Problem 00 First of all, carefully reread Chapter 4 and read Chapter 5 in Eldén.

Problem 01 (30 points) Let $A \in \mathbb{R}^{m \times m}$ be a *symmetric* matrix. You will need to know the following facts.

- As you have already learned in MAT 22A or MAT 67, an *eigenvector* of A is a nonzero vector $\mathbf{x} \in \mathbb{C}^m$ such that $A = \lambda \mathbf{x}$ for some $\lambda \in \mathbb{C}$, the corresponding *eigenvalue* where \mathbb{C} denotes the complex numbers; i.e. all numbers of the form z = a + bi where a and b are real numbers and $i = \sqrt{-1}$ is the square root of -1.
- The complex number $\overline{z} = a bi$ is the *complex conjugate* of z = a + bi and if z_1 and z_2 are any two complex numbers we have $\overline{z_1} \, \overline{z_2} = \overline{z_1} \, \overline{z_2}$.
- Finally, the inner product or dot product of two complex vectors \mathbf{x}_1 , $\mathbf{x}_2 \in \mathbb{C}$ is given by $\overline{\mathbf{x}_1}^T \mathbf{x}_2$ so that the two norm of the vector $\mathbf{x} \in \mathbb{C}$ is

$$||\mathbf{x}||_2 \stackrel{\text{def}}{=} \overline{\mathbf{x}}^{\mathrm{T}} \mathbf{x}$$

In the following problem, you may assume that all of the eigenvalues of A are distinct.

(a) (15 points) Prove that all of the eigenvalues of A are real.

[Hint: If λ is a (complex) eigenvalue of A with eigenvector \mathbf{x} , then it's complex conjugate $\overline{\lambda}$ is also an eigenvalue of A with eigenvector $\overline{\mathbf{x}}$.]

Solution to Problem 01 (a) : Suppose $\lambda = \alpha + \beta i$ is a (possibly) complex eigenvalue (i.e., β *could* be zero) with eigenvector $\mathbf{x} \in \mathbb{C}^n$. Then

$$\mathbf{A}\,\mathbf{x} = \lambda\mathbf{x} \tag{1}$$

We can take the complex conjugate of both sides of equation (1) to obtain

$$\overline{\mathbf{A}\mathbf{x}} = \overline{\lambda}\mathbf{x} \tag{2}$$

However, since the matrix A has all real valued entries equation (2) becomes

$$A\overline{\mathbf{x}} = \overline{\lambda}\overline{\mathbf{x}}.\tag{3}$$

Thus, if $\lambda = \alpha + \beta i$ is a complex eigenvalue (i.e., $\beta \neq 0$) then $\overline{\lambda} = \alpha - \beta i$ is a eigenvalue of A with eigenvector $\overline{\mathbf{x}} \in \mathbb{C}^n$.

Now

$$\overline{\mathbf{x}}^{\mathrm{T}}(\mathbf{A}\mathbf{x}) = \overline{\mathbf{x}}^{\mathrm{T}}(\lambda\mathbf{x}) = \lambda(\overline{\mathbf{x}}^{\mathrm{T}}\mathbf{x}) = \lambda \|\mathbf{x}\|_{2},\tag{4}$$

and, since $A = A^T$, we also have

$$\overline{\mathbf{x}}^{\mathrm{T}}(\mathbf{A}\mathbf{x}) = \overline{\mathbf{x}}^{\mathrm{T}}\mathbf{A}^{\mathrm{T}}\mathbf{x} = (\mathbf{A}\overline{\mathbf{x}})^{\mathrm{T}}\mathbf{x} = (\bar{\lambda}\overline{\mathbf{x}})^{\mathrm{T}}\mathbf{x} = \bar{\lambda}\overline{\mathbf{x}}^{\mathrm{T}}\mathbf{x} = \bar{\lambda}\|\mathbf{x}\|_{2}.$$
 (5)

Thus,

$$\lambda \|\mathbf{x}\|_2 = \bar{\lambda} \|\mathbf{x}\|_2,$$

implying that $\lambda = \bar{\lambda}$ and hence, λ must be real; $\lambda \in \mathbb{R}$.

(b) Prove that if \mathbf{x}_1 and \mathbf{x}_2 are eigenvectors corresponding to distinct eigenvalues, then \mathbf{x}_1 and \mathbf{x}_2 are orthogonal.

Solution to Problem 01 (b) : Let $(\mathbf{x}_1, \lambda_1)$ and $(\mathbf{x}_2, \lambda_2)$ be two *distinct* eigenvector, eigenvalue pairs associated with A; i.e.,

$$A\mathbf{x}_1 = \lambda_1 \mathbf{x}_1$$
 and $A\mathbf{x}_2 = \lambda_2 \mathbf{x}_2$.

with $\lambda_1 \neq \lambda_2$. Then, taking the inner product of $AA\mathbf{x}_1$ with \mathbf{x}_2 we find

$$\lambda_1 \mathbf{x}_1^T \mathbf{x}_2 = (A \mathbf{x}_1)^T \mathbf{x}_2$$

$$= \mathbf{x}_1^T A^T \mathbf{x}_2$$

$$= \mathbf{x}_1^T A \mathbf{x}_2 \qquad \text{Why?}$$

$$= \mathbf{x}_1^T (\lambda_2 \mathbf{x}_2)$$

$$= \lambda_2 \mathbf{x}_1^T \mathbf{x}_2$$

Thus

$$(\lambda_1 - \lambda_2) \mathbf{x}_1^{\mathrm{T}} \mathbf{x}_2 = 0.$$

Since, by assumption, $\lambda_1 \neq \lambda_2$ It follows that $\mathbf{x}_1^T \mathbf{x}_2 = 0$; i.e., $\mathbf{x}_1 \mathbf{x}_2$ are orthogonal.

Note that in the above proof of **Problem 01 (b)** we only used the real valued version of the inner product $\mathbf{x}_1^T \mathbf{x}_2$. Why is this OK?

Problem 02 (60 points) Let

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

where ϵ is a small positive number (e.g., 10^{-8}) so that ϵ^2 can be ignored numerically.

- (a) (15 points) Compute the reduced QR factorization $A = \widehat{Q}\widehat{R}$ using the classical Gram-Schmidt algorithm by hand.
- (b) (15 points) Compute the reduced QR factorization $A = \widehat{Q}\widehat{R}$ using the modified Gram-Schmidt algorithm by hand.
- (c) (15 points) Compute the full QR factorization A = QR using the Householder triangularization by hand.
- (d) (15 points) Check the quality of these results by computing the Frobenius norm of $\|\widehat{Q}^T\widehat{Q} I\|_F$ for the results obtained by the CGS and MGS algorithms and $\|\mathbf{O}^{\mathrm{T}}\mathbf{O} - \mathbf{I}\|_{\mathrm{F}}$ for the result obtained by the Householder triangularization.

Solution 2. Let

$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ \mathbf{c} & 0 \\ 0 & \mathbf{c} \end{bmatrix}.$$

Denote the first column of A as A(:,1) = $\begin{bmatrix} 1 & \varepsilon & 0 \end{bmatrix}^T$. Similarly, denote the second column of A as A(:,2) = $\begin{bmatrix} 1 & 0 & \varepsilon \end{bmatrix}^T$. Then $A = \begin{bmatrix} A(:,1) & A(:,2) \end{bmatrix}$. In the work done below, we calculate the QR factorization of the matrix A using three different methods of calculations.

Part (a): Classical Gram Schmidt (reduced QR Factorization)

We begin by calculating the QR factorization using the classical Gram Schmidt algorithm.

The first step of the algorithm we find an orthonormal basis for the span of the first column of A. To do this, we normalize the vector A(:,1) in order to obtain the first column of Q given byQ(:,1). To this end, set $r_{11} = \|\mathbf{a}(:, 1)\|_2$ and define $Q(:, 1) = \frac{1}{r_{11}}A(:, 1)$. In this case,

$$r_{11} = \|\mathbf{A}(:,1)\|_2 = \sqrt{1^2 + \epsilon^2} \approx 1$$

Then, to normalize we set

$$Q(:,1) = \frac{1}{r_{11}}A(:,1) = \begin{bmatrix} 1 \\ \epsilon \\ 0 \end{bmatrix}$$

In the second step of this algorithm, we obtain the orthonormal basis vector for the span of the first two columns of A. Let $\mathbf{q}_1 = Q(:,1), r_{12} = \mathbf{q}_1^T A(:,2) = 1$. So

$$\mathbf{A}(:,2) - r_{12}\mathbf{q}_1 = \begin{bmatrix} 1 \\ 0 \\ \epsilon \end{bmatrix} - \begin{bmatrix} 1 \\ \epsilon \\ 0 \end{bmatrix}$$

Finally, we take the norm of this vector to get $r_{22} = \sqrt{\varepsilon^2 + \varepsilon^2} \approx \sqrt{2}\varepsilon$ and normalize the resulting vector to obtain

$$Q(:,2) = \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}.$$

We have
$$Q = [Q(:,1) \ Q(:,2)]$$
 and $R = \begin{bmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{bmatrix}$.

Part (b): Modified Gram Schmidt (reduced QR factorization)

In the 3 × 2 case, the modified Gram Schmidt process acts identically to the classical Gram Schmidt process. Thus, the reduced QR factorization resulting from the modified Gram Schmidt process is identical to part (a). Note: in the case covered in lecture 9 and 10 where we start with a 4×3 matrix, these two algorithms behave differently. The difference is one very important key in understanding how matrix computations work on computers.

Part (c): Householder Triangularization

In order to obtain the Householder triangularization of the matrix A given above, I need to find a sequence of orthogonal matrices such that $Q_2Q_1A = R$ where R is upper triangular. Once I find the matrices Q_1 and Q_2 , the Q factor from the full QR factorization is given by $Q = Q_1^T Q_2^T$. To begin, we define

$$Q_1 = F = I_3 - 2 \frac{\mathbf{v} \mathbf{v}^T}{\mathbf{v}^T \mathbf{v}}$$

In general, when computing this transformation for the jth Householder reflector, we take special notice of the diagonal element in the jth row and jth column. In particular, we define v, based on a vector involving the then we will be able to calculate this. The auxiliary vector \mathbf{x} to be the vector whose coefficients start at the diagonal element and continue down to the last row. Thus, we begin with

$$\mathbf{v} = \operatorname{sgn}(x_1) \|\mathbf{x}\|_2 \mathbf{e}_1 + \mathbf{x}$$

For this first vector, we set

$$\mathbf{x} = \begin{bmatrix} 1 \\ \epsilon \\ 0 \end{bmatrix}.$$

Then, $x_1 = 1$ and sgn $(x_1) = 1$. The vector **v** is given by

$$\mathbf{v} = 1(1 + \epsilon^2) \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 1 \\ \epsilon \\ 0 \end{bmatrix} = \begin{bmatrix} 2 \\ \epsilon \\ 0 \end{bmatrix}.$$

Then, the projector is given by

$$Q_{1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{2(1 + \epsilon^{2})} \begin{bmatrix} 2 \\ \epsilon \\ 0 \end{bmatrix} \begin{bmatrix} 2 & \epsilon & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \frac{1}{2(1+\epsilon^2)} \begin{bmatrix} 4 & 2\epsilon & 0 \\ 2\epsilon & \epsilon^2 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\approx \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} - \begin{bmatrix} 2 & \epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$= \begin{bmatrix} -1 & -\epsilon & 0 \\ -\epsilon & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

Then, we can multiply A on the left by Q_1 to find

$$Q_1 A = \begin{bmatrix} -1 & -\epsilon & 0 \\ -\epsilon & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ \epsilon & 0 \\ 0 & \epsilon \end{bmatrix}$$

$$= \left[\begin{array}{cc} -1 - \epsilon^2 & -1 \\ 0 & -\epsilon \\ 0 & \epsilon \end{array} \right]$$

$$\approx \left[\begin{array}{cc} -1 & -1 \\ 0 & -\epsilon \\ 0 & \epsilon \end{array} \right]$$

Notice after the first multiplication by Q_1 , all subdiagonal elements of in the first column have been zeroed out. This will be true in general (given that I use the proper construction of the matrix F).

Next, we define

$$Q_2 = \begin{bmatrix} I \\ F \end{bmatrix}$$
.

In this case, we are defining a second, different auxiliary matrix $F \in \mathbb{R}^{2 \times 2}$. We remember that

$$F = I - 2 \frac{\mathbf{v} \mathbf{v}^{\mathrm{T}}}{\mathbf{v}^{\mathrm{T}} \mathbf{v}}$$

with $\mathbf{v} \in \mathbb{R}^2$. To construct \mathbf{v} we use the formula

$$\mathbf{v} = \text{sgn}(x_1) \|\mathbf{x}\|_2 \mathbf{e}_1 + \mathbf{x}$$

with

$$\mathbf{x} = \begin{bmatrix} -\epsilon \\ \epsilon \end{bmatrix} = \epsilon \begin{bmatrix} -1 \\ 1 \end{bmatrix}.$$

Then, $x_1 = -\epsilon$ and sgn $(x_1) = -1$. The vector **v** is given by

$$\mathbf{v} = -1(\sqrt{2}\epsilon) \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \epsilon \begin{bmatrix} -1 \\ 1 \end{bmatrix} = \epsilon \begin{bmatrix} -(\sqrt{2}+1) \\ 1 \end{bmatrix}.$$

To find F explicitly, we start by finding

$$\mathbf{v}^{\mathrm{T}}\mathbf{v} = \epsilon^{2} \left[-(\sqrt{2} + 1) \quad 1 \right] \begin{bmatrix} -(\sqrt{2} + 1) \\ 1 \end{bmatrix} = \epsilon^{2} \left((1 + \sqrt{2})^{2} + 1 \right) = 2\epsilon^{2} (2 + \sqrt{2})$$

Then we compute

$$\frac{2}{\mathbf{v}^{\mathrm{T}}\mathbf{v}} = \frac{2}{2\epsilon^{2}(2+\sqrt{2})}$$
$$= \frac{2-\sqrt{2}}{2\epsilon^{2}}$$

Now, we compute

$$\mathbf{v}\mathbf{v}^{\mathrm{T}} = \epsilon^{2} \begin{bmatrix} -(\sqrt{2}+1) \\ 1 \end{bmatrix} \begin{bmatrix} -(\sqrt{2}+1) & 1 \end{bmatrix}$$
$$= \epsilon^{2} \begin{bmatrix} (1+\sqrt{2})^{2} & -(1+\sqrt{2}) \\ -(1+\sqrt{2}) & 1 \end{bmatrix}$$
$$= \epsilon^{2} \begin{bmatrix} 3+2\sqrt{2} & -(1+\sqrt{2}) \\ -(1+\sqrt{2}) & 1 \end{bmatrix}$$

Using all of these together, we get

$$\frac{2}{\mathbf{v}^{\mathrm{T}}\mathbf{v}} \cdot \mathbf{v}\mathbf{v}^{\mathrm{T}} = \frac{2 - \sqrt{2}}{2} \begin{bmatrix} 3 + 2\sqrt{2} & -(1 + \sqrt{2}) \\ -(1 + \sqrt{2}) & 1 \end{bmatrix}$$
$$= \frac{1}{2} \begin{bmatrix} 2 + \sqrt{2} & -\sqrt{2} \\ -\sqrt{2} & 2 - \sqrt{2} \end{bmatrix}$$
$$= \begin{bmatrix} 1 + \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 1 - \frac{1}{\sqrt{2}} \end{bmatrix}$$

Finally, we compute F to see

$$F = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 1 + \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 1 - \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

With this, we define the second orthogonal matrix for our householder QR factorization as

$$Q_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

Then

$$Q = Q_1 Q_2 = \begin{bmatrix} -1 & \frac{\varepsilon}{\sqrt{2}} & -\frac{\varepsilon}{\sqrt{2}} \\ -\varepsilon & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}$$

and

$$R = Q_2^T Q_1^T A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} -1 & -1 \\ 0 & -\varepsilon \\ 0 & \varepsilon \end{bmatrix} = \begin{bmatrix} -1 & -1 \\ 0 & -\sqrt{2}\varepsilon \\ 0 & 0 \end{bmatrix}$$

Part (d): Checking results

Note that we ignore the term involving ε^2 .

For Parts (a) and (b)

$$\widehat{Q}^{T}\widehat{Q} = \begin{bmatrix} 1 & \varepsilon & 0 \\ 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ \varepsilon & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} = \begin{bmatrix} 1 & -\frac{\varepsilon}{\sqrt{2}} \\ -\frac{\varepsilon}{\sqrt{2}} & 1 \end{bmatrix}$$

So $\|Q^TQ\|_F = \sqrt{2}$.

For Part (c), $Q^TQ = I$ and $||Q^TQ||_F = \sqrt{2}$.

Problem 03 Let $E \in \mathbb{R}^{m \times m}$ that extracts the "even part" of an m-vector: $E\mathbf{x} = (\mathbf{x} + F\mathbf{x})/2$, where $F \in \mathbb{R}^{m \times m}$ flips $\mathbf{x} = [x_1, \dots, x_m]^T$ to $\mathbf{x} = [x_m, \dots, x_1]^T$.

- (a) (15 points) Is E an orthogonal projector, an oblique projector, or not a projector at all?
- **(b)** (10 points) What are its entries?

Solution 03 Note that

$$F = \begin{bmatrix} 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & \cdots & 1 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 1 & \cdots & 0 & 0 \\ 1 & 0 & \cdots & 0 & 0 \end{bmatrix}$$

So $F^2 = I$. We have

$$E = \frac{1}{2} (I + F).$$

In this problem, we want to determine if P is a projector, and orthogonal projector, an oblique projector or no projector at all. To begin, consider

$$E^{2} = \left(\frac{1}{2}(I+F)\right)\left(\frac{1}{2}(I+F)\right),$$

$$= \frac{1}{4}(I+F)(I+F),$$

$$= \frac{1}{4}(I+2F+F^{2}),$$

$$= \frac{1}{2}(I+F).$$

Thus, E is certainly a projector. Now, we check to see if E is an orthogonal projector $E^{T} = E$:

$$E^{T} = \left(\frac{1}{2}(I+F)\right)^{T}$$
$$= \frac{1}{2}(I^{T}+F^{T})$$
$$= \frac{1}{2}(I+F)$$
$$= E$$

Thus, we see E is an orthogonal projector.

Problem 04 Take m = 50, n = 12. Using MATLAB's linspace, define t to be the m-vector corresponding to linearly spaced grid points from 0 to 1. Using MATLAB's vander and fliplr, define A to be the $m \times n$ matrix associated with least squares fitting on this grid by a polynomial of order n - 1. Take \mathbf{b} to be the function $\cos(4t)$ evaluated on the grid. Now, calculate and print (to 16 digit precision) the least squares coefficient vector \mathbf{x} by the following three methods.

- (a) (10 points) Solving the normal equation explicitly computing $(A^{T}A)^{-1}$.
- **(b)** (10 points) Using the MATLAB implementation CGS.m of the classical Gram-Schmidt algorithm CGS, which can be downloaded from CANVAS.
- (c) (10 points) Using the MATLAB implementation MGS.m of the modified Gram-Schmidt algorithm MGS, which can be downloaded from CANVAS.
- (d) (10 points) QR factorization using MATLAB's qr, which is based on the Householder triangularization.
- (e) (10 points) $x = A \setminus b$ in MATLAB, which is also based on QR factorization.
- (f) (10 points) The calculations above will produce five lists of twelve coefficients. In each list, use the "\textcolor{color}{words}" function in LaTeX

 $\text{textcolor}\{\text{red}\}\{\text{This sentence will be in red.}\} \rightarrow \text{This sentence will be in red.}\}$

to highlight the digits that appear to be incorrect; i.e., affected by rounding error.

- Comment on the differences you observe.
- Do the normal equations exhibit instability?

Although, explanations for what you observe are welcome, you are not *required* to explain your observations.

Solution 4. **Part (a) - (e):** The following script uses MATLAB to find the solution of the least squares problem described above:

```
clear, clc
%Homework 4: Problem 4
m = 50;
                                %row size
                               %column size
n = 12;
t = linspace(0,1,50); %initialize data points
b = cos(4*t)';
                              %initialize right hand side
A = fliplr(vander(t)); %Create proper vandermonde matrix
A = A(:, 1:12);
                               %Look at the first 12 columns only
%Part a: Solve the normal equations explicitly.
                          %%Solve least squares using normal Equations
xe = (A'*A) \setminus A'*b;
%Part b:
[Qc,Rc] = cgs(A); %Produce QR factorization of A with CGS
xc = Rc \backslash Qc' *b;
                           %Solve least squares using QR factorization
%Part c:
[Qm,Rm] = mgs(A);
                     %Produce QR factorization of A with MGS
xm = Rm \setminus (Qm' *b);
                          %Solve least squares using QR factorization
%Part d:
                          %Produce QR factorization of A with Householder
[Q,R] = qr(A);
xq = R \setminus (Q' *b);
                           %Solve least squares using QR factorization
%Part e:
x = A \ b;
                           %Solve using Matlab's built in function
result = [xe, xc, xm, xq, x]; %store the results for analysis
%latex( result, '%.16f','nomath') %print out the matrix to imbed in LaTeX
```

Part (f):

```
 \begin{pmatrix} 0.9999999634647418 & 0.9999990670158116 & 0.999999982202629 & 1.0000000009966088 & 1.000000009966106 \\ 0.0000107827037206 & 0.0002108241903418 & 0.0000003796458411 & -0.0000004227430637 & -0.0000004227436872 \\ -8.0004011015430194 & -8.0066898460667062 & -8.0000111270150818 & -7.9999812356851816 & -7.9999812356666231 \\ 0.0058555638629514 & 0.0828387680521701 & 0.0001189741011661 & -0.0003187632377173 & -0.0003187634658793 \\ 10.6222430224333948 & 10.1420533742784755 & 10.6660964456584750 & 10.6694307959322110 & 10.6694307974530318 \\ -6.2491444977349602 & -9.9267214131541550 & -5.6894048476673298 & -5.6470756271635336 & -5.6470756111814699 \\ 1.0259850489674136 & 5.7582921668654308 & 0.0019601704091591 & -0.0753160244828912 & -0.0753160517019097 \\ 0.3937358967959881 & -3.0069476849166676 & 1.6025526748224943 & 1.69536096395387863 \\ 0.9619717866880819 & 1.9695201725990046 & 0.0728948058089976 & 0.0060321088498510 & 0.0060320877023453 \\ -0.7725797541788779 & -0.6131912136261235 & -0.4020666717498082 & -0.3742417035212904 & -0.3742416950861735 \\ 0.1598681622708682 & 0.0337539279557859 & 0.0930520683479290 & 0.0880405760897516 & 0.0880405746252086 \\ \hline \end{tabular}
```

Note: Consider the system of equations given by

$$Ax = b$$

with $\mathbf{b} \notin \text{range}(A)$. To solve least squares using QR factorization of a matrix we first recall the normal equations:

$$A^{T}Ax = A^{T}b$$
.

Then, we know the least squares solution is given by

$$\hat{\mathbf{x}} = (\mathbf{A}^{\mathrm{T}} \mathbf{A})^{-1} \mathbf{A}^{\mathrm{T}} \mathbf{b}.$$

Using the QR factorization of A, we can write this solution as follows:

$$\begin{split} \hat{\mathbf{x}} &= \left((\mathbf{Q} \mathbf{R})^{\mathrm{T}} (\mathbf{Q} \mathbf{R}) \right)^{-1} (\mathbf{Q} \mathbf{R})^{\mathrm{T}} \mathbf{b}, \\ &= \left(\mathbf{R}^{\mathrm{T}} \mathbf{Q}^{\mathrm{T}} \mathbf{Q} \mathbf{R} \right)^{-1} \mathbf{R}^{\mathrm{T}} \mathbf{Q}^{\mathrm{T}} \mathbf{b}, \\ &= \mathbf{R}^{-1} (\mathbf{R}^{\mathrm{T}})^{-1} \mathbf{R}^{\mathrm{T}} \mathbf{Q}^{\mathrm{T}} \mathbf{b}, \\ &= \mathbf{R}^{-1} \mathbf{Q}^{\mathrm{T}} \mathbf{b}. \end{split}$$

The MATLAB script above mirrors these ideas in solving the least squares problem using the QR factorization

Explanation of the error: Solving the normal equation in MATLAB applies LU decomposition with pivoting. It's numerically stable but $\kappa(A^TA)$ is large. Standard Gram–Schmidt is numerically unstable. Modified Gram–Schmidt is numerically stable.