

Chapter-1: Basic Concepts

Problems

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1. Expand e^x as a Maclaurin series. Estimate the value of $e^{0.5}$, e^2 and e^5 using this series to get 1 per cent accuracy with respect to the exact values. How many terms are required to achieve this accuracy level? Repeat the problem by using a Taylor series expansion of e^x about $x = 2.5$? Comment on your results.

Solution:

2. Expand $f(x) = \sqrt{x}$ about $x = 1, 2$ and 4 to second order. Plot the function and the approximation and comment on your results.

Solution:

Taylor series expansion of the function $f(x) = \sqrt{x}$ around the point $x=a$

$$f(x) = f(a) + \frac{\partial f(a)}{\partial x} \cdot (x - a) + \frac{1}{2} \cdot \frac{\partial^2 f(a)}{\partial x^2} \cdot (x - a)^2 + \text{Higher order terms}$$

Second order approximation or quadratic approximation of the function around the point $x=a$ will be

$$f(x) = f(a) + \frac{\partial f(a)}{\partial x} \cdot (x - a) + \frac{1}{2} \cdot \frac{\partial^2 f(a)}{\partial x^2} \cdot (x - a)^2$$

We need the first and second order derivatives for the Taylor series expansion:

$$\frac{\partial f}{\partial x} = \frac{1}{2\sqrt{x}} \quad \text{and} \quad \frac{\partial^2 f}{\partial x^2} = -\frac{1}{4} \cdot x^{-1.5}$$

Now 2nd order approximation of the function around the point $x=1$

$$f(x) = 1 + \frac{1}{2\sqrt{1}} \cdot (x - 1) + \frac{1}{2} \cdot \left(-\frac{1}{4}\right) \cdot (x - 1)^2$$

$$\Rightarrow f(x) = 0.5 + 0.5x - 0.125(x - 1)^2$$

2nd order approximation of the function around the point $x=2$

$$f(x) = \sqrt{2} + \frac{1}{2\sqrt{2}} \cdot (x - 2) + \frac{1}{2} \cdot \left(-\frac{1}{4}\right) 2^{-1.5} \cdot (x - 2)^2$$

$$\Rightarrow f(x) = 0.7071 + 0.3535x - 0.24845(x - 2)^2$$

2nd order approximation of the function around the point $x=4$

$$f(x) = \sqrt{4} + \frac{1}{2\sqrt{4}} \cdot (x - 4) + \frac{1}{2} \left(-\frac{1}{4}\right) 4^{-1.5} \cdot (x - 4)^2 \Rightarrow f(x) = 1 + 0.25x - \frac{1}{64} \cdot (x - 4)^2$$

Plots:

There are four plots i.e. $f(x)$ vs. x ; $f(x)$ at $x=1$ vs. x ; $f(x)$ at $x=2$ vs. x ; and $f(x)$ at $x=4$ vs. x and these four plots are shown in the Matlab as (f vs. x) ; (f1 vs. x) ; (f2 vs. x) ; (f4 vs. x) respectively.

Comment:

From plots it is observed that the 2nd order approximated functions are matching with the original function in the neighbourhoods of the given points or around those points but then the approximated functions diverge from the original one away from the points. This means they are good approximations of the original function locally but not globally.

Thus Taylor's series expansion is local and differs from point to point for most functions. Methods derived from Taylor's series are good locally. The local nature of Taylor's series expansions is very important.

3. Expand the following function in a Taylor series about (1,1) up to two terms:

$$f(x) = x_1 e^{(x_1 + x_2^3)}$$

Solution:

4. Expand the following function in a Taylor series about (1,2) up to two terms

$$f(\mathbf{x}) = x_1^4 + x_2^4 + 4x_1^3 x_2^3$$

Solution:

At any point (x^*) the Taylor series expansion is as

$$f(x) = f(x^*) + \nabla f'(x - x^*) + \frac{1}{2} (x - x^*)' H(x - x^*) + R \dots \dots \dots (1)$$

$$\text{given } f(x) = x_1^4 + x_2^4 + 4x_1^3 x_2^3 \dots \dots \dots (2)$$

$$f(1,2) = 1^4 + 2^4 + 4 * 1^3 * 2^3 = 49$$

$$\nabla f(x_1, x_2) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix}' = \begin{pmatrix} 4x_1^3 + 12x_1^2x_2^3 \\ 4x_2^3 + 12x_1^3x_2^2 \end{pmatrix}' \dots\dots\dots (3)$$

$$\nabla f(1,2) = \begin{pmatrix} 4 * 1^3 + 12 * 1^2 * 2^3 \\ 4 * 2^3 + 12 * 1^3 * 2^2 \end{pmatrix}' = \begin{pmatrix} 100 \\ 80 \end{pmatrix}' \dots\dots\dots (4)$$

$$H(x_1, x_2) = \begin{pmatrix} 12x_1^2 + 24x_1x_2^3 & 36x_1^2x_2^2 \\ 36x_1^2x_2^2 & 12x_2^2 + 24x_1^3x_2 \end{pmatrix} \dots\dots\dots (5)$$

$$H(1,2) = \begin{pmatrix} 204 & 144 \\ 144 & 96 \end{pmatrix} \dots\dots\dots (6)$$

hence

$$f(x) = 49 + \begin{pmatrix} 100 \\ 80 \end{pmatrix}' \begin{pmatrix} (x_1 - 1) \\ (x_2 - 2) \end{pmatrix} + \frac{1}{2} \begin{pmatrix} (x_1 - 1) \\ (x_2 - 2) \end{pmatrix}' \begin{pmatrix} 204 & 144 \\ 144 & 96 \end{pmatrix} \begin{pmatrix} (x_1 - 1) \\ (x_2 - 2) \end{pmatrix}' \dots\dots\dots (7)$$

or

$$f(x) = 102x_1^2 + 48x_2^2 + 144x_1x_2 - 392x_1 - 256x_2 + 371 \dots\dots\dots Ans.$$

5. Expand the Rosenbrock function $f(\mathbf{x}) = 100(x_2 - x_1^2) + (1 - x_1)^2$ about (1,1) as a Taylor series retaining (a) two terms and (b) three terms. Compare these approximations in the vicinity of (1, 1) with the actual function. Comment on your results.

Solution:

Given the Rosenbrock function $f(\mathbf{x}) = 100(x_2 - x_1^2) + (1 - x_1)^2$ (Eq. (1)) which to be expanded about (1,1) as a Taylor series retaining (a) 2 terms &(b) 3 terms. We can write the Taylor's series in matrix notation for a function of n variables as

$$f(\mathbf{x}) = f(\mathbf{x}^*) + \nabla f^T(\mathbf{x} - \mathbf{x}^*) + 1/2(\mathbf{x} - \mathbf{x}^*)^T \mathbf{H}(\mathbf{x} - \mathbf{x}^*) + R$$

Where R is the higher order terms (that are neglected) and n=2

Here,

$$\mathbf{x} = (x_1, x_2), \mathbf{x}^* = (x_1^*, x_2^*) = (\mathbf{1}, \mathbf{1}), (\mathbf{x} - \mathbf{x}^*) = [(x_1 - 1) \quad (x_2 - 1)]$$

$$f(\mathbf{x}^*) = f(x_1^*, x_2^*) = 0$$

$$\nabla f(\mathbf{x}^*) = \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2} \right) = (-200, 100)$$

$$\mathbf{H}(\mathbf{x}^*) = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_1 \partial x_2} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix} = \begin{bmatrix} -198 & 0 \\ 0 & 0 \end{bmatrix}$$

(a) Therefore retaining 2 terms the Taylor series expansion is:

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{x}^*) + \nabla f^T(\mathbf{x} - \mathbf{x}^*) \\ &= 0 + \begin{bmatrix} -200 \\ 100 \end{bmatrix} [(x_1 - 1) \quad (x_2 - 1)] \\ f(\mathbf{x}) &= -200(x_1 - 1) + 100(x_2 - 1) \dots \dots \dots \text{Eqn (2)} \end{aligned}$$

(b) Therefore retaining 3 terms the Taylor series expansion is:

$$\begin{aligned} f(\mathbf{x}) &= f(\mathbf{x}^*) + \nabla f^T(\mathbf{x} - \mathbf{x}^*) + \frac{1}{2}(\mathbf{x} - \mathbf{x}^*)^T \mathbf{H}(\mathbf{x} - \mathbf{x}^*) \\ &= 0 + \begin{bmatrix} -200 \\ 100 \end{bmatrix} [(x_1 - 1) \quad (x_2 - 1)] + \frac{1}{2} \begin{bmatrix} (x_1 - 1) \\ (x_2 - 1) \end{bmatrix} \begin{bmatrix} -198 & 0 \\ 0 & 0 \end{bmatrix} \\ &\quad \cdot [(x_1 - 1) \quad (x_2 - 1)] \\ f(\mathbf{x}) &= -200(x_1 - 1) + 100(x_2 - 1) - 99(x_1 - 1)^2 \dots \dots \dots \text{Eqn(3)} \end{aligned}$$

Now we are considering the equations (1),(2) &(3) in the vicinity of (1,1), say at $\mathbf{x} = (1 + \delta, 1 + \delta)$ where δ being a real number such that $|\delta| \ll 1$.

$$\begin{aligned} \text{From Eq (1), } f(\mathbf{x}) &= 100 [(1 + \delta) - (1 + \delta)^2] + [1 - (1 + \delta)]^2 \\ &= -100\delta - 99\delta^2 \end{aligned}$$

$$\begin{aligned} \text{From Eq (2), } f(\mathbf{x}) &= -200[(1 + \delta) - 1] + 100[(1 + \delta) - 1] \\ &= -100\delta \end{aligned}$$

$$\begin{aligned} \text{From Eq (3), } f(\mathbf{x}) &= -200[(1 + \delta) - 1] + 100[(1 + \delta) - 1] - 99[(1 + \delta) - 1]^2 \\ &= -100\delta - 99\delta^2 \end{aligned}$$

Comparing these approximations we conclude that evaluation of the Taylor Series expansion of function $f(x)$ in the vicinity of (x^*) is more accurate (rather exact) when we retain 3 terms than in the case when we retain 2 terms.

6. Find a cubic polynomial with minimum at 5 and max at -5.

Solution:

Let $f(x)$ is the cubic polynomial for which min is at 5 and max at -5.

For the function to be minimum or maximum,

$$f'(x) = 0$$

Since $f(x)$ is a cubic polynomial $f'(x)$ is a quadratic polynomial

Roots of $f'(x)=0$ are $x=5$ and $x=-5$ (since min at 5 and max at -5)

$$\begin{aligned}\Rightarrow f'(x) &= (x+5)(x-5) \\ &= x^2 - 25\end{aligned}$$

On integrating $f'(x)$, gives

$$f(x) = \frac{x^3}{3} - 25x + \text{constant}$$

Let constant of integration = 0

So $f(x) = \frac{x^3}{3} - 25x$ is the polynomial whose min at 5 and max at -5

$$(f''(x) = 2x,$$

$$f''(5) = 10 > 0 \text{ so } x=5 \text{ is the minimum point}$$

$$f''(-5) = -10 < 0 \text{ so } x=-5 \text{ is the maximum point)}$$

7. Find the stationary points of the following function and determine if they are minimum, maximum or points of inflexion.

$$f(x) = x^4 - 6x^3 + 3x^2 + 10x$$

Graphically verify your results.

Solution: Given,

$$f(x) = x^4 - 6x^3 + 3x^2 + 10x$$

Differentiating the function,

$$f'(x) = 4x^3 - 18x^2 + 6x + 10$$

$$f''(x) = 12x^2 - 36x + 6$$

For determination of the stationary points we need to equate $f'(x) = 0$

$$f'(x) = 0$$

$$\Rightarrow 4x^3 - 18x^2 + 6x + 10 = 0 \dots\dots\dots(1)$$

Solving Equation (1) we get $x=3.962$, -0.57 and 1.11

So, the stationary points of the given function are 3.962 , -0.57 and 1.11

We need to find if they are minimum points, maximum points or points of inflexion. So, we determine the values of $f''(x)$ at the stationary points.

$$f''(x) = 51.74 > 0 \text{ at } x=3.962$$

$$f''(x) = 30.4 > 0 \text{ at } x=-0.57$$

$$f''(x) = -19.15 < 0 \text{ at } x=1.11$$

From these values of $f''(x)$ we can comment that there are two local minimum points (at $x=3.962$ and -0.57) and one local maximum point (at $x=1.11$). A global minimum or maximum for $f(x)$ does not exist since the domains as well as the function are not bounded.

Now,

$$f(x) = -40.04 \text{ at } x=3.962$$

$$f(x) = -3.51 \text{ at } x=-0.57$$

$$f(x) = 8.11 \text{ at } x=1.11$$

So, we can say that one local minimum is at $x=3.962$ and the value of $f(x)$ at that local minimum point is -40.04 . Another local minimum is at $x=-0.57$ and the value of $f(x)$ at that local minimum point is -3.51 . The local maximum is at $x=1.11$ and the value of $f(x)$ at that local maximum point is 8.11 .

Graphical determination

Since the domain and the function $f(x)$ are unbounded, (i.e., x and $f(x)$ are allowed to have any value between $-\infty$ and $+\infty$) there is no global minimum or maximum for the function. Figure 1 is showing a plot between $f(x)$ and x , for the x values are ranging between -1.25 to 5.25 . We can find that one local minimum is at $x=3.962$ and the value of $f(x)$ at local minimum point is -40.04 , another local minimum is at $x=-0.57$ and the value of $f(x)$ at local minimum point is -3.51 and the local maximum is at $x=1.11$ and the value of $f(x)$ at local maximum point is 8.11 .

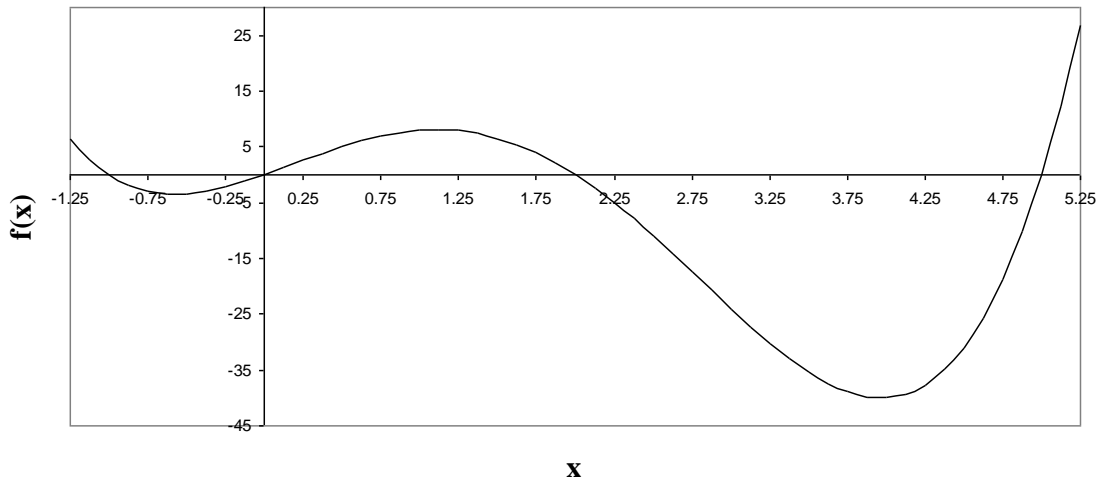


Figure 1: Graph of the given function

8. What are the stationary points of the function f as a function of the scalar c .

$$f(x) = cx_1^2 + \frac{1}{2}x_2^2 - 2x_1x_2 - 4x_2.$$

For what value or values of c is the point a minima, maxima or a point of inflection?

Solution:

9. Find the stationary points of the function

$$f(x_1, x_2) = (x_1^2 - x_2^2)e^{-(x_1^2 + x_2^2)}$$

Determine if the points are minimum, maximum or points of inflexion. Plot the function to verify your results. Conduct an exhaustive search of the design space by creating a grid in terms of the two design

variables and write a computer program to find the minimum and maximum points. Comment on your results.

Solution:

We calculate the gradient and set it to zero

$$\nabla f = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \end{pmatrix} = 0$$

$$\frac{\partial f}{\partial x_1} = 2x_1 e^{-(x_1^2+x_2^2)}(1 - x_1^2 + x_2^2) = 0$$

$$\frac{\partial f}{\partial x_2} = -2x_2 e^{-(x_1^2+x_2^2)}(1 + x_1^2 - x_2^2) = 0$$

Solving the above two equations for x_1 and x_2 we get the following feasible stationary points

x_1	0	0	0	1	-1
x_2	0	1	-1	1	0

The Hessian is calculated as

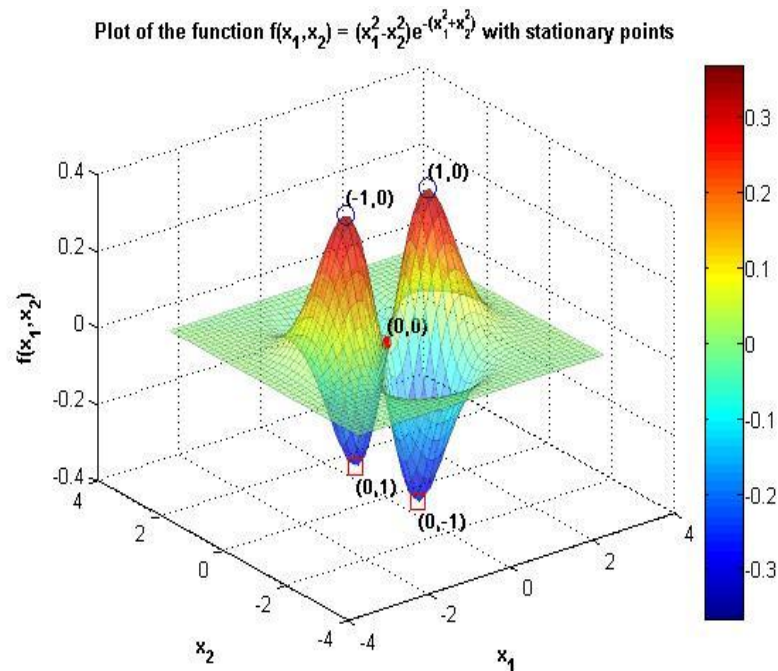
$$H = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} \end{bmatrix}$$

$$\frac{\partial^2 f}{\partial x_1^2} = 2e^{-(x_1^2+x_2^2)}(2x_1^4 - 2x_1^2x_2^2 - 5x_1^2 + x_2^2 + 1)$$

$$\frac{\partial^2 f}{\partial x_2^2} = -2e^{-(x_1^2+x_2^2)}(2x_2^4 - 2x_1^2x_2^2 - 5x_2^2 + x_1^2 + 1)$$

$$\frac{\partial^2 f}{\partial x_1 \partial x_2} = \frac{\partial^2 f}{\partial x_2 \partial x_1} = 4x_1x_2 e^{-(x_1^2+x_2^2)}(x_1^2 - x_2^2)$$

x_1	x_2	H	Eigen values of H	Conclusion
0	0	$\begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$	2, -2	Hessian Indefinite. Hence (0, 0) is a saddle point $f(0,0) = 0$
0	1	$\begin{bmatrix} 4/e & 0 \\ 0 & 4/e \end{bmatrix}$	4/e, 4/e	Hessian Positive Definite. Hence (0, 1) is a minimum point $f(0,1) = -0.3679$
0	-1	$\begin{bmatrix} 4/e & 0 \\ 0 & 4/e \end{bmatrix}$	4/e, 4/e	Hessian Positive Definite. Hence (0, -1) is a minimum point $f(0, -1) = -0.3679$
1	0	$\begin{bmatrix} -4/e & 0 \\ 0 & -4/e \end{bmatrix}$	-4/e, -4/e	Hessian Negative Definite. Hence (1, 0) is a maximum point $f(1,0) = 0.3679$
-1	0	$\begin{bmatrix} -4/e & 0 \\ 0 & -4/e \end{bmatrix}$	-4/e, -4/e	Hessian Negative Definite. Hence (-1, 0) is a maximum point $f(-1,0) = 0.3679$



This verifies that the points that were calculated earlier are indeed the stationary points with respective maxima, minima and saddle point conditions. For finding the solution using exhaustive search more number of grid points are required

MATLAB Program for searching the maxima and minima:

%This program searches for the maxima and minima

```
clear;clc;

x1=-3:0.1:3;

x2=x1;

fmax(1)=0;

fmin(1)=0;

kk=1;mm=1;

changemin=0;

changemax=0;

for ii=1:length(x1)

    for jj=1:length(x2)
```

```
f(ii,jj)=(x1(ii)^2-x2(jj)^2)*exp(-(x1(ii)^2+x1(jj)^2));
```

```
if f(ii,jj)>fmax(kk)
```

```
    if changemax==1
```

```
        kk=1;
```

```
        fmax=[];
```

```
        pmax=[];
```

```
        changemax=0;
```

```
    end
```

```
    fmax(kk)=f(ii,jj);
```

```
    pmax(kk,:)=[x1(ii) x2(jj)];
```

```
elseif f(ii,jj)==fmax(kk)
```

```
    kk=kk+1;
```

```
    changemax=1;
```

```
    fmax(kk)=f(ii,jj);
```

```
    pmax(kk,:)=[x1(ii) x2(jj)];
```

```
end
```

```
if f(ii,jj)<fmin(mm)
```

```
    if changemin==1
```

```
        mm=1;
```

```
        fmin=[];
```

```
        pmin=[];
```

```
        change=0;
```

```
    end
```

```
    fmin(mm)=f(ii,jj);
```

```
pmin(mm,:)= [x1(ii) x2(jj)];  
  
elseif f(ii,jj)==fmin(mm)  
  
    mm=mm+1;  
  
    changemin=1;  
  
    fmin(mm)=f(ii,jj);  
  
    pmin(mm,:)= [x1(ii) x2(jj)];  
  
end  
  
end  
  
end  
  
disp('The maxima points are');  
  
disp(pmax);  
  
disp('The corresponding maxima values are');  
  
disp(fmax);  
  
disp('The minima points are');  
  
disp(pmin);  
  
disp('The corresponding minima values are');  
  
disp(fmin);
```

OUTPUT:

The maxima points are

-1 0

1 0

The corresponding maxima values are

0.3679 0.3679

The minima points are

0 -1

0 1

The corresponding minima values are

0.3679 -0.3679

10. Solve the following problem using optimality criteria:

Minimize $f(x_1, x_2) = x_1^4 + x_2^4$ **subject to** $x_1 + 8x_2 = 32$.

Solution:

$$\frac{\partial L}{\partial x_1} = 4x_1^3 + v = 0$$

$$\frac{\partial L}{\partial x_2} = 4x_2^3 + 8v = 0$$

$$\frac{\partial L}{\partial v} = x_1 + 8x_2 - 32 = 0$$

From equations on solving these equations

$$v = -4x_1^3$$

$$4x_2^3 + 8(-4x_1^3) = 0$$

$$x_2 = 2x_1$$

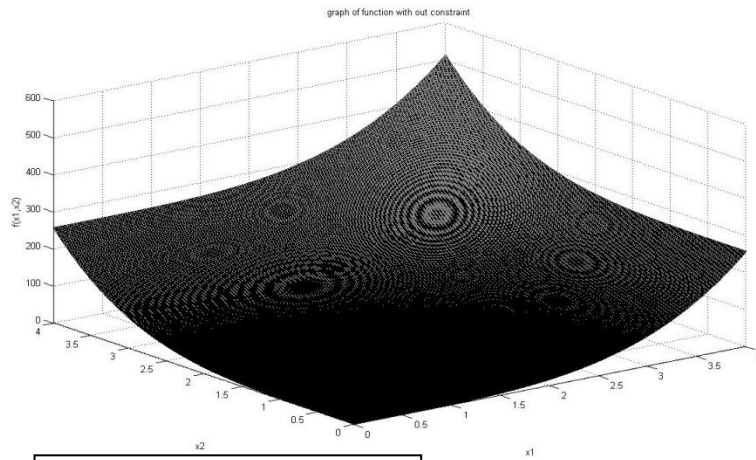
$$x_1 + 8(2x_1) - 32 = 0$$

$$= \frac{32}{17} = 1.882$$

$$x_2 = \frac{64}{17} = 3.764$$

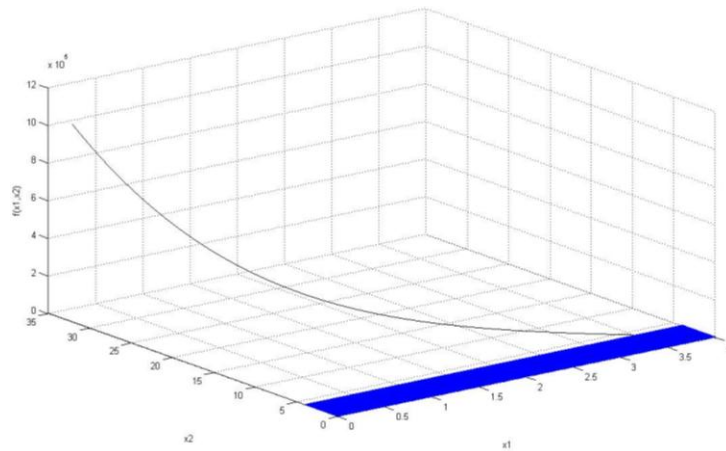
The optimal value of the function is given at (1.882 , 3.764)

$$f(x_1^*, x_2^*) = 17.71626$$



No constrain, Function Curve

From the above figure we can understand that the optimum value of the function comes at(1.882,3.764)while the minimum valu of the function with out constreints is at(0,0)



Constrained Function Curve

11. Solve the problem using optimality criteria

Minimize e^x subject to $1 - x^2 \geq 0$

Solution: First we need to convert the inequality constraint into the desired form:- $x_2 - 1 \leq 0$

The inequality is transformed to equality by adding a positive number. $x_2 - 1 + s^2 = 0$

Here s is called a slack variable and can have any real value. Obviously, $s^2 \geq 0$

Now the constrained optimization problem is converted into unconstrained problem using Lagrangian function as:

$$L = e^x + u(x^2 - 1 + s^2)$$

The Lagrange multipliers for each inequality constraint must be non-negative. *i.e.* $u \geq 0$. If the inequality constraint is inactive at the optimum, $u = 0$. If the inequality constraint is active then $u \geq 0$.

Next, we set the gradient of the Lagrange function to zero

$$\frac{\partial L}{\partial x} = e^x + 2ux = 0$$

$$\frac{\partial L}{\partial u} = x^2 - 1 + s^2 = 0$$

$$\frac{\partial L}{\partial s} = 2us = 0$$

Now, we consider the various possibilities created by the switching condition $us = 0$

Case I:

$$s = 0, u \neq 0$$

$$e^x + 2ux = 0 \Rightarrow u = \frac{e^{-1}}{2}, -\frac{e^{+1}}{2}$$

$$x^2 - 1 = 0 \Rightarrow x = \pm 1$$

$$us = 0$$

Solving these equations yields $x = \pm 1$, $s^2 = 0$, $u = \frac{e^{-1}}{2}, -\frac{e^{+1}}{2}$. This solution corresponds to a case where the inequality is active.

Case II: