Part A. (Data fitting)

The following problem frequently arises in the fitting of experimental data, and in the approximation of a given function. Suppose we are given \( m \) pairs of data points \((x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)\). The problem of discrete approximation (in the least squares sense) is to find a linear combination of prescribed functions \( \phi_1, \phi_2, \ldots, \phi_n \) whose values at the points \( x_i \in [a, b], 1 \leq i \leq m \), approximate the values \( y_1, y_2, \ldots, y_m \) as well as possible. More precisely, the problem is to find a function of the form \( f(x) = \alpha_1 \phi_1(x) + \cdots + \alpha_n \phi_n(x) \) such that

\[
\sum_{i=1}^{m} |y_i - f(x_i)|^2 \leq \sum_{i=1}^{m} |y_i - g(x_i)|^2
\]

(1)

for all functions \( g \in \text{Span}(\phi_1, \phi_2, \ldots, \phi_n) \).

Note that usually the number \( m \) of “observations” \((x_i, y_i)\) is (much) greater than the number \( n \) of basis functions \( \phi_k \) used to approximate the data. In the remainder we assume \( m > n \).

1. Formulate problem (1) as a linear least squares problem. That is, find a matrix \( A \) and a right-hand side vector \( b \in \mathbb{R}^m \) such that problem (1) can be written as

\[
\|b - Ax\|_2 = \min
\]

where \( x = [\alpha_1 \alpha_2 \ldots \alpha_n]^T \).

2. Suppose now that we take \( \phi_k(x) = x^{k-1}, 1 \leq k \leq n \). Write \( A \) out explicitly (the resulting matrix is called a Vandermonde-type matrix). Assuming that \( x_i \neq x_j \) for \( i \neq j \), show that \( A \) has full rank: \( \text{rank}(A) = n \). (Hint: Use the fact that a nonzero polynomial of degree \( n \) cannot have more than \( n \) roots).

3. Consider the problem of finding the best fit with a quadratic function \( f(x) = \alpha_1 + \alpha_2 x + \alpha_3 x^2 \) for the following data:

<table>
<thead>
<tr>
<th>( x_i )</th>
<th>8</th>
<th>10</th>
<th>12</th>
<th>16</th>
<th>20</th>
<th>30</th>
<th>40</th>
<th>60</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>( y_i )</td>
<td>0.88</td>
<td>1.22</td>
<td>1.64</td>
<td>2.72</td>
<td>3.96</td>
<td>7.66</td>
<td>11.96</td>
<td>21.56</td>
<td>43.16</td>
</tr>
</tbody>
</table>

Write a Matlab code that solves the corresponding least squares problem in two ways, first by solving the normal equations and then by (pivoted) QR factorization. The code should first form the matrices \( C = A^T A \) and the right-hand sides \( b \) and \( d = A^T b \); then the Cholesky algorithm should be used to solve \( Cx = d \). Use \texttt{ chol } to compute the Cholesky factorization of \( C \) and \texttt{ format long } to display the computed solution with 15 digits. Next, compute the solution using the pivoted QR factorization; this is just the backslash operator applied to the overdetermined system \( Ax = b \). Compare the two solutions. Finally, plot the data points and the graph of the quadratic approximation in a Matlab (x,y)-plot. Turn in all your m-files and the corresponding output (the result of your runs).

4. A good approximate solution \( \hat{x} \) of the previous problem is given by \( \hat{\alpha}_1 = -1.919, \hat{\alpha}_2 = 0.2782 \), and \( \hat{\alpha}_3 = 0.001739 \). Compute the residual \( r = d - C\hat{x} \) corresponding to this approximate solution. Explain your finding. (Hint: use the fact that

\[
\kappa^{-1} \frac{\|r\|_2}{\|d\|_2} \leq \frac{\|x - \hat{x}\|_2}{\|x\|_2} \leq \kappa \frac{\|r\|_2}{\|d\|_2}
\]

(2)

where \( \kappa := \|C\|_2\|C^{-1}\|_2 \). Here \( C \) is any nonsingular \( n \times n \) matrix and \( \hat{x} \) is an approximate solution to \( Cx = d \). Keep in mind that equality is possible on either side of (2).
Part B. (General least squares problems)

1. Let $A \in \mathbb{R}^{m \times n}$, with rank($A$) = $n$, let $A = QR$ be the (full) QR factorization of $A$, with $Q \in \mathbb{R}^{m \times m}$ orthogonal and $R \in \mathbb{R}^{m \times n}$ upper trapezoidal. Also, let $A = Q_1 R_1$ be the reduced QR factorization of $A$ with $Q_1 \in \mathbb{R}^{m \times n}$ having orthonormal columns and $R_1 \in \mathbb{R}^{m \times n}$ upper triangular. Show that $R_1$ is nonsingular, and that the columns $q_1, \ldots, q_n$ of $Q_1$ form an orthonormal basis for Ran($A$), the column space of $A$. Also, find an orthonormal basis for Null($A^T$), the null space of $A^T$.

2. Use $\beta = 10$ and $t = 3$ digit arithmetic to compute $A^T A$ where

$$A = \begin{bmatrix} 1.07 & 1.10 \\ 1.07 & 1.11 \\ 1.07 & 1.15 \end{bmatrix}.$$  

Note that $A$ has full rank. Is the computed $A^T A$ positive definite?

3. Now use $\beta = 10$ and $t = 3$ digit arithmetic to compute the QR factorization of the same matrix $A$ by means of Householder transformations. Discuss your results.

4. Let $A \in \mathbb{R}^{m \times n}$, with rank($A$) = $n$, and let $b \in \mathbb{R}^m$. Let $A = Q_1 R_1$ be a reduced QR decomposition of $A$, where $Q_1 \in \mathbb{R}^{m \times n}$ has orthonormal columns and $R_1 \in \mathbb{R}^{n \times n}$ is upper triangular and nonsingular. Show that a reduced QR factorization of the augmented matrix $A_+ = [A \ b]$ is given by

$$A_+ = [Q_1 \ q_{n+1}] \begin{bmatrix} R_1 & z \\ 0 & \rho \end{bmatrix}$$

where $z = Q_1^T b$. Also, show that $\rho = \|b - Ax^*\|_2$ where $x^*$ is the solution to the least squares problem $\|b - Ax\|_2 = \min$.  

Part C. (Singular Value Decomposition)

1. Recall the relationship that exists between the singular values and singular vectors of an $m \times n$ matrix $A$ and the eigenvalues and eigenvectors of the square symmetric matrices $A^T A$ and $AA^T$.

2. Let $A \in \mathbb{R}^{m \times n}$, with singular value decomposition $A = U \Sigma V^T$ and rank($A$) = $n$. Express the singular values and singular vectors of the following matrices in terms of those of $A$:

   (a) $(A^T A)^{-1}$,
   (b) $(A^T A)^{-1} A^T$,
   (c) $A(A^T A)^{-1}$,
   (d) $A(A^T A)^{-1} A^T$.

3. Let

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 2 \end{bmatrix}.$$  

Using the SVD, work out (on paper) the values of $\sigma_{\min}(A)$ and $\sigma_{\max}(A)$. Also, draw the image of the unit ball (here it’s just the unit circle) under the linear transformation $y = Ax$. What is the value of $\kappa_2(A)$?

4. Let

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \quad \text{and} \quad b = \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$  

Find the minimum norm solution to $\|b - Ax\|_2 = \min$.  

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5. Let

\[ A = \begin{bmatrix}
-4 & -2 & -4 & -2 \\
2 & -2 & 2 & 1 \\
-800 & 200 & -800 & -401 \\
\end{bmatrix}. \]

Using Matlab, determine the singular values of \( A \), the rank of \( A \), and the Moore-Penrose pseudoinverse \( A^+ \). Also, compute \( \kappa_2( A ) \).

6. For the matrix \( A \) in the previous problem, determine the best rank-1 and rank-2 approximations of \( A \), denoted \( A_1 \) and \( A_2 \). What is \( \kappa_2( A_2 ) \)?

7. Let \( R = (r_{ij}) \) be the \( n \times n \) upper triangular matrix with \( r_{ii} = 1 \) and \( r_{ij} = -1 \) for \( j > i \). Plot the singular values of \( R \) for \( n = 10, \ n = 20, \ n = 50 \) and \( n = 100 \). Also, tabulate the spectral condition number \( \kappa_2( R ) \) for all \( n \) from 1 to 60. What can be said about the numerical rank of \( R \) as \( n \) grows?