## Differential Calculus of Multivariable Functions

## Introduction to Multivariable Functions



## Functions of Two Independent Variables

If $\boldsymbol{z}$ is uniquely determined when the values of $\boldsymbol{x}$ and $\boldsymbol{y}$ are given, we say that $\boldsymbol{z}$ is a single-valued function of $\boldsymbol{x}$ and $\boldsymbol{y}$ and indicate this fact by the notation

$$
z=f(x, y)
$$

Many engineering applications exist that show this functional dependence, for instance the vibration of a string or the temperature of a plate or a cooling fin

$$
T=f(x, y)
$$

It is sometimes useful to visualize the function graphically. The function $\boldsymbol{z}=\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y})$ can be visualized in two different ways:

1. a contour plot
2. a surface plot

## Partial Derivatives



For $\boldsymbol{y}=\boldsymbol{f}(\boldsymbol{x})$ there is only one slope at any point $\boldsymbol{P}$, where the slope of the tangent at $\boldsymbol{P}$ is


$$
\text { slope }=\left.\frac{d y}{d x}\right|_{x=x_{0}}=\left.\lim _{\Delta x \rightarrow 0} \frac{f\left(x_{0}+\Delta x\right)-f\left(x_{0}\right)}{\Delta x}\right|_{a t x=x_{0}}
$$

However for a 3-dimensional surface, $\boldsymbol{z}=\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y})$, the slope varies depending on the direction you move on the surface.


For $\quad z(x, y)=20 e^{\left(-x^{2} / 100\right)} \cos \frac{\pi y}{30} \quad$ find the slope at $P(x=5, y=10)$

Different notations of the partial derivative can be used.

$$
\begin{array}{lll}
\frac{\partial f}{\partial x} & \text { or } & f_{x}
\end{array} \frac{\partial f}{\partial y} \quad \text { or } \quad f_{y}
$$

Higher Orders

$$
\begin{array}{clc}
\frac{\partial^{2} f}{\partial x^{2}} & \text { or } & f_{x x} \\
\frac{\partial^{2} f}{\partial y^{2}} & \text { or } & f_{y y} \\
\frac{\partial^{2} f}{\partial x \partial y} & \text { or } & f_{y x}=f_{x y}
\end{array}
$$

$\longleftarrow$ order of calculation $\quad \longrightarrow$ order of calculation

## Higher Order Partial Derivatives

Partial derivatives of the second order are denoted as

$$
\frac{\partial^{2} f}{\partial x^{2}}, \quad \frac{\partial^{2} f}{\partial y^{2}}, \quad \frac{\partial^{2} f}{\partial x \partial y}, \quad \frac{\partial^{2} f}{\partial y \partial x}
$$

where

$$
\frac{\partial^{2} f}{\partial x^{2}}=\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right), \quad \frac{\partial^{2} f}{\partial x \partial y}=\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)
$$

as so on.
If the function $z=f(x, y)$ together with the partial derivatives $f_{x}, f_{y}, f_{x y}$ and $f_{y x}$ are continuous, then

$$
\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)=\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right)
$$

## Chain Rule for Partial Derivatives



Reading
Trim $12.6 \longrightarrow$ Chain Rules for Partial Derivatives

## Assignment

web page $\longrightarrow$ assignment \#4

## Review of Single Variable Functions

- if we understand for 1 variable, it is easy to understand for 2 or 3 variables
- the changes are straight forward

$$
\frac{d y}{d x}=\frac{d y}{d u} \cdot \frac{d u}{d x}
$$

Using the tree we need to remember $\Rightarrow \quad \begin{gathered}\boldsymbol{y} \\ \mid \\ \boldsymbol{u} \\ \mid \\ \boldsymbol{x}\end{gathered}$
$L \boldsymbol{H} S \rightarrow \frac{d y}{d x} \rightarrow$ implies we are looking at the function $y(x)$
$\boldsymbol{R H S} \rightarrow \frac{d \boldsymbol{y}}{d \boldsymbol{u}} \rightarrow$ implies we are looking at the same $\boldsymbol{y}$ but now the independent variable is $\boldsymbol{u}$, i.e. $y(u)$.

The chain rule relates slopes of the 2 plots

$$
\underbrace{\frac{d y(x)}{d x}}_{\text {slope @ any point } x}=\underbrace{\text { the effect of a change of scale }}_{\lim _{u \rightarrow 0} \frac{\frac{y(u+\Delta u)-y(u)}{\Delta u}}{\frac{d y(u)}{d u}}}
$$

## Chain Rule for Multivariable Functions

1. Given a dependent variable as a function of several independent variables, transform the dependent variable into a new set of independent variables:

$$
\underbrace{\boldsymbol{z}}_{\text {dependent }} \overbrace{(u, v)}^{\rightarrow \text { independent }} \longrightarrow z(x, y)
$$

You will typically be asked to find

$$
\frac{\partial z}{\partial x}, \frac{\partial^{2} z}{\partial x^{2}}, \frac{\partial z}{\partial y}, \frac{\partial^{2} z}{\partial y^{2}}
$$

2. map the dependency of the dependent variable in terms of the independent variables, in our case, $\boldsymbol{z}(\boldsymbol{u}, \boldsymbol{v})$

3. map the dependency of the independent variables in the transformed space in our case, $\boldsymbol{u}(\boldsymbol{x}, \boldsymbol{y})$ and $\boldsymbol{v}(\boldsymbol{x}, \boldsymbol{y})$

4. use the chain rule to form all paths from $\boldsymbol{z} \rightarrow \boldsymbol{x}$ and $\boldsymbol{z} \rightarrow \boldsymbol{y}$

$$
\begin{aligned}
\frac{\partial z}{\partial x} & =\frac{\partial z}{\partial u} \frac{\partial u}{\partial x}+\frac{\partial z}{\partial v} \frac{\partial v}{\partial x} \\
\frac{\partial z}{\partial y} & =\frac{\partial z}{\partial u} \frac{\partial u}{\partial y}+\frac{\partial z}{\partial v} \frac{\partial v}{\partial y}
\end{aligned}
$$

5. How do we find the 2 nd derivative?

- remember $\frac{\partial^{2} z}{\partial x^{2}}=\frac{\partial}{\partial x} \underbrace{\left(\frac{\partial z}{\partial x}\right)}_{\text {we already know how to do this }}$
- replace $z$ at the top of the tree with $\frac{\partial z}{\partial x}$

- find all paths between $\partial \boldsymbol{\partial} / \boldsymbol{\partial} \boldsymbol{x}$
- remember, we may need to do the same for $\boldsymbol{y}$ if asked

$$
\begin{aligned}
\frac{\partial^{2} z}{\partial x^{2}} & =\left[\frac{\partial}{\partial u}\left(\frac{\partial z}{\partial x}\right)\right] \frac{\partial u}{\partial x}+\left[\frac{\partial}{\partial v}\left(\frac{\partial z}{\partial x}\right)\right] \frac{\partial v}{\partial x} \\
\frac{\partial^{2} z}{\partial y^{2}} & =\left[\frac{\partial}{\partial u}\left(\frac{\partial z}{\partial y}\right)\right] \frac{\partial u}{\partial y}+\left[\frac{\partial}{\partial v}\left(\frac{\partial z}{\partial y}\right)\right] \frac{\partial v}{\partial y}
\end{aligned}
$$

for 2nd derivatives, let

$$
\frac{\partial z}{\partial x}=A, \quad \frac{\partial z}{\partial y}=B
$$

$$
\begin{aligned}
\frac{\partial^{2} z}{\partial x^{2}}=\frac{\partial A}{\partial x} & =\frac{\partial A}{\partial u} \frac{\partial u}{\partial x}+\frac{\partial A}{\partial v} \frac{\partial v}{\partial x} \\
& =\frac{\partial}{\partial u}\left(\frac{\partial z}{\partial x}\right)\left(\frac{\partial u}{\partial x}\right)+\frac{\partial}{\partial v}\left(\frac{\partial z}{\partial x}\right)\left(\frac{\partial v}{\partial x}\right)
\end{aligned}
$$

$$
\frac{\partial^{2} z}{\partial y^{2}}=\frac{\partial B}{\partial y}=\frac{\partial B}{\partial u} \frac{\partial u}{\partial y}+\frac{\partial B}{\partial v} \frac{\partial v}{\partial y}
$$

$$
=\frac{\partial}{\partial u}\left(\frac{\partial z}{\partial y}\right)\left(\frac{\partial u}{\partial y}\right)+\frac{\partial}{\partial v}\left(\frac{\partial z}{\partial y}\right)\left(\frac{\partial v}{\partial y}\right)
$$

## Gradients



At each point on a surface $\boldsymbol{z}=\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y})$ we can define two slopes - one in each spatial direction.
From the previous example: $z(x, y)=20 e^{-x^{2} / 100} \cos \pi y / 30$, where
at $P_{x=5, y=10} \quad \frac{\partial f}{\partial x}=-0.78 \quad \frac{\partial f}{\partial y}=-1.41$.
It is useful to combine these into one vector measure of the slope of the surface at $\boldsymbol{P}$. This is called the Gradient Vector.

$$
\operatorname{grad} f=\nabla f \equiv \hat{i} \frac{\partial f}{\partial x}+\hat{j} \frac{\partial f}{\partial y}
$$

where the "del operator" $-\nabla$ is defined in 2D as: $\quad \nabla=\hat{i} \frac{\partial}{\partial \boldsymbol{x}}+\hat{\boldsymbol{j}} \frac{\partial}{\partial \boldsymbol{y}}$

$$
\left.\operatorname{grad} f\right|_{P}=\left.\nabla f\right|_{P}=\hat{i} \frac{\partial f}{\partial x}+\hat{j} \frac{\partial f}{\partial y}=\hat{i}(-0.78)+\hat{j}(-1.41)
$$

$$
f=z=20 e^{-x^{2} / 100} \cos \left(\frac{\pi y}{30}\right)
$$

The meaning is clear on a contour plot

The magnitude of the gradient vector is

$$
\left|\nabla f_{a t P}\right|=\sqrt{(-1.41)^{2}+(-0.78)^{2}}=1.61
$$


slope in this direction is

$$
\left.\frac{\partial f}{\partial x}\right|_{P}=-0.78
$$

The gradient vector, $\boldsymbol{\nabla} \boldsymbol{f}$ is:

- a vector at $\boldsymbol{P}$ that is perpendicular to the contour at $\boldsymbol{P}$
- points uphill in the direction in which slope increases the most at $\boldsymbol{P}$
- its magnitude is $\left|\nabla f_{a t P}\right|=1.61$. If we move 1 unit in the $\nabla f$ direction, then $z$ increases by 1.61 units. This is the biggest slope in any direction at $\boldsymbol{P}$.

The gradient comes up in many applications because things tend to move down the gradient.
Examples:

1. If we release a ball at point $\boldsymbol{P}$ from rest it will roll down the gradient

- the direction will be in the negative $\nabla f$ direction
- how far it rolls will depend on the magnitude $\left|\nabla f_{a t P}\right|$

2. Heat flow in a cooling fin

- in the cross section of the fin, $T=f(x, y)$
- the heat flow at some point $P$ is in the $\nabla f$ direction
- how much heat depends on the magnitude $\left|\nabla f_{a t P}\right|$
- Fourier's law in 2D is $\overrightarrow{\boldsymbol{q}}=-\boldsymbol{k} \boldsymbol{\nabla} \boldsymbol{T}$

3. Lava flowing from a volcano

- Mauna Loa and Kilauea on the Big Island of Hawaii are highly active
- the gradient can be used to predict to path of lava flowing to the sea



## Functions of 3 or More Independent Variables

The procedure can be extended to any number of independent variables. In Mechanical Engineering, the biggest number is usually 4 . You may have more in abstract applications.

Examples: Solving for the transient temperature response in a room

$$
T=f(x, y, z, t)
$$

Includes 3 spatial variables and 1 time variable. Graphical representation becomes difficult.
Possible graphical representations include:

- multiple contour plots
- level surfaces (surfaces of constant value)
- "slice" - show $\boldsymbol{T}$ vs. $\boldsymbol{z}$ and fixed locations $\left(\boldsymbol{x}_{0}, \boldsymbol{y}_{0}\right)$. Need many "slices" for full representation


## Gradient in 3-D

For both $\boldsymbol{T}=\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ and $\boldsymbol{T}=\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}, \boldsymbol{t})$ the vector gradient is

$$
\nabla f=\hat{i} \frac{\partial f}{\partial x}+\hat{j} \frac{\partial f}{\partial y}+\hat{k} \frac{\partial f}{\partial z}
$$

with the del operator

$$
\nabla=\hat{i} \frac{\partial}{\partial x}+\hat{j} \frac{\partial}{\partial y}+\hat{k} \frac{\partial}{\partial z}
$$

since the gradient vector is a measure in space only. $\nabla f$ is a vector in 3-D space. If $T=$ $f(x, y, z, t)$ then $\nabla f$ will change with time.

## Example 2.1

Find the temperature variation inside a spherical lead shield enclosing a small radioactive sphere. The temperature will vary with radius. Suppose for example, that

$$
T=f(x, y, z)=\frac{1}{\sqrt{x^{2}+y^{2}+z^{2}}}
$$

where $0.05 \leq x, y, z \leq 2$

## Directional Derivatives



We know how to find a vector that points in the direction of the maximum and minimum change on slope but how do we account for the rate of change in slope in any other arbitrary direction. For this we introduce the directional derivative.

THEOREM: let $\boldsymbol{f}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ be continuous and possess partial derivatives $f_{x}, f_{y}, f_{z}$ throughout some neighborhood of the point $\boldsymbol{P}_{0}\left(\boldsymbol{x}_{0}, \boldsymbol{y}_{0}, z_{0}\right)$. Let $f_{x}, f_{y}$ and $\boldsymbol{f}_{z}$ be continuous at $\boldsymbol{P}_{0}$. Then the directional derivative at $\boldsymbol{P}_{\mathbf{0}}$ exists for a unit vector $\hat{\boldsymbol{v}}=\left(\boldsymbol{v}_{\boldsymbol{x}}, \boldsymbol{v}_{\boldsymbol{y}}, \boldsymbol{v}_{\boldsymbol{z}}\right)$ in the direction of $\boldsymbol{v}$, such that

To find the gradient along a line segment $s$

$$
\begin{aligned}
\frac{d f}{d s} & =\underbrace{\frac{d f}{d x}}_{f_{x}} \underbrace{\frac{d x}{d s}}_{v_{x}}+\frac{d f}{d y} \frac{d y}{d s}+\frac{d f}{d z} \frac{d z}{d s} \\
& =f_{x} v_{x}+f_{y} v_{y}+f_{z} v_{z}
\end{aligned}
$$

where $f$ is expressed in terms of $s$, where $s$ is a measure of directed distance along a vector and the unit vector is $\hat{\boldsymbol{v}}=\left(v_{x}, v_{y}, v_{z}\right)$. First set $s=0$ at $P_{0}=\left(x_{0}, y_{0}, z_{0}\right)$.

To find $\boldsymbol{f}$ in this transformed space, we can write

$$
\begin{aligned}
x & =x_{0}+v_{x} s \\
y & =y_{0}+v_{y} s \\
z & =z_{0}+v_{z} s
\end{aligned}
$$

Note: we start at $\boldsymbol{P}_{\mathbf{0}}\left(\boldsymbol{x}_{\mathbf{0}}, \boldsymbol{y}_{0}, \boldsymbol{z}_{\mathbf{0}}\right)$ and attach a vector in the $\hat{\boldsymbol{v}}\left(\boldsymbol{v}_{\boldsymbol{x}}, \boldsymbol{v}_{\boldsymbol{y}}, \boldsymbol{v}_{\boldsymbol{z}}\right)$ direction with a magnitude of $s$

Then

$$
\begin{aligned}
\frac{\partial f}{\partial s} & =\frac{\partial f}{\partial x} \frac{\partial x}{\partial s}+\frac{\partial f}{\partial y} \frac{\partial y}{\partial s}+\frac{\partial f}{\partial z} \frac{\partial z}{\partial s} \\
& =\frac{\partial f}{\partial x} v_{x}+\frac{\partial f}{\partial y} v_{y}+\frac{\partial f}{\partial z} v_{z} \\
& =D_{v} f \\
& =\text { directional derivative in direction } v
\end{aligned}
$$

The directional derivative of $\boldsymbol{f}$ at $\boldsymbol{P}_{\mathbf{0}}$ in the direction $\boldsymbol{v}$ can also be defined as the average rate of change of $\boldsymbol{f}$ with respect to distance as $\boldsymbol{P}_{\mathbf{1}}$ approaches $\boldsymbol{P}_{\mathbf{0}}$ along $\boldsymbol{s}$.

$$
\frac{\partial f}{\partial s}=\lim _{\Delta s \rightarrow 0} \frac{\Delta f}{\Delta s}=\lim _{P_{1} \rightarrow P_{0}} \frac{f\left(x_{1}, y_{1}, z_{1}\right)-f\left(x_{0}, y_{0}, y_{0}\right)}{\sqrt{\left(x_{1}-x_{0}\right)^{2}+\left(y_{1}-y_{0}\right)^{2}+\left(z_{1}-z_{0}\right)^{2}}}
$$

This can be expressed as a scalar product of the gradient of $f$ and the vector $\boldsymbol{v}$.

$$
D_{v} f=\nabla f \cdot \hat{v}
$$

this can be thought of as the projection of $\nabla f$ onto the vector $v$.



This is another application of the gradient.
The basic idea is that the $\nabla \boldsymbol{f}$ is perpendicular to a contour line in 2D and perpendicular to a level surface in 3D. Therefore the $\nabla \boldsymbol{f}$ vector will be perpendicular to a tangent line or plane. We will use this to find the tangent line or plane at a point.

$$
z=20 e^{-x^{2} / 100} \cos \left(\frac{\pi y}{30}\right)
$$

Find the plane tangent to the surface at point $P(x=5, y=10)$.
one way is to use the Taylor series, keeping only the linear terms

$$
z=7.79-0.78(x-5)-1.41(y-10)
$$

another way is to use the gradient ideas described above. We can write the equation of the hill as

$$
\left.\begin{array}{rl}
F(x, y, z)=20 e^{-x^{2} / 100} \cos \left(\frac{\pi y}{30}\right)-z \\
\hookrightarrow & \begin{array}{l}
\text { move } z \text { to the righthand side } \\
\text { if } F=0 \Rightarrow \text { on surface }
\end{array} \\
\text { if } F<0 \Rightarrow \text { outside } \\
\text { if } F>\Rightarrow \text { inside }
\end{array}\right]
$$

In 3D the level surface $\boldsymbol{F}=\mathbf{0}$ defines the hill surface

$$
\begin{aligned}
\nabla F= & \hat{i} \frac{\partial F}{\partial x}+\hat{j} \frac{\partial F}{\partial y}+\hat{k} \frac{\partial F}{\partial z} \\
= & \hat{i} \\
& {\left[20 e^{-x^{2} / 100}\left(-\frac{2 x}{100}\right) \cos \left(\frac{\pi y}{30}\right)\right] } \\
& +\hat{j}\left[20 e^{-x^{2} / 100}-\left(\frac{\pi}{30}\right) \sin \left(\frac{\pi y}{30}\right)\right]+\hat{k}(-1)
\end{aligned}
$$

at $P(5,10,7.79)$

$$
\left.\nabla F\right|_{a t P}=\hat{i}(-0.78)+\hat{j}(-1.41)+\hat{k}(-1)
$$

$\left.\boldsymbol{\nabla} \boldsymbol{F}\right|_{a t}{ }_{P}$ is perpendicular to the $\boldsymbol{F}=\mathbf{0}$ surface and also perpendicular to a tangent plane at $\boldsymbol{P}$. We have:

- a point on the plane $P(5,10,7.79)$
- a vector normal to the plane $\vec{N}=\nabla \boldsymbol{F}$

Therefore the equation of the tangent plane is

$$
\begin{aligned}
& N_{x}\left(x-x_{P}\right)+N_{y}\left(y-y_{P}\right)+N_{z}\left(z-z_{P}\right)=0 \\
&-0.78(x-5)-1.41(y-10)-1(z-7.79)=0 \\
& z=7.79-0.78(x-5)-1.41(y-10)
\end{aligned}
$$

This is the same as the Taylor series.

Tangent Plane : $A\left(x-x_{0}\right)+B\left(y-y_{0}\right)+C\left(z-z_{0}\right)=0$

$$
\text { Normal Line }: \frac{x-x_{0}}{A}=\frac{y-y_{0}}{B}=\frac{z-z_{0}}{C}
$$

where

$$
A=f_{x}\left(x_{0}, y_{0}\right), \quad B=f_{y}\left(x_{0}, y_{0}\right), \quad C=-1
$$

## Extrema of Functions



## Reading

Trim $12.10 \longrightarrow$ Relative Maxima and Minima
$12.11 \longrightarrow$ Absolute Maxima and Minima

## Assignment

web page $\longrightarrow$ assignment \#5

## Review of Functions of One Variable

The critical points are identified by the $x$-values where $f^{\prime} \rightarrow 0$ or where $f^{\prime}$ does not exist. We apply the 2 nd derivative test at these critical points:


1. at $\boldsymbol{P}_{1}: f^{\prime}=0$ and $f^{\prime \prime}=0$
2. at $\boldsymbol{P}_{2}: f^{\prime}=0$ and $f^{\prime \prime}<0$
3. at $P_{3}: f^{\prime}=0$ and $f^{\prime \prime}>0$
4. at $P_{4}: f^{\prime}$ and $f^{\prime \prime}$ do no exist, i.e. $\rightarrow \infty$

The absolute max/min in the range $\boldsymbol{a} \rightarrow \boldsymbol{b}$ is either at one of the critical points or at the end points of the domain, Note: end points must be checked.

- we can see from the figure, that the absolute minimum in the range $\boldsymbol{a} \rightarrow \boldsymbol{b}$ is at $\boldsymbol{f}(\boldsymbol{a})$ and that the absolute maximum in the range $\boldsymbol{a} \rightarrow \boldsymbol{b}$ is at $\boldsymbol{x}=\boldsymbol{P}_{\mathbf{2}}$
- if the test fails, we can always plot up $\boldsymbol{y}=\boldsymbol{f}(\boldsymbol{x})$ to see what it looks like
- sometimes it is easier to use plots or an understanding of the physics associated with the problem to decide rather that formal tests


## Functions of Two Variables

We will examine $\boldsymbol{z}=f(x, y)$ where $\nabla f=0$, i.e. the "flat" portion of the curved surface. The critical points are where

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

In this instance, the 2nd derivative tests involve $\frac{\partial^{2} f}{\partial x^{2}}$ and $\frac{\partial^{2} f}{\partial y^{2}}$ and $\frac{\partial^{2} f}{\partial x \partial y}$.
Possible max/min locations include:

1. Peak Shape: Relative maximum at $\frac{\partial f}{\partial x}=\frac{\partial f}{\partial y}=0$

$$
\frac{\partial^{2} f}{\partial x^{2}}<0 \quad \text { and } \quad \frac{\partial^{2} f}{\partial y^{2}}<0
$$

The $\boldsymbol{x}$ - and $\boldsymbol{y}$-slopes are decreasing +ve to -ve
2. Bowl Shape: Relative minimum at $\frac{\partial f}{\partial x}=\frac{\partial f}{\partial y}=0$

$$
\frac{\partial^{2} f}{\partial x^{2}}>0 \quad \text { and } \quad \frac{\partial^{2} f}{\partial y^{2}}>0
$$

The $\boldsymbol{x}$ - and $\boldsymbol{y}$-slopes are increasing -ve to +ve
3. Saddle Shape: "saddle point" at $\frac{\partial f}{\partial x}=\frac{\partial f}{\partial y}=0$, there is no clear min or max at $\frac{\partial f}{\partial x}=$ $\frac{\partial f}{\partial y}=0$. It looks like a max in $x$ and a min in $y$.

$$
\frac{\partial^{2} f}{\partial x^{2}}<0 \quad \text { but } \quad \frac{\partial^{2} f}{\partial y^{2}}>0
$$

4. Bowl Shape on $\boldsymbol{x}$ and $\boldsymbol{y}$ axes, but decreasing in the $\boldsymbol{s}$ direction This is where the $\frac{\partial^{2} f}{\partial x \partial y}$ derivative comes in.

If the critical point is at $\boldsymbol{P}$ and

$$
\left.\frac{\partial f}{\partial x}\right|_{P}=0,\left.\quad \frac{\partial f}{\partial y}\right|_{P}=0
$$

or either or both are undefined at $\boldsymbol{P}$, then compute

$$
\begin{aligned}
& A=\left.\frac{\partial^{2} f}{\partial x^{2}}\right|_{P} \\
& B=\left.\frac{\partial^{2} f}{\partial x \partial y}\right|_{P} \\
& C=\left.\frac{\partial^{2} f}{\partial y^{2}}\right|_{P} \\
& D=B^{2}-A C \\
& \text { if } D<0 \text { and } A<0 \Rightarrow \text { relative max at } P \\
& \text { if } D<0 \text { and } A>0 \Rightarrow \text { relative min at } P \\
& \text { if } D>0 \Rightarrow \text { saddle point at } P \\
& \text { if } D=0
\end{aligned}
$$

To find the absolute max/min in the interval:

- check $f(\boldsymbol{x}, \boldsymbol{y})$ values at all critical points and on all the boundary points i.e. edges of the interval
- the boundary points are more of an issue in 2D than the 1 D case


## Example 2.2

Find the max. or min. point for the function

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

in the domain $x^{2}+y^{2} \leq 1$.



Problem Statement: An open rectangular box is to have a volume of $0.5 \mathrm{~m}^{\mathbf{3}}$.
Choose the dimensions $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$ for minimum material to make the box.
Solution Procedure: Let the material needed be equal to the total surface area $S$.

$$
\begin{equation*}
S=x y+2 y z+2 x z=F(x, y, z) \tag{1}
\end{equation*}
$$

We want the minimum of $\boldsymbol{f}$, subject to a constrained equation.

$$
\begin{equation*}
V=x y z=0.5 \tag{2}
\end{equation*}
$$

Method 1: apply the constraint by substituting (2) into (1)
From (2)

$$
z=0.5 /(x y)
$$

Therefore,

$$
S=x y+2 y\left(\frac{0.5}{x y}\right)+2 x\left(\frac{0.5}{x y}\right)=x y+\frac{1}{x}+\frac{1}{y}
$$

now we want the minimum of $f(x, y)$, where

$$
S=f(x, y)
$$

For a minimum

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

$$
\begin{array}{ll}
\frac{\partial f}{\partial x}=0 \Rightarrow y-\frac{1}{x^{2}}=0 & x^{2} y=1 \\
\frac{\partial f}{\partial y}=0 \Rightarrow x-\frac{1}{y^{2}}=0 & x y^{2}=1
\end{array}
$$

Solve by dividing out. This gives

$$
x=1 \quad y=1
$$

From Eq. (2)

$$
x y z=0.5 \Rightarrow z=0.5
$$

From Eq. (1), $S_{m i n}=3 \boldsymbol{m}^{2}$.

We can apply the 2 nd derivative test to see if this is really a minimum.

$$
\begin{aligned}
\frac{\partial^{2} f}{\partial x^{2}} & =\left.\frac{2}{x^{3}}\right|_{a t x=1, y=1}=2=A \\
\frac{\partial^{2} f}{\partial x \partial y} & =1=B \\
\frac{\partial^{2} f}{\partial y^{2}} & =\left.\frac{2}{y^{3}}\right|_{a t x=1, y=1}=2=C
\end{aligned}
$$

Check $\boldsymbol{D}=\boldsymbol{B}^{2}-\boldsymbol{A}$. If $\boldsymbol{D}<\mathbf{0}$ and $\boldsymbol{A}>0$ then we have a minimum

$$
D=B^{2}-A C=1-4=-3
$$

Therefore we have a local minimum.
The minimum at $x=1, y=1$ corresponds to $z=0.5$ and $S_{m i n}=3 \mathrm{~m}^{2}$.
The method is straight forward as long as the substitution step of (2) into (1) is easy. Note: sometimes this step is difficult or impossible to allow for a straight forward reduction of (2)/(1) into one $f(x, y)$ form.

## Example 2.3

Maximize $\boldsymbol{F}(\boldsymbol{x}, \boldsymbol{y})=\boldsymbol{x}+\boldsymbol{y}$ subject to a constraint equation. $\boldsymbol{x}^{2}+\boldsymbol{y}^{2}=4$
or $\quad G(x, y)=x^{2}+y^{2}-4=0$


## Extend These Ideas to 3-D Functions

Find the max $/ \min$ of $\boldsymbol{F}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ subject to a constraint $\boldsymbol{G}(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})=\mathbf{0}$.

1. form the Lagrangian function

$$
L=F+\lambda G
$$

where the Lagrange multiplier, $\boldsymbol{\lambda}$, is an unknown parameter at this point.
2. $\min / \max \Rightarrow \nabla L=0$. i.e. $\nabla \boldsymbol{F}$ is parallel to $\nabla G$.

Note $L=L(x, y, z, \lambda)$.

Therefore

$$
\begin{equation*}
\frac{\partial L}{\partial x}=0 \quad \text { (1) } \quad \frac{\partial L}{\partial y}=0 \quad(2) \quad \frac{\partial L}{\partial z}=0 \quad \text { (3) } \quad \frac{\partial L}{\partial \lambda}=0 \tag{4}
\end{equation*}
$$

3. Leads to 4 equations for 4 unknowns - solve for the max/min location - $(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ and the value of $\boldsymbol{\lambda}$, which relates the change in the max/min value of $\boldsymbol{F}$ for small increases or decreases in the constraint.

It should be noted that the solution can sometimes be difficult, since the 4 equations are non-linear.
4. once we have $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}$ location, we can evaluate $\boldsymbol{F}$ at the $\mathrm{min} / \mathrm{max}$ value.
5. the 2 nd derivative test of $\boldsymbol{F}$ is possible, but often not necessary.

## Example 2.4

Minimize $\boldsymbol{F}=\boldsymbol{x} \boldsymbol{y}+2 \boldsymbol{y} \boldsymbol{z}+2 \boldsymbol{x} \boldsymbol{z}$ (surface area), subject to:

$$
x \cdot y \cdot z=0.5 m^{3} \text { or } \boldsymbol{G}=\boldsymbol{x} \cdot \boldsymbol{y} \cdot \boldsymbol{z}-0.5=0
$$

## Method of Least Squares



## Reading

Trim $12.13 \longrightarrow$ Least Squares

## Assignment

web page $\longrightarrow$ assignment \#6

We will demonstrate the method through example.
Given four data points from an experiment

$$
\begin{array}{lllll}
\boldsymbol{x}_{\boldsymbol{i}} & 0 & 1 & 4 & 6 \\
\boldsymbol{y}_{\boldsymbol{i}} & 2 & 3 & 3 & 1
\end{array}
$$

where $N=4$ is the number of data points.
Fit the "best" quadratic curve through the data.

$$
g(x)=A+B x+C x^{2}
$$

The curve can take any form we want. Often, these is some physical basis to guide us in determining which form of the curve to use. Sometimes we might use trial and error for a few different curve shapes.


The question remains - how good is the fit? At each $\boldsymbol{x}_{\boldsymbol{i}}$ data point, we must compute the difference
(residual). At $\boldsymbol{x}_{\boldsymbol{i}}$

$$
R_{i}=\underbrace{g\left(x_{i}\right)}_{\text {curve fit value at } x_{i}}-\underbrace{y_{i}}_{\text {data value at } x_{i}}
$$

The "best" curve would have minimum $\boldsymbol{R}_{\boldsymbol{i}}$ summed over all data points. However, some $\boldsymbol{R}_{\boldsymbol{i}}$ 's are +'ve and some are -'ve. The cancellation effect can be misleading, giving a false indication of a good fit. To avoid this, we need to square $\boldsymbol{R}_{i}$, so all are +'ve. Therefore the "best" curve is based on the minimum $\boldsymbol{R}_{i}^{2}$, summed over all points.

The sum of the square of the residuals is given as

$$
S=\sum_{i=1}^{N}\left[g\left(x_{i}\right)-y_{i}\right]^{2}=\sum_{i=1}^{N}\left[A+B x_{i}+C x_{i}^{2}-y_{i}\right]^{2}
$$

$\boldsymbol{x}_{i}$ and $\boldsymbol{y}_{i}$ are the given data points. The unknowns here are $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$. i.e. $\boldsymbol{S}=\boldsymbol{S}(\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C})$. The best fit will have the minimum value of $\boldsymbol{S}$. For minimum $\boldsymbol{S}$

$$
\frac{\partial S}{\partial A}=0 \quad \frac{\partial S}{\partial B}=0 \quad \frac{\partial S}{\partial C}=0
$$

We need to solve three equations to find the best values for our three unknowns, $A, B, C$.

The physical meaning of this is - on average, a data point is 0.0464 away from the $\boldsymbol{g}(\boldsymbol{x})$ curve - which is considered a good fit. (similar to a RMS type average).


The procedure can be used for any curve shape, however, it is sometimes convenient to change the variable first.

If we want to fit the data $x_{i}$ and $y_{i}$ to $\boldsymbol{g}(\boldsymbol{x})=\boldsymbol{A} \boldsymbol{e}^{B x}$, it is easier to take the $\ln$, i.e.

$$
\begin{aligned}
& \text { data } x_{i}, \quad Y_{i}=\ln y_{i} \\
& \ln g(x)=\ln A+B x \\
& \Rightarrow \quad G(x)=A^{*}+B x
\end{aligned}
$$

We will fit a line $\boldsymbol{A}^{*}+\boldsymbol{B} \boldsymbol{x}$ to $\boldsymbol{x}_{\boldsymbol{i}}, \boldsymbol{Y}_{\boldsymbol{i}}$ data.

