Lecture 13: Differential Operations on Vectors

Reading:
Kreyszig Sections: 9.8, 9.9 (pages410–413, 414–416)

Generalizing the Derivative

The number of different ideas, whether from physical science or other disciplines, that can be understood with reference to the “meaning” of a derivative from the calculus of scalar functions, is very very large. Our ideas about many topics, such as price elasticity, strain, stability, and optimization, are connected to our understanding of a derivative.

In vector calculus, there are generalizations to the derivative from basic calculus that act on a scalar and give another scalar back:

**gradient** ($\nabla$): A derivative on a scalar that gives a vector.

**curl** ($\nabla \times$): A derivative on a vector that gives another vector.

**divergence** ($\nabla \cdot$): A derivative on a vector that gives scalar.

Each of these have “meanings” that can be applied to a broad class of problems.

The gradient operation on $f(\vec{x}) = f(x, y, z) = f(x_1, x_2, x_3)$,

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

(13-1)
has been discussed previously. The curl and divergence will be discussed below.
An example of a scalar potential, due to three point charges in the plane, is visualized. Methods for computing a gradient are presented.

1: This is the 2D $1/r$-potential; here $potential$ takes four arguments: two for the location of the charge and two for the position where the “test” charge “feels” the potential.

2-4: These are three fixed charge potentials, arranged at the vertices of an equilateral triangle.

5: $gradfield$ is an example of a function that takes a scalar function of $x$ and $y$ and returns a vector with component derivatives: the gradient vector of the scalar function of $x$ and $y$.

6: However, the previous example only works for functions of $x$ and $y$ explicitly. This expands $gradfield$ to other Cartesian coordinates other than $x$ and $y$.

7: $ThreeHolePotential$ is the superposition of the three potentials defined in 2–4.

8: Plot3D is used to visualize the superposition of the potentials due to the three charges.

9: $ContourPlot$ is an alternative method to visualize this scalar field. The option $ColorFunction$ points to an example of a Pure Function—a method of making functions that do not operate with the usual “square brackets.” Pure functions are indicated with the & at the end; the # is a place-holder for the pure function’s argument.
Divergence and Its Interpretation

The divergence operates on a vector field that is a function of position, \( \vec{v}(x, y, z) = \vec{v}(\vec{x}) = (v_1(\vec{x}), v_2(\vec{x}), v_3(\vec{x})) \), and returns a scalar that is a function of position. The scalar field is often called the divergence field of \( \vec{v} \), or simply the divergence of \( \vec{v} \).

\[
\text{div } \vec{v}(\vec{x}) = \nabla \cdot \vec{v} = \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z} = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot (v_1, v_2, v_3) = \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot \vec{v}
\]  

Think about what the divergence means.
A visualization gradient field of the potential defined in the previous example is presented. The divergence of the gradient $\nabla \cdot \nabla \phi = \nabla^2 \phi$ (i.e., the result of the Laplacian operator $\nabla^2$) is computed and visualized.

1: We use our previously defined function $\text{gradfield}$ to compute the gradient of $\text{ThreeHolePotential}$ everywhere in the plane.

2: $\text{PlotVectorField}$ is in the $\text{VectorFieldPlots}$ package. Because a gradient produces a vector field from a scalar potential, arrows are used at discrete points to visualize it.

3: The divergence operates on a vector and produces a scalar. Here, we define a function, $\text{divergence}$, that operates on a 2D-vector field of $x$ and $y$ and returns the sum of the component derivatives. Therefore, taking the divergence of the gradient of a scalar field returns a scalar field that is naturally associated with the original—its physical interpretation is (minus) the rate at which gradient vectors “diverge” from a point.

4–5: We compute the divergence of the gradient of the scalar potential. This is used to visualize the Laplacian field of $\text{ThreeHolePotential}$.
Coordinate Systems

The above definitions are for a Cartesian \((x, y, z)\) system. Sometimes it is more convenient to work in other (spherical, cylindrical, etc) coordinate systems. In other coordinate systems, the derivative operations \(\nabla\), \(\nabla \cdot\), and \(\nabla \times\) have different forms. These other forms can be derived, or looked up in a mathematical handbook, or specified by using the MATHEMATICA® package “VectorAnalysis.”
Examples of Coordinate Transformations obtained from the VectorAnalysis package are presented.

It is no surprise that many of these differential operations already exist in Mathematica packages.

1:
<< "VectorAnalysis"

Converting between coordinate systems

The spherical coordinates expressed in terms of the cartesian x,y,z

CoordinatesFromCartesian[
{x, y, z}, Spherical[r, theta, phi]]

\[
\begin{align*}
&\{\sqrt{x^2 + y^2 + z^2}, \\
&\text{ArcCos}\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right), \\
&\text{ArcTan}\left(\frac{x}{y}\right)\}\n\end{align*}
\]

The cartesian coordinates expressed in terms of the spherical r & \theta

CoordinatesToCartesian[
{r, theta, phi}, Spherical[r, theta, phi]]

\[
\begin{align*}
&\{r \cos(\phi) \sin(\theta), \\
&r \sin(\phi) \sin(\theta), \\
&r \cos(\theta)\}\n\end{align*}
\]

The equation of a line through the origin in spherical coordinates

Simplify[
CoordinatesFromCartesian[{a t, b t, c t},
Spherical[r, theta, phi]], t > 0]

1–2: CoordinatesFromCartesian from the VectorAnalysis package transforms three Cartesian coordinates, named in the first argument-list, into one of many coordinate systems named by the second argument.

3: CoordinatesToCartesian transforms one of many different coordinate systems, named in the second argument, into the three Cartesian coordinates, named in the first argument (which is a list).

4: For example, this would be the equation of a line radiating from the origin in spherical coordinates.
We compute distances from Boston to Paris along different routes.

1–3: CityData provides downloadable data. The data includes—among many other things—the latitude and longitude of many cities in the database. This show that Marseilles is north of Boston (which I found to be surprising).

4–5: SphericalCoordinatesofCity takes the string-argument of a city name and uses CityData to compute its spherical coordinates (i.e., \((r_{\text{earth}}, \theta, \phi)\)) are same as (average earth radius = 6378.1 km, latitude, longitude). We use Degree which is numerically \(\pi/180\).

6: LatLong takes the string-argument of a city name and uses CityData to return a list-structure for its latitude and longitude. We will use this function below.

7–8: CartesianCoordinatesofCity uses a coordinate transform and SphericalCoordinatesofCity.

9–10: If we imagine traveling through the earth instead of around it, we would use the Norm of the difference of the Cartesian coordinates of two cities.

11–12: Comparing the great circle route using SphericalDistance (from the Geodesy package) to the Euclidean distance, is a result that surprises me. It would save only about 55 kilometers to dig a tunnel to Paris—sigh.

13: SpheroidalDistance accounts for the earth’s extra waistline for computing great-circle distances.
A $1/r^n$-potential is used to demonstrate how to obtain gradients and divergences in other coordinate systems.

1: `SimplePot` is the simple $1/r^n$ potential in Cartesian coordinates.

2: `Grad` is defined in the `VectorAnalysis`: in this form it takes a scalar function and returns its gradient in the coordinate system defined by the second argument.

3: An alternate form of `SimplePot` is defined in terms of a single coordinate; if $r$ is the spherical coordinate $r^2 = x^2 + y^2 + z^2$ (referring back to a Cartesian $(x,y,z)$), then this is equivalent the function in 1.

4: Here, the gradient of $1/r$ is obtained in spherical coordinates; it is equivalent to the gradient in 2, but in spherical coordinates.

5: Here, the gradient of $1/r$ is obtained in cylindrical coordinates, but it is not equivalent to 2 nor 4 because in cylindrical coordinates, $(r, \theta, z)$, $r^2 = x^2 + y^2$, even though the form appears to be the same.

6: Here, the gradient of $1/r$ is obtained in prolate spheroidal coordinates.

7: We define a function for the $x$-$y$-$z$ gradient of the $1/r^n$ scalar potential. `Evaluate` is used in the function definition, so that `Grad` is not called each time the function is used.

8: The Laplacian ($\nabla^2(1/r^n)$) has a particularly simple form, $n(n-1)/r^{2+n}$.

9: By inspection of $\nabla^2(1/r^n)$ or by direct calculation, it follows that $\nabla^2(1/r)$ vanishes identically.
The curl is the vector-valued derivative of a vector function. As illustrated below, its operation can be geometrically interpreted as the rotation of a field about a point.

For a vector-valued function of \((x, y, z)\):

\[
\vec{v}(x, y, z) = \vec{v}(\vec{x}) = (v_1(\vec{x}), v_2(\vec{x}), v_3(\vec{x})) = v_1(x, y, z)\hat{i} + v_2(x, y, z)\hat{j} + v_3(x, y, z)\hat{k}
\]  

(13-3)

the curl derivative operation is another vector defined by:

\[
\text{curl } \vec{v} = \nabla \times \vec{v} = \left( \frac{\partial v_3}{\partial y} - \frac{\partial v_2}{\partial z}, \frac{\partial v_1}{\partial z} - \frac{\partial v_3}{\partial x}, \frac{\partial v_2}{\partial x} - \frac{\partial v_1}{\partial y} \right)
\]  

(13-4)

or with the memory-device:

\[
\text{curl } \vec{v} = \nabla \times \vec{v} = \det \begin{pmatrix} \hat{i} & \hat{j} & \hat{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ v_1 & v_2 & v_3 \end{pmatrix}
\]  

(13-5)

For an example, consider the vector function that is often used in Brakke’s Surface Evolver program:

\[
\vec{w} = \frac{z^n}{(x^2 + y^2)(x^2 + y^2 + z^2)^{\frac{n}{2}}} (y\hat{i} - x\hat{j})
\]  

(13-6)

This will be shown below, in a Mathematica® example, to have the property:

\[
\nabla \times \vec{w} = \frac{n z^{n-1}}{(x^2 + y^2 + z^2)^{\frac{1}{2} + \frac{n}{2}}} (x\hat{j} + y\hat{j} + z\hat{k})
\]  

(13-7)

which is spherically symmetric for \(n = 1\) and convenient for turning surface integrals over a portion of a sphere, into a path-integral, over a curve, on a sphere.
LeavingKansas is the family of vector fields indicated by 13-6.

2–3: The function will be singular for \( n > 1 \) along the \( z \)-axis. This singularity will be reported during the numerical evaluations for visualization. There are two visualizations—the second one is over a sub-region but is equivalent because of the cylindrical symmetry of LeavingKansas. The singularity in the second case could be removed easily by excluding points near \( z = 0 \), but Mathematica® seems to handle this fine without doing so.

4–6: This demonstrates the assertion, that for Eq. 13-7, the curl has cylindrical symmetry for arbitrary \( n \), and spherical symmetry for \( n = 1 \).

7–8: This demonstrates that the divergence of the curl of \( \vec{w} \) vanishes for any \( n \); this is true for any differentiable vector field.
One important result that has physical implications is that the curl of a gradient is always zero: 
\[ f(\vec{x}) = f(x, y, z) \]
\[ \nabla \times (\nabla f) = 0 \]  
(13-8)

Therefore if some vector function \( \vec{F}(x, y, z) = (F_x, F_y, F_z) \) can be derived from a scalar potential, \( \nabla f = \vec{F} \), then the curl of \( \vec{F} \) must be zero. This is the property of an exact differential \( df = (\nabla f) \cdot (dx, dy, dz) = \vec{F} \cdot (dx, dy, dz) \). Maxwell's relations follow from equation 13-8:

\[
0 = \frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} = \frac{\partial^2 f}{\partial z \partial y} - \frac{\partial^2 f}{\partial y \partial z} \\
0 = \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} = \frac{\partial^2 f}{\partial x \partial z} - \frac{\partial^2 f}{\partial z \partial x} \\
0 = \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} = \frac{\partial^2 f}{\partial y \partial x} - \frac{\partial^2 f}{\partial x \partial y} 
\]  
(13-9)

Another interpretation is that gradient fields are curl-free, irrotational, or conservative.

The notion of “conservative” means that, if a vector function can be derived as the gradient of a scalar potential, then integrals of the vector function over any path is zero for a closed curve—meaning that there is no change in “state;” energy is a common state function.

Here is a picture that helps visualize why the curl invokes names associated with spinning, rotation, etc.
Figure 13-10: Consider a small paddle wheel placed in a set of stream lines defined by a vector field of position. If the $v_y$ component is an increasing function of $x$, this tends to make the paddle wheel want to spin (positive, counter-clockwise) about the $\hat{k}$-axis. If the $v_x$ component is a decreasing function of $y$, this tends to make the paddle wheel want to spin (positive, counter-clockwise) about the $\hat{k}$-axis. The net impulse to spin around the $\hat{k}$-axis is the sum of the two. Note that this is independent of the reference frame because a constant velocity $\vec{v} = \text{const.}$ and the local acceleration $\vec{a} = \nabla f$ can be subtracted because of Eq. 13-10.

Another important result is that divergence of any curl is also zero, for $\vec{v}(\vec{x}) = \vec{v}(x, y, z)$:

$$\nabla \cdot (\nabla \times \vec{v}) = 0 \quad (13-10)$$
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