数值算法 Homework 06

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姓名: 雍崔扬
学号: 21307140051

Problem 01

Suppose that a tall-skinny matrix $A \in \mathbb{R}^{m\times n}$ is upper bidiagonal (i.e., $a_{ij} \neq 0$ if and only if $i-j \in \{-1,0\}$)
Design an algorithm based on Givens rotations to solve the ridge regression problem
$\min \|Ax-b\|_2^2 + \lambda\|x\|_2^2$
where λ is a given positive number.

- **观察:** 之所以设置 $A \in \mathbb{R}^{m\times n}$，可能是因为我们目前掌握的仅仅是实数域上的 Givens 变换.

Solution:
岭回归问题，即带 l_2 惩罚项的最小二乘问题，本质上是标准的最小二乘问题:

$$\min_x \|Ax-b\|_2^2 + \lambda\|x\|_2^2$$
$$\Leftrightarrow$$
$$\min_x \left\| \begin{bmatrix} A \\ \sqrt{\lambda} I_n \end{bmatrix} x - \begin{bmatrix} b \\ 0_n \end{bmatrix} \right\|_2^2$$
$$\Leftrightarrow$$
$$\min_x \|\tilde{A}x - \tilde{b}\|_2^2$$
$$\text{where } \tilde{A} = \begin{bmatrix} A \\ \sqrt{\lambda} I_n \end{bmatrix} \in \mathbb{R}^{(m+n)\times n} \text{ and } \tilde{b} = \begin{bmatrix} b \\ 0_n \end{bmatrix} \in \mathbb{R}^{m+n}$$

等价问题的法方程为:

$$\begin{bmatrix} A \\ \sqrt{\lambda} I_n \end{bmatrix}^H \begin{bmatrix} A \\ \sqrt{\lambda} I_n \end{bmatrix} x = \begin{bmatrix} A \\ \sqrt{\lambda} I_n \end{bmatrix}^H \begin{bmatrix} b \\ 0_n \end{bmatrix}$$
$$\Leftrightarrow$$
$$(A^H A + \lambda I_n)x = A^H b$$

因此岭回归解 $x_{\text{Ridge}} := (A^H A + \lambda I_n)^{-1} A^H b$

Algorithm 1

考虑到 $\tilde{A}$ 的特殊结构，我们可以很方便地通过 Givens 变换得到其 QR 分解.
为直观地展示这一事实，我们考虑 $\begin{cases} m = 4 \\ n = 3 \end{cases}$ 的例子:

$$\tilde{A} = \begin{bmatrix} A \\ \sqrt{\lambda} I_n \end{bmatrix} = \left[\begin{array}{ccc} * & * & \\ & * & * \\ & & * \\ 0 & 0 & 0 \\ \hline * & & \\ & * & \\ & & * \end{array}\right]$$

$$\Rightarrow G_{1,5}\tilde{A} = \left[\begin{array}{ccc} * & * & \\ & * & * \\ & & * \\ 0 & 0 & 0 \\ \hline 0 & * & \\ & * & \\ & & * \end{array}\right] \Rightarrow G_{2,6}G_{2,5}(G_{1,5}\tilde{A}) = \left[\begin{array}{ccc} * & * & \\ & * & * \\ & & * \\ 0 & 0 & 0 \\ \hline 0 & 0 & * \\ & 0 & * \\ & & * \end{array}\right] \Rightarrow G_{3,7}G_{3,6}G_{3,5}(G_{2,6}G_{2,5}G_{1,5}\tilde{A}) = \left[\begin{array}{ccc} * & * & \\ & * & * \\ & & * \\ 0 & 0 & 0 \\ \hline 0 & 0 & 0 \\ & 0 & 0 \\ & & 0 \end{array}\right]$$

这样我们就得到 $\tilde{A}$ 的 QR 分解为:

$$\tilde{A} = \tilde{Q}\tilde{R} \text{ where } \begin{cases} \tilde{R} = G_{3,7}G_{3,6}G_{3,5}(G_{2,6}G_{2,5}G_{1,5}\tilde{A}) \in \mathbb{R}^{(m+n)\times n} \\ \tilde{Q} = G_{1,5}^T G_{2,5}^T G_{2,6}^T G_{3,5}^T G_{3,6}^T G_{3,7}^T \in \mathbb{R}^{(m+n)\times(m+n)} \end{cases}$$

我们取 $\begin{cases} Q = \tilde{Q}(1:m+n, 1:n) \in \mathbb{R}^{(m+n)\times n} \\ R = \tilde{R}(1:n, 1:n) \in \mathbb{R}^{n\times n} \end{cases}$ 便得到 $\tilde{A}$ 的精简 QR 分解.

使用回代法求解上三角方程组 $Rx = Q^T\tilde{b}$ 即可得到 $\min_x \|\tilde{A}x - \tilde{b}\|_2^2$ 问题的解.

(1) Helper Functions

生成尺寸为 $m \times n$ $(m \geq n)$ 的上双对角矩阵 A 的函数:

```
function A = Upper_Bidiagonal(m, n)
    % Generates an upper bidiagonal matrix of size m x n
    % where m >= n. The main diagonal and the upper diagonal
    % contain random elements, and the remaining elements are zeros.
    %
    % Inputs:
    %   m - number of rows
    %   n - number of columns
    %
    % Output:
    %   A - resulting m x n upper bidiagonal matrix

    % Check if m is greater than or equal to n
    if m < n
        error('m must be greater than or equal to n');
    end

    % Construct the upper bidiagonal matrix
    A = diag(rand(n, 1)) + diag(rand(n-1, 1), 1);

    % Add rows of zeros to make it m x n
    A = [A; zeros(m - n, n)];
end
```

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
```

回代法的 Matlab 代码如下:

```
function x = Backward_Sweep(U, y)
    % 回代法求解 Ux = y
    n = length(y);
    for i = n:-1:2
        y(i) = y(i) / U(i, i);  % 对角线归一化
        y(1:i-1) = y(1:i-1) - y(i) * U(1:i-1, i);  % 消去
    end
    y(1) = y(1) / U(1, 1);  % 处理第一行
    x = y;  % 返回结果
end
```

(2) 核心算法

生成增广矩阵 $\tilde{A} = \begin{bmatrix} A \\ \sqrt{\lambda} I_n \end{bmatrix}$ 并使用 Givens 变换计算其精简 QR 分解的函数 `Augmented_System_Fast_QR`:

$A \in \mathbb{R}^{m\times n}$ is an upper bidiagonal matrix where $m \geq n$, $\lambda \in \mathbb{R}$ is a positive number

function: $[Q, R] = \text{Augmented\_System\_Fast\_QR}(A, \lambda)$

$$\tilde{A} = \begin{bmatrix} A \\ \sqrt{\lambda} I_n \end{bmatrix}$$

$$\tilde{Q} = I_n$$

for $j = 1 : n-1$

for $i = 1 : j$

$$[c, s] = \text{Givens}(\tilde{A}(j, j), \tilde{A}(m+i, j))$$

$$\tilde{A}([j, m+i], j : j+1) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \tilde{A}([j, m+i], j : j+1)$$

$$\tilde{Q}(1 : m+n, [j, m+i]) = \tilde{Q}(1 : m+n, [j, m+i]) \begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T$$

end

end

for $i = 1 : n$ (Handling the case of $j = n$)

$$[c, s] = \text{Givens}(\tilde{A}(n, n), \tilde{A}(m+i, n))$$

$$\tilde{A}([n, m+i], n) = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \tilde{A}([n, m+i], n)$$

$$\tilde{Q}(1 : m+n, [n, m+i]) = \tilde{Q}(1 : m+n, [n, m+i]) \begin{bmatrix} c & s \\ -s & c \end{bmatrix}^T$$

end

$$Q = \tilde{Q}(1 : m+n, 1 : n)$$

$$R = \tilde{A}(1 : n, 1 : n)$$

end

其 Matlab 代码为:

```
function [Q, R] = Augmented_System_Fast_QR(A, lambda)
    % Augmented_System_Fast_QR performs QR decomposition using Givens rotations.
    %
    % Inputs:
    %   A      - An upper bidiagonal matrix of size m x n (m >= n).
    %   lambda - A positive scalar value.
    %
    % Outputs:
    %   Q - Orthogonal matrix of size (m+n) x n resulting from the QR decomposition.
    %   R - Upper triangular matrix of size n x n.

    [m, n] = size(A); % Get dimensions of matrix A

    % Check if m is greater than or equal to n
    if m < n
        error('Matrix A must have m >= n.');
    end

    % Construct the augmented matrix
    % \tilde{A} = [A; sqrt(lambda) * I_n]
    I_n = eye(n); % Identity matrix of size n
    A_tilde = [A; sqrt(lambda) * I_n]; % Augmented matrix

    % Initialize \tilde{Q} as the identity matrix of size (m + n) x (m + n)
    Q_tilde = eye(m + n);

    % Perform Givens rotations for j = 1 to n-1
    for j = 1:n-1
        for i = 1:j
```

```
            % Compute Givens rotation parameters
            [c, s] = Givens(A_tilde(j, j), A_tilde(m + i, j));

            % Apply the Givens rotation to the augmented matrix
            A_tilde([j, m + i], j:j + 1) = [c, s; -s, c] * A_tilde([j, m + i], j:j +
1);

            % Apply the Givens rotation to the orthogonal matrix \tilde{Q}
            Q_tilde(1:m + n, [j, m + i]) = Q_tilde(1:m + n, [j, m + i]) * [c, s; -s,
c]';
        end
    end

    % Handle the case for j = n
    for i = 1:n
        % Compute Givens rotation parameters
        [c, s] = Givens(A_tilde(n, n), A_tilde(m + i, n));

        % Apply the Givens rotation to the augmented matrix
        A_tilde([n, m + i], n) = [c, s; -s, c] * A_tilde([n, m + i], n);

        % Apply the Givens rotation to the orthogonal matrix \tilde{Q}
        Q_tilde(1:m + n, [n, m + i]) = Q_tilde(1:m + n, [n, m + i]) * [c, s; -s, c]';
    end

    % Extract Q from \tilde{Q}
    Q = Q_tilde(1:m + n, 1:n);

    % Extract R from the upper triangular portion of \tilde{A}
    R = A_tilde(1:n, 1:n);
end
```

计算岭回归解的函数 `Solve_Upper_Bidiagonal_Ridge_Regression`:

```
function x = Solve_Upper_Bidiagonal_Ridge_Regression(A, b, lambda)
    % Solve_Upper_Bidiagonal_Ridge_Regression solves the ridge regression problem
    % for an upper bidiagonal matrix A using QR decomposition.
    %
    % Inputs:
    %   A      - An upper bidiagonal matrix of size m x n (m >= n).
    %   b      - A column vector of size m x 1 representing the dependent variable.
    %   lambda - A positive scalar for regularization.
    %
    % Outputs:
    %   x      - The estimated coefficients for the ridge regression.

    [m, n] = size(A); % Get dimensions of matrix A

    % Check if m is greater than or equal to n
    if m < n
        error('Matrix A must have m >= n.'); % Ensure the matrix A has more rows than
columns
    end

    % Augment the response vector b with zeros to match the size of A
    b_tilde = [b; zeros(n, 1)];

    % Perform reduced QR decomposition using the Augmented System approach
    [Q, R] = Augmented_System_Fast_QR(A, lambda);
```

```
    % Solve the upper triangular system using backward substitution
    x = Backward_Sweep(R, Q' * b_tilde); % Calculate the coefficients

end
```

(3) 运行结果

我们将 $x_{\text{Ridge}} = (A^TA + \lambda I_n)^{-1}A^Tb$ 作为精确解,
与 `Solve_Upper_Bidiagonal_Ridge_Regression` 得到的计算解进行对比.
函数调用如下:

```
rng(51);
m = 1000;
n = 500;
lambda = 1;     % Regularization parameter for ridge regression

% Generate an upper bidiagonal matrix A of size m x n
A = Upper_Bidiagonal(m, n);

% Generate random dependent variable vector b of size m x 1
b = rand(m, 1);

% Solve ridge regression using the custom function
x = Solve_Upper_Bidiagonal_Ridge_Regression(A, b, lambda);

% Calculate the exact solution for comparison (using explicit inversion)
x_exact = (A' * A + lambda * eye(n, n)) \ (A' * b);

% Display the norm of the difference between x and x_exact (Frobenius norm)
disp("计算解与精确解之差的 Frobenius 范数:")
disp(norm(x - x_exact, "fro"));
```

运行结果:

```
计算解与精确解之差的 Frobenius 范数:
   2.3420e-14
```

将 `lambda` 的值从 `1` 改到 `0.1`, 再次运行得到:

```
计算解与精确解之差的 Frobenius 范数:
   3.0359e-14
```

这验证了上述算法的正确性.

对比: Algorithm 2

回忆起等价问题的法方程为:

$$(A^TA + \lambda I_n)x = A^Tb$$

注意到 A 作为一个实上双对角矩阵, 能够保证 $A^TA + \lambda I_n$ 是一个对称正定三对角阵.
我们可以利用 Givens 变换方便地得到 $A^TA + \lambda I_n$ 的 QR 分解.

为直观地展示这一事实, 我们考虑 $\begin{cases} m \geq n \\ n = 4 \end{cases}$ 的例子:

$$A^TA+\lambda I_n=\begin{bmatrix} * & * & & \\ * & * & * & \\ & * & * & * \\ & & * & * \end{bmatrix}$$

$$G_{1,2}(A^TA+\lambda I_n)=\begin{bmatrix} * & * & * & \\ 0 & * & * & \\ & * & * & * \\ & & * & * \end{bmatrix}$$

$$G_{2,3}[G_{1,2}(A^TA+\lambda I_n)]=\begin{bmatrix} * & * & * & \\ 0 & * & * & * \\ & 0 & * & * \\ & & * & * \end{bmatrix}$$

$$G_{3,4}[G_{2,3}G_{1,2}(A^TA+\lambda I_n)]=\begin{bmatrix} * & * & * & \\ 0 & * & * & * \\ & 0 & * & * \\ & & 0 & * \end{bmatrix}$$

$$A^TA+\lambda I_n=QR \text{ where } \begin{cases} R=G_{3,4}[G_{2,3}G_{1,2}(A^TA+\lambda I_n)] \\ Q=G_{1,2}^TG_{2,3}^TG_{3,4}^T \end{cases}$$

(1) 核心算法

求解法方程系数矩阵 $A^TA+\lambda I_n$ 的 QR 分解的函数 `Normal_Equation_Fast_QR`:

```
function [Q, R] = Normal_Equation_Fast_QR(A, lambda)
    % Normal_Equation_Fast_QR performs QR decomposition on the normal equation
    % matrix of a linearly constrained least squares problem using Givens rotations.
    %
    % Inputs:
    %   A      - An upper bidiagonal matrix of size m x n, where m >= n.
    %   lambda - A positive scalar regularization parameter for ridge regression.
    %
    % Outputs:
    %   Q - An orthogonal matrix of size n x n resulting from the QR decomposition.
    %   R - An upper triangular matrix of size n x n, representing the R factor
    %       in the QR decomposition of the regularized normal equation matrix.

    % Get the dimensions of matrix A
    [~, n] = size(A);

    % Construct the regularized normal equation matrix for ridge regression
    % R starts as (A' * A + lambda * I), where I is the n x n identity matrix
    R = A' * A + lambda * eye(n);

    % Initialize Q as the identity matrix of size n x n
    Q = eye(n);

    % Apply Givens rotations to create an upper triangular matrix R
    % Iterate over each column up to n-1 to zero out sub-diagonal elements
    for j = 1:n-1
        % Compute the Givens rotation parameters (c, s) to zero out R(j+1, j)
        [c, s] = Givens(R(j, j), R(j+1, j));

        % Apply the Givens rotation to the submatrix R(j:j+1, j:j+1)
        % This operation zeros out the (j+1, j) entry of R
        R(j:j+1, j:j+1) = [c, s; -s, c] * R(j:j+1, j:j+1);

        % Update Q with the transpose of the Givens rotation to maintain orthogonality
```

```
        Q(1:n, j:j+1) = Q(1:n, j:j+1) * [c, s; -s, c]';
    end
end
```

计算岭回归解的函数 `Solve_Upper_Bidiagonal_Ridge_Regression`:

```
function x = Solve_Upper_Bidiagonal_Ridge_Regression(A, b, lambda)
    % Solve_Upper_Bidiagonal_Ridge_Regression solves the ridge regression problem
    % for an upper bidiagonal matrix A using QR decomposition.
    %
    % Inputs:
    %   A      - An upper bidiagonal matrix of size m x n (m >= n).
    %   b      - A column vector of size m x 1 representing the dependent variable.
    %   lambda - A positive scalar for regularization.
    %
    % Outputs:
    %   x      - The estimated coefficients for the ridge regression.

    [m, n] = size(A); % Get dimensions of matrix A

    % Check if m is greater than or equal to n
    if m < n
        error('Matrix A must have m >= n.'); % Ensure the matrix A has more rows than
columns
    end

    % Perform reduced QR decomposition using the Augmented System approach
    [Q, R] = Normal_Equation_Fast_QR(A, lambda);

    % Solve the upper triangular system using backward substitution
    x = Backward_Sweep(R, Q' * (A' * b)); % Calculate the coefficients

end
```

(2) 运行结果

我们将 $x_{\text{Ridge}} = (A^TA + \lambda I_n)^{-1}A^Tb$ 作为精确解,
与 `Solve_Upper_Bidiagonal_Ridge_Regression` 得到的计算解进行对比.
函数调用:

```
rng(51);
m = 1000;
n = 500;
lambda = 1;     % Regularization parameter for ridge regression

% Generate an upper bidiagonal matrix A of size m x n
A = Upper_Bidiagonal(m, n);

% Generate random dependent variable vector b of size m x 1
b = rand(m, 1);

% Solve ridge regression using the custom function
x = Solve_Upper_Bidiagonal_Ridge_Regression(A, b, lambda);

% Calculate the exact solution for comparison (using explicit inversion)
x_exact = (A' * A + lambda * eye(n, n)) \ (A' * b);

% Display the norm of the difference between x and x_exact (Frobenius norm)
disp("计算解与精确解之差的 Frobenius 范数:")
disp(norm(x - x_exact, "fro"));
```

运行结果:

```
计算解与精确解之差的 Frobenius 范数:
    0.1680
```

将 `lambda` 的值从 `1` 改到 `0.1`，再次运行得到:

```
计算解与精确解之差的 Frobenius 范数:
   45.5396
```

这说明算法 2 的数值稳定性较差，即法方程不适合直接进行数值求解.

Problem 02 (第一个算法有误)

Consider the linearly constrained least squares problem $\min\{\|Ax-b\|_2^2 : Cx=d\}$
In the lecture we use the QR factorization of C^H to eliminate the linear constraint $Cx=d$
and reduce the problem to a standard least squares one.
Design an algorithm based on Gaussian elimination to eliminate the linear constraint.

Solution:
考虑线性等式约束的最小二乘问题:

$$\min_{Cx=d} \|Ax-b\|_2^2 \text{ where } \begin{cases} A\in\mathbb{C}^{m\times n} \text{ and } \mathrm{rank}(A)=n\leq m \\ b\in\mathbb{C}^m \\ C\in\mathbb{C}^{p\times n} \text{ and } \mathrm{rank}(C)=p<n \\ d\in\mathbb{C}^p \end{cases}$$

设根据 Gauss 消元法得到 $C\in\mathbb{C}^{p\times n}$ 的 LU 分解为:

$$C=LU \text{ where } \begin{cases} L\in\mathbb{C}^{p\times p} \\ U=[U_1,U_2]\in\mathbb{C}^{p\times n} \\ U_1\in\mathbb{C}^{p\times p} \text{ is a upper triangular matrix} \\ U_2\in\mathbb{C}^{p\times(n-p)} \end{cases}$$

对应地将 A,x 分块为:

$$\begin{cases} A=[A_1,A_2]\in\mathbb{C}^{m\times n} \\ x=\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\in\mathbb{C}^n \end{cases} \text{ where } \begin{cases} A_1\in\mathbb{C}^{m\times p} \\ A_2\in\mathbb{C}^{m\times(n-p)} \\ x_1\in\mathbb{C}^p \\ x_2\in\mathbb{C}^{n-p} \end{cases}$$

则我们有:

$$Cx=LUx=L[U_1,U_2]\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}=L(U_1x_1+U_2x_2)=d$$
$$\Leftrightarrow$$
$$x_1=U_1^{-1}(L^{-1}d-U_2x_2)$$

于是我们有:

$$
\begin{aligned}
\min_{Cx=d} \|Ax-b\|_2^2 &\Leftrightarrow \min_{Cx=d} \left\| [A_1, A_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - b \right\|_2^2 \\
&\Leftrightarrow \min_{Cx=d} \|A_1x_1 + A_2x_2 - b\|_2^2 \\
&\Leftrightarrow \min_{x_2\in\mathbb{R}^{n-p}} \|A_1U_1^{-1}(L^{-1}d - U_2x_2) + A_2x_2 - b\|_2^2 \\
&\Leftrightarrow \min_{x_2\in\mathbb{R}^{n-p}} \|(A_2 - A_1U_1^{-1}U_2)x_2 - (b - A_1U_1^{-1}L^{-1}d)\|_2^2 \\
&\Leftrightarrow \min_{x_2\in\mathbb{R}^{n-p}} \|\tilde{A}x_2 - \tilde{b}\|_2^2 \\
&\text{where } \begin{cases} \tilde{A} = A_2 - A_1U_1^{-1}U_2 \in \mathbb{C}^{m\times(n-p)} \\ \tilde{b} = b - A_1U_1^{-1}L^{-1}d \in \mathbb{C}^m \end{cases}
\end{aligned}
$$

(1) Helper Functions

生成线性等式约束的最小二乘问题的函数:

```
function [A, b, C, d] = Linearly_Constrained_Least_Squares(n, m, p)
    % Linearly_Constrained_Least_Squares creates a constrained least squares problem.
    %
    % Inputs:
    %   n - Number of variables (size of x).
    %   m - Number of observations (size of b).
    %   p - Number of constraints (size of d).
    %
    % Outputs:
    %   A - A full-rank matrix of size m x n.
    %   b - A vector of size m x 1.
    %   C - A rank-deficient matrix of size p x n.
    %   d - A vector of size p x 1.

    % Check input constraints
    if n > m
        error('Condition n <= m is violated: n must be less than or equal to m.');
    end
    if p >= n
        error('Condition p < n is violated: p must be less than n.');
    end

    % Generate a random full-rank matrix A (m x n)
    A = rand(m, n) + 1i * rand(m, n); % Adding complex components
    A = A * rand(n, n); % Ensure full rank by multiplying with a full-rank matrix

    % Check the rank of A
    if rank(A) ~= n
        error('Rank of A must be n.');
    end

    % Generate a random vector b (m x 1)
    b = rand(m, 1) + 1i * rand(m, 1); % Complex vector

    % Generate a random rank-deficient matrix C (p x n)
    % We can ensure C has rank p < n by making the last (n - p) columns zero
    C_temp = rand(p, p) + 1i * rand(p, p); % Create a random full-rank matrix
    C = [C_temp, zeros(p, n - p)]; % Append zero columns to make it p x n

    % Check the rank of C
    if rank(C) ~= p
        error('Rank of C must be p.');
    end
```

```
    % Generate a random vector d (p x 1)
    d = rand(p, 1) + 1i * rand(p, 1); % Complex vector
end
```

长方矩阵的 Gauss 消去法:

$$
\begin{aligned}
&\text{function: } A = \text{Gaussian\_Elimination}(A)\\
&\qquad [m,n] = \text{size}(A)\\
&\qquad \text{for } k = 1 : \min\{m-1, n-1\}\\
&\qquad\qquad A(k+1:m,k) \leftarrow A(k+1:m,k)/A(k,k)\\
&\qquad\qquad A(k+1:m,k+1:n) \leftarrow A(k+1:m,k+1:n) - A(k+1:m,k)A(k,k+1:n)\\
&\qquad \text{end}\\
&\text{end}
\end{aligned}
$$

长方矩阵 Gauss 消去法的 Matlab 代码如下:

```
function A = Gaussian_Elimination(A)
    % Gaussian_Elimination performs Gaussian elimination on matrix A
    %
    % Inputs:
    %   A - An m x n matrix to be transformed into an upper triangular form.
    %
    % Outputs:
    %   A - The matrix after Gaussian elimination, with zeros below the main diagonal.

    % Get dimensions of A
    [m, n] = size(A);

    % Perform Gaussian elimination
    for k = 1:min(m-1, n-1)
        % Scale the column below the diagonal in the k-th column
        A(k+1:m, k) = A(k+1:m, k) / A(k, k);

        % Update the submatrix to eliminate entries in the k-th column
        A(k+1:m, k+1:n) = A(k+1:m, k+1:n) - A(k+1:m, k) * A(k, k+1:n);
    end
end
```

前代法:

```
function y = Forward_Sweep(L, b)
    % 前代法求解 Ly = b
    n = length(b);
    for i = 1:n-1
        b(i) = b(i) / L(i, i);  % 对角线归一化
        b(i+1:n) = b(i+1:n) - b(i) * L(i+1:n, i);  % 消去
    end
    b(n) = b(n) / L(n, n);  % 处理最后一行
    y = b;  % 返回结果
end
```

回代法:

```matlab
function X = Backward_Sweep(U, Y)
    % 回代法求解 UX = Y
    [n, ~] = size(Y);
    for i = n:-1:2
        Y(i,:) = Y(i,:) / U(i, i);  % 对角线归一化
        Y(1:i-1,:) = Y(1:i-1,:) - U(1:i-1, i) * Y(i,:);  % 消去
    end
    Y(1,:) = Y(1,:) / U(1, 1);  % 处理第一行
    X = Y;  % 返回结果
end
```

以下是基于复数域上的 Householder QR 分解的求解最小二乘问题的函数:
复数域上的 Householder 变换的计算算法已在 Homework 4 Problem 2 中给出:

```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
```

复数域上的 Householder QR 算法已在 Homework 4 Problem 3 中给出:

```
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
```

计算得到 $A \in \mathbb{C}^{m\times n}$ 的 QR 分解 $A = QR$ 之后 (其中 $Q \in \mathbb{C}^{m\times m}$ 为酉矩阵，$R \in \mathbb{C}^{m\times n}$ 的上 $n\times n$ 分块 R_1 为上三角阵)

求解法方程 $A^HAx = R^HRx = A^Hb$ 就等价于求解 $\begin{cases} R^Hy = A^Hb \\ Rx = y \end{cases}$ (分别由前代法和回代法求解)

或者也可考虑精简 QR 分解 $A = Q_1R_1$ (其中 $Q_1 \in \mathbb{C}^{m\times n}$ 由 Q 的前 n 列构成)

则求解法方程 $A^HAx = R_1^HR_1x = R_1^HQ_1^Hb = A^Hb$ 就等价于求解 $R_1x = Q_1^Hb$ (由回代法求解)

```
function x = Householder_Solution(A, b)
    [m, n] = size(A);

    % Step 1: Compute the QR decomposition of A using Householder reflections
    [Q, R] = Complex_Householder_QR(A);

    % Step 2: Solve the system Rx = Q' * b using backward substitution
    x = Backward_Sweep(R(1:n, 1:n), Q(1:m, 1:n)' * b);
end
```

(2) 核心算法

基于 Gauss 消去法的解法:

- ① 计算 $C \in \mathbb{C}^{p\times n}$ $(p < n)$ 的 LU 分解

  $$C = LU \text{ where } \begin{cases} L \in \mathbb{C}^{p\times p} \\ U = [U_1, U_2] \in \mathbb{C}^{p\times n} \\ U_1 \in \mathbb{C}^{p\times p} \text{ is a upper triangular matrix} \\ U_2 \in \mathbb{C}^{p\times(n-p)} \end{cases}$$
- ② 计算 $\begin{cases} \tilde{A} = A_2 - A_1U_1^{-1}U_2 \in \mathbb{C}^{m\times(n-p)} \\ \tilde{b} = b - A_1U_1^{-1}L^{-1}d \in \mathbb{C}^m \end{cases}$
- ③ 计算 $x_2 = \text{Householder\_Solution}(\tilde{A}, \tilde{b})$

  (这里通过调用 Homework 5 Problem 6 的 `Householder_Solution` 函数得到消元后的最小二乘问题的解)
- ④ 计算 $x_1 = U_1^{-1}(L^{-1}d - U_2x_2)$，得到 $x_{\text{Gauss}} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

```
function [x_Gauss, b_tilde, A_tilde] = Gaussian_Method(A, b, C, d)
    % Gaussian_Method eliminates constrained variables in a linearly constrained
    % least squares problem using Gaussian elimination.
    %
    % Inputs:
```

```
    %   A - The original matrix of size m x n, representing the coefficients of the
least squares problem.
    %   b - The original vector of size m x 1, representing the observed values.
    %   C - The constraint matrix of size p x n, representing the constraints on the
variables.
    %   d - The constraint vector of size p x 1, representing the values of the
constraints.
    %
    % Outputs:
    %   x_Gauss - The solution vector after eliminating variables.
    %   b_tilde - The modified vector after eliminating constrained variables.
    %   A_tilde - The modified matrix after eliminating constrained variables.

    % Get dimensions of A and C
    [m, n] = size(A); % m: number of observations, n: number of variables
    [p, ~] = size(C); % p: number of constraints

    % Step 1: Perform Gaussian elimination on C
    C = Gaussian_Elimination(C); % Transform C into an upper triangular matrix

    % Step 2: Extract L and U from the Gaussian elimination of C
    L = eye(p) + tril(C(1:p, 1:p), -1); % Construct the lower triangular matrix L with
elimination factors
    U = triu(C(1:p, 1:n));              % Extract the upper triangular matrix U

    % Step 3: Compute the modified vector b_tilde based on the elimination
    % d_tilde = U(1:p, 1:p) \ (L \ d);
    d_tilde = Forward_Sweep(L, d);
    d_tilde = Backward_Sweep(U(1:p, 1:p), d_tilde);
    b_tilde = b - A(1:m, 1:p) * d_tilde; % Adjust b by removing the effect of the
constraints

    % Step 4: Compute the modified matrix A_tilde to reflect the elimination
    % U_tilde = U(1:p, 1:p) \ U(1:p, p+1:n);
    U_tilde = Backward_Sweep(U(1:p, 1:p), U(1:p, p+1:n));
    A_tilde = A(1:m, p+1:n) - A(1:m, 1:p) * U_tilde; % Adjust A to eliminate variables
according to constraints

    % Step 5: Solve for x2 using the modified A_tilde and b_tilde
    x2 = Householder_Solution(A_tilde, b_tilde); % Solve the least squares problem for
the remaining variables

    % Step 6: Compute x1 from d_tilde and U_tilde
    x1 = d_tilde - U_tilde * x2; % Calculate x1 based on the relationship with x2

    % Combine x1 and x2 into the final solution vector
    x_Gauss = [x1; x2]; % Concatenate x1 and x2 to form the complete solution vector
end
```

(3) 对比: Lagrange 乘子法

考虑线性等式约束的最小二乘问题:

$$\min_{Cx=d} \|Ax-b\|_2^2 \text{ where } \begin{cases} A \in \mathbb{C}^{m\times n} \text{ and } \operatorname{rank}(A) = n \le m \\ b \in \mathbb{C}^m \\ C \in \mathbb{C}^{p\times n} \text{ and } \operatorname{rank}(C) = p < n \\ d \in \mathbb{C}^p \end{cases}$$

注意到目标函数 $f(x) = \|Ax-b\|_2^2$ 是关于 x 的凸函数，而问题只有线性等式约束 $Cx = d$
因此这是一个标准形式的凸优化问题，其最优解即为 KKT 点.

定义其 Lagrange 函数 $L(x, \lambda)$ 为:

$$
\begin{aligned}
L(x, \lambda) &= f(x) - \lambda^H (Cx - d) \\
&= \|Ax - b\|_2^2 - \lambda^H (Cx - d) \\
\hline
\mathrm{dom}\{L\} &= \mathbb{C}^n \times \mathbb{C}^p
\end{aligned}
$$

Lagrange 函数 $L(x, \lambda)$ 关于 x 的梯度为:

$$
\begin{aligned}
\nabla_x L(x, \lambda) &= \nabla_x \{\|Ax - b\|_2^2 - \lambda^H (C\beta - h)\} \\
&= -A^H \cdot 2(b - Ax) - (\lambda^H C)^H \\
&= -2A^H b + 2A^H Ax - C^H \lambda
\end{aligned}
$$

KKT 条件为:

$$
\begin{cases}
\nabla_x L(x, \lambda) = -2A^H b + 2A^H Ax - C^H \lambda = 0_n & \text{①} \\
Cx = d & \text{②}
\end{cases}
$$

① 式左乘 $(A^H A)^{-1}$ 可得 $-2(A^H A)^{-1} A^H b + 2x - (A^H A)^{-1} C^H \lambda = 0_n$
于是有 $x = (A^H A)^{-1} A^H b + \frac{1}{2}(A^H A)^{-1} C^H \lambda$
代入 ② 式即得 $Cx = C(A^H A)^{-1} A^H b + \frac{1}{2} C(A^H A)^{-1} C^H \lambda = d$
解得 $\lambda_{\mathrm{KKT}} = 2[C(A^H A)^{-1} C^H]^{-1}[d - C(A^H A)^{-1} A^H b]$
因此我们有:

$$
\begin{aligned}
x_{\mathrm{Lagrange}} &= x_{\mathrm{KKT}} \\
&= (A^H A)^{-1} A^H b + \frac{1}{2}(A^H A)^{-1} C^H \lambda_{\mathrm{KKT}} \\
&= (A^H A)^{-1} A^H b + \frac{1}{2}(A^H A)^{-1} C^H \cdot 2[C(A^H A)^{-1} C^H]^{-1}[d - C(A^H A)^{-1} A^H b] \\
&= x_{\mathrm{ls}} - (A^H A)^{-1} C^H [C(A^H A)^{-1} C^H]^{-1}(Cx_{\mathrm{ls}} - d)
\end{aligned}
$$

其中 $x_{\mathrm{ls}} := (A^H A)^{-1} A^H b$
我们将 x_{Lagrange} 视为问题的精确解，与计算解 x_{Gauss} 进行比较.

以下是基于 Lagrange 乘子法的解法:
(简单起见，我们直接使用 Matlab 内置的 `\` 运算来求逆)

```
% Function to solve the constrained least squares problem using the Lagrangian method
function x_Lagrange = Lagrangian_Method(A, b, C, d)
    % Calculate the least squares solution without constraints
    x_ls = (A' * A) \ (A' * b); % Normal equation solution for least squares

    % Intermediate calculation to prepare for the constrained adjustment
    tmp = C * ((A' * A) \ C'); % Project the constraints into the least squares space

    % Adjust the least squares solution for the constraints
    x_Lagrange = x_ls - (A' * A) \ (C' * (tmp \ (C * x_ls - d)));
    % Apply the Lagrangian adjustment based on the constraints
end
```

(4) 运行结果

我们通过对比基于 Gauss 消去法的解 x_{Gauss} 和基于 Lagrange 乘子法的解 x_{Lagrange} (视为精确解) 来检验我们结果的正确性.
函数调用:

```
rng(51);
m = 500; % Number of observations
n = 50;  % Number of variables
p = 10;  % Number of constraints
```

```
% Generate the linearly constrained least squares problem
[A, b, C, d] = Linearly_Constrained_Least_Squares(n, m, p);

% Apply Gaussian elimination method to eliminate constraints
[x_Gauss, b_tilde, A_tilde] = Gaussian_Method(A, b, C, d);

% Apply Lagrangian method to solve the same constrained problem
x_Lagrange = Lagrangian_Method(A, b, C, d);

% Display the Frobenius norm of the difference between the two solutions
disp("Gauss 消去法得到的解和精确解 (Lagrange 乘子法得到的解) 之差的 Frobenius 范数:");
disp(norm(x_Gauss - x_Lagrange, "fro"));
```

运行结果:

```
Gauss 消去法得到的解和精确解 (Lagrange 乘子法得到的解) 之差的 Frobenius 范数:
   2.5071e-10
```

这验证了上述算法的正确性.

Problem 03

The least squares problem $\min \|Ax-b\|_2^2$ is equivalent to an augmented linear system:

$$\begin{bmatrix} I_{m\times m} & A \\ A^H & 0_{n\times n} \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0_n \end{bmatrix}$$

which is Hermitian and indefinite.
Similar augmented linear systems exist for the linearly constrained least squares problem
$\min\{\|Ax-b\|_2^2 : Cx = d\}$
Can you figure it out?

- **TA:** 第三题增广系统可以进一步改写到不含有 A^HA: (也是由 **KKT 条件**导出的)

$$\begin{cases} \nabla_x L(x,\lambda) = -2A^Hb + 2A^HAx + C^H\lambda = 0_n \\ Cx = d \end{cases}$$

$$\Rightarrow$$

$$\begin{cases} r + Ax = b \\ A^Hr + C^H\lambda = 0_n \\ Cx = d \end{cases}$$

$$\Rightarrow$$

$$\begin{bmatrix} I_{m\times m} & A & \\ A^H & 0_{n\times n} & C^H \\ & C & 0_{p\times p} \end{bmatrix} \begin{bmatrix} r \\ x \\ \lambda \end{bmatrix} = \begin{bmatrix} b \\ 0_n \\ d \end{bmatrix}$$

Solution:
考虑线性等式约束的最小二乘问题:

$$\min_{Cx=d} \|Ax-b\|_2^2 \text{ where } \begin{cases} A \in \mathbb{C}^{m\times n} \text{ and } \operatorname{rank}(A) = n \le m \\ b \in \mathbb{C}^m \\ C \in \mathbb{C}^{p\times n} \text{ and } \operatorname{rank}(C) = p < n \\ d \in \mathbb{C}^p \end{cases}$$

注意到目标函数 $f(x) = \|Ax-b\|_2^2$ 是关于 x 的凸函数，而问题只有线性等式约束 $Cx = d$
因此这是一个标准形式的凸优化问题，其最优解即为 KKT 点.

定义其 Lagrange 函数 $L(x,\lambda)$ 为:

$$
\begin{aligned}
L(x,\lambda) &= f(x) + \lambda^H(Cx-d) \\
&= \|Ax-b\|_2^2 + \lambda^H(Cx-d) \\
\hline
\mathrm{dom}\{L\} &= \mathbb{C}^n \times \mathbb{C}^p
\end{aligned}
$$

Lagrange 函数 $L(x,\lambda)$ 关于 x 的梯度为:

$$
\begin{aligned}
\nabla_x L(x,\lambda) &= \nabla_x\{\|Ax-b\|_2^2 + \lambda^H(C\beta - h)\} \\
&= -A^H \cdot 2(b-Ax) + (\lambda^H C)^H \\
&= -2A^Hb + 2A^HAx + C^H\lambda
\end{aligned}
$$

KKT 条件为:

$$
\begin{cases}
\nabla_x L(x,\lambda) = -2A^Hb + 2A^HAx + C^H\lambda = 0_n & ① \\
Cx = d & ②
\end{cases}
$$

我们便可得到**增广线性系统**:

$$
\begin{bmatrix} 2A^HA & C^H \\ C & 0_{p\times p} \end{bmatrix}
\begin{bmatrix} x \\ \lambda \end{bmatrix}
=
\begin{bmatrix} 2A^Hb \\ d \end{bmatrix}
$$

更进一步，我们可以求解上述方程组:
① 式左乘 $(A^HA)^{-1}$ 可得 $-2(A^HA)^{-1}A^Hb + 2x + (A^HA)^{-1}C^H\lambda = 0_n$
于是有 $x = (A^HA)^{-1}A^Hb - \frac{1}{2}(A^HA)^{-1}C^H\lambda$
代入 ② 式即得 $Cx = C(A^HA)^{-1}A^Hb - \frac{1}{2}C(A^HA)^{-1}C^H\lambda = d$
解得 $\lambda_{\mathrm{KKT}} = 2[C(A^HA)^{-1}C^H]^{-1}[C(A^HA)^{-1}A^Hb - d]$
因此我们有:

$$
\begin{aligned}
x_{\mathrm{Lagrange}} &= x_{\mathrm{KKT}} \\
&= (A^HA)^{-1}A^Hb - \frac{1}{2}(A^HA)^{-1}C^H\lambda_{\mathrm{KKT}} \\
&= (A^HA)^{-1}A^Hb - \frac{1}{2}(A^HA)^{-1}C^H \cdot 2[C(A^HA)^{-1}C^H]^{-1}[C(A^HA)^{-1}A^Hb - d] \\
&= x_{\mathrm{ls}} - (A^HA)^{-1}C^H[C(A^HA)^{-1}C^H]^{-1}(Cx_{\mathrm{ls}} - d)
\end{aligned}
$$

其中 $x_{\mathrm{ls}} := (A^HA)^{-1}A^Hb$

即上述增广线性系统的解为:

$$
\begin{bmatrix} x_{\mathrm{KKT}} \\ \lambda_{\mathrm{KKT}} \end{bmatrix}
=
\begin{bmatrix} x_{\mathrm{ls}} - (A^HA)^{-1}C^H[C(A^HA)^{-1}C^H]^{-1}(Cx_{\mathrm{ls}} - d) \\ 2[C(A^HA)^{-1}C^H]^{-1}[C(A^HA)^{-1}A^Hb - d] \end{bmatrix}
$$

Problem 04

Implement the Arnoldi process based on CGS/CGS2/MGS/MGS2 and visualize the loss of orthogonality.
You can randomly generate a 1000×1000 matrix and generate a 30-dimensional Krylov subspace.
(Optional) Design an algorithm to perform the Arnoldi process based on Householder orthogonalization.
Hint: use the left-looking variant.

Algorithm 1

记 $Q := [q_1,\dots,q_r]$ (其中 $1 \le r \le \mathrm{rank}(Y)$)
根据 $AQ = QH$ (其中 $H \in \mathbb{C}^{r\times r}$ 为 Hessenberg 阵)，因而有 $Aq_j = \sum_{i=1}^{j+1} h_{i,j}q_i$
由于 Q 列标准正交，故我们有 $q_k^HAq_j = \sum_{i=1}^{j+1} h_{i,j}q_k^Hq_i = 0 + h_{k,j}\cdot 1 = h_{k,j}\ (1 \le k \le j)$
最后有 $h_{j+1,j}q_{j+1} = Aq_j - \sum_{i=1}^{j} h_{i,j}q_i$
得到 $AQ = QH + \mathrm{rank\text{-}one}$
其中 $\mathrm{rank\text{-}one}$ 代表遗留的秩一矩阵，仅在最后一列有非零元素.
它的存在是因为 Aq_r 不一定能完全表示为 $q_1,\dots,q_r$ 的线性组合.

$$A[q_1,q_2,\dots,q_r]=[Aq_1,Aq_2,\dots,Aq_r]=[q_1,q_2,\dots,q_r]\begin{bmatrix} h_{11} & h_{21} & \cdots & h_{1r} \\ h_{21} & h_{22} & \cdots & h_{2r} \\ & \ddots & \ddots & \vdots \\ & & h_{r,r-1} & h_{r,r} \end{bmatrix}+\text{rank-one}$$

基于 Gram-Schmidt 正交化的 Arnoldi 过程:

$$\begin{array}{l}
\text{Given square matrix } A\in\mathbb{C}^{n\times n}\text{, vector } b\in\mathbb{C}^n \text{ and integer } 1\le r\le n \\
\hline
\text{function: } [Q,H]=\text{Gram_Schmidt_Arnoldi}(A,b,\text{tolerance},\text{modified},\text{reorthogonalized}) \\
\qquad n=\dim(A) \\
\qquad Q=\text{zeros}(n,n) \\
\qquad Q(1:n,1)=\dfrac{b}{\|b\|_2} \\
\qquad H=\text{zeros}(n,n) \\
\qquad \delta=\text{zeros}(n,1) \\
\hline
\qquad \text{if reorthogonalized} == \text{TRUE} \\
\qquad\qquad \text{max_iter}=2 \\
\qquad \text{else} \\
\qquad\qquad \text{max_iter}=1 \\
\qquad \text{end} \\
\hline
\qquad \text{for } k=1:r-1 \\
\qquad\qquad Q(1:n,k+1)=AQ(1:n,k) \\
\qquad\qquad \text{if modified} == \text{TRUE (MGS: Modified Gram-schmidt)} \\
\qquad\qquad\qquad \text{for iter} = \text{1:max_iter} \\
\qquad\qquad\qquad\qquad \text{for } i=1:k \\
\qquad\qquad\qquad\qquad\qquad \delta(i)=Q(1:n,i)^H Q(1:n,k+1) \\
\qquad\qquad\qquad\qquad\qquad H(i,k)=H(i,k)+\delta(i) \\
\qquad\qquad\qquad\qquad\qquad Q(1:n,k+1)=Q(1:n,k+1)-\delta(i)Q(1:n,i) \\
\qquad\qquad\qquad\qquad \text{end} \\
\qquad\qquad\qquad \text{end} \\
\qquad\qquad \text{else (CGS: Classic Gram-Schmidt)} \\
\qquad\qquad\qquad \text{for iter} = \text{1:max_iter} \\
\qquad\qquad\qquad\qquad \delta(1:k)=Q(1:n,1:k)^H Q(1:n,k+1) \\
\qquad\qquad\qquad\qquad H(1:k,k)=H(1:k,k)+\delta(1:k) \\
\qquad\qquad\qquad\qquad Q(1:n,k+1)=Q(1:n,k+1)-Q(1:n,1:k)\delta(1:k) \\
\qquad\qquad\qquad \text{end} \\
\qquad\qquad \text{end} \\
\qquad\qquad H(k+1,k)=\|Q(1:n,k+1)\|_2 \\
\qquad\qquad \text{if } H(k+1,k)<\text{tolerance} \quad \text{(indicates linear dependence)} \\
\qquad\qquad\qquad r=k \\
\qquad\qquad\qquad \text{break} \\
\qquad\qquad \text{else} \\
\qquad\qquad\qquad Q(1:n,k+1)=\dfrac{1}{H(k+1,k)}Q(1:n,k+1) \\
\qquad\qquad \text{end} \\
\qquad \text{end} \\
\hline
\qquad H(1:r,r)=Q(1:n,1:r)^H(AQ(1:n,r)) \quad \text{(fill the last column)} \\
\hline
\qquad Q=Q(1:n,1:r) \\
\qquad H=H(1:r,1:r) \\
\text{end}
\end{array}$$

其 Matlab 代码为:

```
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(n, n); % 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

% If the rank is full, 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
```

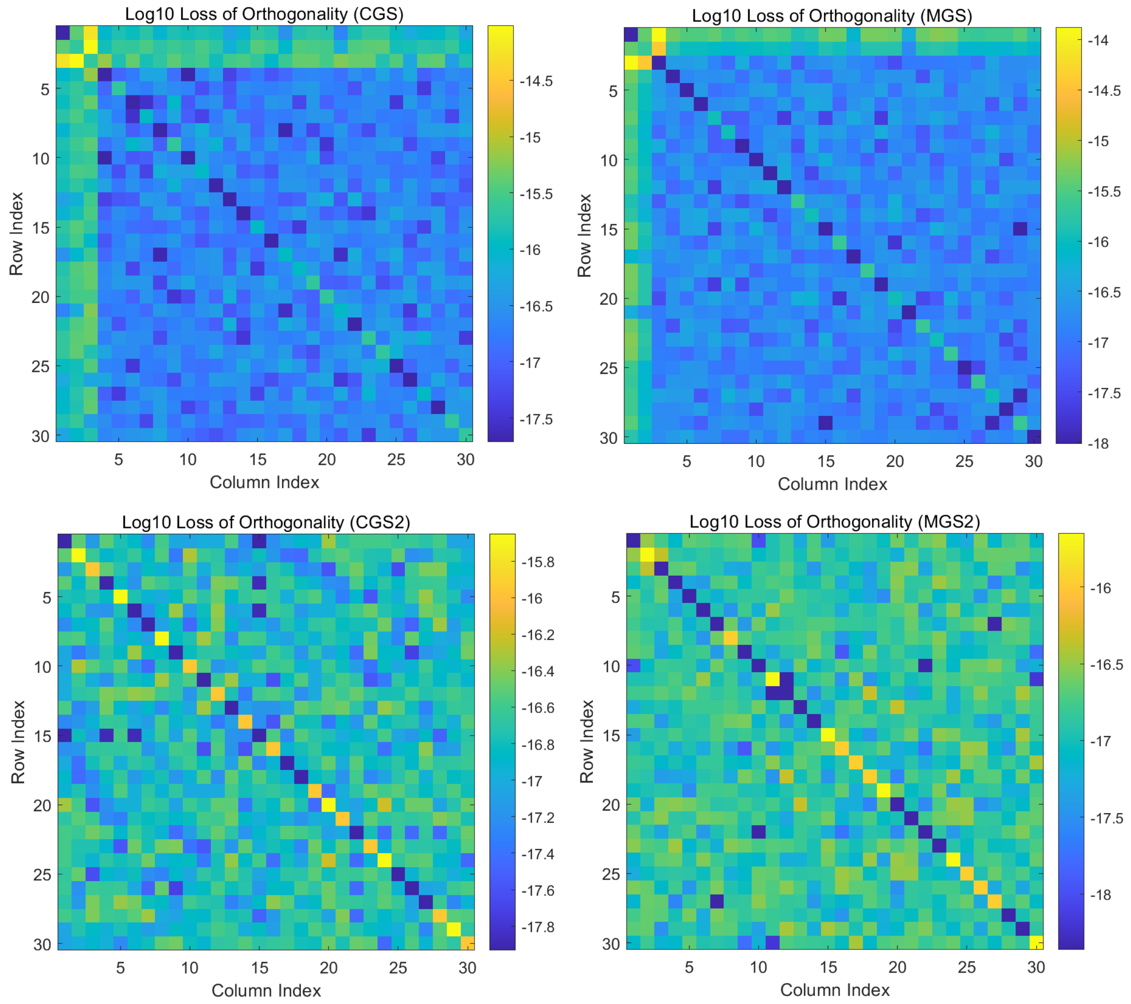
可视化正交性损失的函数 `visualize_orthogonality_loss`:

```
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 = 1000; % Size of the square matrix
r = 30;   % Dimension of the Krylov subspace

% Generate a random complex matrix A and vector b
A = rand(n, n) + 1i * rand(n, n);
b = rand(n, 1) + 1i * rand(n, 1);
```

```matlab
% Apply the Arnoldi process with different methods
[Q_CGS, H_CGS] = Gram_Schmidt_Arnoldi(A, b, r, 1e-10, false, false);
visualize_orthogonality_loss(Q_CGS, 'Log10 Loss of Orthogonality (CGS)');
disp("CGS:")
leftover_CGS = A * Q_CGS(:, end) - Q_CGS(:, 1:end) * H_CGS(1:end, end);
residual_CGS = A * Q_CGS - Q_CGS * H_CGS;
residual_CGS(:, end) = residual_CGS(:, end) - leftover_CGS;
disp(norm(residual_CGS, "fro") / norm(A, "fro"));

[Q_CGS2, H_CGS2] = Gram_Schmidt_Arnoldi(A, b, r, 1e-10, false, true);
visualize_orthogonality_loss(Q_CGS2, 'Log10 Loss of Orthogonality (CGS2)');
disp("CGS2:")
leftover_CGS2 = A * Q_CGS2(:, end) - Q_CGS2(:, 1:end) * H_CGS2(1:end, end);
residual_CGS2 = A * Q_CGS2 - Q_CGS2 * H_CGS2;
residual_CGS2(:, end) = residual_CGS2(:, end) - leftover_CGS2;
disp(norm(residual_CGS2, "fro") / norm(A, "fro"));

[Q_MGS, H_MGS] = Gram_Schmidt_Arnoldi(A, b, r, 1e-10, true, false);
visualize_orthogonality_loss(Q_MGS, 'Log10 Loss of Orthogonality (MGS)');
disp("MGS:")
leftover_MGS = A * Q_MGS(:, end) - Q_MGS(:, 1:end) * H_MGS(1:end, end);
residual_MGS = A * Q_MGS - Q_MGS * H_MGS;
residual_MGS(:, end) = residual_MGS(:, end) - leftover_MGS;
disp(norm(residual_MGS, "fro") / norm(A, "fro"));

[Q_MGS2, H_MGS2] = Gram_Schmidt_Arnoldi(A, b, r, 1e-10, true, true);
visualize_orthogonality_loss(Q_MGS2, 'Log10 Loss of Orthogonality (MGS2)');
disp("MGS2:")
leftover_MGS2 = A * Q_MGS2(:, end) - Q_MGS2(:, 1:end) * H_MGS2(1:end, end);
residual_MGS2 = A * Q_MGS2 - Q_MGS2 * H_MGS2;
residual_MGS2(:, end) = residual_MGS2(:, end) - leftover_MGS2;
disp(norm(residual_MGS2, "fro") / norm(A, "fro"));
```



Algorithm 2

记 $Q := [q_1, \dots, q_r]$ (其中 $1 \le r \le \operatorname{rank}(Y)$)
Arnoldi 过程的基本框架是 $AQ = QH + \text{rank-one}$
其中 $H \in \mathbb{C}^{r\times r}$ 为 Hessenberg 阵，而 rank-one 代表遗留的秩一矩阵，仅在最后一列有非零元素.
它的存在是因为 Aq_r 不一定能完全表示为 $q_1, \dots, q_r$ 的线性组合.

我们可以通过扩充一列，将 H 扩充为上三角阵，使用 Householder QR 去做:

$$A[q_1, q_2, \dots, q_r] = [Aq_1, Aq_2, \dots, Aq_r] = [q_1, q_2, \dots, q_r] \begin{bmatrix} h_{11} & h_{21} & \cdots & h_{1r} \\ h_{21} & h_{22} & \cdots & h_{2r} \\ & \ddots & \ddots & \vdots \\ & & h_{r,r-1} & h_{r,r} \end{bmatrix} + \text{rank-one}$$

$$[q_1, Aq_1, Aq_2, \dots, Aq_r] = [q_1, q_2 \dots, q_r] \begin{bmatrix} 1 & h_{11} & h_{21} & \cdots & h_{1r} \\ & h_{21} & h_{22} & \cdots & h_{2r} \\ & & \ddots & \ddots & \vdots \\ & & & h_{r,r-1} & h_{r,r} \end{bmatrix} + \text{rank-one}$$

值得注意的是，我们并不是直接生成 $[q_1, Aq_1, Aq_2, \dots, Aq_r]$ 然后应用 Householder QR
而是使用 **left-looking** 的变体，即存储每步的 Householder 变换
(具体来说可使用 **Matrix Computation 算法** $5.1.2$,
但注意其 Householder 变换的计算顺序与实际作用在新加入的向量的顺序相反)
当添加新的向量时，对其应用之前的 Householder 变换，再计算该步需要进行的 Householder 变换.

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

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

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

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

复数域上使用 Householder 变换计算 Arnoldi 过程的函数:
(注意其中应用 $(I - WY^H)^H = I - YW^H$ 左乘新加入的向量，而不是用 $I - WY$ 左乘新加入的向量，这个 bug 找了很久)

```
function [Q, H] = Complex_Householder_Arnoldi(A, b, r, tolerance)
    % This function performs the Complex Householder Arnoldi process.
    % Input:
    %   A         : The input matrix (n x n)
    %   b         : The input vector (n x 1)
    %   r         : The number of desired orthonormal vectors
    %   tolerance : Tolerance for stopping criterion
    % Output:
    %   Q         : Orthonormal basis of the Krylov subspace (n x r)
    %   H         : Upper Hessenberg matrix (r x (r+1))

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

    % Initialize matrices
    Y = zeros(n, r); % Matrix to store Householder vectors
    W = zeros(n, r); % Matrix to store Householder weights
    H = zeros(n, r + 1); % Matrix to store the upper Hessenberg matrix
    Q = zeros(n, r);     % Matrix to store the orthonormal basis vectors

    % Main loop to construct the Arnoldi process
    for k = 1:r
        if k == 1
            % First iteration: Apply Householder transformation to b
            [v, beta] = Complex_Householder(b); % Get the Householder vector and scalar
beta
            Y(:, 1) = v;                        % Store the Householder vector in Y
            W(:, 1) = -beta * v;                % Store the modified vector W
            v = zeros(n, 1);                    % Reset v for future use

            H(1, 1) = norm(b, 2) * b(1) / abs(b(1)); % Store the norm of b in H(1,1)
            Q(:, 1) = W(:, 1) * Y(1, 1)';       % Compute the first orthonormal vector
for Q
            Q(1, 1) = Q(1, 1) + 1;              % Adjust the first element of Q to
maintain orthonormality

        else
            % Subsequent iterations
            z = A * Q(:, k-1);                % Matrix-vector product for the next
Krylov subspace vector
```

```
            z = z + Y(:, 1:k-1) * (W(:, 1:k-1)' * z); % Adjust z with contributions
from W and Y

            % Store the computed values in H
            H(1:k-1, k) = z(1:k-1);           % Fill the upper part of the current
column in H
            H(k, k) = norm(z(k:n), 2) * z(k) / abs(z(k)); % Compute the norm of the
remainder of z and store in H

            % Check for convergence based on the tolerance
            if abs(H(k, k)) < tolerance
                r = k - 1;                     % Adjust the rank if the value is below
tolerance
                break                          % Exit the loop if convergence is
achieved
            end

            % Apply Householder transformation to the part of z
            [v(k:n), beta] = Complex_Householder(z(k:n)); % Generate the Householder
vector and beta for z(k:n)
            Y(:, k) = v;                          % Store the Householder vector in Y
            W(:, k) = -beta * (v + W(:, 1:k-1) * (Y(:, 1:k-1)' * v)); % Update W based
on the new Householder vector
            v = zeros(n, 1);                      % Reset v after use
            Q(:, k) = W(:, 1:k) * Y(k, 1:k)';     % Compute the k-th orthonormal vector
for Q
            Q(k, k) = Q(k, k) + 1;                % Adjust the diagonal of Q to
maintain orthonormality
        end
    end

    % If the rank r is full, compute the last column of H
    z = A * Q(:, r);                 % Matrix-vector product for the last vector in Q
    z = z + W(:, 1:r) * (Y(:, 1:r)' * z); % Adjust z with contributions from W and Y
    H(1:r, r+1) = Q(:, 1:r)' * z;    % Store the last column in H by projecting z onto Q

    % Trim H and Q to their final sizes based on the computed rank
    H = H(1:r, 2:r + 1);             % Keep only the relevant portion of H
    Q = Q(:, 1:r);                   % Keep only the relevant portion of Q
end
```

复数域上的 Householder 变换的计算算法已在 Homework 4 Problem 2 中给出:

```
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
```

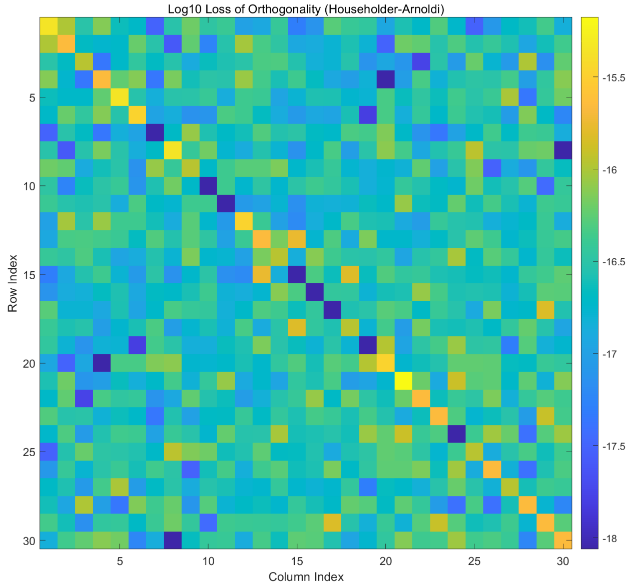
```
    if sigma < 1e-10
        beta = 0; % If sigma is close to zero, set beta to zero (no transformation
needed)
    else
        % Determine gamma to account for the argument of complex number x(1)
        if abs(x(1)) < 1e-10
            gamma = 1; % If x(1) is close to zero, set gamma to 1
        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
```

函数调用:

```
rng(51);
n = 1000; % Size of the square matrix
r = 30;   % Dimension of the Krylov subspace
tolerance = 1e-10;

% Generate a random complex matrix A (n x n) and vector b (n x 1)
A = rand(n, n) + 1i * rand(n, n); % Create a random complex matrix with real and
imaginary parts
b = rand(n, 1) + 1i * rand(n, 1); % Create a random complex vector with real and
imaginary parts

% Call the Complex Householder Arnoldi process to compute Q and H
[Q, H] = Complex_Householder_Arnoldi(A, b, r, tolerance);

% Visualize the loss of orthogonality in the Q matrix
visualize_orthogonality_loss(Q, 'Log10 Loss of Orthogonality (Householder-Arnoldi)');

% Compute the "leftover" term for the last column of the residual
leftover = A * Q(:, end) - Q(:, 1:end) * H(1:end, end);

% Calculate the residual matrix between AQ and QH, ensuring the last column accounts
for the leftover term
residual = A * Q - Q * H;
residual(:, end) = residual(:, end) - leftover; % Adjust the last column with the
leftover term

% Display the Frobenius norm of the residual matrix, normalized by the Frobenius norm
of A
disp("Householder (left-looking):")
disp(norm(residual, "fro") / norm(A, "fro"));
```

运行结果:

```
Householder (left-looking):
   9.4769e-16
```



Problem 05

Write a program to solve rank deficient least squares problems.
You may assume that the rank is given.
Test your program with a low-rank least squares problem.
Try it with a general full-rank least squares solver and compare the results.

- **TA:** 第五题也可以用选主元的 QR 分解求解秩亏损的最小二乘问题

Solution:

(1) Helper Functions

Gram-Schmidt QR 分解算法已经在 Homework 5 Problem 1 中给出了:

```
function [Q, R] = Gram_Schmidt_QR(A, tolerance, modified, reorthogonalized)
    % This function performs the Gram-Schmidt QR factorization of a matrix A
    % It supports both classical and modified versions of the GS algorithm,
    % and it allows for reorthogonalization to improve numerical stability.
    %
    % Inputs:
    %   - A: The m x n matrix to be factorized
    %   - tolerance: The threshold below which a vector is considered linearly
dependent
    %   - modified: Boolean flag to choose between Classical Gram-Schmidt (CGS)
    %               or Modified Gram-Schmidt (MGS)
    %   - reorthogonalized: Boolean flag to perform reorthogonalization (improves
numerical stability)
    %
    % Outputs:
    %   - Q: An m x r orthonormal matrix (r is the rank of A, or the number of
orthogonal vectors)
    %   - R: An r x n upper triangular matrix
```

```
    [m, n] = size(A);  % Get the size of matrix A (m rows, n columns)
    r = 0;  % Initialize rank of A
    Q = zeros(m, m);  % Preallocate Q as an m x m zero matrix
    R = zeros(m, n);  % Preallocate R as an m x n zero matrix
    delta = zeros(m, 1);  % Temporary vector for storing projection coefficients

    % Set the number of orthogonalization iterations based on the reorthogonalized flag
    if reorthogonalized
        max_iter = 2;  % If reorthogonalization is enabled, perform two passes
    else
        max_iter = 1;  % Otherwise, perform only one pass
    end

    % Main loop over each column of matrix A (for each column k)
    for k = 1:min(m,n)
        % Initialize the k-th column of Q as the k-th column of A
        Q(1:m, r+1) = A(1:m, k);

        % If modified Gram-Schmidt (MGS) is selected
        if modified
            for iter = 1:max_iter  % Repeat orthogonalization based on max_iter
                for i = 1:r  % Loop over previously computed columns of Q
                    delta(i) = Q(1:m, i)' * Q(1:m, r+1);  % Compute projection of Q_k
on Q_i
                    R(i, k) = R(i, k) + delta(i);  % Update the corresponding entry in
R
                    Q(1:m, r+1) = Q(1:m, r+1) - delta(i) * Q(1:m, i);  % Subtract
projection from Q_k
                end
            end
        else  % Classical Gram-Schmidt (CGS)
            for iter = 1:max_iter
                delta(1:r) = Q(1:m, 1:r)' * Q(1:m,r+1);  % Compute projections in one
step
                R(1:r, k) = R(1:r, k) + delta(1:r);  % Update R
                Q(1:m, r+1) = Q(1:m, r+1) - Q(1:m, 1:r) * delta(1:r);  % Subtract the
projection from Q_k
            end
        end

        % Compute the 2-norm of the current column of Q (for normalization)
        R(r+1, k) = norm(Q(1:m, r+1), 2);

        % Check if the norm is smaller than the tolerance, indicating linear dependence
        if R(r+1, k) < tolerance
            R(r+1, k) = 0;  % Set R entry to zero if linearly dependent
        else
            Q(1:m, r+1) = Q(1:m, r+1) / R(r+1, k);  % Normalize the vector
            r = r + 1;  % Increment the rank
        end

    end

    % Additional step: if the number of columns n is greater than m,
    % compute the remaining upper triangular part of R using the orthonormal Q matrix
    if n > m
        for k = m+1:n
            % Compute the projections of columns of A onto the previously computed
orthonormal columns of Q
            R(1:r, k) = Q(1:m, 1:r)' * A(1:m, k);
```

```
        end
    end

    % Reduce the size of Q and R to the actual rank r of A
    Q = Q(1:m, 1:r);  % Return the first r columns of Q
    R = R(1:r, 1:n);  % Return the first r rows of R
end
```

`Rotate()` 函数用于将一个矩阵绕矩阵中心旋转 180°，最后再进行简单转置 (即不取复共轭):

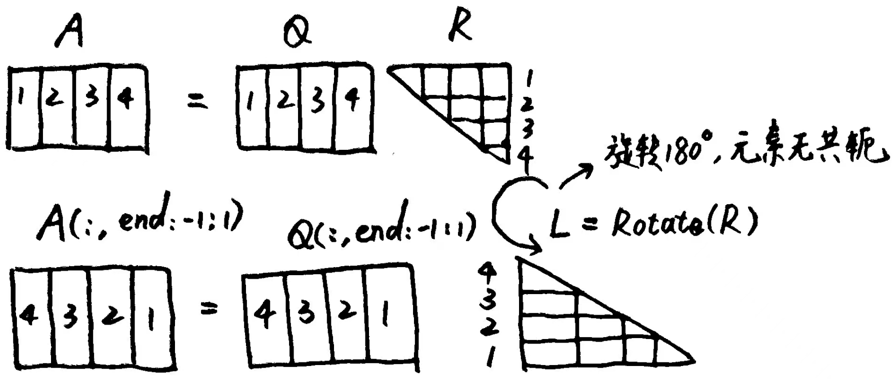
```
function B = Rotate(A)
    % Rotate computes the 90-degree counterclockwise rotation of a matrix A.
    %
    % Inputs:
    %   A - The input matrix to be rotated (size m x n).
    %
    % Outputs:
    %   B - The rotated matrix (size n x m).

    [m, n] = size(A);  % Get the dimensions of the input matrix A

    B = zeros(n, m);  % Initialize the output matrix B with zeros (size n x m)

    % Loop through each element of A to fill in the rotated matrix B
    for i = 1:m
        for j = 1:n
            % Place the element from A into its new position in B
            B(n - j + 1, m - i + 1) = A(i, j);
        end
    end

    % Note: In MATLAB, the operation A' is the complex conjugate transpose,
    % while A.' is the simple transpose.
    % In this function, B = B.';
    % ensures we only transpose the matrix without taking the complex conjugate.
    B = B.';  % Transpose the resulting matrix to correct the orientation

end
```

回代法:

```
function X = Backward_Sweep(U, Y)
    % 回代法求解 UX = Y
    [n, ~] = size(Y);
    for i = n:-1:2
        Y(i,:) = Y(i,:) / U(i, i);  % 对角线归一化
        Y(1:i-1,:) = Y(1:i-1,:) - U(1:i-1, i) * Y(i,:);  % 消去
    end
    Y(1,:) = Y(1,:) / U(1, 1);  % 处理第一行
    X = Y;  % 返回结果
end
```

(2) 基于 QR 的 RQ 算法

基于已有的 QR 算法，我们可以方便地得到 QL 分解，进而得到 RQ 分解:



因此对 $A^H(:, end:-1:1)$ 作 QR 分解: $A^H(:, end:-1:1) = QR$

便可得 A^H 的 QL 分解: $A^H = \tilde{Q}\tilde{L}$ 其中 $\begin{cases} \tilde{Q} = Q(:, end:-1:1) \\ \tilde{L} = Rotate(R) \end{cases}$

共轭转置后 进而可得 A 的 RQ 分解 $A = \tilde{L}^H \tilde{Q}^H$

上述算法的 Matlab 代码为:

```
function [R, Q] = Gram_Schmidt_RQ(A, tolerance, modified, reorthogonalized)
    % Gram_Schmidt_RQ computes the RQ factorization of matrix A using
    % the Gram-Schmidt process.
    %
    % Inputs:
    %   A - The input matrix to be factorized (size m x n).
    %   tolerance - Threshold for the modified Gram-Schmidt process.
    %   modified - Boolean indicating whether to use modified Gram-Schmidt.
    %   reorthogonalized - Boolean indicating whether to reorthogonalize.
    %
    % Outputs:
    %   R - Upper triangular matrix (size n x n).
    %   Q - Orthogonal matrix (size m x n).

    A = A';  % Transpose A to prepare for RQ factorization

    % Call the Gram-Schmidt QR function on the reversed matrix
    [Q, R] = Gram_Schmidt_QR(A(:, end:-1:1), tolerance, modified, reorthogonalized);

    Q = Q(:, end:-1:1);  % Reverse the columns of Q to match RQ format
    R = Rotate(R);       % Apply rotation to R for final format

    Q = Q';  % Transpose Q back to original dimensions
    R = R';  % Transpose R back to original dimensions
end
```

(3) 亏秩最小二乘问题的求解

考虑亏秩最小二乘问题 $\min_x \|Ax - b\|_2^2$
其中 $b \in \mathbb{C}^m$ 为给定向量，而 $A \in \mathbb{C}^{m\times n}$ 为秩 $r < \min(m, n)$ 的矩阵.

假设我们已通过一次 QR 分解和一次 RQ 分解得到了秩 r 矩阵 $A \in \mathbb{C}^{m\times n}$ 的分解 $A = Q_1 R Q_2$
其中 $Q_1 \in \mathbb{C}^{m\times r}$ 为列标准正交的矩阵，$R \in \mathbb{C}^{r\times r}$ 为满秩的上三角阵，$Q_2 \in \mathbb{C}^{r\times n}$ 为行标准正交的矩阵.
则我们有:

$$
\begin{aligned}
\min_x \|Ax-b\|_2^2 &\Leftrightarrow \min_x \|Q_1 R Q_2 x - b\|_2^2 \\
&\Leftrightarrow \min_x \left\| \begin{bmatrix} Q_1 & Q_1^{\perp} \end{bmatrix} \begin{bmatrix} R \\ 0_{(m-r)\times r} \end{bmatrix} Q_2 x - b \right\|_2^2 \\
&\Leftrightarrow \min_x \left\| \begin{bmatrix} R \\ 0_{(m-r)\times r} \end{bmatrix} Q_2 x - \begin{bmatrix} Q_1^H b \\ (Q_1^{\perp})^H b \end{bmatrix} \right\|_2^2 \\
&\Leftrightarrow \min_x \|R Q_2 x - Q_1^H b\|_2^2 \\
&\Leftrightarrow \min_x \|Q_2 x - R^{-1} Q_1^H b\|_2^2
\end{aligned}
$$

因此 $x = Q_2^H R^{-1} Q_1^H b$ 是亏秩最小二乘问题 $\min_x \|Ax-b\|_2^2$ 的一个特解.
下面我们给出求解亏秩最小二乘问题 $\min_x \|Ax-b\|_2^2$ 的特解 $x = Q_2^H R^{-1} Q_1^H b$ 的 Matlab 函数:

```
function [x, r] = Rank_Deficient_Solver(A, b)
    % Solve_Rank_Deficient_Least_Squares computes the least squares solution
    % for a potentially rank-deficient matrix A using the Gram-Schmidt process.
    %
    % Inputs:
    %   A - The input matrix (size m x n), which may be rank deficient.
    %   b - The right-hand side vector (size m x 1).
    %
    % Outputs:
    %   x - The least squares solution vector (size n x 1).
    %   r - The rank of the matrix R obtained during the process.

    % Step 1: Perform QR factorization of A using the Gram-Schmidt process
    [Q1, R_tmp] = Gram_Schmidt_QR(A, 1e-10, true, true);

    % Step 2: Get the size of R_tmp to determine the effective rank
    [r, ~] = size(R_tmp);  % r will be the number of rows in R_tmp

    % Step 3: Perform RQ factorization on R_tmp
    [R, Q2] = Gram_Schmidt_RQ(R_tmp, 1e-10, true, true);

    % Step 4: Solve the triangular system R * b_tilde = Q1' * b
    b_tilde = Backward_Sweep(R, Q1' * b);  % Backward substitution

    % Step 5: Compute the final solution x using Q2
    x = Q2' * b_tilde;  % Project the solution back

end
```

(4) 满秩求解器

复数域上的 Householder 变换的计算算法已在 Homework 4 Problem 2 中给出:

```
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
```

复数域上的 Householder QR 算法已在 Homework 4 Problem 3 中给出:

```
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
```

计算得到 $A \in \mathbb{C}^{m\times n}$ 的 QR 分解 $A = QR$ 之后 (其中 $Q \in \mathbb{C}^{m\times m}$ 为酉矩阵，$R \in \mathbb{C}^{m\times n}$ 的上 $n\times n$ 分块 R_1 为上三角阵)

求解法方程 $A^HAx = R^HRx = A^Hb$ 就等价于求解 $\begin{cases} R^Hy = A^Hb \\ Rx = y \end{cases}$ (分别由前代法和回代法求解)

或者也可考虑精简 QR 分解 $A = Q_1R_1$ (其中 $Q_1 \in \mathbb{C}^{m\times n}$ 由 Q 的前 n 列构成)

则求解法方程 $A^HAx = R_1^HR_1x = R_1^HQ_1^Hb = A^Hb$ 就等价于求解 $R_1x = Q_1^Hb$ (由回代法求解)

```
function x = Householder_Full_Rank_Solver(A, b)
    [m, n] = size(A);

    % Step 1: Compute the QR decomposition of A using Householder reflections
    [Q, R] = Complex_Householder_QR(A);

    % Step 2: Solve the system Rx = Q' * b using backward substitution
    x = Backward_Sweep(R(1:n, 1:n), Q(1:m, 1:n)' * b);
end
```

(5) 运行结果

我们比较 Matlab 内置求解器、亏秩求解器和满秩求解器应用于亏秩最小二乘问题的效果.
函数调用:

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

% Define dimensions
m = 300;  % Number of rows in matrix A
n = 50;   % Number of columns in matrix A
r = 25;   % Rank of matrix A

% Generate a rank-r complex matrix A
A = (rand(m, r) + 1i * rand(m, r)) * (rand(r, n) + 1i * rand(r, n));
b = rand(m, 1) + 1i * rand(m, 1);  % Generate a random complex vector b

% Ensure the rank of A is exactly r
assert(rank(A) == r);

% Solve the linear system Ax = b for the exact solution
x_exact = A \ b;  % Use MATLAB's backslash operator for solving
object_value_exact = norm(A * x_exact - b, 2);  % Calculate the exact objective value
disp('Exact solution objective value:');
disp(object_value_exact);

% Solve for the rank-deficient case
[x_deficient, r_deficient] = Rank_Deficient_Solver(A, b);  % Custom solver for rank-deficient case
object_value_deficient = norm(A * x_deficient - b, 2);  % Calculate the objective value for deficient case
disp('Rank-deficient solution objective value:');
disp(object_value_deficient);

% Solve for the full rank case using Householder transformations
x_full_rank = Householder_Full_Rank_Solver(A, b);  % Custom solver for full rank case
object_value_full_rank = norm(A * x_full_rank - b, 2);  % Calculate the objective value for full rank case
disp('Full rank solution objective value:');
disp(object_value_full_rank);
```

运行结果:

```
警告: 秩亏, 秩 = 25, tol =  1.703841e-10。
Exact solution objective value:
    6.7824

Rank-deficient solution objective value:
    6.7824

Full rank solution objective value:
    7.4224
```

Problem 06 (optional)

Implement the Lanczos process.
Make sure you are using a short recurrence instead of using the naive Arnoldi process.

Solution:
当 A 是对称阵时，Arnoldi 过程得到的 $T := Q^T AQ$ 是一个对称三对角阵.
理论上，我们可将 Arnoldi 过程简化为 **Lanczos 过程** (考虑到 T 的很多上三角元为零)
给定对称阵 $A \in \mathbb{R}^{n\times n}$ 和单位向量 $q_1 \in \mathbb{R}^n$
我们记:

$$\widetilde{T}_k = \begin{bmatrix} \alpha_1 & \beta_1 & & & \\ \beta_1 & \alpha_2 & \beta_2 & & \\ & \beta_2 & \alpha_3 & \ddots & \\ & & \ddots & \ddots & \beta_{k-1} \\ & & & \beta_{k-1} & \alpha_k \\ & & & & \beta_k \end{bmatrix}$$

记 $Q_k := [q_1, \dots, q_k]$ (其中 $1 \leq k \leq \mathrm{rank}(\mathcal{K}(A, q_1, n))$)
(其中 Krylov 子空间 $\mathcal{K}(A, q_1, n) = \mathrm{span}\{q_1, Aq_1, \dots, A^{n-1}q_1\}$)
根据 $AQ_k = Q_{k+1}\widetilde{T}_k$ 可知 $Aq_k = \beta_{k-1}q_{k-1} + \alpha_k q_k + \beta_k q_{k+1}$
由于 $q_1, \dots, q_{k+1}$ 标准正交，故我们有 $q_k^T Aq_k = \alpha_k$
最后有 $\beta_k q_{k+1} = Aq_k - \alpha_k q_k - \beta_{k-1}q_{k-1}$

Matlab 代码如下:

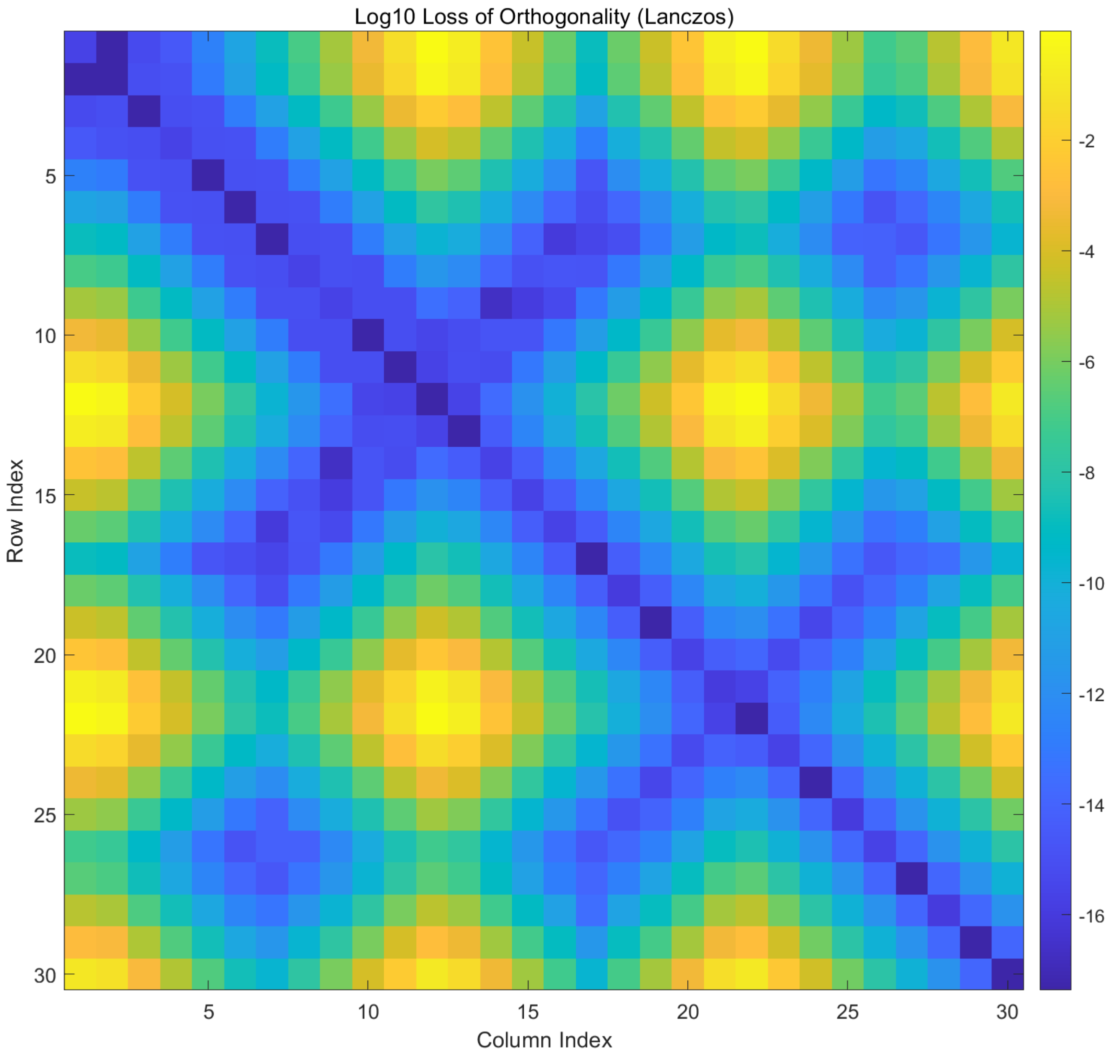
```
function [Q, T] = Lanczos(A, b, r, tolerance)
    % Lanczos Algorithm to compute the tridiagonal matrix T and orthonormal basis Q
    %
    % Input:
    %   A   - A symmetric matrix (n x n)
    %   b   - A vector (n x 1)
    %   r   - Number of Lanczos iterations
    %
    % Output:
    %   Q   - Orthogonal basis vectors (n x m)
    %   T   - Tridiagonal matrix (m x m)

    % Initialize variables
    n = size(A, 1);  % Get the size of matrix A
    Q = zeros(n, r);  % Initialize orthogonal basis matrix Q with zeros (n x r)
    T = zeros(r, r);  % Initialize tridiagonal matrix T with zeros (r x r)

    % Normalize the initial vector b to create the first orthogonal basis vector
    Q(:, 1) = b / norm(b);
```

```
    % Start the Lanczos iterations
    for j = 1:r
        % Compute the matrix-vector product of A and the j-th basis vector
        z = A * Q(:, j);

        % Compute the diagonal entry of T (the Rayleigh quotient)
        T(j, j) = Q(:, j)' * z;

        if j == 1
            % For the first iteration, adjust z by subtracting the first term
            z = z - T(j, j) * Q(:, j);
        else
            % For subsequent iterations, subtract the contributions from the last two
basis vectors
            z = z - T(j, j) * Q(:, j) - T(j-1, j) * Q(:, j-1);
        end

        % Compute the off-diagonal entry of T and check for convergence
        T(j, j+1) = norm(z, 2);  % Norm of the vector z is the off-diagonal element
        T(j+1,j) = T(j, j+1);    % Since T is symmetric

        if norm(z, 2) < tolerance
            % If the norm of z is below the tolerance, reduce the number of iterations
            r = j-1;
            break;  % Exit the loop if convergence is achieved
        else
            % If not converged, normalize z to create the next basis vector
            Q(:, j+1) = z / T(j, j+1);
        end
    end

    % Return results by truncating Q and T to the size of the computed basis
    Q = Q(:, 1:r);  % Truncate Q to include only the computed basis vectors
    T = T(1:r, 1:r);  % Truncate T to the size of the computed matrix
end
```

函数调用:

```
rng(51);
n = 1000;
r = 30;
A = rand(n, n);
A = (A + A') / 2;
b = rand(n, 1);

% Perform the Lanczos algorithm on matrix A with vector b
% r specifies the number of iterations, and 1e-10 is the tolerance for convergence
[Q, T] = Lanczos(A, b, r, 1e-10);

% Visualize the loss of orthogonality of the vectors in Q
visualize_orthogonality_loss(Q, 'Log10 Loss of Orthogonality (Lanczos)');
```

可视化正交性损失:



Problem 07 (optional)

Implement the GTH algorithm and verify its componentwise accuracy by some examples.

Solution:
给定实方阵 $A \in \mathbb{R}^{n\times n}$，其列和均为 1，即 $1_n^T A = 1_n^T$
我们的目标是对 A 进行 LU 分解.

首先对 $A^T - I_n$ 进行 Gauss 消元，得到 $A^T - I_n = LU$
直观起见，考虑 $n = 4$ 的例子:
(注意到 $A^T - I_n$ 的行和均为 0，非对角元均为正值，对角元均为负值)

$$
\begin{aligned}
A^T - I_n &= \begin{bmatrix} - & + & + & + \\ + & - & + & + \\ + & + & - & + \\ + & + & + & - \end{bmatrix} \\
&= \begin{bmatrix} 1 & & & \\ - & 1 & & \\ - & & 1 & \\ - & & & 1 \end{bmatrix} \begin{bmatrix} - & + & + & + \\ & - & + & + \\ & + & - & + \\ & + & + & + \end{bmatrix} \\
&= \begin{bmatrix} 1 & & & \\ - & 1 & & \\ - & & 1 & \\ - & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & - & 1 & \\ & - & & 1 \end{bmatrix} \begin{bmatrix} - & + & + & + \\ & - & + & + \\ & & - & + \\ & & + & - \end{bmatrix} \\
&= \begin{bmatrix} 1 & & & \\ - & 1 & & \\ - & & 1 & \\ - & & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & - & 1 & \\ & - & & 1 \end{bmatrix} \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & - & 1 \end{bmatrix} \begin{bmatrix} - & + & + & + \\ & - & + & + \\ & & - & + \\ & & & 0 \end{bmatrix} \\
&= L_3^{-1} L_2^{-1} L_1^{-1} U \\
&= LU
\end{aligned}
$$

(消元结束时，上三角阵最后一行全为零，这是显然的，因为行和为零)
我们发现只有对角元位置会发生相消，而且这个相消是可以避免的.
注意到 $A^T - I_n$ 的行和均为 0，且列 Gauss 消元会保留 "行和均为 0" 的性质.
因此我们每步 Gauss 消元结束后都要修正对角元，
即将同一行的正元素加起来再取负，便得到对角元的更精确的计算结果.

上述算法的 Matlab 代码为:

```
function [L, U] = GTH(A)
    % GTH performs Gaussian elimination to decompose a matrix A into lower
    % triangular matrix L and upper triangular matrix U.
    %
    % Input:
    %   A - A square matrix to be decomposed.
    %
    % Output:
    %   L - Lower triangular matrix with ones on the diagonal.
    %   U - Upper triangular matrix.

    % Get the size of matrix A
    [n, ~] = size(A);

    % Perform Gaussian elimination
    for i = 1:n-1

        % Normalize the column below the pivot element
        A(i+1:n, i) = A(i+1:n, i) / A(i, i);

        % Update the submatrix to eliminate elements below the pivot
        A(i+1:n, i+1:n) = A(i+1:n, i+1:n) - A(i+1:n, i) * A(i, i+1:n);

        % Computation for the diagonal elements
        for k = i+1:n
            % Update the diagonal element in the k-th row
            A(k, k) = 0;
            A(k, k) = - sum(A(k, i+1:n));
        end
```

```
        % Output every 100 iterations
        if mod(i, 100) == 0
            fprintf('Iteration %d completed\n', i);
        end

    end

    % Extract L and U
    L = tril(A, -1) + eye(n);
    U = triu(A);

end
```

得到 $A^T - I_n = LU$ 后，我们有:
(注意到 L 是单位下三角阵，因而是满秩的)

$$A^T - I_n = LU$$
$$\Leftrightarrow$$
$$A - I_n = U^T L^T$$
$$\Leftrightarrow$$
$$A = (U^T + L^{-T})L^T = \tilde{L}\tilde{U} \text{ where } \begin{cases} \tilde{L} := U^T + L^{-T} \\ \tilde{U} := L^T \end{cases}$$

这样我们就得到了 A 的 LU 分解 $A = \tilde{L}\tilde{U}$，可以验证其逐元素绝对误差接近机器精度.
函数调用:

```
rng(51);
n = 2000;
A = rand(n, n);

% Normalize each row of the matrix A using L1 norm
for j = 1:n
    A(:, j) = A(:, j) / norm(A(:, j), 1);
end

% Perform Gaussian elimination using the GTH function
[U_GTH, L_GTH] = GTH(A' - eye(n));
U_GTH = U_GTH';
L_GTH = L_GTH' + U_GTH \ eye(n);

% Calculate the difference between the reconstructed matrix and A
difference_GTH = L_GTH * U_GTH - A;

% Display the maximum absolute error from the reconstruction
disp("Maximum pointwise absolute residual:")
disp(max(abs(difference_GTH(:))));
```

运行结果:

```
Maximum pointwise absolute residual:
   8.9214e-16
```