens 变换到 Q
        Q(:, k:k+1) = Q(:, k:k+1) * G';
```

```
    end
    R = H;  % 上三角矩阵
end
```

- ③ 最终我们得到 $A = Q_1 H = Q_1(Q_2 R) = Q_1 Q_2 R$
因此 A 的 QR 分解为 $A = QR$，其中 $Q = Q_1 Q_2$，它不必显式计算，可由 Q_1 直接代入步骤 ② 中累积 Givens 变换得到.

Matlab 代码如下:

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

    % 1. 使用 Givens 变换将稀疏矩阵 A 上 Hessenberg 化为 H，得到 A = Q1 * H
    [Q, H] = Upper_Hessenberg(A);

    % 2. 使用 Givens 变换对上 Hessenberg 矩阵 H 进行 QR 分解，得到 H = Q2 * R，累积 Q = Q1 * Q2
    [Q, R] = Hessenberg_QR(Q, H);

end
```

主函数调用:

```
rng(51)
n = 1000;
% 初始化一个全零矩阵
A = zeros(n, n);

% 填充第一列，除去第一个元素
A(2:n, 1) = rand(n-1, 1);  % 第一列的随机数

% 填充第一行，除去第一个元素
A(1, 2:n) = rand(1, n-1);  % 第一行的随机数

% 填充主对角线
A(1:n+1:end) = rand(n, 1);  % 对角线上的随机数

% 使用快速 QR 分解
[Q, R] = Efficient_QR(A);

% 计算 A 与 QR 的差异
QR_approx = Q * R;
F_norm_diff = norm(A - QR_approx, 'fro');

% 输出误差
disp(['Frobenius norm of the difference ||A - QR||_F = ', num2str(F_norm_diff)]);
```

输出结果:

```
Frobenius norm of the difference ||A - QR||_F = 4.31e-14
```

最开始的错误解法:

$$A = \begin{bmatrix} \alpha_1 & \gamma_2 & \gamma_3 & \cdots & \gamma_{n-1} & \gamma_n \\ \beta_2 & \alpha_2 & & & & \\ \beta_3 & & \alpha_3 & & & \\ \vdots & & & \ddots & & \\ \beta_{n-1} & & & & \alpha_{n-1} & \\ \beta_n & & & & & \alpha_n \end{bmatrix} \in \mathbb{R}^{n\times n}$$

- ① 首先我们使用初等置换矩阵将 A 的列进行重排，得到一个上 Hessenberg 矩阵 $\tilde{A}$.

$$P = \begin{bmatrix} e_n^T \\ e_1^T \\ e_2^T \\ \vdots \\ e_{n-2}^T \\ e_{n-1}^T \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 1 \\ 1 & 0 & & & & \\ & 1 & 0 & & & \\ & & \ddots & \ddots & & \\ & & & 1 & 0 & \\ & & & & 1 & 0 \end{bmatrix}$$

$$\tilde{A} = AP = \begin{bmatrix} \gamma_2 & \gamma_3 & \cdots & \gamma_{n-1} & \gamma_n & \alpha_1 \\ \alpha_2 & 0 & & & & \beta_2 \\ & \alpha_3 & 0 & & & \beta_3 \\ & & \ddots & \ddots & & \vdots \\ & & & \alpha_{n-1} & 0 & \beta_{n-1} \\ & & & & \alpha_n & \beta_n \end{bmatrix}$$

其中置换矩阵 P 无需显式生成，$\tilde{A} = PA$ 也无需显式计算
只需将 A 的第 1 列放到最后一列，其余各列往前移动一列即可得到 $\tilde{A}$.

- ② 然后使用 Givens 变换对上 Hessenberg 矩阵 $\tilde{A}$ 进行上三角化，得到 $\tilde{A} = QR$
得到 $A = \tilde{A}P^T = QRP^T$
但这不能化为 QR 分解的形式，因为 RP^T 并不是一个上三角阵.

Problem 5

Let $Q \in \mathbb{R}^{n\times n}$ be an orthogonal matrix (下列的结论对一般的酉矩阵 $U \in \mathbb{C}^{n\times n}$ 并不一定成立)
Show that Q can be factorized as the product of finitely many Householder reflections,
and if, in addition, $\det(Q) = 1$, Q can be factorized as the product of finitely many Givens rotations.

Solution:
(1) 证明正交阵 $Q \in \mathbb{R}^{n\times n}$ 可以分解为有限个 Householder 变换矩阵的乘积:

- ① 首先我们可使用 Householder QR 分解，
找到 $n-1$ 个 Householder 矩阵 $H_1, \dots, H_{n-1} \in \mathbb{R}^{n\times n}$ 使得 $R = H_{n-1}\cdots H_1 Q$
其中 R 为上三角阵.
- ② 其次我们可以证明 R 是对角阵，且对角元只可能为 ± 1
根据 $R^TR = (H_{n-1}\cdots H_1Q)^T(H_{n-1}\cdots H_1Q) = Q^TH_1^T\cdots H_{n-1}^TH_{n-1}\cdots H_1Q = I_n$ 可知 R 为正交阵.
记 $R = [r_{ij}]_{i,j=1}^n = [r_1, \dots, r_n]$，我们希望证明 $r_i = \pm e_i \ (i = 1, \dots, n)$ (其中 e_i 代表 $\mathbb{R}^n$ 的第 i 个标准单位基向量)

  (数学归纳法)
  首先显然有 $r_1 = \pm e_1$ 成立
  假设对于 $k \in \mathbb{Z}_+$ 有 $r_i = \pm e_i \ (i = 1, \dots, k)$
  则根据 $r_i \perp r_{k+1} \ (i = 1, \dots, k)$ 可知 $r_{i,k+1} = 0 \ (i = 1, \dots, k)$
  再根据 R 为上三角阵可知 $r_{i,k+1} = 0 \ (i = k+2, \dots, n)$
  最后根据 $\|r_{k+1}\|_2 = 1$ 可知 $r_{k+1,k+1} = \pm 1$，即 $r_{k+1} = \pm e_{k+1}$
  根据归纳原理得证 R 是对角阵，且对角元只可能为 ± 1
- ③ 最后我们证明 R 可分解为有限个 Householder 矩阵.
任意给定的 $i = 1, \dots, n$
若 $r_{i,i} = -1$，则我们可取 $w := -e_i$，定义 Householder 变换 $\tilde{H}_i := I_n - 2ww^T = I_n - 2e_ie_i^T$
记 $E_{i,i} = e_ie_i^T$ 为 (i,i) 位置为 1，其余位置为 0 的 n 阶方阵
于是我们有:

$$\tilde{H}_iR = (I_n - 2e_ie_i^T)R = R - 2r_{i,i}E_{i,i} = R + 2E_{i,i}$$

  显然 $R + 2E_{i,i}$ 在 (i,i) 位置的元素为 1
  换言之，Householder 变换 $\tilde{H}_i$ 将 R 变为 $R + 2E_{i,i}$，即将其 (i,i) 位置的元素 -1 变为了 1.

  由于 R 仅有有限个对角元为 -1 (记其个数为 m，指标为 $i_1, \dots, i_m$)，
  故我们可找到有限个 Householder 变换 $\tilde{H}_{i_1}, \dots, \tilde{H}_{i_m}$ 使得 $\tilde{H}_{i_m}\cdots\tilde{H}_{i_1}R = I_n$

综上所述，我们有:

$$
\begin{aligned}
R &= H_{n-1}\cdots H_1 Q \\
\tilde{H}_{i_m}\cdots\tilde{H}_{i_1}R &= I_n \\
&\Rightarrow \\
Q &= (H_{n-1}\cdots H_1)^T R \\
&= H_1\cdots H_{n-1}(\tilde{H}_{i_m}\cdots\tilde{H}_{i_1})^T I_n \\
&= H_1\cdots H_{n-1}\tilde{H}_{i_1}\cdots\tilde{H}_{i_m}
\end{aligned}
$$

其中 m 是 R 的对角元中 -1 的个数.
这样就将正交阵 Q 表示为有限个 Householder 变换的乘积.

---

(2) 证明满足 $\det(Q)=1$ 的正交阵 $Q\in\mathbb{R}^{n\times n}$ 可以分解为有限个 Givens 变换矩阵的乘积:

- ① 首先我们可使用 Givens QR 分解,
找到 $(n-1)+\cdots+1=\frac{n(n-1)}{2}$ 个 Givens 变换 $G_1,\dots,G_{\frac{1}{2}n(n-1)}\in\mathbb{R}^{n\times n}$ 使得 $R=G_{\frac{1}{2}n(n-1)}\cdots G_1 Q$
其中 R 为上三角阵.
由于 Givens 变换的行列式为 1，故我们有 $\det(R)=\det(Q)=1$
- ② 其次我们可以证明 R 是对角阵，且对角元只可能为 ± 1
证明过程同 (1) ②
- ③ 最后根据 $\det(R)=1$ 可知 R 仅有偶数个对角元为 -1
任意给定的 $i,j\in\{1,\dots,n\}$ 满足 $i\neq j$ (不妨设 $i<j$)
若 $r_{i,i}=r_{j,j}=-1$，则我们可取 $\theta=\pi$
定义 Givens 变换:

$$
\begin{aligned}
\tilde{G}_{i,j} &= I_n+[\cos(\theta)-1](e_ie_i^T+e_je_j^T)+\sin(\theta)e_ie_j^T-\sin(\theta)e_je_i^T \quad (\text{note that } \theta=\pi) \\
&= I_n-2(e_ie_i^T+e_je_j^T)
\end{aligned}
$$

记 $E_{i,i}=e_ie_i^T$ 为 (i,i) 位置为 1，其余位置为 0 的 n 阶方阵
则我们有:

$$
\begin{aligned}
\tilde{G}_{i,j}R &= [I_n-2(e_ie_i^T+e_je_j^T)]R \\
&= R-2r_{i,i}E_{i,i}-2r_{j,j}E_{j,j} \\
&= R+2E_{i,i}+2E_{j,j}
\end{aligned}
$$

显然 $R+2E_{i,i}+2E_{j,j}$ 在 (i,i) 和 (j,j) 位置的元素为 1
换言之，Givens 变换 $\tilde{G}_{i,j}$ 将 R 变为 $R+2E_{i,i}+2E_{j,j}$，即将其 (i,i) 和 (j,j) 位置的元素 -1 变为了 1.
由于 R 仅有有限偶数个对角元为 -1 (记其个数为 $2m$，指标为 $i_1,\dots,i_m,j_1,\dots,j_m$),
故我们可找到有限个 Givens 变换 $\tilde{G}_{i_1,j_1},\dots,\tilde{G}_{i_m,j_m}$ 使得 $\tilde{G}_{i_m,j_m}\cdots\tilde{G}_{i_1,j_1}R=I_n$

综上所述，我们有:

$$
\begin{aligned}
R &= G_{\frac{1}{2}n(n-1)}\cdots G_1 Q \\
\tilde{G}_{i_m,j_m}\cdots\tilde{G}_{i_1,j_1}R &= I_n \\
&\Rightarrow \\
Q &= (G_{\frac{1}{2}n(n-1)}\cdots G_1)^T R \\
&= G_1\cdots G_{\frac{1}{2}n(n-1)}(\tilde{G}_{i_m,j_m}\cdots\tilde{G}_{i_1,j_1})^T I_n \\
&= G_1\cdots G_{\frac{1}{2}n(n-1)}\tilde{G}_{i_1,j_1}\cdots\tilde{G}_{i_m,j_m}
\end{aligned}
$$

其中 $2m$ 是 R 的对角元中 -1 的个数.
这样就将正交阵 Q 表示为有限个 Givens 变换的乘积.

Problem 6 (optional)

本题可参考文章 **A Storage-Efficient WY Representation for Products of Householder Transformations** 的算法 2
而 Problem 7 可参考上述文章的 Compact WY 表示.
(Block Householder Triangularization)
Design a block algorithm (either left-looking or right-looking) for Householder triangularization.
For simplicity, you may assume that the number of columns of the matrix is a multiple of the block size.

- **Background:**
  给定矩阵 $V \in \mathbb{C}^{n\times r}$
  定义推广形式的 Householder 变换 $H := I_n - 2VV^\dagger$
  根据 Moore-Penrose 逆的性质容易验证 H 是 **Hermite 酉矩阵**.

  特殊地，若 V 列满秩，则 Moore-Penrose 逆 $V^\dagger = (V^HV)^{-1}V^H$
  此时 $H = I_n - 2V(V^HV)^{-1}V^H$
- **Lemma:**

  考虑列满秩矩阵 $X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \in \mathbb{C}^{m\times r}$ (其中 X_1 为 r 阶复方阵)

  若定义:

$$Y := I_r + (X_2X_1^{-1})^H(X_2X_1^{-1})$$
$$\text{Denote } Y = Q\Lambda Q^H \text{ as the spectral decomposition, define } Y^{\frac{1}{2}} = Q\Lambda^{\frac{1}{2}}Q^H$$
$$R := Y^{\frac{1}{2}}A_1$$
$$V := \begin{bmatrix} X_1 + R \\ X_2 \end{bmatrix}$$
$$H := I_n - 2V(V^HV)^{-1}V^H$$

  则我们有:

$$HA = \begin{bmatrix} -R \\ 0_{(m-r)\times r} \end{bmatrix}$$

Solution:
基于 **Lemma** 的分块 Householder 变换的 Matlab 代码如下:

```
function [V, beta] = Block_Complex_Householder(X)
    % Block_Complex_Householder computes a block Householder transformation
    % for a given complex matrix X. The transformation aims to introduce zeros
    % below the diagonal of the upper-left r x r block of the matrix.

    [m, r] = size(X);  % Get the dimensions of the matrix X
    % Compute the matrix Z which is used to define the Householder transformation
    Z = X(r+1:m, 1:r) / X(1:r, 1:r);

    % Construct the symmetric matrix Y, which is used to calculate the Householder vector
    Y = eye(r, r) + Z' * Z;

    % Compute the eigenvectors (Q) and eigenvalues (Lambda) of Y
    [Q, Lambda] = eig(Y);

    % Calculate the square root of the matrix Y
    Y_sqrt = Q * sqrt(Lambda) * Q';

    % Compute the upper triangular matrix R that will be used for the transformation
    R = Y_sqrt * X(1:r, 1:r);

    % Initialize V as a copy of X
    V = X;

    % Update the upper-left r x r block of V by subtracting R, introducing zeros below the
diagonal
    V(1:r, 1:r) = V(1:r, 1:r) - R;

    % Compute the scaling factor beta for the Householder transformation
    beta = 2 * eye(r, r) / (V' * V);
end
```

复数域上的 Householder 变换的计算算法已在 Problem 2 中给出.
最终的分块 Householder QR 算法的 Matlab 代码如下:

```
function [Q, R] = Block_Complex_Householder_QR(A, r)
```

```
    % Block_Complex_Householder_QR computes the QR decomposition of a
    % complex matrix A using a block-wise approach with complex Householder
    % reflections.
    %
    % Inputs:
    %   A - An m x n complex matrix to be decomposed.
    %   r - The block size for the Householder transformation.
    %
    % Outputs:
    %   Q - An m x m unitary matrix such that Q*R = A.
    %   R - An m x n upper triangular matrix.

    [m, n] = size(A);  % Get the dimensions of matrix A
    Q = eye(m);        % Initialize Q as the identity matrix of size m
    R = A;             % Start with R equal to A
    m_block = floor(m / r);  % Calculate the number of complete blocks in m
    n_block = floor(n / r);  % Calculate the number of complete blocks in n

    % Loop over the blocks
    for k = 1:min(m_block-1, n_block)
        index1 = (k-1) * r + 1;  % Starting index for the current block in R
        index2 = k * r;          % Ending index for the current block in R

        % Apply the Block Complex Householder transformation to the current block
        [V, beta] = Block_Complex_Householder(R(index1 : m, index1 : index2));

        % Update the R matrix using the Householder transformation
        R(index1:m, index1:n) = R(index1:m, index1:n) - V * (beta * (V' * R(index1:m,
index1:n)));

        % Update the Q matrix to reflect the transformations applied to R
        Q(1:m, index1:m) = Q(1:m, index1:m) - ((Q(1:m, index1:m) * V) * beta) * V';
    end

    % Process the leftover elements that do not fit into a complete block
    leftover_index = min(m_block-1, n_block) * r + 1;
    for k = leftover_index : min(m-1, n)
        % Apply Complex Householder transformation for the remaining elements
        [v, beta] = Complex_Householder(R(k:m, k));

        % Update R for the last elements
        R(k:m, k:n) = R(k:m, k:n) - (beta * v) * (v' * R(k:m, k:n));

        % Update Q for the last elements
        Q(1:m, k:m) = Q(1:m, k:m) - (Q(1:m, k:m) * v) * (beta * v');
    end
end
```

复述 Problem 3 中使用 `imagesc()` 检查并可视化 Q 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
```

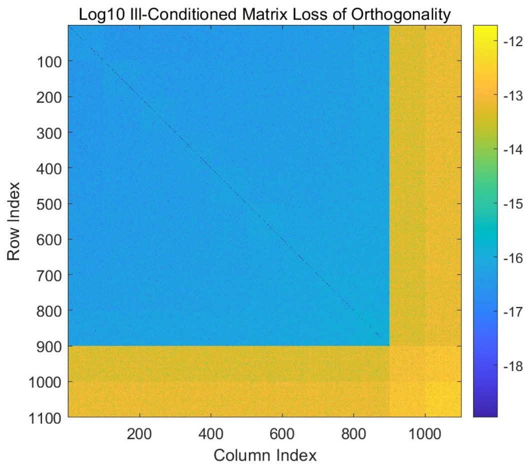
函数调用:

```
rng(51);
```

```
m = 1100;
n = 1000;
r = 100; % Block zize
A = randn(m, n) + 1i * randn(m, n);

% Apply Block Householder QR algorithm
[Q, R] = Block_Complex_Householder_QR(A, r);

% Check if Q * R is close to A
disp('Frobenius norm of A - Q * R:');
disp(norm(Q * R - A, 'fro'))

% Visualize loss of orthogonality for ill-conditioned matrix
visualize_orthogonality_loss(Q, 'Log1Ill-Conditioned Matrix Loss of Orthogonality');
```

输出结果:

```
Frobenius norm of A - Q * R:
   6.6750e-09
```



一开始错误的做法:

考虑列满秩矩阵 $X = \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \in \mathbb{R}^{m\times r}$ (其中 X_1 为 r 阶实方阵)

若定义:

$$
\begin{gathered}
L := \text{Cholesky}(X^TX) \\
(\text{so that } LL^T = X^TX = X_1^TX_1 + X_2^TX_2 \text{ and } L \text{ is a lower triangle matrix}) \\
V := \begin{bmatrix} X_1 + L^T \\ X_2 \end{bmatrix} \\
H := I_n - 2V(V^TV)^{-1}V^T
\end{gathered}
$$

则我们有:

$$
HA = \begin{bmatrix} -L^T \\ 0_{(m-r)\times r} \end{bmatrix}
$$

但上述命题并不成立.

Matrix Computation Section $5.2.3$ 似乎有相关内容.
但邵老师的提示是使用 Problem 7 的结论，得到多个 Householder 变换后复合.

Problem 7 (optional)

Let $w_1, \dots, w_k \in \mathbb{C}^n$ be unit vectors.
Try to find a matrix $T \in \mathbb{C}^{k\times k}$ such that:

$$(I_n - 2w_1w_1^H)\cdots(I_n - 2w_kw_k^H) = I_n - [w_1, \dots, w_k]T[w_1, \dots, w_k]^H$$

Solution:

$$\begin{aligned}
&(I_n - 2w_1w_1^H)\cdots(I_n - 2w_kw_k^H) \\
&= I_n - \sum_{i=1}^k 2w_iw_i^H - \sum_{m=2}^k \sum_{1\le i_1<\cdots<i_m\le k} (2w_{i_1}w_{i_1}^H)\cdots(2w_{i_m}w_{i_m}^H) \\
&= I_n - \sum_{i=1}^k 2w_iw_i^H - \sum_{m=2}^k 2^m \sum_{1\le i_1<\cdots<i_m\le k} [(w_{i_1}^H w_{i_2})\cdots(w_{i_{m-1}}^H w_{i_m})](w_{i_1}w_{i_m}^H) \\
&= I_n - \sum_{i=1}^k 2w_iw_i^H - \sum_{1\le i<j\le k} 2^2 \left\{ w_i^H w_j + \sum_{p=1}^{j-i-1} 2^p \sum_{i<i_2<\cdots<i_{p+1}<j} (w_i^H w_{i_2})(w_{i_2}^H w_{i_3})\cdots(w_{i_p}^H w_{i_{p+1}})(w_{i_{p+1}}^H w_j) \right\}(w_iw_j^H)
\end{aligned}$$

因此 $T = [t_{ij}] \in \mathbb{C}^{k\times k}$ 是一个上三角阵，其元素满足:

$$t_{ij} := \begin{cases} 0 & \text{if } i > j \\ 2 & \text{if } i = j \\ 4w_i^H w_j & \text{if } j = i+1 \\ 4w_i^H w_j + 4\sum_{p=1}^{j-i-1} 2^p \sum_{i<i_2<\cdots<i_{p+1}<j} (w_i^H w_{i_2})(w_{i_2}^H w_{i_3})\cdots(w_{i_p}^H w_{i_{p+1}})(w_{i_{p+1}}^H w_j) & \text{if } j \ge i+2 \end{cases}$$

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

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

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

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

Problem 8 (optional)

(Matrix Computation, Golub & Van Loan, 3rd Edition Section $12.5.1$**)**
Design an efficient algorithm to compute the QR factorization of $QR + uv^T$,
where $Q \in \mathbb{R}^{m\times m}$ is an orthogonal matrix, $R \in \mathbb{R}^{m\times n}$ is an upper triangular matrix and $u \in \mathbb{R}^m, v \in \mathbb{R}^n$ are column vectors.

- uv^T 的精简 QR 分解为 $uv^T = \frac{u}{\|u\|_2} \cdot (\|u\|_2 v^T)$，尽管这没什么用.
- 此算法在 Matlab 有内置函数: (grupdate: QR 分解的秩 1 更新)

Solution:
假设我们已有 $A \in \mathbb{R}^{m\times n}$ 的 QR 分解 $A = QR$
现要求 $A + uv^T$ 的 QR 分解 $A + uv^T = \tilde{Q}\tilde{R}$ (其中 $u \in \mathbb{R}^m, v \in \mathbb{R}^n$ 为给定向量)

记 $w = Q^T u \in \mathbb{R}^{m\times m}$，则我们有:

$$A + uv^T = Q(R + Q^T uv^T) = Q(R + wv^T)$$

我们计算 $m-1$ 个 Givens 变换 $G_{m-1}, \dots, G_1$ (其中 G_k 是作用在第 $k, k+1$ 列的 Givens 变换) 使得:

$$G_1 \cdots G_{m-1} w = \pm \|w\|_2 e_1$$

其中 e_1 是 $\mathbb{R}^m$ 的第 1 个标准单位基向量.
容易看出 $H = G_1 \cdots G_{m-1} R$ 是一个上 Hessenberg 矩阵
为直观地展示这一事实，我们考虑 $\begin{cases} m = 5 \\ n = 4 \end{cases}$ 的例子:

$$w = \begin{bmatrix} * \\ * \\ * \\ * \\ * \end{bmatrix} \quad R = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & & * \\ & & & 0 \end{bmatrix}$$
$$G_4 w = \begin{bmatrix} * \\ * \\ * \\ * \\ 0 \end{bmatrix} \quad G_4 R = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & & * \\ & & & * \end{bmatrix}$$
$$G_3(G_4 w) = \begin{bmatrix} * \\ * \\ * \\ 0 \\ 0 \end{bmatrix} \quad G_3(G_4 R) = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & & * & * \\ & & * & * \\ & & & * \end{bmatrix}$$
$$G_2(G_3 G_4 w) = \begin{bmatrix} * \\ * \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad G_2(G_3 G_4 R) = \begin{bmatrix} * & * & * & * \\ & * & * & * \\ & * & * & * \\ & & * & * \\ & & & * \end{bmatrix}$$
$$G_1(G_2 G_3 G_4 w) = \begin{bmatrix} * \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \quad G_1(G_2 G_3 G_4 R) = \begin{bmatrix} * & * & * & * \\ * & * & * & * \\ & * & * & * \\ & & * & * \\ & & & * \end{bmatrix}$$

现考虑:

$$\begin{aligned} \tilde{H} &= G_1 \cdots G_{m-1}(R + wv^T) \\ &= G_1 \cdots G_{m-1} R + (G_1 \cdots G_{m-1} w) v^T \\ &= H + (\pm \|w\|_2 e_1) v^T \end{aligned}$$

由于 $H \in \mathbb{R}^{m \times n}$ 是上 Hessenberg 矩阵，$\pm \|w\|_2 e_1 v^T$ 是仅第一行有非零元素的 $m \times n$ 矩阵
因此 $\tilde{H} = H \pm \|w\|_2 e_1 v^T$ 也是上 Hessenberg 矩阵.
我们可以构造 $m-1$ 个 Givens 变换 $G_{1,2}, \ldots, G_{m-1,m}$ 将 $\tilde{H}$ 上三角化:

$$G_{m-1,m} \cdots G_{1,2} \tilde{H} = \tilde{R}$$

于是我们有:

$$\begin{aligned} A + uv^T &= Q(R + Q^T uv^T) \quad (\text{note that } w := Q^T u) \\ &= Q(R + wv^T) \\ &= Q(G_1 \cdots G_{m-1})^T \tilde{H} \\ &= QG_{m-1}^T \cdots G_1^T (G_{m-1,m}, \ldots, G_{1,2})^T \tilde{R} \\ &= QG_{m-1}^T \cdots G_1^T G_{1,2}^T \cdots G_{m-1,m}^T \tilde{R} \\ &= \tilde{Q} \tilde{R} \quad (\tilde{Q} := QG_{m-1}^T \cdots G_1^T G_{1,2}^T) \end{aligned}$$

基于上述讨论，我们给出 QR 分解的秩 1 更新算法:

Given $Q \in \mathbb{R}^{m\times m}, R \in \mathbb{R}^{m\times n}, u \in \mathbb{R}^m, v \in \mathbb{R}^n$

---

function: $[Q, R] = \text{QR\_rank\_one\_update}(Q, R, u, v)$

$w = Q^T u$

for $k = m-1 : -1 : 1$

$[c, s] = \text{Givens}(w(k), w(k+1))$

$$w(k:k+1) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} w(k:k+1)$$

$$R(k:k+1, \min(k,n):n) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} R(k:k+1, \min(k,n):n)$$

$$Q(1:m, k:k+1) = Q(1:m, k:k+1)\begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T$$

end

$R = R + wv^T \quad$ (This is a upper Hessenberg matrix)

for $k = 1 : \min(m-1, n)$

$[c, s] = \text{Givens}(R(k,k), R(k+1,k))$

$$R(k:k+1, \min(k,n):n) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} R(k:k+1, \min(k,n):n)$$

$$Q(1:m, k:k+1) = Q(1:m, k:k+1)\begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T$$

end

end

简单起见，假设 $m \approx n$
那么这个算法将 $O(n^3)$ 级别的时间复杂度降为 $O(n^2)$ 级别.
其 Matlab 代码为:

```
function [Q, R] = QR_rank_one_update(Q, R, u, v)
    % Inputs:
    % Q - Orthogonal matrix (m x m)
    % R - Upper triangular matrix (m x n)
    % u - Vector (m x 1)
    % v - Vector (n x 1)
    %
    % Outputs:
    % Q - Updated orthogonal matrix
    % R - Updated upper triangular matrix (Hessenberg form)

    m = size(Q, 1);
    n = size(R, 2);

    % Step 1: Compute w = Q' * u
    w = Q' * u;

    % Step 2: Apply Givens rotations to zero out elements in w
    for k = m-1:-1:1
        % Apply Givens rotation to elements w(k) and w(k+1)
        [c, s] = Givens(w(k), w(k+1));

        % Update w(k:k+1) using Givens rotation
        G = [c s; -s c];  % Givens matrix
        w(k:k+1) = G * w(k:k+1);

        % Update R(k:k+1, min(k,n):n) using Givens rotation
        R(k:k+1, min(k,n):n) = G * R(k:k+1, min(k,n):n);

        % Update Q(1:m, k:k+1) using Givens rotation
        Q(1:m, k:k+1) = Q(1:m, k:k+1) * G';
    end

    % Step 3: Update R with rank-one update
    R = R + w * v';
```

```
    % Step 4: Apply Givens rotations to restore upper triangular form
    for k = 1:min(m-1, n)
        % Apply Givens rotation to elements R(k, k) and R(k+1, k)
        [c, s] = Givens(R(k, k), R(k+1, k));

        % Update R(k:k+1, min(k,n):n) using Givens rotation
        R(k:k+1, min(k,n):n) = [c s; -s c] * R(k:k+1, min(k,n):n);

        % Update Q(1:m, k:k+1) using Givens rotation
        Q(1:m, k:k+1) = Q(1:m, k:k+1) * [c s; -s c]';
    end
end
```

其中计算 Givens 变换的算法为:

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

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
```

函数调用:

```
rng(51);
m = 800;
n = 1000;
A = randn(m, n);
u = randn(m, 1);
v = randn(n, 1);

% 计算 A 的 QR 分解
[Q, R] = qr(A);

% 使用快速算法计算秩一更新后的矩阵 A + u * v' 的 QR 分解
[Q1, R1] = QR_rank_one_update(Q, R, u, v);

% Check if Q * R is close to A
```

```
disp('Frobenius norm:');
disp(norm(Q1 * R1 - (A + u * v'), 'fro'))
```

输出结果:

```
Frobenius norm:
   4.0786e-12
```