Lectures 1 and 2

Mathematical Background

1) Differential calculus

a) The gradient (of a scalar field).

The gradient is a generalization of the notion of derivative to multidimensional spaces. Consider a scalar field, defined in a, say, 3D space:

\[ f = f(x, y, z) = f(\vec{r}). \]

For an infinitesimal change of \( \Delta f = f(\vec{r} + \Delta \vec{r}) - f(\vec{r}) \) we can write

\[ \Delta f = \frac{\partial f}{\partial x} \Delta x + \frac{\partial f}{\partial y} \Delta y + \frac{\partial f}{\partial z} \Delta z, \]

which can be written as a scalar product:

\[ \Delta f = \left( \frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} + \frac{\partial f}{\partial z} \right) \Delta \vec{r}. \]

Clearly, this depends on \( \Delta \vec{r} \) and the first bracketed is only a property of the field itself, and is called its gradient

\[ \nabla f = \left( \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z} \right). \]

("del f")
Meaning of the gradient: the gradient is a vector in its proper meaning. What is the meaning of this vector?

Property 1: \( \nabla f \) at any surface of constant \( f \).

Proof: consider a surface \( S : f(\vec{r} \in S) = \text{const} \).
For two points \( A \) and \( B \) that are infinitesimally close, we have

\[
\Delta f = f(A) - f(B) = \nabla f \cdot \Delta \vec{r}_{AB} = 0.
\]

Since this is true for any \( B \)-point on the vicinity of \( A \), \( \nabla f \) must be \( \perp \) to the surface at that point, and any point on \( S \), as the choice of \( A \) is arbitrary.

Property 2: \( \nabla f \) points in the direction of the fastest growth of \( f \).

Proof: \( \Delta f = \nabla f \cdot \Delta \vec{r} = |\nabla f| \cdot |\Delta \vec{r}| \cdot \cos \theta \),

where \( \theta \) is the angle between \( \Delta \vec{r} \) and \( \nabla f \).

Thus for fixed \( |\Delta \vec{r}| \), \( \Delta f \) is maximal for \( \theta = 0 \) or \( \theta = \pi \), i.e. \( \Delta \vec{r} \parallel \nabla f \). Thus the direction of \( \nabla f \) coincides with the direction of the fastest growth of \( f \), \( |\nabla f| \), giving the rate of growth.
To illustrate this, let us calculate \( \nabla f \) for \( e^{-r^2} \) (the Gaussian) in 2D:
\[
f(x, y) = e^{-x^2 - y^2}.
\]

Equipotential curves: \( f(x, y) = \text{const} \Rightarrow r = \text{const} \Rightarrow \text{circles} \).

We see that \( \nabla f \) must point radially by property of the function.

Check:
\[
\nabla f = \left( \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right).
\]
\[
\frac{\partial f}{\partial x} = -2x \cdot e^{-x^2-y^2} \quad \Rightarrow \quad \nabla f = -2x e^{-x^2} (x, y) = -2x e^{-r^2}, \text{ as expected.}
\]

b) \( \nabla \) operator.

\( \nabla f \) can be formally written as
\[
\nabla f = \left( \frac{\partial f}{\partial x}, \frac{\partial f}{\partial y} \right), \text{ which represents the gradient as a result of a differential operator,} \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y} \right) \text{ acting on } f. \text{ Thus defined vector differential operator } \nabla \text{ is called "del" for brevity.}
The convention that everyone uses is that it is always acts to the right.

1) The divergence

It allows to compactly write other differential operators on vectors. The divergence is an example:

\[ \vec{F} = \vec{F}(x, y, z) \text{ vector field}, \]

\[ \text{div } \vec{F} = \nabla \cdot \vec{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}. \]

(Scalar field)

\[ \left( \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \right) (x F_x + y F_y + z F_z) = \]

\[ = \frac{\partial F_x}{\partial x} \ldots \rightarrow \text{laterally works as a scalar product.} \]

**Meaning:**

Divergence of a vector field at a point measures net "piercing" done by the vector field to an infinitesimal surface around the point.

"A lot of net piercing" \( \text{div } \vec{F} \) no net piercing \( \text{div } \vec{F} = 0 \).

C.f. point charge E-field.
Example: \( \mathbf{F} = \mathbf{r} \), \( \text{div} \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = 3 \).

2) The curl:

There is another way we can apply \( \nabla \times \) to a vector field:

\[
\text{curl} \, \mathbf{F} = \nabla \times \mathbf{F} = \begin{vmatrix}
\hat{i} & \hat{j} & \hat{k} \\
\frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\
F_x & F_y & F_z
\end{vmatrix} = \hat{x} \left( \frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) - \\
\hat{y} \left( \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} \right) + \\
\hat{z} \left( \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right).
\]

Meaning: the curl shows whether a vector field "curls around" a point.

Example: \( \mathbf{F} = (-xy, 0, 0) \).

\[
\nabla \times \mathbf{F} = \hat{z} \left( -\frac{\partial F_y}{\partial y} \right) = \hat{z} \mathbf{F}.
\]
Second derivatives

\[ \frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x} \left( \frac{\partial f}{\partial x} \right) \]

\[ \frac{\partial^2 f}{\partial y^2} = \frac{\partial}{\partial y} \left( \frac{\partial f}{\partial y} \right) \]

\[ \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x} \left( \frac{\partial f}{\partial y} \right) \]

\[ \frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial y} \left( \frac{\partial f}{\partial x} \right) \]

(see Frenkel and Smit, page 86)
\[ \text{div} (\text{curl} \, \mathbf{F}) = \mathbf{F} \cdot (\nabla \times \mathbf{F}) = 0. \]

\[ \nabla \times (\nabla \times \mathbf{F}) = \nabla (\nabla \cdot \mathbf{F}) - (\nabla \times \mathbf{F}) \cdot \mathbf{F} = \nabla \left( \nabla \cdot \mathbf{F} \right) - \Delta \mathbf{F}. \]

Laplacian of a vector is understood as Laplacian of each component:

\[ \Delta \mathbf{F} = (\Delta f_x, \Delta f_y, \Delta f_z). \]

4) **Triple products**

There are also useful relations for \( \nabla \) acting on various products:

\[ \nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) + \mathbf{a} \cdot (\nabla \times \mathbf{b}). \]

\[ \nabla \times (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \times (\nabla \times \mathbf{a}) + \mathbf{a} \times (\nabla \times \mathbf{b}). \]

\[ \nabla \cdot (\mathbf{a} \cdot \nabla \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) + \mathbf{a} \cdot (\nabla \times \mathbf{b}). \]

\[ \nabla \times (\mathbf{a} \cdot \nabla \mathbf{b}) = \mathbf{b} \times (\nabla \times \mathbf{a}) + \mathbf{a} \times (\nabla \times \mathbf{b}). \]

\[ \text{div} : \nabla \cdot (\mathbf{a} \mathbf{a}) = \mathbf{a} \cdot (\nabla \mathbf{a}) + \Delta \mathbf{a}. \]

\[ \nabla \cdot (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \cdot (\nabla \times \mathbf{a}) + \mathbf{a} \cdot (\nabla \times \mathbf{b}). \]

\[ \nabla \times (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \times (\nabla \times \mathbf{a}) - \mathbf{a} \cdot (\nabla \times \mathbf{b}). \]
curl:
\[
\nabla \times (\mathbf{a} \mathbf{b}) = \nabla \cdot (\mathbf{a} \mathbf{b}) - \mathbf{a} \times \nabla \mathbf{b}
\]
\[
\nabla \times (\mathbf{a} \times \mathbf{b}) = \mathbf{b} \times (\nabla \times \mathbf{a}) + \mathbf{a} \times (\nabla \times \mathbf{b}) =
\]
\[
= (\mathbf{b} \cdot \mathbf{a}) \mathbf{a} - \mathbf{a} (\mathbf{a} \cdot \mathbf{b}) + \mathbf{a} (\mathbf{b} \cdot \mathbf{a}) - (\mathbf{b} \cdot \mathbf{a}) \mathbf{b}.
\]