738616

SCHOOL OF ENGINEERING

DATA MODELLING AND SIMULATION

Lecture 10: Optimisation-II

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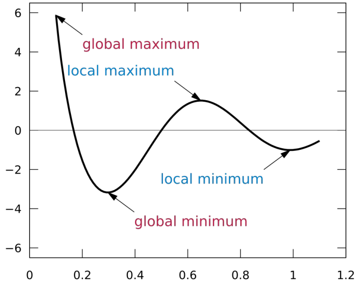
Recap

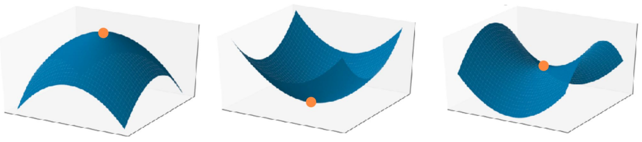
- Maxima,
- Minima,
- Stationary points,
- Saddle points,
- Function of two variables
- Objective function
- Constraints
- Optimisation of unconstrained functions
    - Taylor's theorem
- Hessian Matrix

$$\frac{dy}{dx} = 0$$

$$\frac{d^2y}{dx^2} = \text{positive/negative}$$



f(x)



local maximum

local minimum

saddle point (transition state)

f(x,y)

These generate a set of rules and conditions that can be summarised as follows,

1) A necessary condition for the function f(x, y) to have a stationary value at (a, b) is that

$\frac{\partial f}{\partial x} = 0$ and $\frac{\partial f}{\partial y} = 0$ at (a, b)

2) If $\frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2 > 0$ and $\frac{\partial^2 f}{\partial x^2}$ *or* $\frac{\partial^2 f}{\partial y^2} < 0$ at (a, b)

then the stationary point is a local maximum.

3) If $\frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2 > 0$ and $\frac{\partial^2 f}{\partial x^2}$ *or* $\frac{\partial^2 f}{\partial y^2} > 0$ at (a, b)

then the stationary point is a local minimum.

4) If $\frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2 < 0$ then the stationary point is a saddle point.

5) If $\frac{\partial^2 f}{\partial x^2}\frac{\partial^2 f}{\partial y^2} - \left(\frac{\partial^2 f}{\partial x \partial y}\right)^2 = 0$ then we cannot draw a conclusion as to whether the point is a maximum, minimum or saddle point and further investigation is required.

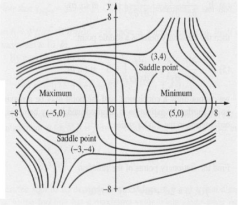
$$H = \begin{pmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{pmatrix}$$

$|H| > 0$ and $\frac{\partial^2 f}{\partial x^2} > 0$ then the point is a MINIMUM.

$|H| > 0$ and $\frac{\partial^2 f}{\partial x^2} < 0$ then the point is a MAXIMUM.

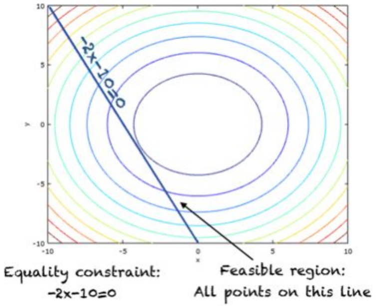
$|H| < 0$ then the point is a SADDLE POINT.

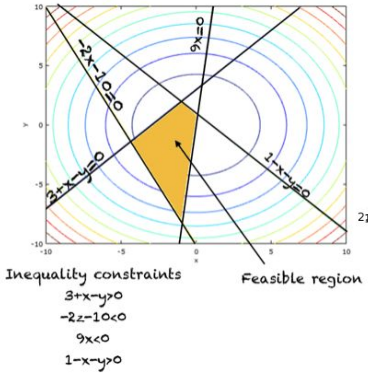
$|H| < 0$ then the point is a SADDLE POINT.

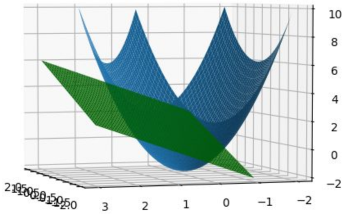


Optimisation of Constrained Functions

➔ Find the stationary points of f(x,y) that is subject to one or more constraint conditic

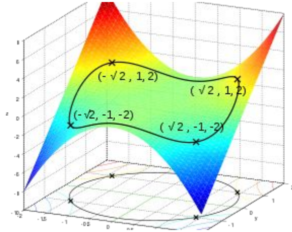


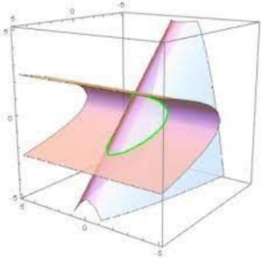


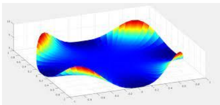


For example

- Minimise material used but be constrained by a particular volume
- Maximise production but we have budget constraints







Commonly used methods

Substitution Approach | Total Differential Approach | Lagrange Multiplier

1. Substitution Approach

$\text{Constraints} \longrightarrow \boxed{\text{Objective function}} \longrightarrow \boxed{\text{Composite Function}}$

Example 1. Solve the following optimisation problem using the substitution approach,

$$\min_{(x,y)} \quad f(x,y)=x^2+5xy+y^2, \quad \textit{subject to } g(x,y)=x-y-5=0$$

Our objective function is $f(x,y)=x^2+5xy+y^2$

Our constraint is $g(x,y)=x-y-5=0$

Rearrange the constraint →

$$x=y+5$$

Substitute into obj. function

$$f(y)=(y+5)^2+5y(y+5)+y^2$$

$$=7y^2+35y+25$$

→ Differentiate and equate to zero

$$f(y)=7y^2+35y+25$$

$$\frac{df}{dy}=14y+35=0$$

Solving gives,

$Y^*=-2.5$ and therefore, $X^*=2.5$

We can use the second derivative test in order to determine whether this is a minimum or a maximum stationary point. This gives,

$\frac{d^2f}{dy^2}=14$, which is positive and hence a MINIMUM

2. Total Differential Approach

Differentiate → Objective function
Differentiate → Constraints
Partial differentiation

Example 2. Solve the following optimisation problem using the total differential approach,

$$\min_{(x,y)} \quad f(x,y)=x^2+5xy+y^2, \quad \textit{subject to} \;\; g(x,y)=x-y-5=0$$

Our objective function is $f(x,y)=x^2+5xy+y^2$

Our constraint is $g(x,y)=x-y-5=0$

Partial differentiation →

$\frac{\partial f}{\partial x}=2x+5y$ and $\frac{\partial f}{\partial y}=5x+2y$

$\frac{\partial g}{\partial x}=1$ and $\frac{\partial g}{\partial y}=-1$

Rearrange →

$\partial f=(2x+5y)\partial x$ and $\partial f=(5x+2y)\partial y$

$$(2x+5y)\partial x=(5x+2y)\partial y$$

$$\frac{\partial y}{\partial x}=\frac{(2x+5y)}{(5x+2y)}$$

$\partial g=1\partial x$ and $\partial g=-1\partial y$

$$\partial x=-\partial y$$

$$\frac{\partial y}{\partial x}=-1$$

Equating the results →

$$\frac{(2x+5y)}{(5x+2y)}=-1$$

Rearranging gives

$$-(5x+2y)=1(2x+5y)$$

$$-5x-2y=2x+5y$$

$$-7x=7y$$

$$x=-y$$

Substituting this into the constraint

$$g(x,y)=x-y-5=0$$

$$g(y)=-y-y-5=0$$

$$-2y=5$$

$$Y^*=-2.5$$

Therefore,

$$X^*=2.5$$

3. Lagrange Multiplier

Introduce a new variable Lagrange Multiplier Greek letter lambda, λ.

$$L(x,y,\lambda) = f(x,y) + \lambda[c - g(x,y)]$$

Example 3. Solve the following optimisation problem using the Lagrange Multiplier approach,

$$\min_{(x,y)} \quad f(x,y) = x^2 + 5xy + y^2, \quad \textit{subject to} \;\; g(x,y) = x - y - 5 = 0$$

Our objective function is $f(x,y) = x^2 + 5xy + y^2$

Our constraint is $g(x,y) = x - y - 5 = 0$

Lagrangian

rearrange the constraint to equal zero then $c = 0$

$$L(x,y,\lambda) = f(x,y) - \lambda[g(x,y)]$$

$$L(x,y,\lambda) = x^2 + 5xy + y^2 - \lambda[x - y - 5]$$

$$L(x,y,\lambda) = x^2 + 5xy + y^2 - \lambda x + \lambda y + 5\lambda$$

Partial derivative with respect to each of the variables and equate them to zero

$$\frac{\partial L}{\partial x} = 2x + 5y - \lambda = 0$$

$$\frac{\partial L}{\partial y} = 5x + 2y + \lambda = 0$$

$$\frac{\partial L}{\partial \lambda} = -x + y + 5 = 0$$

solve

$$\begin{pmatrix} 2 & 5 & -1 \\ 5 & 2 & 1 \\ -1 & 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \\ \lambda \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -5 \end{pmatrix}$$

$$X^* = 2.5, \; Y^* = -2.5$$

Using the inverse matrix method, Cramer's rule or Gaussian elimination or matlab

Example 4. Solve the following optimisation problem using the Lagrange Multiplier approach,

$$f(x,y,z) = x^2 + y^2 + z^2$$

Subject to two constraints:

$$z^2 = x^2 + y^2$$

$$x + y - z + 1 = 0$$

set up the problem using the definition of the Lagrangian,

$$L = f(x,y,z) + \lambda_1[c - g(x,y,z)] + \lambda_2[c - h(x,y,z)]$$

$$L(x, y, z, \lambda_1, \lambda_2) = x^2 + y^2 + z^2 - \lambda_1 x^2 - \lambda_1 y^2 + \lambda_1 z^2 - \lambda_2 x - \lambda_2 y + \lambda_2 z - \lambda_2$$

Now we find the partial derivative with respect to each of the variables and equate them to zero,

$$\frac{\partial L}{\partial x} = 2x - 2\lambda_1 x - \lambda_2 = 0 \qquad \text{(eq.1)}$$

$$\frac{\partial L}{\partial y} = 2y - 2\lambda_1 y - \lambda_2 = 0 \qquad \text{(eq.2)}$$

$$\frac{\partial L}{\partial z} = 2z + 2\lambda_1 z + \lambda_2 = 0 \qquad \text{(eq.3)}$$

$$\frac{\partial L}{\partial \lambda_1} = -x^2 - y^2 + z^2 = 0 \qquad \text{(eq.4)}$$

$$\frac{\partial L}{\partial \lambda_2} = -x - y + z - 1 = 0 \qquad \text{(eq.5)}$$

From Eq 3:

$\lambda_2 = -2z - 2\lambda_1 z$

Sub into Eq. 1 and Eq. 2:

$2x - 2\lambda_1 x + 2z + 2\lambda_1 z = 0$

$2y - 2\lambda_1 y + 2z + 2\lambda_1 z = 0$

Rearrange both for λ_1:

$$\lambda_1 = \frac{2x + 2z}{2x - 2z}$$

$$\lambda_1 = \frac{2y + 2z}{2y - 2z}$$

Therefore,

$$\frac{2x + 2z}{2x - 2z} = \frac{2y + 2z}{2y - 2z}$$

$$2yz - 2xz = 0$$

$$2z(y - x) = 0$$

from eq. 4

If $z = 0$, $x^2 + y^2 = 0$, $y = 0$ $x = 0$

which does not satisfy the second (h) constraint.

If $y = x$ will reduce the number of equations to three:

$$y = x$$

$$z^2 = x^2 + y^2$$

$$x + y - z + 1 = 0$$

Substitute the first eq into the second one:

$$z^2 = 2x^2$$

Substitute the first eq into the third one:

$$z = 2x + 1$$

We get:

$$(2x + 1)^2 = 2x^2$$

$$2x^2 + 4x + 1 = 0$$

Use the quadratic formula to find x:

$$x = -1 \pm \frac{\sqrt{2}}{2}$$

Therefore,

$$y = -1 \pm \frac{\sqrt{2}}{2}$$

$$z = -1 \pm \sqrt{2}$$

There two solutions:

$$\left(-1 + \frac{\sqrt{2}}{2}, -1 + \frac{\sqrt{2}}{2}, -1 + \sqrt{2}\right), \left(-1 - \frac{\sqrt{2}}{2}, -1 - \frac{\sqrt{2}}{2}, -1 - \sqrt{2}\right)$$

Substituting both into $f(x, y, z) = x^2 + y^2 + z^2$ we get:

$$f\left(-1 + \frac{\sqrt{2}}{2}, -1 + \frac{\sqrt{2}}{2}, -1 + \sqrt{2}\right) = 6 - 4\sqrt{2} \qquad \text{MINIMUM}$$

$$f\left(-1 - \frac{\sqrt{2}}{2}, -1 - \frac{\sqrt{2}}{2}, -1 - \sqrt{2}\right) = 6 + 4\sqrt{2} \qquad \text{MAXIMUM}$$

Practice Problems

1) Find the stationary values of the following constrained function using the substitution, total differential and Lagrange Multiplier approaches.

   a) $f(x,y) = 2x^2 + 3y^2$ subject to $g(x,y) = 2x + y = 50$
   b) $f(x,y) = 3x^2 + xy - 2y^2 + 10$ subject to $g(x,y) = x - y = 50$

2) Find the optimum of $f = x^2 + xy + y^2$ subject to constraint $x + y = 1$ using the substitution, total differential and Lagrange Multiplier approaches.