Assignment #1: Review of Numerical Methods and Basics of Optimization

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Course : Numerical Optimization
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1. Consider the following function and do the following (by hand):

$$f(\mathbf{x}) = 2x_1^2 - 3x_2^2 + 4x_1x_2 + (x_3+2)^2 + 4x_1$$

(a) What are the gradient and Hessian of $f(\mathbf{x})$?

$$\nabla^T f(\mathbf{x}) = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \frac{\partial f}{\partial x_3} \end{bmatrix} = \begin{bmatrix} 4x_1 + 4x_2 + 4 \\ -6x_2 + 4x_1 \\ 2x_3 + 4 \end{bmatrix}$$

$$\mathbf{H}(\mathbf{x}) = \nabla(\nabla^T f(\mathbf{x})) = \begin{bmatrix} \frac{\partial^2 f(\mathbf{x})}{\partial x_1^2} & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_2} & \frac{\partial^2 f(\mathbf{x})}{\partial x_1 \partial x_3} \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_2^2} & \frac{\partial^2 f(\mathbf{x})}{\partial x_2 \partial x_3} \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_3 \partial x_1} & \frac{\partial^2 f(\mathbf{x})}{\partial x_3 \partial x_2} & \frac{\partial^2 f(\mathbf{x})}{\partial x_3^2} \end{bmatrix} = \begin{bmatrix} 4 & 4 & 0 \\ 4 & -6 & 0 \\ 0 & 0 & 2 \end{bmatrix}$$

(b) What are the stationary point(s) of $f(x)$?

The gradient of function at the stationary point is zero. Let stationary point $\mathbf{x}^*$

$$\to \nabla f(\mathbf{x}^*) = \mathbf{0}$$

$$\to \begin{bmatrix} 4x_1^* + 4x_2^* + 4 \\ -6x_2^* + 4x_1^* \\ 2x_3^* + 4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 4 & 4 & 4 \\ 4 & -6 & 0 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} x_1^* \\ x_2^* \\ x_3^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ -4 \end{bmatrix}$$

By Gaussian elimination process,

$$\rightarrow \begin{bmatrix} 4 & 4 & 4 \\ 4 & -6 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1^* \\ x_2^* \\ x_3^* \end{bmatrix} = \begin{bmatrix} 8 \\ 0 \\ -2 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 1 & 1 & 0 \\ 0 & -10 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1^* \\ x_2^* \\ x_3^* \end{bmatrix} = \begin{bmatrix} 2 \\ -8 \\ -2 \end{bmatrix}$$

$$\rightarrow \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1^* \\ x_2^* \\ x_3^* \end{bmatrix} = \begin{bmatrix} 1.2 \\ 0.8 \\ -2 \end{bmatrix}$$

$$\therefore \mathbf{x}^* = \begin{bmatrix} 1.2 \\ 0.8 \\ -2 \end{bmatrix}$$

(c) Is the Hessian positive-definite?

To determine if Hessian is positive-definite, the eigenvalues of Hessian should be evaluated. Let $\mathbf{x}^*$ eigenvector and λ eigenvalues

$$\rightarrow (\mathbf{H} - \lambda \mathbf{I})\mathbf{x}^* = \mathbf{0}$$

$$\rightarrow \begin{bmatrix} 4-\lambda & 4 & 0 \\ 4 & -6-\lambda & 0 \\ 0 & 0 & 2-\lambda \end{bmatrix} \begin{bmatrix} x_1^* \\ x_2^* \\ x_3^* \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$\rightarrow det(\mathbf{H} - \lambda \mathbf{I}) = 0$$

$$\rightarrow (\lambda - 2)(\lambda^2 + 2\lambda - 40) = 0$$

The product of the roots of the second-order equation is negative, so the eigenvalues of the characteristic equation must have different signs.
Therefore the Hessian is indeterminate, rather than positive-definite

2. Let $f(x) = \sin(x)$ be a function that you are interested in optimizing. Please answer the following questions completely:

(a) What are the necessary conditions for a solution to be an optimum of $f(x)$?

If $\mathbf{x}^*$ is a local minimizer of a function f which is continuously differentiable near $\mathbf{x}^*$, then:

$$\nabla f(\mathbf{x}^*) = 0$$

That is, the gradient of f at $\mathbf{x}^*$ must be zero if $\mathbf{x}^*$ is a local minimizer.
Proof by Contradiction,

Assume $\mathbf{x}^*$ is a local minimizer of $f(\mathbf{x})$, but:

$$\nabla f(\mathbf{x}^*) \neq 0$$

Using a second-order Taylor expansion:

$$f(\mathbf{x}^* + \mathbf{p}) = f(\mathbf{x}^*) + \nabla f(\mathbf{x}^*)^\top \mathbf{p} + \frac{1}{2}\mathbf{p}^\top H(f(\mathbf{x}))\mathbf{p}$$

Let $\mathbf{p} = -\gamma \nabla f(\mathbf{x}^*)$, for some small $\gamma > 0$. Then:

$$f(\mathbf{x}^* + \mathbf{p}) = f(\mathbf{x}^*) - \gamma \|\nabla f(\mathbf{x}^*)\|_2^2 + \mathcal{O}(\gamma^2)$$

For sufficiently small γ, the second-order term is negligible, so:

$$f(\mathbf{x}^* + \mathbf{p}) < f(\mathbf{x}^*)$$

This contradicts the assumption that $\mathbf{x}^*$ is a local minimizer.

$$\therefore \quad \nabla f(\mathbf{x}^*) = 0$$

In this case, $f(x)$ is univariate function so $\frac{df(x^*)}{dx}$ should be zero to be local minimum at x^*. The necessary condition for a local maximum follows in the same way.

(b) Using the necessary conditions obtained in (a), and considering the interval $0 \leq x \leq 2\pi$, obtain the stationary point(s)?

$$
\begin{aligned}
f(x) &= \sin x \\
\frac{df(x)}{dx} &= \cos x \\
\text{Set } \frac{df(x^*)}{dx} &= 0 \Rightarrow \cos x = 0 \\
&\Rightarrow x_1^* = \frac{\pi}{2}, \quad x_2^* = \frac{3\pi}{2}
\end{aligned}
$$

(c) Confirm whether the above point(s) are inflection points, maxima, or minima. If they are maxi- mum (or minimum) points, are they global maximum (or minimum) in the given interval?

$$
\begin{aligned}
\frac{d^2 f(x)}{dx^2} &= -\sin x \\
\text{At } x_1^* = \frac{\pi}{2} : \frac{d^2 f(x)}{dx^2} &= -\sin\left(\frac{\pi}{2}\right) = -1 < 0 \\
&\Rightarrow x_1^* \text{ is a local maximum} \\
f(x_1^*) &= \sin\left(\frac{\pi}{2}\right) = 1 \\
\text{At } x_2^* = \frac{3\pi}{2} : \frac{d^2 f(x)}{dx^2} &= -\sin\left(\frac{3\pi}{2}\right) = 1 > 0 \\
&\Rightarrow x_2^* \text{ is a local minimum} \\
f(x_2^*) &= \sin\left(\frac{3\pi}{2}\right) = -1
\end{aligned}
$$

$$
\begin{aligned}
f(x_2^*) = -1 < f(0) = 0 < f(x_1^*) = 1 \\
f(x_2^*) = -1 < f(\pi) = 0 < f(x_1^*) = 1
\end{aligned}
$$

$$
\therefore \text{At the given interval, } x^* = \frac{\pi}{2} \text{ is the global maximum, and } x^* = \frac{3\pi}{2} \text{ is the global minimum.}
$$

(d) Plot the function $\sin(x)$ over the interval $0 \leq x \leq 2\pi$. Show all the stationary points on it, and label them appropriately (maximum, minimum, or inflection).

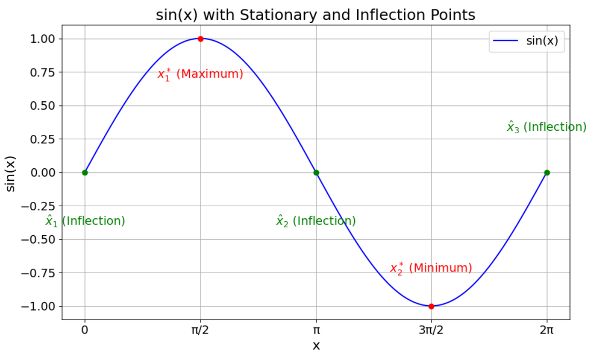

Figure 1: Problem 2.(d) - Graph of $\sin(x)$ with labeled stationary and inflection points.

3. Consider the single variable function $f(x) = e - ax^2$, where a is a constant. This function is often used as a "radial basis function" for function approximation. Please answer the following questions completely:

(a) Is the point $x = 0$ a stationary point for (i) $a > 0$, and (ii) $a < 0$. What happens if $a = 0$? Is $x = 0$ still a stationary point?

$$f'(x) = -2ax \cdot e^{-ax^2}$$

$$f'(0) = 0 \Rightarrow x = 0 \text{ is a stationary point regardless of the sign of } a.$$

$$\text{If } a = 0, \quad f(x) = 0 \quad \text{(constant function).}$$

Since every point on a constant function is a stationary point, $x = 0$ is still a stationary point.

(b) If $x = 0$ is a stationary point, classify it as a minimum, maximum, or an inflection point for (i) $a > 0$,(ii) $a < 0$, and (iii) $a = 0$.

$$\begin{aligned} f''(x) &= -2ae^{-ax^2} + 4a^2x^2e^{-ax^2} = e^{-ax^2}(-2a + 4a^2x^2) \\ &= 4a^2e^{-ax^2}\left(x^2 - \frac{1}{2a}\right) \\ f''(0) &= -2a \end{aligned}$$

$$\begin{cases} < 0 & \text{if } a > 0 \Rightarrow x = 0 \text{ is a local maximum} \\ > 0 & \text{if } a < 0 \Rightarrow x = 0 \text{ is a local minimum} \\ = 0 & \text{if } a = 0 \Rightarrow x = 0 \text{ is an inflection point} \end{cases}$$

(c) Prepare a plot of f(x) for $a = 1$, $a = 2$, and $a = 3$. Plot all three curves on the same figure. By observing the plot, do you think $f(x) = e - ax^2$, $a > 0$ has a global minimum? If so, what is the value of x and $f(x)$ at the minimum?

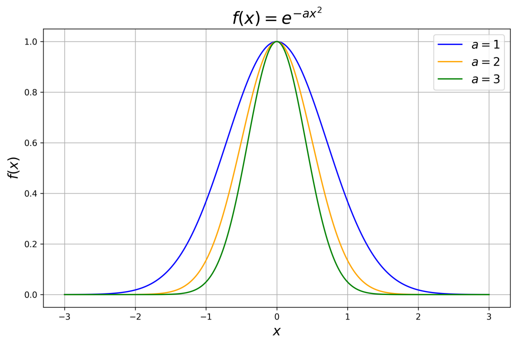

Figure 2: Problem 3.(c) - Graph of e^{-ax^2} with three different positive a values.

I think $f(x)$ would have a global minimum, if certain finite boundary is given. If given boundary is $[-b; b]$, global minimum value will be e^{-ab^2}.

4. Let $A = \begin{bmatrix} 3 & 4 \\ 2 & 1 \end{bmatrix}$

(a) Use the definition to determine whether $\begin{bmatrix} -\pi \\ \pi \end{bmatrix}$ and $\begin{bmatrix} 1 \\ 2 \end{bmatrix}$ are eigenvectors. of A associated with $\lambda = -1$.

$$A\begin{bmatrix}-\pi\\ \pi\end{bmatrix}=\begin{bmatrix}3&4\\2&1\end{bmatrix}\begin{bmatrix}-\pi\\ \pi\end{bmatrix}=\begin{bmatrix}-3\pi+4\pi\\-2\pi+\pi\end{bmatrix}=\begin{bmatrix}\pi\\-\pi\end{bmatrix}=-1\cdot\begin{bmatrix}-\pi\\ \pi\end{bmatrix}$$

Therefore, $\begin{bmatrix}-\pi\\ \pi\end{bmatrix}$ is an eigenvector of A with eigenvalue -1.

$$A\begin{bmatrix}1\\2\end{bmatrix}=\begin{bmatrix}3&4\\2&1\end{bmatrix}\begin{bmatrix}1\\2\end{bmatrix}=\begin{bmatrix}11\\4\end{bmatrix}=2\begin{bmatrix}1\\2\end{bmatrix}+\begin{bmatrix}9\\0\end{bmatrix}$$

$\therefore \begin{bmatrix}1\\2\end{bmatrix}$ is not an eigenvector.

(b) Is either of the given eigenvectors of A associated with $\lambda = 5$?

$$\begin{bmatrix}3&4\\2&1\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix}=5\begin{bmatrix}x_1\\x_2\end{bmatrix}$$

$$\begin{cases}3x_1+4x_2=5x_1\Rightarrow x_1=2x_2\\2x_1+x_2=5x_2\Rightarrow x_1=2x_2\end{cases}$$

$$\begin{bmatrix}x_1\\x_2\end{bmatrix}=x_2\begin{bmatrix}2\\1\end{bmatrix}$$

$\therefore \lambda=5$ is eigenvalue and $\begin{bmatrix}2\\1\end{bmatrix}$ is corresponding eigenvector.

(c) What is the point of this exercise?
If either eigenvector or eigenvalue is known, the other one could be evaluated as well.

5. Use the Bisection, Fixed-Point, Newton's, and Secant methods to find solutions accurate to within 10^{-5} for the following problems:
(a) $x^2-4x+4-ln(x)=0$ for $1\le x\le 2$ and $2\le x\le 4$
(b) $x+1-2sin(\pi x)=0$ for $0\le x\le 0.5$ and $0.5\le x\le 1$
Write a code to solve the above problems using the specified methods. Provide a plot illustrating the convergence of the error versus the number of iterations. For the fixed-point, Newton's, and Secant methods set x_0 to be the minimum point for the specified range. In addition to the plot, show a table with four entries of the values of $x, f(x)$ and the error $f(x)$. You may treat x as $\bar{x}$ in these cases. Out of the four entries, provide the initial value, the final values and two intermediary values during the convergence of the algorithm.

6. Let $f(x,y)=x^3-x+y^3-y$
(a) Graph the surface $z=f(x,y)$.

(b) Verify that the complete list of critical points of f is $\left(-\frac{1}{\sqrt3},-\frac{1}{\sqrt3}\right)$, $\left(-\frac{1}{\sqrt3},\frac{1}{\sqrt3}\right)$, $\left(\frac{1}{\sqrt3},-\frac{1}{\sqrt3}\right)$, $\left(\frac{1}{\sqrt3},\frac{1}{\sqrt3}\right)$

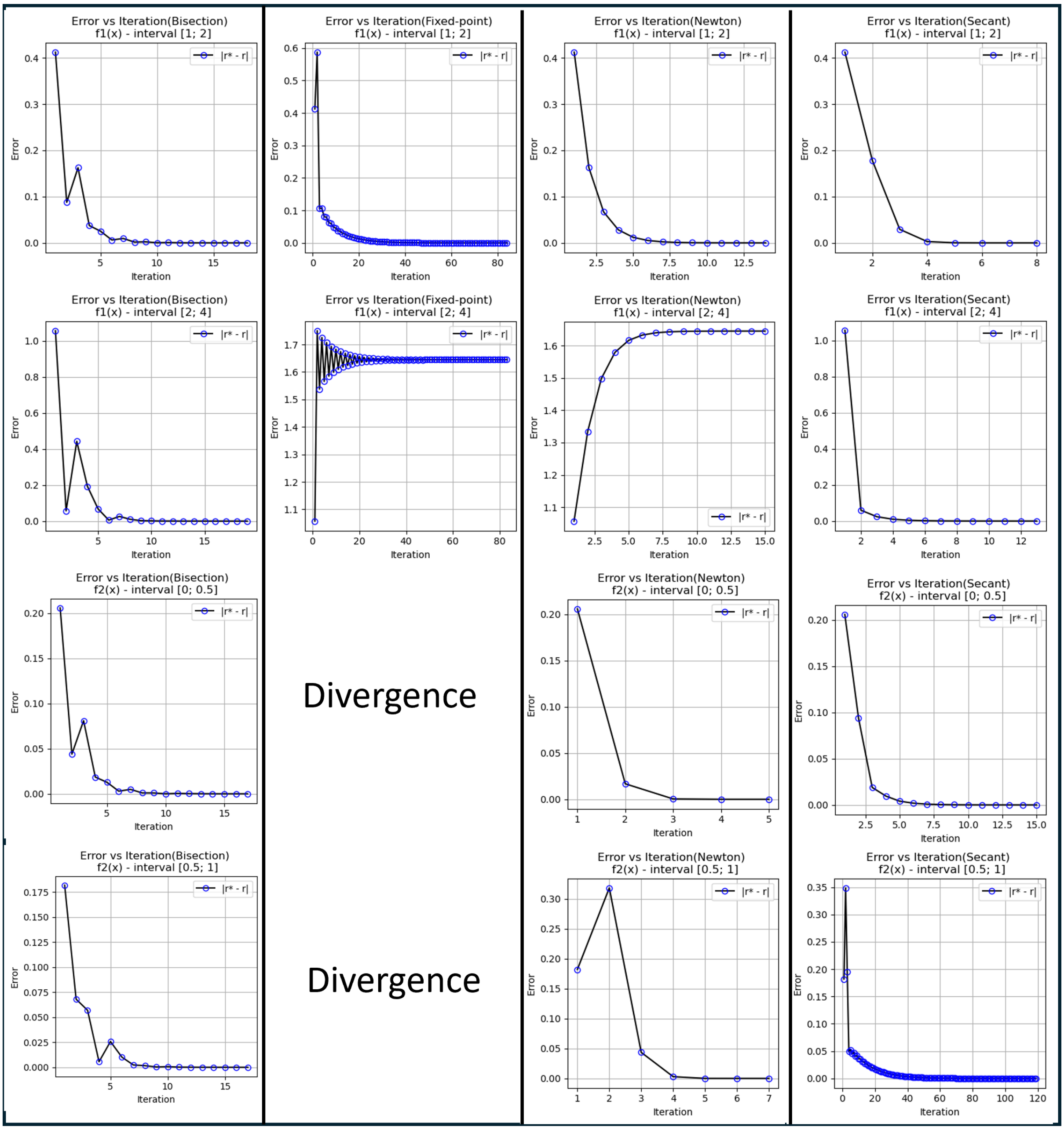

Figure 3: Problem 5 - Error vs Iteration plot of Bisection, Fixed-point iteration, Newton's, Secant method.

Iteration (k)	r	$f(r)$	$\lvert r^* - r\rvert$
0	2.000000	0.693147	1.057104
1	1.306853	0.212831	1.750251
2	1.519684	0.187799	1.537420
Final	1.412396	8.36×10^{-6}	1.644708

Table 1: Problem 5 - Fixed-Point Iteration for $f_1(x)$ on $[2, 4]$

$$\text{First derivatives: } \frac{\partial f}{\partial x} = 3x^2 - 1 = 0, \frac{\partial f}{\partial y} = 3y^2 - 1 = 0$$

Iteration (k)	r	$f(r)$	$\lvert r^* - r\rvert$
0	2.000000	0.693147	1.057104
1	1.722741	0.467044	1.334362
2	1.559309	0.250035	1.497794
Final	1.412397	1.15×10^{-5}	1.644706

Table 2: Problem 5 - Newton's Method for $f_1(x)$ on $[2, 4]$

Iteration (k)	r	$f(r)$	$\lvert r^* - r\rvert$
0	0.000000	1.000000	0.206035
1	1.000000	2.000000	0.793965
2	3.000000	4.000000	2.793965
Final	Diverge	Diverge	Diverge

Table 3: Problem 5 - Fixed-Point Iteration for $f_2(x)$ on $[0, 0.5]$

Iteration (k)	r	$f(r)$	$\lvert r^* - r\rvert$
0	0.000000	1.000000	0.206035
1	0.189280	0.068859	0.016755
2	0.205656	0.001520	0.000379
Final	0.206035	2.68×10^{-13}	3.84×10^{-13}

Table 4: Problem 5 - Newton's Method for $f_2(x)$ on $[0, 0.5]$

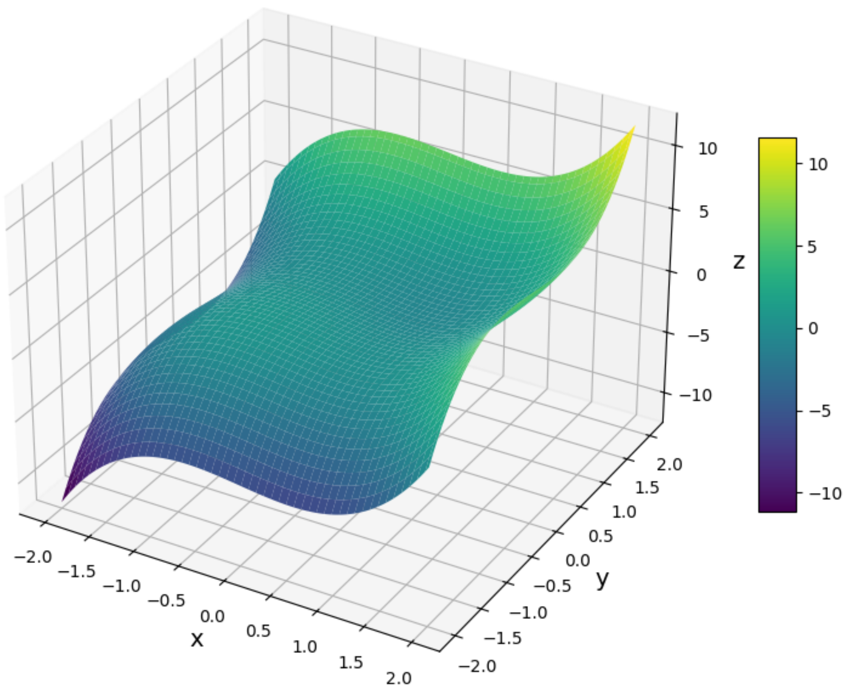

Figure 4: Problem 6.(a) - Graph of $f(x, y) = x^3 - x + y^3 - y$

$$\text{Critical points: } \left(\pm\frac{1}{\sqrt{3}}, \pm\frac{1}{\sqrt{3}}\right)$$

(c) Calculate the Hessian matrix

$$\text{Hessian: } H = \begin{bmatrix} 6x & 0 \\ 0 & 6y \end{bmatrix}$$

$$\text{At } \left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right) : H = \begin{bmatrix} 2\sqrt{3} & 0 \\ 0 & 2\sqrt{3} \end{bmatrix}, \lambda_1, \lambda_2 > 0 \Rightarrow \text{Local Min}$$

$$\text{At } \left(-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right) : H = \begin{bmatrix} -2\sqrt{3} & 0 \\ 0 & -2\sqrt{3} \end{bmatrix}, \lambda_1, \lambda_2 < 0 \Rightarrow \text{Local Max}$$

$$\text{At } \left(\pm\frac{1}{\sqrt{3}}, \mp\frac{1}{\sqrt{3}}\right) : H = \begin{bmatrix} \pm 2\sqrt{3} & 0 \\ 0 & \mp 2\sqrt{3} \end{bmatrix}, \text{Eigenvalues of opposite sign} \Rightarrow \text{Saddle Point}$$

(d) Fill in the following table.

Critical points	Hessian at (x, y)	Eigenvalues of Hessian at (x, y)	Concavity at (x, y)
$\left(-\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right)$	$\begin{bmatrix} -2\sqrt{3} & 0 \\ 0 & -2\sqrt{3} \end{bmatrix}$	$-2\sqrt{3}, -2\sqrt{3}$	Concavity
$\left(-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$	$\begin{bmatrix} -2\sqrt{3} & 0 \\ 0 & 2\sqrt{3} \end{bmatrix}$	$-2\sqrt{3}, 2\sqrt{3}$	Saddle
$\left(\frac{1}{\sqrt{3}}, -\frac{1}{\sqrt{3}}\right)$	$\begin{bmatrix} 2\sqrt{3} & 0 \\ 0 & -2\sqrt{3} \end{bmatrix}$	$2\sqrt{3}, -2\sqrt{3}$	Saddle
$\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)$	$\begin{bmatrix} 2\sqrt{3} & 0 \\ 0 & 2\sqrt{3} \end{bmatrix}$	$2\sqrt{3}, 2\sqrt{3}$	Convexity

(e) Examine the table carefully and explain how eigenvalues of Hessian matrices can help you classify the concavity of the surface at each critical point.

If eigenvalues are all positive, the function has local minimum and convexity at that point.
If eigenvalues are all negative, the function has local maximum and concavity at that point.
If eigenvalues are mixed with positive and negative, the function has saddle point.

7. Find the critical points of $f(x, y) = x^2 + y^3 - x^2y + xy^2$ and classify them all by using the eigenvalues of the appropriate Hessian matrices.

The partial derivatives are:

$$\frac{\partial f}{\partial x} = -2xy + 2x + y^2$$
$$\frac{\partial f}{\partial y} = -x^2 + 2xy + 3y^2$$

We solve the coupled equation:

$$\frac{\partial f}{\partial x} = 0, \quad \frac{\partial f}{\partial y} = 0$$

$$\frac{\partial f}{\partial x} = 2x - 2xy + y^2 = 0 \rightarrow 2x(1-y) + y^2 = 0 \rightarrow x = \frac{y^2}{2(y-1)}$$

$$\frac{\partial f}{\partial y} = 3y^2 - x^2 + 22xy = 0 \rightarrow 3y^2 - \frac{y^4}{4(y-1)^2} + \frac{2y^3}{2(y-1)} = 0 \rightarrow y^2\left(3 - \frac{y^2}{4(y-1)^2} + \frac{y}{y-1}\right) = 0$$

$$\to y^2\left(12(y-1)^2 - y^2 + 4y(y-1)\right) = 0 \to y^2(15y^2 - 28y + 12) = 0 \to y^2(3y-2)(5y-6) = 0$$

$$\to y_1 = 0, \quad y_2 = \frac{2}{3}, \quad y_3 = \frac{6}{5}$$

- Critical point: $(x, y) = (-\frac{2}{3}, \frac{2}{3})$
- Critical point: $(x, y) = (0, 0)$
- Critical point: $(x, y) = (\frac{18}{5}, \frac{6}{5})$

Hessian matrix at (x, y) :

$$H(x,y) = \begin{bmatrix} 2-2y & -2x+2y \\ -2x+2y & 2x+6y \end{bmatrix}$$

At the critical point $(x, y) = (-\frac{2}{3}, \frac{2}{3})$:
Hessian :

$$H = \begin{bmatrix} \frac{2}{3} & \frac{8}{3} \\ \frac{8}{3} & \frac{8}{3} \end{bmatrix}$$

Eigenvalues:

$$\frac{5}{3} - \frac{\sqrt{73}}{3}, \frac{5}{3} + \frac{\sqrt{73}}{3}$$

Classification: Saddle point

At the critical point $(x, y) = (0, 0)$:
Hessian matrix:

$$H = \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}$$

Eigenvalues:

$$2, 0$$

Classification: Indeterminate

At the critical point $(x, y) = (\frac{18}{5}, \frac{6}{5})$:
Hessian matrix:

$$H = \begin{bmatrix} -\frac{2}{5} & -\frac{24}{5} \\ -\frac{24}{5} & \frac{72}{5} \end{bmatrix}$$

Eigenvalues:

$$7 - \frac{\sqrt{1945}}{5}, 7 + \frac{\sqrt{1945}}{5}$$

Classification: Saddle point