Vector Calculus

Exercise

Dresden Summer School in Systems Biology 2018

For a function $f(x)$ in one variable x (for example a concentration field along a line), you are familiar with the ordinary derivative $\frac{d}{dx}f(x)$ and the corresponding rules of calculus, e.g. how to differentiate a function of the form $f(x) = x^n$.

a) If necessary, recapitulate the rules of calculus (product rule, chain rule). What does it mean for a function if $\frac{d}{dx}f(x) = 0$ at some point x?

Spatial models generally contain more than one dimension, which are represented by a space vector $\mathbf{r} = (x, y, z)^T$. Besides scalar fields (e.g. concentration values in space $c(\mathbf{r})$), also vector fields – a vector of scalar fields – are often needed to formulate a model. The standard rules of calculus, as well as the usual vector algebra hold for those quantities, but a clever notation is needed to depict these operations. For this, one introduces the vector of partial derivatives (the gradient or nable operator)

$$\nabla \equiv \begin{pmatrix} \partial_x \\ \partial_y \\ \partial_z \end{pmatrix} = (\partial_x, \partial_y, \partial_z)^T$$

and the aim of the following exercises is to familiarize yourself with this object.

b)
- Write out the components of the gradient of a function $\nabla f(\mathbf{r})$.
- How can $\nabla f(\mathbf{r})$ be used to identify local extrema of $f(\mathbf{r})$?
- Isolines or isosurfaces of $f(\mathbf{r})$ are lines or surfaces where $f(\mathbf{r})$ is constant. How is the direction of $\nabla f(\mathbf{r})$ related to those lines and surfaces?
- What information is contained in the length of the gradient vector $|\nabla f(\mathbf{r})|$?
- If you can't find a general answer to those questions, consider as a test case the function $f(\mathbf{r}) = x^2 + y^2$. Visualize it and calculate the corresponding quantities, to investigate how they are related to $f(\mathbf{r})$.

c) Connecting the gradient operator with a vector field by a scalar product defines the divergence $\nabla \cdot \mathbf{v} = \partial_x v_x(\mathbf{r}) + \partial_y v_y(\mathbf{r}) + \partial_z v_z(\mathbf{r})$. This operator tells you about the source density within a flow field, i.e. if mass is generated or lost at certain points. To understand this better, consider the two flow fields $\mathbf{v}_1 = (x, y, 0)^T$ and $\mathbf{v}_2 = (y, x, 0)^T$.

- Calculate the divergence of $\mathbf{v}_1$ and $\mathbf{v}_2$.
- Try to understand the result qualitatively by plotting $\mathbf{v}_1$ and $\mathbf{v}_2$ in a computer program or by sketching it on paper.
- Try to understand it quantitatively by calculating the total flux Q through some closed box of side-length 1. Denoting the normal on the surface of this box by $\mathbf{n}$, the integral to calculate Q has the form[1]:

$$Q = \oint \mathbf{v} \cdot \mathbf{n} dA = \int_0^1 dz \left(\int_0^1 [-v_x(0) + v_x(1)] dy + \int_0^1 [-v_y(0) + v_y(1)] dx \right).$$

- Conclude your answers to the questions in *c)* by looking up the so called 'divergence theorem' to find out how the first integral is related to $\nabla \cdot \mathbf{v}$.

d) The operation $\nabla \times \mathbf{v}$, which connects a vector field and the gradient operator by a cross-product '$\times$' is called the curl ($\boldsymbol{\omega} = \nabla \times \mathbf{v}$ is called vortex strength) of $\mathbf{v}$. Consider a flow field of the form $\mathbf{v}_3 = \boldsymbol{\Omega} \times \mathbf{r}$ with a constant vector $\boldsymbol{\Omega} = (0, 0, \Omega)^T$ pointing in z-direction and the space vector $\mathbf{r} = (x, y, z)^T$.

[1] This is the general form of a surface integral over a vector field. You may ask google if you want to learn more about it.

- Calculate the components of $\mathbf{v}_3$ and sketch this flow field.
- Determine the components of $\boldsymbol{\omega} = \nabla \times \mathbf{v}_3$.
- Use those results to give a qualitative description of the effect of the curl operator.
- Determine the source density of this flow field $\nabla \cdot \mathbf{v}_3$. Did you expect this result from your sketch of $\mathbf{v}_3$?

As an additional information: Note that the curl of a vector field $\nabla \times \mathbf{v}$ enters in another important integral theorem: the Stokes theorem. It formally reads

$$\int (\nabla \times \boldsymbol{v}) \cdot \mathbf{n} \, dA = \oint \mathbf{v} \cdot d\mathbf{l},$$

where the area integral on the left is the same type as in question *c*) and the right integral is calculated along the curve which makes up the boundary of this area.

e) The answers to *b*) and *c*) essentially suffice to understand the diffusion equation and in the following we give you some ideas how this works.

- Given a concentration field $c(\mathbf{r})$ and a diffusion constant D, Fick's law relates heterogeneities in the field $c(\mathbf{r})$ to diffusive fluxes that tend to homogenize it. This flux $\mathbf{j}$ (number of particles per area and time or 'flow $\mathbf{v}$ per volume') is given by

$$\mathbf{j} = -D\nabla c(\mathbf{r}).$$

  Interpret this equation based on your answers to question *b*).

Now one can calculate the source density (the divergence) of $\mathbf{j}$, which is related to the local change in concentration per time, to get the diffusion equation:

$$\frac{\partial c(\mathbf{r}, t)}{\partial t} = -\nabla \cdot \mathbf{j} = D\nabla \cdot [\nabla c(\mathbf{r})]$$

From your answers to the previous questions this equation can now be paraphrased in the following way: At all points in space, where the diffusive fluxes have a non-vanishing source density (right hand side), the concentration has to change in time (left hand side).

- As a practical example, sketch a one-dimensional concentration field $c(x) = e^{-x^2}$ and determine in what regions on the x-axis the concentration would increase in time and where it would decrease in time if diffusion would take place. To determine those regions, the diffusion equation tells you that you simply have to find out where the second derivative of $c(x)$ is larger or smaller than zero. Add the corresponding regions to your sketch of the concentration field! You should now be able to observe the homogenizing nature of diffusive processes.