

## 2. Differentiation of scalar fields

*What is the gradient of a scalar field? Why is the gradient perpendicular to level contours? What is its relation to ‘slope’? How do we take derivatives in other directions? How do we decide which points are maxima, minima or saddles (using the Hessian)?*

### 2.1 The gradient of a scalar field

Consider the level curves of a scalar field in 2D.

Clearly the gradient or slope is different depending on the path taken over the contours. We can calculate the gradient or rate of change of slope along any path. So clearly the differential (derivative) of a *scalar* field must itself be a *vector* (it has magnitude and direction).

**Definition: gradient vector**

$$\text{grad } \phi = \frac{\partial \phi}{\partial x} \mathbf{i} + \frac{\partial \phi}{\partial y} \mathbf{j} + \frac{\partial \phi}{\partial z} \mathbf{k}$$

**Key properties of  $\text{grad } \phi$ :**

- (i) The quantity  $\text{grad } \phi(x, y, z)$  is a vector field.
- (ii) Its magnitude  $|\text{grad } \phi|$  is the maximum rate of change of  $\phi$ .
- (iii) It points in the direction of the maximal rate of change of  $\phi$ ; i.e. along the **normal vector** to the level surface  $\phi = \text{const.}$

To help us understand  $\text{grad } \phi$ , let us consider a **directional derivative**  $D_{\mathbf{a}}$  of a scalar field  $\phi(x, y, z)$  at a point  $\mathbf{p}$  in a direction  $\mathbf{a}$

$$D_{\mathbf{a}}\phi(\mathbf{p}) = \left. \frac{d\phi(\mathbf{r}(t))}{dt} \right|_{t=0}, \quad \mathbf{r}(t) = \mathbf{p} + t\hat{\mathbf{a}}$$

We can find the directional derivative  $D_{\mathbf{a}}\phi(\mathbf{p})$  from the slope of a scalar function  $f(t) = \phi(\mathbf{r}(t))$  along the line  $\mathbf{r}(t) = \mathbf{p} + t\hat{\mathbf{a}}$  at  $t = 0$ . Some algebra (see additional material) shows

$$D_{\mathbf{a}}\phi = \hat{\mathbf{a}} \cdot \text{grad } \phi$$

This leads us to write the gradient more abstractly as:

**Definition  $\nabla$**  ‘*del*’ is the **vector differential operator**

$$\nabla = \frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{k} = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$$

**Worked example 2.1** Calculate  $\text{grad } \phi$  where

$$\phi = 2xy + ax + z^2 \quad (a = \text{constant}).$$

*Evaluate at the origin and at the point  $(a, a, a)$ . Find the directional derivative in the direction  $\mathbf{a} = (1, 1, 1)$  at these two points.*

## 2.2 Applications of gradient

### 1. Equation for the tangent plane to a surface

$\nabla f$  is perpendicular to level surfaces of fields  $f(x, y, z)$ . So therefore if we can write a surface as  $f(x, y, z) = c$ , then the normal is

$$\mathbf{n} = \nabla f,$$

so the equation for the tangent plane at a point  $P$  with position vector  $\mathbf{r} = \mathbf{r}_0$  is

$$(\mathbf{r} - \mathbf{r}_0) \cdot \mathbf{n} = 0, \quad \Rightarrow \quad (\mathbf{r} - \mathbf{r}_0) \cdot \nabla f|_{\mathbf{r}=\mathbf{r}_0} = 0$$

**Worked example 2.2** *Show that the equation for the tangent plane to a sphere, centre  $\mathbf{0}$ , of radius  $a$ , at a point  $(x_0, y_0, z_0)$  is*

$$xx_0 + yy_0 + zz_0 = a^2$$

*When is the direction of the unit normal to the surface not defined?*

### 2. Temperature and pressure

- If  $\phi$  is a temperature field, then heat flows in the direction  $-\nabla\phi$
- Similarly, if  $\phi$  is a pressure field, the wind blows in the direction  $-\nabla\phi$  in which pressure decreases the most (think of a weather map!)

### 3. Force and potential energy

We know from 1D that ' $F = dV/dx$ ' where  $V$  is a potential (the work associated with moving against a potential energy  $-V$ ).

How does this apply in more dimensions?

$$\mathbf{F} = \text{grad } V$$

i.e. force is in the direction of maximum increase in potential.

This applies quite generally, e.g.

- in elasticity and stress analysis where  $V$  is the strain energy and  $\mathbf{F}$  the corresponding stress;
- to electrostatic force  $\mathbf{E}$  between two particles of charge  $Q_1$  and  $Q_2$  being the gradient of the electrostatic potential  $f$  (measured in volts)

$$\mathbf{E} = Q_1 Q_2 4\pi\epsilon_0 \left( \frac{\mathbf{r}}{|\mathbf{r}|^3} \right), \quad f = -Q_1 Q_2 4\pi\epsilon_0 \frac{1}{|\mathbf{r}|}$$

(cf. example 2.3 to follow) where  $\epsilon_0$  is the dielectric constant;

- to gravitational force  $\mathbf{F}$  where  $V \propto 1/r$  is the gravitational potential.

**Worked example 2.3** *A space ship moves in the gravitational field of a planet with gravitational potential*

$$\phi = \frac{k}{|\mathbf{r}|} \quad (\text{where } k = \text{const})$$

*Find the magnitude and direction of the force  $\text{grad } \phi$  acting on the ship at position  $\mathbf{r}$ .*

## 2.3 Stationary points of scalar fields

$\nabla f = \mathbf{0}$  defines the points at which the field  $f(x, y, z)$  is flat

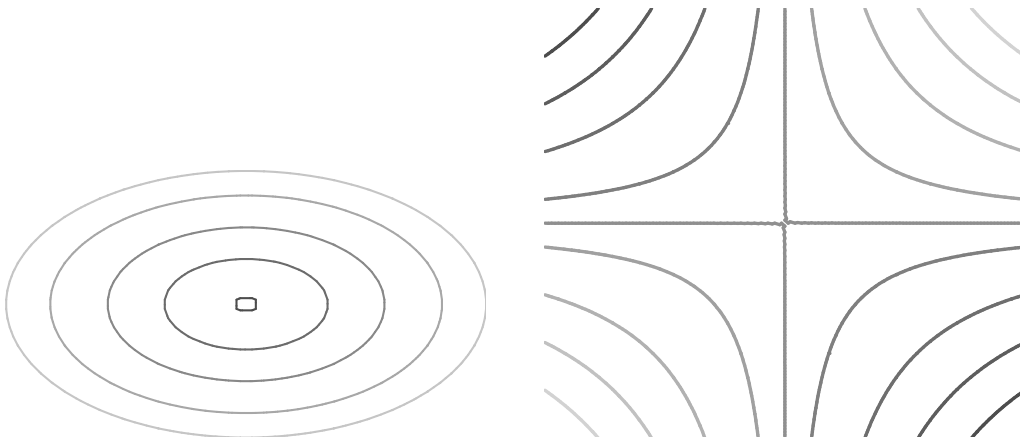
i.e. its stationary (extremum) points =  $(x_0, y_0, z_0)$  such that

$$0 = \nabla f = \left( \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right) \Big|_{x=x_0, y=y_0, z=z_0}$$

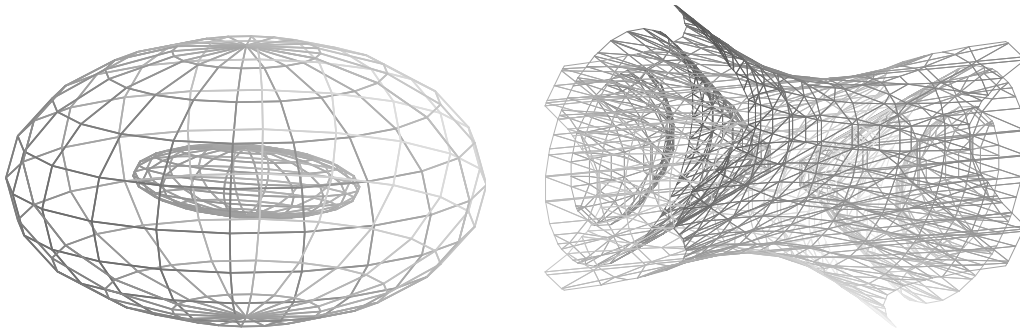
$\Rightarrow f_x = f_y = f_z = 0$  (conditions for a stationary point from EMaI)

In 2D we know there are three kinds of stationary points. Maxima, minima and saddles.

Note that the contours of the level sets  $f = \text{const.}$  are degenerate at stationary points (the unit normal vector  $\hat{\mathbf{n}} = \nabla f / |\nabla f|$  is not defined). The nearby level curves look like ellipses or hyperbolae.



Similarly, for 3D scalar field  $f(x, y, z)$ , the level surfaces are degenerate at stationary points. The surfaces look like ellipsoids or hyperboloids.



**Worked example 2.4** *Calculate all the extrema of the following scalar fields*

(a)  $f(x, y) = x^3 + y^2 - 3(x + y) + 1,$

(b)  $f(x, y, z) = x^2 - 3y^2 + 2z^2 + 3x + 2z + 7.$

## 2.5 Summary

- $\text{grad } \phi$  is defined by

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

- Key properties:
  - (i) The quantity  $\nabla \phi(x, y, z)$  is a vector field.
  - (ii) Its magnitude  $|\nabla \phi|$  is the maximum rate of change of  $\phi$ .
  - (iii) It points in the direction of the maximal rate of change of  $\phi$ ; i.e. along the **normal vector** to the level surface  $\phi = \text{const.}$
- The directional derivative

$$D_{\mathbf{a}} \phi = \hat{\mathbf{a}} \cdot \nabla \phi$$

- Stationary (extremal) points of a vector function  $f(x, y, z)$  can be found from

$$\mathbf{0} = \nabla f = \left( \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right)$$

**Extra: Proof that the direction of  $\text{grad } \phi$  is along the normal vector to the level surface  $\phi = \text{const}$  (non examinable)**

Consider any arbitrary curve  $C$  in 3D parametrised by  $t$  lying inside a level surface  $\phi = c$ . Such a curve can be written as

$$\mathbf{r}(t) = x(t)\mathbf{i} + y(t)\mathbf{j} + z(t)\mathbf{k}$$

where, by definition

$$\phi(\mathbf{r}(t)) = \phi(x(t), y(t), z(t)) = c \quad (2.1)$$

$$\Rightarrow \left. \frac{d\phi}{dt} \right|_{\mathbf{r}(t)} = 0$$

Now, a tangent vector to the  $C$  can be written as

$$\frac{d\mathbf{r}}{dt}(t) = \frac{dx}{dt}(t)\mathbf{i} + \frac{dy}{dt}(t)\mathbf{j} + \frac{dz}{dt}(t)\mathbf{k}.$$

Differentiating (2.1) using the chain rule we find

$$\frac{d\phi(\mathbf{r}(t))}{dt} = \frac{\partial \phi}{\partial x} \frac{dx}{dt}(t) + \frac{\partial \phi}{\partial y} \frac{dy}{dt}(t) + \frac{\partial \phi}{\partial z} \frac{dz}{dt}(t) = 0$$

$$\Rightarrow (\text{grad } \phi) \cdot \frac{d\mathbf{r}}{dt} = 0$$

In other words  $\text{grad } \phi$  is orthogonal to the tangent to any curve lying in the surface  $\{\phi = c\}$ .

Therefore it defines the normal vector to the level set.



**Extra: Proof that the magnitude  $|\text{grad } \phi|$  gives the maximum rate of change of  $\phi$  (non-examinable)**

To see this we need to define the concept of a directional derivative

**Definition.** *The directional derivative  $D_{\mathbf{a}}$  of a scalar field  $\phi(x, y, z)$  at a point  $P$  is the differential of  $\phi$  at  $P$  in the direction of the unit vector  $\hat{\mathbf{a}}$ .*

$$D_{\mathbf{a}}\phi = \lim_{t \rightarrow 0} \frac{\phi(\mathbf{p}_0 + t\hat{\mathbf{a}}) - \phi(\mathbf{p}_0)}{t} = \frac{d\phi(\mathbf{r}(t))}{dt}, \quad \mathbf{r}(t) = \mathbf{p}_0 + t\hat{\mathbf{a}}$$

where  $\mathbf{p}_0$  is the position vector of  $P$ .

**Sub-result.** First we prove that

$$D_{\mathbf{a}}\phi = \frac{d\phi}{dt} = \hat{\mathbf{a}} \cdot \text{grad } \phi$$

**Proof.** Equation for the straight line through  $P$  in direction  $\hat{\mathbf{a}}$  is

$$\mathbf{r}(t) = x(t)\mathbf{i} + y(t)\mathbf{j} + z(t)\mathbf{k} = \mathbf{p}_0 + t\hat{\mathbf{a}}$$

So

$$\frac{d\mathbf{r}(t)}{dt} = \hat{\mathbf{a}}.$$

Applying the chain rule

$$\begin{aligned} D_{\mathbf{a}}\phi &= \frac{d\phi(\mathbf{r}(t))}{dt} = \frac{\partial\phi}{\partial x} \frac{dx}{dt} + \frac{\partial\phi}{\partial y} \frac{dy}{dt} + \frac{\partial\phi}{\partial z} \frac{dz}{dt} \\ &= \left( \frac{\partial\phi}{\partial x}, \frac{\partial\phi}{\partial y}, \frac{\partial\phi}{\partial z} \right) \cdot \left( \frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt} \right) \\ &= \text{grad } \phi \cdot \hat{\mathbf{a}} \quad \square \end{aligned}$$

**Main proof.** So

$$\frac{d\phi(\mathbf{r}(t))}{dt} = \hat{\mathbf{a}} \cdot \text{grad } \phi = |\text{grad } \phi| \cos \theta$$

When is  $\frac{d\phi}{dt}$  a maximum? When  $\hat{\mathbf{a}}$  is parallel to  $\text{grad } \phi$  so

$$\left| \frac{d\phi(t)}{dt} \right| = |\text{grad } \phi|$$

i.e. magnitude of  $\text{grad } \phi$  gives maximum rate of change of  $\phi$ .

## Classification of stationary points (non-examinable)

**Q)** How do we decide whether a stationary point is a maximum, minimum or a saddle?

**A)** By using the notion of curvature. Since gradient — the first derivative — in some way measures slope, we should expect that somehow the rate of change of slope — the curvature — should be a second derivative. Since the function is a scalar and its slope a vector, then what should the curvature be? ... a matrix!

**Definition** *The matrix of second-derivatives (matrix of curvatures) of a scalar function is called the **Hessian**  $H$*

$$H(x, y, z) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial x \partial z} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} & \frac{\partial^2 f}{\partial y \partial z} \\ \frac{\partial^2 f}{\partial z \partial x} & \frac{\partial^2 f}{\partial z \partial y} & \frac{\partial^2 f}{\partial z^2} \end{bmatrix}$$

The Hessian can be written more compactly in 3D (or 2D) as  $H_{ij} = f_{r_i r_j}$  where  $r = (x, y, z)$  (or  $r = (x, y)$ ), that is

$$H(x, y, z) = \begin{bmatrix} f_{xx} & f_{xy} & f_{xz} \\ f_{yx} & f_{yy} & f_{yz} \\ f_{zx} & f_{zy} & f_{zz} \end{bmatrix} \quad \text{or, in 2D} \quad H(x, y) = \begin{bmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{bmatrix}$$

But how does this help? E.g. Consider the case where the Hessian is diagonal.

$$H = \begin{bmatrix} h_{xx} & 0 \\ 0 & h_{yy} \end{bmatrix}$$

Then  $h_{xx} > 0$  implies that in the  $x$ -direction, the function ‘curves up’. If  $h_{yy} > 0$  also, then the function curves up in the  $y$ -direction too.

... thus we have a *minimum*. Similarly if  $h_{xx} < 0$  and  $h_{yy} < 0$  we have a *maximum*.

Finally, if  $h_{xx}$  and  $h_{yy}$  are of opposite signs, then we have that in one co-ordinate direction the function curves up, and in another it curves down. This is the definition of a *saddle point*.

In the case that  $H$  is diagonal; these concepts go over to 3 dimensions also. Minimum if each diagonal entry is positive, maximum if each entry is negative, and a saddle point otherwise.

But what if  $H$  is not diagonal. Now, we know from Eng Maths I, that for ‘most’ matrices we can apply a co-ordinate transform to put the matrix in **diagonal form**. The resulting diagonal matrix has as its entries the **eigenvalues of  $H$** ,  $\{\lambda_1, \lambda_2, \lambda_3\}$ . That is, there is a co-ordinate transform such that

$$H = V^{-1}\Lambda V, \quad \text{where} \quad \Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}$$

After all this we arrive at the criterion for determining the nature of extrema

- All eigenvalues of the Hessian positive  $\Rightarrow$  a **minimum**
- All eigenvalues of the Hessian negative  $\Rightarrow$  a **maximum**
- Some positive, some negative eigenvalues  $\Rightarrow$  a **saddle point**  
(the number of positive eigenvalues, corresponds to the number of ‘uphill’ directions).
- If there is a zero eigenvalue of the Hessian then we have no information

[Nb. Since the Hessian is a real symmetric matrix, all its eigenvalues are real numbers]

**Worked example 2.5 (extra - non-examinable)** *Classify as maxima, minima or saddles, all the stationary points found in Worked example 2.4*