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ADVANCED COMPUTATIONAL TECHNIQUES IN ENGINEERING

Assignment 1

Question 1

Part 1

The goal is to find the parameters that minimise the sum of the absolute deviations between the raw material price and its prediction, hence the optimisation program can be written as:

$$min \sum_{n=1}^{6} | z(n) - ax(n) - by(n) - c |$$

The optimisation variables in this form are only the three parameters a, b, c.
However, the program is not linear due to the absolute value. To write the program as a linear one, it is possible to define a new variable for each deviation and to apply a trick.

$$l(n) = z(n) - ax(n) - by(n) - c \quad n = 1, \dots ,6$$

$$l(n) = l^{+}(n) - l^{-}(n)$$
$$|l(n)| = l^{+}(n) + l^{-}(n)$$

$$l^{+}(n) \geq 0$$
$$l^{-}(n) \geq 0$$

So now the program can be written as:

$$min \sum_{n=1}^{6} l^{+}(n) + l^{-}(n)$$

$$s.t.$$

$$\begin{aligned} &l(n) = z(n) - ax(n) - by(n) - c && n = 1, \dots ,6 \\ &l(n) = l^{+}(n) - l^{-}(n) && n = 1, \dots ,6 \\ &l^{+}(n) \geq 0 && n = 1, \dots ,6 \\ &l^{-}(n) \geq 0 && n = 1, \dots ,6 \end{aligned}$$

In this program, there are 15 optimisation variables, but it is now linear and can be solved through the simplex method.
Hence, by manipulating the constraint equations and using the data provided by the question, the simplex table, **Table 1**, can be built. It is noticeable also that to reach the standard form, the program must be transformed into a maximisation problem by changing the sign of the objective function. Hence, we can write the objective function equation which corresponds to the first row in the simplex table:

$$h + \sum_{n=1}^{6} l^{+}(n) + l^{-}(n) \; = 0$$

	$l^+(1)$	$l^-(1)$	$l^+(2)$	$l^-(2)$	$l^+(3)$	$l^-(3)$	$l^+(4)$	$l^-(4)$	$l^+(5)$	$l^-(5)$	$l^+(6)$	$l^-(6)$	a	b	c	$=$
h	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0
L_1	1	-1	0	0	0	0	0	0	0	0	0	0	9	1	1	5
L_2	0	0	1	-1	0	0	0	0	0	0	0	0	13	8	1	2
L_3	0	0	0	0	1	-1	0	0	0	0	0	0	17	3	1	9
L_4	0	0	0	0	0	0	1	-1	0	0	0	0	8	5	1	10
L_5	0	0	0	0	0	0	0	0	1	-1	0	0	10	9	1	4
L_6	0	0	0	0	0	0	0	0	0	0	1	-1	15	2	1	6

Table 1

Part 2

To find the parameters that minimise the largest absolute deviation between the raw material price and its prediction is possible to define the following program by using the infinity norm:

$$min \ \left|\left|Z - a\mathrm{X} - b\mathrm{Y} - \mathbf{1}c\right|\right|_{\infty}$$

$$\mathrm{Z} = \begin{bmatrix} 5 \\ 2 \\ 9 \\ 10 \\ 4 \\ 6 \end{bmatrix} \quad \mathrm{X} = \begin{bmatrix} 9 \\ 13 \\ 17 \\ 8 \\ 10 \\ 15 \end{bmatrix} \quad \mathrm{Y} = \begin{bmatrix} 1 \\ 8 \\ 3 \\ 5 \\ 9 \\ 2 \end{bmatrix} \quad \mathbf{1} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$

The program is not linear. To transform it into a linear one is possible to define a new variable P.

$$min \ \ P$$

$$s.t.$$

$$Z - a\mathrm{X} - b\mathrm{Y} - \mathbf{1}c \leq \mathbf{1}P$$
$$-Z + a\mathrm{X} + b\mathrm{Y} + \mathbf{1}c \leq \mathbf{1}P$$

In this form, the optimisation variables are a, b, c, P and the program can be solved by using the $linprog$ MATLAB function as shown in **Figure 1**.

```
%% Vectors set up

Z=[5;2;9;10;4;6];        % vector of obsrved prices of raw material

X=[9;13;17;8;10;15];     % vector of observed quantity of product A sold

Y=[1;8;3;5;9;2];         % vector of observed quantity of product B sold

%% linprog usage

f=[0;0;0;1]; % coefficients of the optimisation variables in the objective function

% Definition of inequalities constraints
uno=ones(6,1);
A=[-X,-Y,-uno,-uno;
   +X,+Y,+uno,-uno];
b=[-Z;Z];

% Optimisation
theta=linprog(f,A,b);
```

Figure 1

The results are:

$$a = -0.1831 \quad b = -0.32394 \quad c = 10.0282 \quad \text{Maximum deviation} = 3.0563$$

In **Figure 2** is possible to see the predicted prices using the optimum variables and the observed prices. The data point which shows the maximum deviation is highlighted in orange.

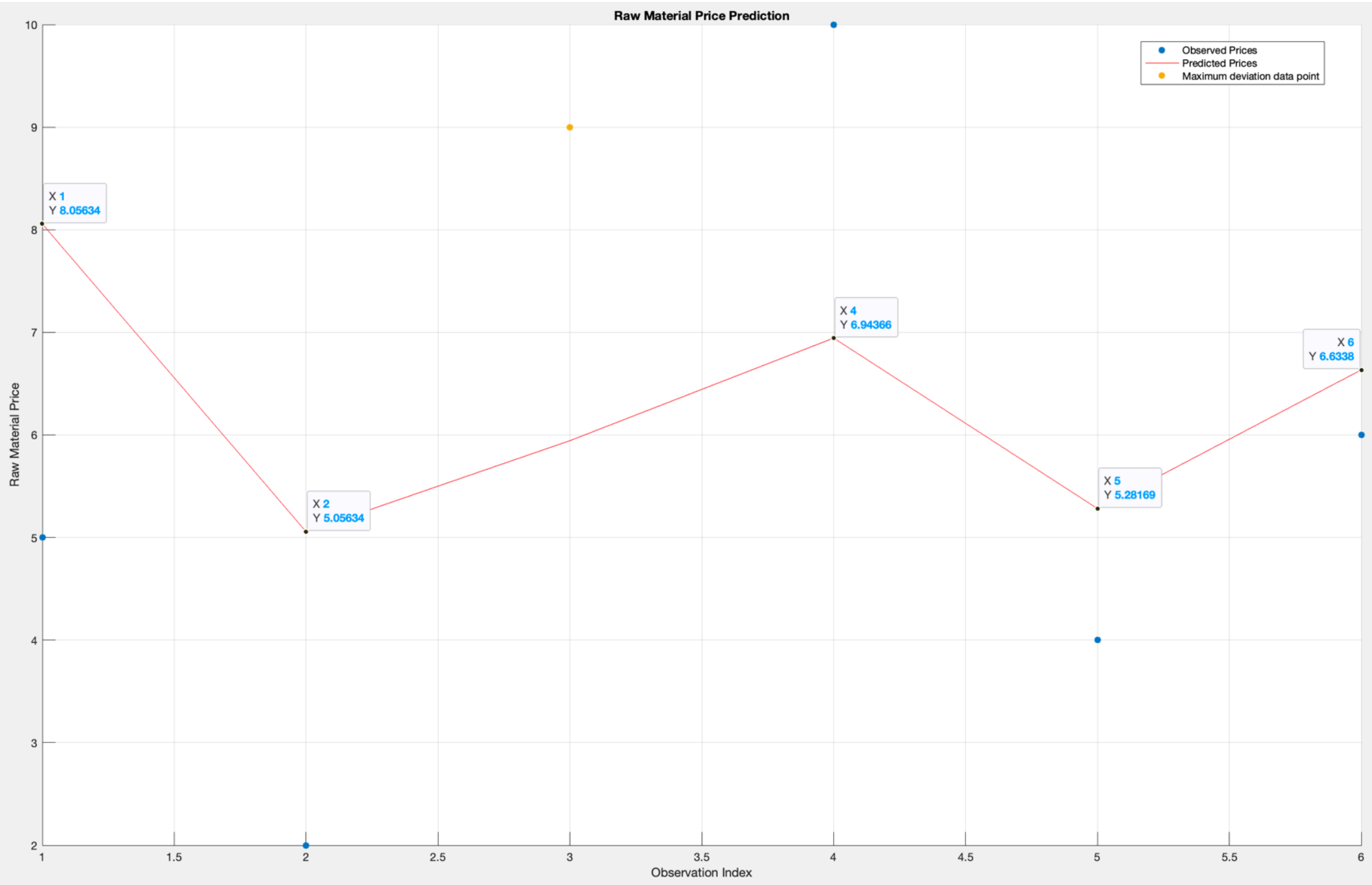

Figure 2

Part 3

The minimisation of the squared deviations between the raw material price and its prediction is carried out through the Least Square procedure.

$$min \sum_{n=1}^{6} (z(n) - ax(n) - by(n) - c)^2$$

From here we can write the linear system of the Least Square procedure.

$$\theta = \begin{bmatrix} a \\ b \\ c \end{bmatrix} \quad A = \begin{bmatrix} 9 & 1 & 1 \\ 13 & 8 & 1 \\ 17 & 3 & 1 \\ 8 & 5 & 1 \\ 10 & 9 & 1 \\ 15 & 2 & 1 \end{bmatrix} \quad Z = \begin{bmatrix} 5 \\ 2 \\ 9 \\ 10 \\ 4 \\ 6 \end{bmatrix}$$

$$A\theta = Z \quad \rightarrow \quad \begin{bmatrix} 9 & 1 & 1 \\ 13 & 8 & 1 \\ 17 & 3 & 1 \\ 8 & 5 & 1 \\ 10 & 9 & 1 \\ 15 & 2 & 1 \end{bmatrix} \begin{bmatrix} a \\ b \\ c \end{bmatrix} = \begin{bmatrix} 5 \\ 2 \\ 9 \\ 10 \\ 4 \\ 6 \end{bmatrix}$$

To solve the system the normal equation can be used.

$$\theta^* = (A'A)^{-1}A' Z$$

The results are:

$$a = -0.0481 \quad b = -0.4233 \quad c = 8.5530$$

The minimum of the square deviations sum is 36.783

Question 2

In this question, the area of a triangle must be maximised respecting some constraints.
The sides of the triangle are x, y, z.
The constraints are:

$$x = y$$
$$x + y + z = 100$$

Hence, the triangle is isosceles, and the perimeter must be equal to 100.
The objective function to be maximised is the area A, where h is the height of the triangle:

$$A = \frac{z\,h}{2}$$

However, by using the constraints equations and the Heron or Pythagoras formula, **Appendix 1**, is possible to reduce A to the expressions:

$$A = 10\,(50 - x)\,\sqrt{x - 25}$$

Now we can define the program as a one-optimisation problem.

$$max \quad 10\,(50 - x)\,\sqrt{x - 25}$$

By plotting the objective function, in **Figure 3,** some considerations can be made.

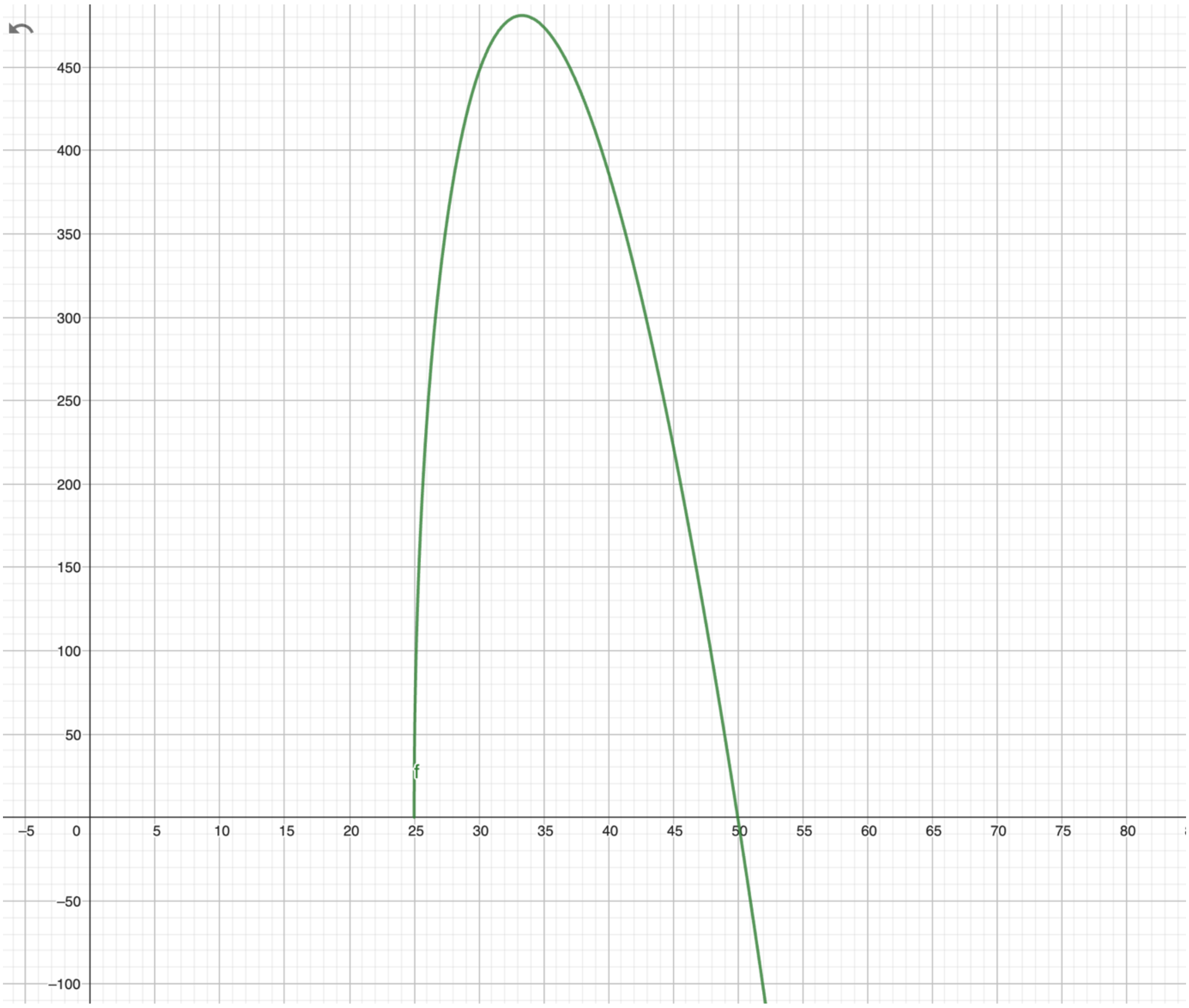

Figure 3

First, it is visible that the two equal sides of the triangle cannot be lower than 25. Indeed, if $x = 25$ then $z = 50$ due to the constraint on the perimeter. This is the limit case where the angles of the triangle and the height are equal to zero. The dual case is where $x = 50$ and $z = 0$. Consequently, the interval of x corresponding to a meaningful result is $25 \leq x \leq 50$.

Successive Parabolic Interpolation method

The first approach to solve the problem is by using the Successive Parabolic Interpolation method. Since in this method the objective function is minimised, the first step is to change the sign of the objective function that we want to maximise.

```
fun=@(x)(-10*(50-x)*sqrt(x-25)); % function to minimise ( Area changed in sign)
```

Following, the three initial points on which the first parabola is interpolated are chosen: $x1 = 25$ and $x3 = 50$ define the search interval, $x2 = 45$ is the initial guess. The parameters to stop the optimisation, **Appendix 2**, are the maximum number of iterations $n = 70$ and the tolerance on the length of the interval $tol = 1$ which is representative of the goodness of the result.

```
%% Successive parabolic interpolation

% Interval and initial guess definition
x1=25;
x2=45;
x3=50;

n=70; %maximum number of interations
tol=1;% tolerance on the lenght of the interval

tic
xmin_parab=parab(fun,x1,x2,x3,n,tol)
toc
```

Figure 4

The optimal sides of the triangle found by the optimisation routine are $x = 33.33$ $y = 33.33$ and $z = 33.33$, so it is an equilateral triangle. The value of the area is $A = 481.13$. The optimisation routine can find the minimum in 58 $iterations$ and roughly $7ms$.

Newton's Method

In this method, after the choice of the initial guess, it is needed to evaluate the first and second derivatives of the objective function at each iteration. The derivatives are computable algebraically and are:

$$f'(x) = -\sqrt{x - 25} + \frac{(50 - x)}{2\sqrt{x - 25}} \qquad f''(x) = \frac{(50 - 3x)}{4(x - 25)^{3/2}}$$

The parameters to stop the optimisation routine are the maximum number of iterations $n = 30$ and the tolerance on the magnitude of the first derivative of the objective function $tol = 10^{-3}$.

```
%% Newton's Method

x0_guess=45; %initial guess
tol=1e-3;    %tolerance on the magnitude of the gradient
n=30;        %maximum number of iterations

tic
xmin_newton=Newton(x0_guess,n,tol)
toc
```

Figure 5

The initial guess is equal to the one used for the Successive Interpolation method to compare the two methods. As shown in **Figure 6** optimisation routine is defined by:

$$x(k+1) = x(k) - \frac{f'\big(x(k)\big)}{f''\big(x(k)\big)}$$

```
function xx=Newton(x0,n,t)

xx=zeros(n,1);
i=1;
xx(1)=x0;

while abs(df(xx(i)))>t && i<n % condition to respect to continue to search

    xx(i+1)=xx(i)-df(xx(i))./ddf(xx(i));
    i=i+1;

end
```

Figure 6

The results of the optimisation are the same as before, but the Newton's method carries out only 6 $iterations$ and a computational time around $2ms$. Consequently, the Newton's method, as expected, is much more effective. Indeed, it converges quadratically since the initial guess is close to the minimizer and the function is well approximated by a parabola.

Appendix

Question 2

Since $x=y$ the triangle is Isosceles

Heron Formula or Pitagora $\longrightarrow x^2 = h^2 + \frac{z^2}{4} \Rightarrow h^2 = x^2 - \frac{z^2}{4} \quad A = \frac{1}{2} z \cdot h = \frac{1}{2} z \sqrt{x^2 - \frac{z^2}{4}} = \frac{z}{4}\sqrt{4x^2 - z^2}$

$$s = \frac{a+b+c}{2} \qquad A = \sqrt{s(s-x)(s-y)(s-z)} \underset{x=y}{=} \frac{z}{4}\sqrt{4x^2 - z^2}$$

$\max \ \frac{z}{4}\sqrt{4x^2 - z^2}$ $\rightarrow$ We can reduce it to one computational dimension problem

s.t.

$2x + z = 100 \Rightarrow z = 100 - 2x$

$$\Downarrow$$

$$\frac{100-2x}{4}\sqrt{4x^2 - (100^2 + 4x^2 - 400x)} = \frac{100-2x}{4}\sqrt{400x - 100^2} = 5(50-x)\sqrt{4x-100} = 10(50-x)\sqrt{x-25}$$

Appendix 1

```
while i<n && (c-a)>t % conditions to be satisfied to continue to iterate

    x= b - ((fb-fc) *(b-a)^2 - (fb-fa)*(b-c)^2) / ...
    (2* ( (fb-fc) * (b-a) - (fb-fa) * (b-c) )) ; %minimum of the interpolated parabola

    fx=f(x);
    xx(i)=x;

    if (x>b)

        if (fx > fb)
            c = x;
            fc = fx;
        else
            a = b;
            fa = fb;
            b = x;
            fb = fx;
        end

    else

        if (fx > fb)
            a = x;
            fa = fx;
        else
            c = b;
            fc = fb;
            b = x;
            fb = fx;
        end

    end
```

Appendix 2