Assignment 2

(Be sure to observe the rules about handing in homework)

1. Solve:

\[
\begin{align*}
    x_1 + x_2 - x_3 &= -3 \\
    6x_1 + 2x_2 + 2x_3 &= 2 \\
    -3x_1 + 4x_2 + x_3 &= 1
\end{align*}
\]

with \( \text{(a) (10 pts) naive Gauss elimination,} \quad \text{(b) (10 pts) Gauss with partial pivoting} \)

*You need to show all of the steps manually. MATLAB code alone is not acceptable.

Solution

(a) The system is first expressed as an augmented matrix:

\[
\begin{bmatrix}
    1 & 1 & -1 & -3 \\
    6 & 2 & 2 & 2 \\
    -3 & 4 & 1 & 1 \\
\end{bmatrix}
\]

Forward elimination:

\(a_{21}\) is eliminated by multiplying row 1 by \(-6/1 = -6\) and adding the result to row 2. \(a_{31}\) is eliminated by multiplying row 1 by \(3/1 = 3\) and adding the result to row 3.

\[
\begin{bmatrix}
    1 & 1 & -1 & -3 \\
    0 & -4 & 8 & 20 \\
    0 & 7 & -2 & -8 \\
\end{bmatrix}
\]

\(a_{32}\) is eliminated by multiplying row 2 by \(-7/(-4) = 1.75\) and adding the result to row 3.

\[
\begin{bmatrix}
    1 & 1 & -1 & -3 \\
    0 & -4 & 8 & 20 \\
    0 & 0 & 12 & 27 \\
\end{bmatrix}
\]

Back substitution:

\[
x_3 = \frac{27}{12} = 2.25
\]

\[
x_2 = \frac{20 - 8(2.25)}{-4} = -0.5
\]

\[
x_1 = \frac{-3 - (-1)(2.25) - 1(-0.5)}{1} = -0.25
\]
(b) The system is first expressed as an augmented matrix:

\[
\begin{bmatrix}
1 & 1 & -1 & -3 \\
6 & 2 & 2 & 2 \\
-3 & 4 & 1 & 1 \\
\end{bmatrix}
\]

Forward elimination: First, we pivot by switching rows 1 and 2:

\[
\begin{bmatrix}
6 & 2 & 2 & 2 \\
1 & 1 & -1 & -3 \\
-3 & 4 & 1 & 1 \\
\end{bmatrix}
\]

Multiply row 1 by \(-\frac{1}{6}\) = -0.167 and add the result to row 2 to eliminate \(a_{21}\). Multiply row 1 by \(\frac{3}{6} = 0.5\) and add the result to row 3 to eliminate \(a_{31}\).

\[
\begin{bmatrix}
6 & 2 & 2 & 2 \\
0 & 0.67 & -1.34 & -3.34 \\
0 & 5 & 2 & 2 \\
\end{bmatrix}
\]

Pivot:

\[
\begin{bmatrix}
6 & 2 & 2 & 2 \\
0 & 5 & 2 & 2 \\
0 & 0.67 & -1.34 & -3.34 \\
\end{bmatrix}
\]

Multiply row 2 by \(-0.67/5 = -0.134\) and add the result to row 3 to eliminate \(a_{32}\).

\[
\begin{bmatrix}
6 & 2 & 2 & 2 \\
0 & 5 & 2 & 2 \\
0 & 0 & -1.6 & -3.6 \\
\end{bmatrix}
\]

Back substitution:

\[
x_3 = \frac{-3.6}{-1.6} = 2.25
\]

\[
x_2 = \frac{2 - 2(2.25)}{5} = -0.5
\]

\[
x_1 = \frac{2 - 2(2.25) - 2(-0.5)}{6} = -0.25
\]
2. (a) (10 pts) Solve the following system of equations by LU decomposition without pivoting. Show explicitly the $L$ and $U$ matrices found during the process.

\[
\begin{align*}
8x_1 + 4x_2 - x_3 &= 11 \\
-2x_1 + 3x_2 + x_3 &= 4 \\
2x_1 - x_2 + 6x_3 &= 7
\end{align*}
\]

(b) (15 pts) Determine the matrix inverse in three steps (column by column) as taught in class. Check your results by verifying that $[A][A]^{-1} = I$. You may use MATLAB to verify your results.

**Solution**

(a) The coefficient $a_{21}$ is eliminated by multiplying row 1 by $f_{21} = 2/8 = 0.25$ and adding the result to row 2. $a_{31}$ is eliminated by multiplying row 1 by $f_{31} = -(2/8) = -0.25$ and adding the result to row 3. The factors $f_{21}$ and $f_{31}$ can be stored in $a_{21}$ and $a_{31}$.

\[
\begin{bmatrix}
8 & 4 & -1 \\
-0.25 & 4 & 0.75 \\
0.25 & -2 & 6.25
\end{bmatrix}
\]

$a_{32}$ is eliminated by multiplying row 2 by $f_{32} = 2/4 = 0.5$ and adding the result to row 3. The factor $f_{32}$ can be stored in $a_{32}$.

\[
\begin{bmatrix}
8 & 4 & -1 \\
-0.25 & 4 & 0.75 \\
0.25 & -0.5 & 6.625
\end{bmatrix}
\]

Therefore, the $LU$ decomposition is

\[
\begin{bmatrix}
L & \\
U
\end{bmatrix} = \begin{bmatrix}
1 & 0 & 0 \\
-0.25 & 1 & 0 \\
0.25 & -0.5 & 1
\end{bmatrix}
\begin{bmatrix}
8 & 4 & -1 \\
0 & 4 & 0.75 \\
0 & 0 & 6.625
\end{bmatrix}
\]

Forward substitution: $[L]{d} = {b}$

\[
\begin{pmatrix}
1 & 0 & 0 \\
-0.25 & 1 & 0 \\
0.25 & -0.5 & 1
\end{pmatrix}\begin{bmatrix}
d_1 \\
d_2 \\
d_3
\end{bmatrix} = \begin{bmatrix}11 \\
4 \\
7
\end{bmatrix}
\]

Solving yields $d_1 = 11$, $d_2 = 6.75$, and $d_3 = 7.625$

Back substitution:

\[
\begin{pmatrix}
8 & 4 & -1 \\
0 & 4 & 0.75 \\
0 & 0 & 6.625
\end{pmatrix}\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix} = \begin{bmatrix}11 \\
6.75 \\
7.625
\end{bmatrix}
\]

\[
x_3 = \frac{7.625}{6.625} = 1.1509 \\
x_2 = \frac{6.75 - 0.75(1.1509)}{4} = 1.4717 \\
x_1 = \frac{11 - 4(1.4717) + 1(1.1509)}{8} = 0.783
\]
(b) The first column of the inverse can be computed by using $[L][d] = \{b\}$

\[
\begin{bmatrix}
1 & 0 & 0 \\
-0.25 & 1 & 0 \\
0.25 & -0.5 & 1
\end{bmatrix}
\begin{bmatrix}
d_1 \\
d_2 \\
d_3
\end{bmatrix}
= \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}
\]

This can be solved for $d_1 = 1$, $d_2 = 0.25$, and $d_3 = -0.125$. Then, we can implement back substitution

\[
\begin{bmatrix}
8 & 4 & -1 \\
0 & 4 & 0.75 \\
0 & 0 & 6.625
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3
\end{bmatrix}
= \begin{bmatrix} 1 \\ 0.25 \\ -0.125 \end{bmatrix}
\]

to yield the first column of the inverse

\[
\{X1\} = \begin{bmatrix} 0.0896 \\ 0.0660 \\ -0.0189 \end{bmatrix}
\]

For the second column use $\{b\}^T = \{0 \ 1 \ 0\}$ which gives $\{d\}^T = \{0 \ 1 \ 0.5\}$. Back substitution then gives $\{X2\}^T = \{-0.1085 \ 0.2358 \ 0.0755\}$.

For the third column use $\{b\}^T = \{0 \ 0 \ 1\}$ which gives $\{d\}^T = \{0 \ 0 \ 1\}$. Back substitution then gives $\{X3\}^T = \{ 0.0330 \ -0.0283 \ 0.1509\}$.

Therefore, the matrix inverse is

\[
[A]^{-1} = \begin{bmatrix}
0.0896 & -0.1085 & 0.0330 \\
0.0660 & 0.2358 & -0.0283 \\
-0.0189 & 0.0755 & 0.1509
\end{bmatrix}
\]

We can verify that this is correct by multiplying $[A][A]^{-1}$ (in MATLAB) to yield the identity matrix.

\[
>> A=[8,4,-1;-2,3,1;2,-1,6] \\
A = \\
8 \ 4 \ -1 \\
-2 \ 3 \ 1 \\
2 \ -1 \ 6 \\
>> AI = inv(A) \\
AI = \\
0.0896 \ -0.1085 \ 0.0330 \\
0.0660 \ 0.2358 \ -0.0283 \\
-0.0189 \ 0.0755 \ 0.1509 \\
>> A*AI \\
an = \\
1.0000 \ -0.0000 \ 0 \\
0.0000 \ 1.0000 \ -0.0000 \\
-0.0000 \ 0 \ 1.0000
\]
3. Use least-squares regression to fit a straight line to

<table>
<thead>
<tr>
<th>x</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
</tr>
</thead>
<tbody>
<tr>
<td>y</td>
<td>1</td>
<td>1.5</td>
<td>2</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>8</td>
<td>10</td>
<td>13</td>
</tr>
</tbody>
</table>

(a) (7 pts) Along with the slope and intercept, compute $S_r$, $S_t$, and the correlation coefficient $r$ as described in lecture slides (slide#9 in Chap-17e.ppt). Plot the data and the straight line. Assess the fit.

(b) (8 pts) Recompute (a), but use polynomial regression to fit a parabola to the data. Compare the results with those of (a) using the correlation coefficient $r$. Which one (a line or a parabola?) does provide a better fit?

**Solution:**
(* Details are in the supplemental excel file *)

(a) The results can be summarized as $y = -2.0139 + 1.4583x$ $(r = 0.956)$

Although the correlation coefficient appears to be close to 1, the straight line does not describe the data as well as a parabola (as will be seen in part (b)).
(b) The results can be summarized as

\[ y = 1.4881 - 0.45184x + 0.191x^2 \quad (r = 0.997) \]

Comparison of the correlation coefficients (line vs. parabola) indicates that the quadratic fit does a much better job of fitting the data.

![Graph showing linear and quadratic fits](image)

4. Given the data

<table>
<thead>
<tr>
<th>x</th>
<th>5</th>
<th>10</th>
<th>15</th>
<th>20</th>
<th>25</th>
<th>30</th>
<th>35</th>
<th>40</th>
<th>45</th>
<th>50</th>
</tr>
</thead>
<tbody>
<tr>
<td>y</td>
<td>17</td>
<td>24</td>
<td>31</td>
<td>33</td>
<td>37</td>
<td>37</td>
<td>40</td>
<td>40</td>
<td>42</td>
<td>41</td>
</tr>
</tbody>
</table>

use least-squares regression to fit
(a) **(10 pts)** a power equation, and
(b) **(10 pts)** a saturation-growth-rate equation.

Plot the data along with all the curves. Is any one of the curves superior? If so, justify by using the correlation coefficient \( r \).

(* Note that correlation coefficient \( r \) must be calculated using the original data and the fitted non-linear function. In other words, do not use the transformed values for the calculation of the correlation coefficient *)

(*Important Note: Do not use package programs to find the answers. However, you may use the MATLAB programs to check the correctness of your answers.*)
Solution:

(a) **Power equation:** We regress $\log_{10} y$ versus $\log_{10} x$ to give 

$$ \log_{10} y = 0.998 + 0.3851 \log_{10} x $$

Therefore, $\alpha_2 = 10^{0.998} = 9.953$ and $\beta_2 = 0.3851$, and the power model is

$$ y = 9.953 x^{0.3851} $$

The model and the data can be plotted as

![Power Equation Plot](image)

(b) **Saturation-growth-rate:** We regress $1/y$ versus $1/x$ to give

$$ \frac{1}{y} = 0.02 + 0.1974 \frac{1}{x} $$

Therefore, $\alpha_3 = 1/0.02 = 50.09$ and $\beta_3 = 0.1974 * (50.09) = 9.89$, and the saturation-growth-rate model is

$$ y = \frac{x}{9.89 + x} $$

The model and the data can be plotted as

![Saturation-Growth-Rate Plot](image)

**Comparison of fits:** The **linear fit** is obviously inadequate. Although the **power fit** follows the general trend of the data, it is also inadequate because (1) the residuals do not appear to be randomly distributed around the best fit line and (2) it has a lower $r^2$ than the **saturation model**.

Using the $r$ values, we can conclude that the **saturation model** represents the **best fit**.
5. (10 pts) Given the data

<table>
<thead>
<tr>
<th>x</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>5</th>
<th>7</th>
<th>8</th>
</tr>
</thead>
<tbody>
<tr>
<td>f(x)</td>
<td>3</td>
<td>6</td>
<td>19</td>
<td>99</td>
<td>291</td>
<td>444</td>
</tr>
</tbody>
</table>

Calculate $f(4)$ using Newton’s interpolating polynomials of order 1 through 4, i.e. you will calculate $f_1(4)$, $f_2(4)$, $f_3(4)$, and $f_4(4)$. In each case, choose your base points to attain good accuracy (Hint: around the point of interest, i.e. 4). What do your results indicate regarding the order of the polynomial used to generate the data in the table?

Solution:

First, order the points so that they are as close to and as centered about the unknown as possible

- $x_0 = 3$ \hspace{1cm} $f(x_0) = 19$
- $x_1 = 5$ \hspace{1cm} $f(x_1) = 99$
- $x_2 = 2$ \hspace{1cm} $f(x_2) = 6$
- $x_3 = 7$ \hspace{1cm} $f(x_3) = 291$
- $x_4 = 1$ \hspace{1cm} $f(x_4) = 3$

Next, the divided differences can be computed and displayed in the format of Fig. 18.5,

<table>
<thead>
<tr>
<th>$i$</th>
<th>$x_i$</th>
<th>$f(x_i)$</th>
<th>$f[x_{i+1}, x_i]$</th>
<th>$f[x_{i+2}, x_{i+1}, x_i]$</th>
<th>$f[x_{i+3}, x_{i+2}, x_{i+1}, x_i]$</th>
<th>$f[x_{i+4}, x_{i+3}, x_{i+2}, x_{i+1}, x_i]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>3</td>
<td>19</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>5</td>
<td>99</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>2</td>
<td>6</td>
<td>31</td>
<td>9</td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>7</td>
<td>291</td>
<td>57</td>
<td>13</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>3</td>
<td>48</td>
<td>9</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

The first through fourth-order interpolations can then be implemented as

- $f_1(4) = 19 + 40(4 - 3) = 59$
- $f_2(4) = 59 + 9(4 - 3)(4 - 5) = 50$
- $f_3(4) = 50 + 1(4 - 3)(4 - 5)(4 - 2) = 48$
- $f_4(4) = 48 + 0(4 - 3)(4 - 5)(4 - 2)(4 - 7) = 48$

Clearly this data was generated with a cubic polynomial since the difference between the 4th and the 3rd-order versions is zero.
6. (10 pts) Repeat the question above (Q.5) using Lagrange polynomials of order 1 through 3.

Solution:

First order:
\[ x_0 = 3 \quad f(x_0) = 19 \]
\[ x_1 = 5 \quad f(x_1) = 99 \]
\[ f_1(4) = \frac{4 - 5}{3 - 5}f(x_0) + \frac{4 - 3}{5 - 3}f(x_1) = 59 \]

Second order:
\[ x_0 = 3 \quad f(x_0) = 19 \]
\[ x_1 = 5 \quad f(x_1) = 99 \]
\[ x_2 = 2 \quad f(x_2) = 6 \]
\[ f_2(4) = \frac{4 - 5}{3 - 5}f(x_0) + \frac{4 - 3}{5 - 3}f(x_1) + \frac{4 - 2}{2 - 5}f(x_2) = 50 \]

Third order:
\[ x_0 = 3 \quad f(x_0) = 19 \]
\[ x_1 = 5 \quad f(x_1) = 99 \]
\[ x_2 = 2 \quad f(x_2) = 6 \]
\[ x_3 = 7 \quad f(x_3) = 291 \]
\[ f_3(4) = \frac{4 - 5}{3 - 5}f(x_0) + \frac{4 - 3}{5 - 3}f(x_1) + \frac{4 - 2}{2 - 5}f(x_2) + \frac{4 - 7}{7 - 5}f(x_3) = 48 \]