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)? How do we do constrained optimisation (using Lagrange multipliers)?

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

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

What is grad ϕ?

(i) Its magnitude gives the slope (rate of change) of ϕ, when moving along a certain direction. This direction is the **normal vector** to the surface $\phi = const.$

Proof. Consider any arbitrary curve C parametrised by t lying inside a level set $\phi = c$. Such a curve can be written as

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

where, by definition

$$\phi(x(t), y(t), z(t)) = c \tag{2.1}$$

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

$$\boldsymbol{r}'(t) = \frac{dx}{dt}(t)\boldsymbol{i} + \frac{dy}{dt}(t)\boldsymbol{j} + \frac{dz}{dt}(t)\boldsymbol{k}.$$

Differentiating (2.1) using the chain rule we find

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

$$\Rightarrow \quad (\text{grad}\,\phi) \cdot \boldsymbol{r}' = 0$$

In other words grad ϕ is orthogonal to the tangent to any curve lying in the surface $\{\phi = c.\}$. Therefore it defines the normal vector to the level set.

(ii) Its magnitude gives the rate of change of ϕ. To see this we need to define the concept of a directional derivative

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

$$D_{\boldsymbol{a}}\phi = \lim_{t \to 0} \frac{\phi(\boldsymbol{p}_0) - \phi(\boldsymbol{p}_0 + t\hat{\boldsymbol{a}})}{t}$$

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

We can show that

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

Proof. An equation for the straight line through P in the direction $\hat{\boldsymbol{a}}$ is

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

So $\boldsymbol{r}'(t) = \hat{\boldsymbol{a}}$. Applying the chain rule

$$\begin{aligned} D_{\boldsymbol{a}}\phi &= \frac{d\phi}{dt} = \frac{\partial \phi}{\partial x}x' + \frac{\partial \phi}{\partial y}y' + \frac{\partial \phi}{\partial z}z' \\ &= \left(\frac{\partial \phi}{\partial x}, \frac{\partial \phi}{\partial y}, \frac{\partial \phi}{\partial z}\right) \cdot (x', y', z') \\ &= \operatorname{grad} \phi \cdot \hat{\boldsymbol{a}} \qquad \square \end{aligned}$$

Now, since

$$\hat{\boldsymbol{a}} \cdot \operatorname{grad} \phi = |\operatorname{grad} \phi||\hat{\boldsymbol{a}}| \cos\theta = |\operatorname{grad} \phi| \cos\theta$$

we have that $D_{\boldsymbol{a}}$ is largest when $\theta = 0$, and in this case $|D_{\boldsymbol{a}}\phi| = |\operatorname{grad}\phi|$. Thus:

$|\operatorname{grad} \phi|$ points in direction $\theta = 0$ in which ϕ **increases** the most.

(iii) Clearly the gradient is not a constant in space. E.g. consider the contours of a ski slope.

In fact, $\operatorname{grad} \phi(x, y, z)$ defines a vector field. To stress that $\operatorname{grad} \phi$ is a vector field, we have a special notation

$$\operatorname{grad} \phi = \boldsymbol{\nabla}\phi, \qquad \text{where}$$

Definition $\boldsymbol{\nabla}$ *'del' is the* **vector differential operator**

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

Worked example 2.1 *Calculate grad ϕ where*

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

Evaluate at the origin and at the point (a, a, a). Find the directional derivative in the direction of the vector $(1, 1, 1)$ at each of these two points.

2.2 Applications of gradient

1. Equation for the tangent plane to a surface

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

$$\hat{\boldsymbol{n}} = \frac{\boldsymbol{\nabla} f}{|\boldsymbol{\nabla} f|},$$

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

$$(\boldsymbol{r} - \boldsymbol{r}_0) \cdot \hat{\boldsymbol{n}} = 0, \quad \Rightarrow \quad (\boldsymbol{r} - \boldsymbol{r}_0) \cdot \boldsymbol{\nabla} f|_{r=r_0} = 0$$

Worked example 2.2 *Show that the equation for the tangent plane to a sphere 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?

3. Temperature and pressure

- If ϕ is a temperature field, then heat flows in the direction $-\boldsymbol{\nabla}\phi$

- Similarly, if ϕ is a pressure field, the wind blows in the direction $-\boldsymbol{\nabla}\phi$ in which pressure decreases the most (think of a weather map!)

4. Force and potential energy

We know from 1D that '$F = dV/dx$' where V is potential (the work associated with moving against a potential energy $-V$) . How does this apply in more dimensions?

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

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 F the corresponding stress;
- to electrostatic force $\boldsymbol{E}$ between two particles of opposite charge Q_1 and Q_2 being the gradient of the electrostatic potential f (measured in volts)

$$\begin{aligned} \boldsymbol{E} &= Q_1 Q_2 4\pi\epsilon_0 \left(\frac{\boldsymbol{r}}{|\boldsymbol{r}|^3}\right) \\ f &= -Q_1 Q_2 4\pi\epsilon_0 \frac{1}{|\boldsymbol{r}|} \end{aligned}$$

  (cf. example 2.3 to follow) where ϵ_0 is the dielectric constant;
- to gravitational force F where V is the gravitational potential.

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

$$\phi = \frac{k}{|\boldsymbol{r}|} \qquad \textit{where } k = \textit{const})$$

Calculate the magnitude and direction of the force gradϕ acting on the ship at a distance $\boldsymbol{r}$ from the centre of the planet. Calculate *the maximum potential energy reached if the ship is constrained to move on the plane*

$$(x - a) + y = b, \quad a,\, b = \mathit{const.}$$

What happens if $a = -b$?

2.3 Stationary points of multi-valued functions

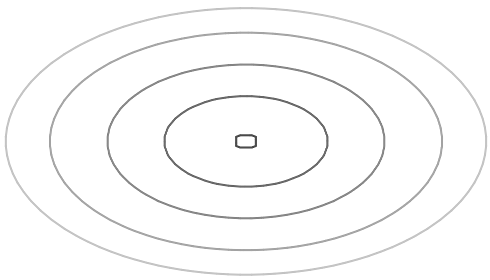
$\boldsymbol{\nabla} f = \mathbf{0}$ defines the points at which the function $f(x, y, z)$ is flat, i.e. its stationary (extremum) points $= (x_0, y_0, z_0)$ such that

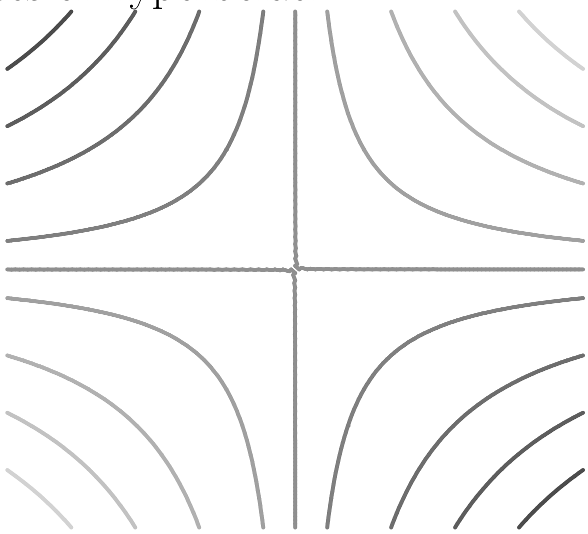
$$0 = \boldsymbol{\nabla} f = \left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}\right)\Bigg|_{x=x_0, y=y_0, z=z_0} = (f_x, f_y, f_z)|_{x=x_0, y=y_0, z=z_0}$$

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

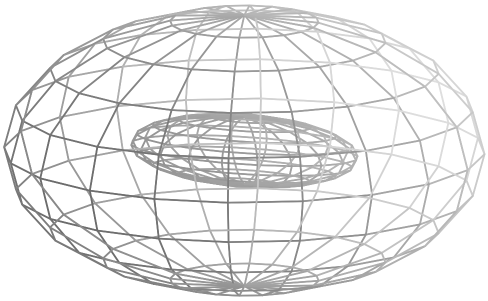
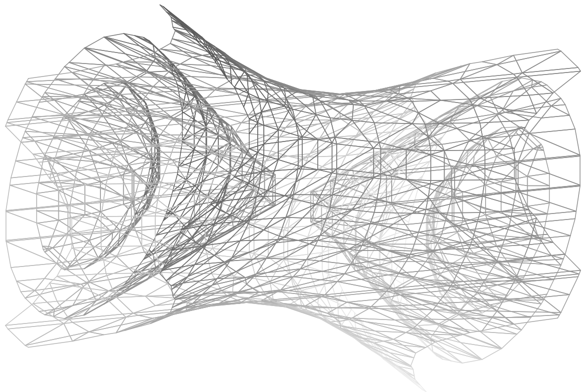
In 2D we know there are three kinds of stationary points. Maxima, minima and saddles.

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





Similarly, in 3D, 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 functions*

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

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

Q) But 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

$$H(x, y, z) = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial xy} & \frac{\partial^2 f}{\partial xz} \\ \frac{\partial^2 f}{\partial yx} & \frac{\partial^2 f}{\partial yy} & \frac{\partial^2 f}{\partial yz} \\ \frac{\partial^2 f}{\partial zx} & \frac{\partial^2 f}{\partial zy} & \frac{\partial^2 f}{\partial z^2} \end{bmatrix}$$

The Hessian can be written more simply 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.

$$H = \begin{bmatrix} h_{11} & 0 \\ 0 & h_{22} \end{bmatrix}$$

Then $h_{11} > 0$ implies that in the x-direction, the function 'curves up'. If h_{22} >0 also, then the function curves up in the y-direction too:

... thus we have a *minimum*. Similarly if $h_{11} < 0$ and $h_{22} < 0$ we have a *maximum*:

Finally, if h_{11} and h_{12} 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 postive, 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

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

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 *Classify as maxima, minima or saddles, all the stationary points found in Worked example 2.4*

Worked example 2.6 *In 2D a set of criteria for determining whether a stationary point is a maximum, minimum or saddle can be written as*

- *Minimum if* $f_{xx}f_{yy} - (f_{xy})^2 > 0$ *and* $f_{xx} > 0$

- *Maximum if* $f_{xx}f_{yy} - (f_{xy})^2 > 0$ *and* $f_{xx} < 0$
- *Saddle if* $f_{xx}f_{yy} - (f_{xy})^2 < 0$

Show that this is equivalent to the condition on the eigenvalues of the Hessian.

2.4. Constrained optimisation; Lagrange multipliers

Consider constrained optimisation in 2D (3D and greater similar):

How to maximise (or minimise) $\quad f(x, y), \quad$ subject to $\quad g(x, y) = 0$?

Answer: find stationary points of

$$h(x, y, \mu) = f(x, y) + \mu g(x, y),$$

where μ is an arbitrary **Lagrange multiplier** which is an arbitrary constant that can take on any real value.

But why does this work?

Worked example 2.7 *Find the maximum and minimum values of*

$$f(x, y) = 4x + y + y^2$$

where (x, y) *lies on the circle* $x^2 + y^2 + 2x + y = 1$

The same ideas work in 3D (see next worked example). That is, to maximise (or minimise) $f(x, y, z)$, subject to $g(x, y, z) = 0$, we find the stationary points of

$$h(x, y, z, \mu) = f(x, y, z) + \mu g(x, y, z)$$

Worked example 2.8 *Find the dimensions of the rectangular box* **of maximum capacity** *whose total surface area is 108*m^2.

The same ideas work where more than one constraint is active. That is to find extrema of $f(x, y, z)$, subject to $g_1(x, y, z) = 0$, and $g_2(x, y, z) = 0$ we find the stationary points of

$$h(x, y, z, \mu_1, \mu_2) = f(x, y, z) + \mu_1 g_1(x, y, z) + \mu_2 g_2(x, y, z).$$