

homework 20241022

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第一题

$$1. \min \|Ax - b\|_2^2 + \lambda \|x\|_2^2 = \min \left\| \begin{bmatrix} A \\ \sqrt{\lambda} I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_2^2$$

转化为法方程: $\begin{bmatrix} A \\ \sqrt{\lambda} I \end{bmatrix}^T \begin{bmatrix} A \\ \sqrt{\lambda} I \end{bmatrix} x = \begin{bmatrix} A^T b \\ 0 \end{bmatrix}$, 即 $(A^T A + \lambda I)x = A^T b$.

$A_{m \times n}$

$$A^T A = \begin{bmatrix} \text{matrix} & 0 \\ 0 & \text{matrix} \end{bmatrix} = \begin{bmatrix} \text{matrix} & \\ & \text{matrix} \end{bmatrix} \text{ 是对角矩阵.}$$

对于增广矩阵 $[A^T A + \lambda I | A^T b] = \left[\begin{array}{c|c} \text{matrix} & \text{vector} \end{array} \right]$

依次对 $r_1, r_2, r_3, \dots, r_{m-1}, r_m$ 进行 Givens 变换, 使右边成为上三角阵.

即 $\left[\begin{array}{c|c} \text{matrix} & \text{vector} \end{array} \right] \xrightarrow[\text{n-1次}]{\text{若干次 Givens 变换}} \left[\begin{array}{c|c} \text{matrix} & \text{vector} \end{array} \right] =: [R | b']$

问题转化为求解 $Rx = b'$, R 是上三角阵

第二题

2. 对线性约束 $Cx=d$, 若添加/删除 $[C|d]$

运用选主元高斯消元, 可得:

$$[C|d] \rightarrow [C_1 C_2 | d']$$

$$\begin{bmatrix} A \\ \hline \end{bmatrix} \begin{bmatrix} x \\ \hline \end{bmatrix} = \begin{bmatrix} b \\ \hline \end{bmatrix}$$

$$\begin{bmatrix} C \\ \hline \end{bmatrix} \begin{bmatrix} d \\ \hline \end{bmatrix} \xrightarrow{\text{Gauss elimination}} \begin{bmatrix} C_1 & C_2 \\ \hline \end{bmatrix} \begin{bmatrix} d' \\ \hline \end{bmatrix}$$

$$\begin{bmatrix} C \\ \hline \end{bmatrix} \begin{bmatrix} x \\ \hline \end{bmatrix} = \begin{bmatrix} d \\ \hline \end{bmatrix}$$

其中 C_1 是上三角阵, 是可逆的 (选主元确保).

按照 $C = [C_1 C_2]$, 将 x 相应地分割为 $\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$. 则 $[C_1 C_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = d'$.

$$\text{解得 } x_1 = C_1^{-1}(d' - C_2 x_2), \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} C_1^{-1}(d' - C_2 x_2) \\ x_2 \end{bmatrix}.$$

按照 $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$, 将 A 相应地分割为 $[A_1 A_2]$, 则求解 $\min \| [A_1 A_2] \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - b \|_2$

$$\min \| A_1 C_1^{-1}(d' - C_2 x_2) + A_2 x_2 - b \|_2 = \min \| (A_2 - A_1 C_1^{-1} C_2) x_2 + A_1 C_1^{-1} d' - b \|_2$$

$$\text{令 } \tilde{A} = A_2 - A_1 C_1^{-1} C_2, \quad \tilde{b} = A_1 C_1^{-1} d' - b, \quad \tilde{x} = x_2$$

问题转化为无约束的最小二乘问题 $\min \| \tilde{A} \tilde{x} - \tilde{b} \|_2$.

第三题

3. 用 Lagrange 乘子法: $L(x, \lambda) = \frac{1}{2} \|Ax - b\|_2^2 + \lambda^*(Cx - d)$. $A \in \mathbb{C}^{m \times n}$, $C \in \mathbb{C}^{p \times n}$, $\lambda \in \mathbb{C}^p$, $(n \leq m)$.

$$L(x, \lambda) = \frac{1}{2} (Ax - b)^*(Ax - b) + \lambda^*(Cx - d)$$

$$= \frac{1}{2} (x^* A^* Ax - x^* A^* b - b^* Ax + b^* b) + \lambda^*(Cx - d)$$

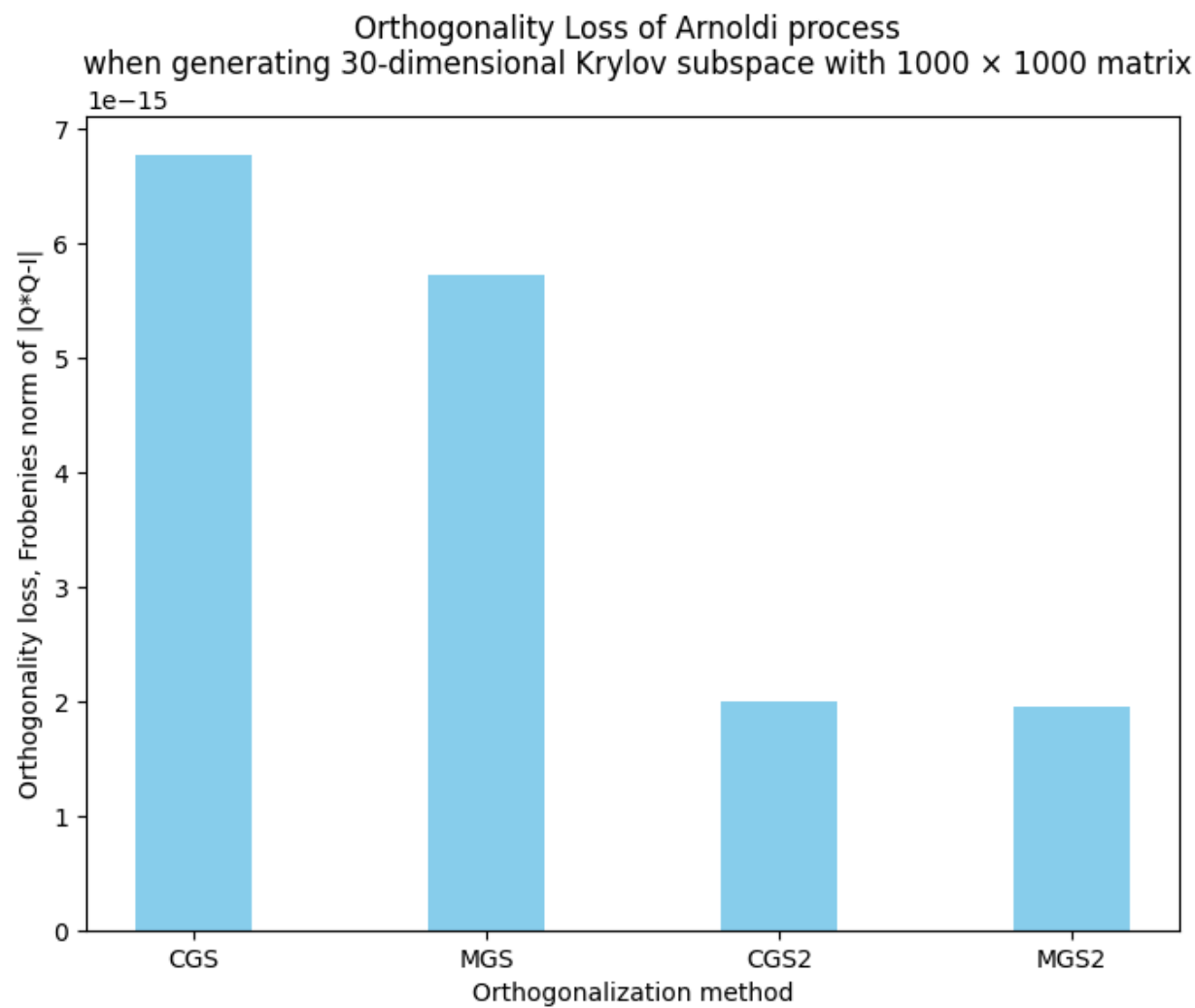
$$L^*(x, \lambda) = \frac{1}{2} (A^* Ax - 2A^* b) + C^* \lambda = A^*(Ax - b) + C^* \lambda = 0.$$

记 $Ax - b = -r$. 有 $\begin{cases} b - Ax = r \\ A^* r - C^* \lambda = 0 \\ Cx = d \end{cases} \Leftrightarrow \begin{bmatrix} I & A & 0 \\ A^* & 0 & C^* \\ 0 & C & 0 \end{bmatrix} \begin{bmatrix} r \\ x \\ \lambda \end{bmatrix} = \begin{bmatrix} b \\ 0 \\ d \end{bmatrix}$

再令 $\tilde{\lambda} = -\lambda$. 则有 $\begin{bmatrix} I & A & 0 \\ A^* & 0 & C^* \\ 0 & C & 0 \end{bmatrix} \begin{bmatrix} r \\ x \\ \tilde{\lambda} \end{bmatrix} = \begin{bmatrix} b \\ 0 \\ d \end{bmatrix}$ 系数矩阵是 Hermitian 阵

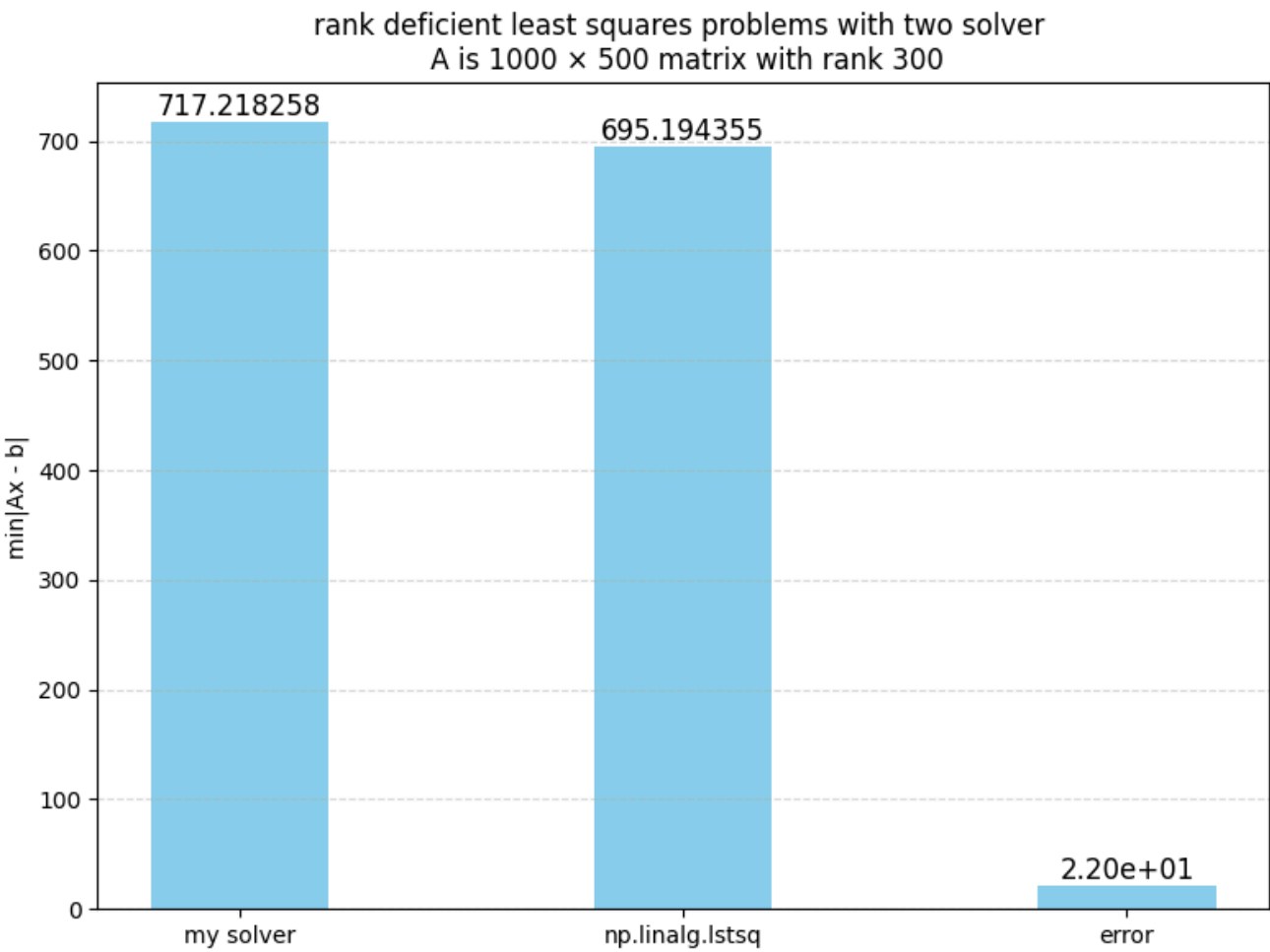
第四题

代码文件 `Arnoldi_precess.py`



第五题

代码文件 rank_deficient_ls.py



附录

```
# part of Arnoldi_precess.py
def Arnoldi_precess(A, b, k, modified, reortho):
    """
    Arnoldi process for matrix A and vector v, using CGS/CGS2/MGS/MGS2 when orthogonaliza
    A[q_1, q_2, ... ,q_k] = [q_1, q_2, ..., q_(k+1)] H
    :param A: matrix A, n x n
    :param b: vector b, iterative initial vector
    :param k: number of iterations
    :param modified: use CGS/CGS2 if modified is not True else use MGS/MGS2
    :param reortho: use CGS/MGS if reortho is not True else use CGS2/MGS2
    :return: Q (n x (k+1) orthogonal matrix), H ((k+1) x k upper hessenberg matrix)
    """
    n = len(b)
    n1, n2 = A.shape
    if n1 != n or n2 != n:
        print(f'input matrix A and vector b have different size, A: {n1} x {n2}, b: {n} x ')
        return None, None

    Q = np.zeros((n, (k+1)))
    H = np.zeros(((k+1), k))
    Q[:, [0]] = b / np.linalg.norm(b, ord=2)

    if modified is not True:
        # Use BLAS2 may be faster, but here use BLAS1 for simplicity
        for i in range(k):
            cur = A @ Q[:, [i]]
            for j in range(i+1):
                H[i, j] = np.dot(cur.T, Q[:, [j]]).item()
            for j in range(i+1):
                cur = cur - H[i, j] * Q[:, [j]]
            if reortho is True:
                correct = [0] * (i+1)
                for j in range(i+1):
                    correct[j] = np.dot(cur.T, Q[:, [j]]).item()
                H[i, j] = H[i, j] + correct[j]
                for j in range(i+1):
                    cur = cur - correct[j] * Q[:, [j]]
            H[i+1, i] = np.linalg.norm(cur, ord=2)

        if H[i+1, i] == 0:
            print(f'cannot continue iteration when generating q_{i+1}, H[{i+1}], {i}')
```

```

42         return Q, H
43
44         Q[:, [i+1]] = cur / H[i+1, i]
45
46     if modified is True:
47         for i in range(k):
48             cur = A @ Q[:, [i]]
49             for j in range(i+1):
50                 H[i, j] = np.dot(cur.T, Q[:, [j]]).item()
51                 cur = cur - H[i, j] * Q[:, [j]]
52                 if reortho is True:
53                     correct = np.dot(cur.T, Q[:, [j]]).item()
54                     H[i, j] = H[i, j] + correct
55                     cur = cur - correct * Q[:, [j]]
56             H[i+1, i] = np.linalg.norm(cur, ord=2)
57
58         if H[i+1, i] == 0:
59             print(f'cannot continue iteration when generating q_{i+1}, H[{i+1}], {i}]')
60             return Q, H
61
62         Q[:, [i+1]] = cur / H[i+1, i]
63
64     return Q, H

```

```

# part of rank_deficient_ls_py
def qr_decomposition_with_pivoting(origin_A, tol=1e-10):
    """
    matrix A is a rank deficient matrix, return QR decomposition with column pivoting
    :param origin_A: matrix A, m x n, m >= n
    :return: Q (m x m, Q*Q = I), R, P (record column exchange)
    """
    A = np.copy(origin_A).astype(float)
    m, n = A.shape
    if m < n:
        print(f'warning, m={m} < n={n}')
        return None, None, None
    exchange = np.arange(n)
    Q = np.zeros((m, m))
    R = np.zeros((m, n))
    col_norms = np.sum(A**2, axis=0)
    rank = 0

    for i in range(n):
        pivot = np.argmax(col_norms[i:]) + i
        if col_norms[pivot] < tol:
            break
        if pivot != i:
            A[:, [i, pivot]] = A[:, [pivot, i]]
            exchange[i], exchange[pivot] = exchange[pivot], exchange[i]
            col_norms[i], col_norms[pivot] = col_norms[pivot], col_norms[i]

        R[i, i] = np.linalg.norm(A[:, [i]], ord=2)
        Q[:, [i]] = A[:, [i]] / R[i, i]
        R[i, i+1:] = Q[:, [i]].T @ A[:, i+1:]

        A[:, i+1:] = A[:, i+1:] - np.outer(Q[:, [i]], R[i, i+1:])
        col_norms[i+1:] = col_norms[i+1:] - R[i, i+1:]**2
        col_norms[col_norms < tol] = 0

        rank = rank + 1

    # make Q orthogonalized square matrix

    for j in range(m):
        if rank == m:
            break
        e = np.zeros(m, dtype=float)

```



```

44     e[j] = 1.0
45
46     for k in range(rank):
47         projection = np.dot(e, Q[:, k])
48         e = e - projection * Q[:, k]
49     norm_e = np.linalg.norm(e, ord=2)
50     if norm_e > tol:
51         Q[:, rank] = e / norm_e
52         rank += 1
53
54     P = np.zeros((n, n), dtype=int)
55     for i in range(n):
56         P[i, exchange[i]] = 1
57
58     return Q, R, P
59
60 # now  $\min \|Ax - b\| \rightarrow \min \|QRPx - b\| \rightarrow \min \|RPx - Q^T b\| \rightarrow \min \|[R1 \ 0]^T y - [c1 \ c2]^T\|$ , in
61 # so  $\min \|Ax - b\| = \min \|R1^T y - c1\| + \|c2\| = \|c2\|$ , thanks to  $R1$ 's rank  $\leq n$ 
62
63 def ls_for_rank_deficient_matrix(A, b, tol=1e-10):
64     Q, R, P = qr_decomposition_with_pivoting(A, tol)
65     c = Q.T @ b
66     rank_R = np.linalg.matrix_rank(R)
67     c2 = c[rank_R:]
68     norm_c2 = np.linalg.norm(c2, ord=2)
69     return norm_c2 ** 2

```