Module 1: A Crash Course in Vectors
Lecture 4: Gradient of a Scalar Function

Objectives
In this lecture you will learn the following

- Gradient of a Scalar Function
- Divergence of a Vector Field
- Divergence theorem and applications

Gradient of a Scalar Function:
Consider a scalar field such as temperature $T(x, y, z)$ in some region of space. The distribution of temperature may be represented by drawing isothermal surfaces or contours connecting points of identical temperatures,

$$T(x, y, z) = \text{constant}$$

One can draw such contours for different temperatures. If we are located at a point $\vec{r}$ on one of these contours and move away along any direction other than along the contour, the temperature would change.

The change $\Delta T$ in temperature as we move away from a point $P(x, y, z)$ to a point $Q(x + \Delta x, y + \Delta y, z + \Delta z)$ is given by

$$\Delta T = \frac{\partial T}{\partial x} \Delta x + \frac{\partial T}{\partial y} \Delta y + \frac{\partial T}{\partial z} \Delta z$$

where the derivatives in the above expression are partial derivatives.

If the displacement from the initial position is infinitesimal, we get
Note that the change $dT$ involves a change in temperature with respect to each of the three directions. We define a vector called the gradient of $T$, denoted by $\nabla T$ or grad $T$ as

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

using which, we get

$$dT = \nabla T \cdot (i dx + j dy + k dz) = \nabla T \cdot d\vec{r}$$

Note that $\nabla T$, the gradient of a scalar $T$ is itself a vector. If $\theta$ is the angle between the direction of $\nabla T$ and $d\vec{r}$,

$$dT = |\nabla T||d\vec{r}| \cos \theta = (\nabla T)_r |d\vec{r}|$$

where $(\nabla T)_r$ is the component of the gradient in the direction of $d\vec{r}$. If $d\vec{r}$ lies on an isothermal surface then $dT = 0$. Thus, $\nabla T$ is perpendicular to the surfaces of constant $T$. When $d\vec{r}$ and $\nabla T$ are parallel, $\cos \theta = 1$ and $dT$ has maximum value. Thus the magnitude of the gradient is equal to the maximum rate of change of $T$ and its direction is along the direction of greatest change.

The above discussion is true for any scalar field $V$. If a vector field can be written as a gradient of some scalar function, the latter is called the potential of the vector field. This fact is of importance in defining a conservative field of force in mechanics. Suppose we have a force field $\vec{F}$ which is expressible as a gradient

$$\vec{F} = \nabla V$$

The line integral of $\vec{F}$ can then be written as follows:

$$\int_a^b \vec{F} \cdot d\vec{l} = \int_a^b \nabla V \cdot d\vec{l} = \int_a^b dV = V_f - V_i$$

where the symbols $a$ and $b$ represent the initial and final positions and in the last step we have used an expression for $dV$ similar to that derived for $dT$ above. Thus the line integral of the force field is independent of the path connecting the initial and final points. If the initial and final points are the same, i.e., if the particle is taken through a closed loop under the force field, we have

$$\oint \vec{F} \cdot d\vec{l} = 0$$

Since the scalar product of force with displacement is equal to the work done by a force, the above is a statement of conservation of mechanical energy. Because of this reason, forces for which one can define a potential function are called conservative forces.

**Example 14**

Find the gradient of the scalar function $V := x^2y + y^2z + z^2x + 2xyz$.

**Solution**:
\[ \nabla V = \hat{i} \frac{\partial V}{\partial x} + \hat{j} \frac{\partial V}{\partial y} + \hat{k} \frac{\partial V}{\partial z} \]

\[ = 2(xy + yz + zx)(\hat{i} + \hat{j} + \hat{k}) \]

**Exercise 1**

Find the gradients of

(i) \(xz - x^2y + y^3x^2\)

(ii) \(x^3 + y^3 + z^3\)

(iii) \(\ln\sqrt{x^2 + y^2 + z^2}\) (Ans. \((x\hat{i} + y\hat{j} + z\hat{k})/(x^2 + y^2 + z^2)\))

Gradient can be expressed in other coordinate systems by finding the length elements in the direction of basis vectors. For example, in cylindrical coordinates the length elements are \(d\rho\), \(\rho d\theta\) and \(dz\) along \(\hat{\rho}\), \(\hat{\theta}\) and \(\hat{z}\) respectively. The expression for gradient is

\[ \nabla V = \hat{\rho} \frac{\partial V}{\partial \rho} + \hat{\theta} \frac{1}{\rho} \frac{\partial V}{\partial \theta} + \hat{z} \frac{\partial V}{\partial z} \]

The following facts may be noted regarding the gradient

1. The gradient of a scalar function is a vector
2. \(\nabla(U + V) = \nabla U + \nabla V\)
3. \(\nabla(UV) = U \nabla (V) + V \nabla (U)\)
4. \(\nabla(V^n) = nV^{n-1} \nabla V\)

**Example 15**

Find the gradient of \(V = e^{-(x^2+y^2)}\) in cylindrical (polar) coordinates.

**Solution:**

In polar variables the function becomes \(V = e^{-\rho^2}\). Thus

\[ \nabla V = \hat{\rho} \frac{\partial e^{-\rho^2}}{\partial \rho} \]

\[ = \hat{\rho} e^{-\rho^2} \cdot (-2\rho) = -2\rho e^{-\rho^2} \]

**Exercise 2**

Find the gradient of the function \(V\) of Example 15 in cartesian coordinates and then transform into polar form to verify the answer.

**Exercise 3**

Find the gradient of the function \(\ln \sqrt{\rho^2 + z^2}\) in cylindrical coordinates.
In spherical coordinates the length elements are $dr, rd\theta$ and $r \sin \theta d\phi$.

Hence the gradient of a scalar function $U$ is given by

$$\nabla V = \hat{r} \frac{\partial V}{\partial r} + \hat{\theta} \frac{1}{r} \frac{\partial V}{\partial \theta} + \hat{\phi} \frac{1}{r \sin \theta} \frac{\partial V}{\partial \phi}$$

**Exercise 4**

Find the gradient of $V = r^2 \cos \theta \cos \phi$

(Ans. $2r \cos \theta \cos \phi \hat{r} - r \sin \theta \cos \phi \hat{\theta} - r \cos \theta \sin \phi \hat{\phi}$.)

**Exercise 5**

A potential function is given in cylindrical coordinates as $\frac{k}{\sqrt{\rho^2 + z^2}}$. Find the force field it represents and express the field in spherical polar coordinates.

(Ans. $-\frac{k}{r^3}$)

**Divergence of a Vector Field**: 

Divergence of a vector field $\vec{F}$ is a measure of net outward flux from a closed surface $S$ enclosing a volume $V$, as the volume shrinks to zero.

$$\text{div} \vec{F} \equiv \nabla \cdot \vec{F} = \lim_{\Delta V \to 0} \frac{\int_S \vec{F} \cdot d\vec{S}}{\Delta V}$$

where $\Delta V$ is the volume (enclosed by the closed surface $S$) in which the point P at which the divergence is being calculated is located. Since the volume shrinks to zero, the divergence is a point relationship and is a scalar.

Consider a closed volume $V$ bounded by $S$. The volume may be mentally broken into a large number of elemental volumes closely packed together. It is easy to see that the flux out of the boundary $S$ is equal to the sum of fluxes out of the surfaces of the constituent volumes. This is because surfaces of boundaries of two adjacent volumes have their outward normals pointing opposite to each other. The following figure illustrates it.
We can generalize the above to closely packed volumes and conclude that the flux out of the bounding surface $\mathcal{S}$ of a volume $V$ is equal to the sum of fluxes out of the elemental cubes. If $\Delta V$ is the volume of an elemental cube with $\Delta \mathcal{S}$ as the surface, then,

$$
\int_{\mathcal{S}} \vec{F} \cdot d\mathcal{S} = \sum \int_{\Delta \mathcal{S}} \vec{F} \cdot d\mathcal{S} = \lim_{\Delta V \to 0} \left( \frac{1}{\Delta V} \int_{\mathcal{S}} \vec{F} \cdot d\mathcal{S} \right) \Delta V
$$

The quantity in the bracket of the above expression was defined as the divergence of $\vec{F}$, giving

$$
\int_{\mathcal{S}} \vec{F} \cdot d\mathcal{S} = \int_{V} \text{div}\vec{F} dV
$$

This is known as the **Divergence Theorem**.

We now calculate the divergence of $\vec{F}$ from an infinitesimal volume over which variation of $\vec{F}$ is small so that one can retain only the first order term in a Taylor expansion. Let the dimensions of the volume element be $\Delta x \times \Delta y \times \Delta z$ and let the element be oriented parallel to the axes.

Consider the contribution to the flux from the two shaded faces. On these faces, the normal is along the $+\hat{j}$ and $-\hat{j}$ directions so that the contribution to the flux is from the $y$-component of $\vec{F}$ only and is given by

$$
[F_y(y + dy) - F_y(y)] dxdz
$$

Expanding $F_y(y + dy)$ in a Taylor series and retaining only the first order term

$$
F(y + dy) = F_y + \frac{\partial F_y}{\partial y} dy
$$

so that the flux from these two faces is

$$
\frac{\partial F_y}{\partial y} dxdydz = \frac{\partial F_y}{\partial y} dV
$$

where $dV = dxdydz$ is the volume of the cuboid.
Combining the above with contributions from the two remaining pairs of faces, the total flux is

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

Thus

\[ \int_S \vec{F} \cdot d\vec{S} = \int \left( \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} \right) dV \]

Comparing with the statement of the divergence theorem, we have

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

Recalling that the operator \( \nabla \) is given by

\[ \nabla = \hat{i} \frac{\partial}{\partial x} + \hat{j} \frac{\partial}{\partial y} + \hat{k} \frac{\partial}{\partial z} \]

and using \( \vec{F} = \hat{i}F_x + \hat{j}F_y + \hat{k}F_z \), we can write \( \text{div} \vec{F} = \nabla \cdot \vec{F} \).

The following facts may be noted:

1. The divergence of a vector field is a scalar
   \[ \nabla \cdot (\vec{F} + \vec{G}) = \nabla \cdot \vec{F} + \nabla \cdot \vec{G} \]
2. \[ \nabla \cdot (\phi \vec{F}) = \phi \nabla \cdot \vec{F} + \nabla \phi \cdot \vec{F} \]
3. In cylindrical coordinates
   \[ \nabla \cdot \vec{F} = \frac{1}{\rho} \frac{\partial}{\partial \rho} (\rho F_\rho) + \frac{1}{\rho} \frac{\partial F_\theta}{\partial \theta} + \frac{\partial F_z}{\partial z} \]
5. In spherical polar coordinates

\[ \nabla \cdot \vec{F} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 F_r) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \theta} (F_\theta \sin \theta) + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} F_\phi \]

6. The divergence theorem is

\[ \oint_S \vec{F} \cdot d\vec{S} = \int_V \nabla \cdot \vec{F} dV \]

**Example 16**

Divergence of \( \vec{r} = \hat{i}x + \hat{j}y + \hat{k}z \)

Divergence of position vector \( \vec{r} \) is very useful to remember.

\[ \nabla \cdot \vec{r} = \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y} + \frac{\partial z}{\partial z} = 1 + 1 + 1 = 3 \]

One can also calculate easily in spherical coordinate since \( \vec{r} \) only has radial component

\[ \nabla \cdot \vec{r} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \cdot r) = \frac{1}{r^2} \cdot 3r^2 = 3 \]

**Exercise 6**

Calculate the divergence of the vector field \( \vec{r}^3 \) using all the three coordinate systems. \hspace{1cm} (Ans. 0)

**Example 17**

A vector field is given by \( \vec{F} = 4xz\hat{i} - y^2\hat{j} + yz\hat{k} \). Find the surface integral of the field from the surfaces of a unit cube bounded by planes \( x = 0, x = 1, y = 0, y = 1, z = 0 \) and \( z = 1 \). Verify that the result agrees with the divergence theorem.

**Solution :**

Divergence of \( \vec{F} \) is

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

\[ = \frac{\partial 4xz}{\partial x} + \frac{\partial (-y^2)}{\partial y} + \frac{\partial yz}{\partial z} \]

\[ = 4z - 2y + y = 4z - y \]

The volume integral of above is
$$\int \nabla \cdot \vec{F} \, dV = \int_0^1 dx \int_0^1 dy \int_0^1 (4x - y) \, dx \, dy \, dz = \frac{3}{2}$$

Consider the surface integral from the six faces individually. For the face AEOD, the normal is along $-\hat{j}$. On this face $y = 0$ so that $\vec{F} = 4xz\hat{x}$. Since $\hat{x} \cdot \hat{j} = 0$, the integrand is zero. For the surface BFGC, the normal is along $\hat{j}$ and on this face $y = 1$. On this face the vector field is $\vec{F} = 4xz\hat{i} - \hat{j} + s\hat{k}$. The surface integral is

$$\int \vec{F} \cdot d\vec{S} = \int \vec{F} \cdot \hat{j} \, dx \, dz$$

$$= -\int_0^1 dx \int_0^1 dz = -1$$

Consider the top face (ABFE) for which the normal is $\hat{k}$ so that the surface integral is $\int F_z dx dy$. On this face $z = 1$ and $F_z = y$. The contribution to the surface integral from this face is

$$\int_0^1 dx \int_0^1 y \, dy = \frac{1}{2}$$

For the bottom face (DOGC) the normal is along $-\hat{k}$ and $z = 0$. This gives $F_z = 0$ so that the integral vanishes.

For the face EFGO the normal is along $-\hat{x}$ so that the surface integral is $-\int F_x dy \, dz$. On this face $x = 0$ giving $F_x = 0$. The surface integral is zero. For the front face ABCD, the normal is along $\hat{x}$ and on this face
\[ x = 1 \text{ giving } F_x = 4z. \text{ The surface integral is} \]
\[
\int_0^1 dx \int_0^1 4z \, dz = 2
\]

Adding the six contributions above, the surface integral is \( 3/2 \) consistent with the divergence theorem.

**Exercise 7**

Verify the divergence theorem by calculating the surface integral of the vector field \( \vec{F} = \hat{i}x^3 + \hat{j}y^3 + \hat{k}z^3 \) for the cubical volume of Example 17. (Ans. Surface integral has value 3)

**Example 18**

In Example 13 we found that the surface integral of a vector field \( x\hat{i} + y\hat{j} + z\hat{k} \) over a cylinder of radius \( R \) and height \( h \) is \( 3\pi R^3 \). Verify this result using the divergence theorem.

**Solution :**

In Example 16 we have seen that the divergence of the field vector is 3. Since the integrand is constant, the volume integral is \( \int \int \int \text{div} \vec{F} \, dV = 3\pi R^3 h \).

**Example 19**

A vector field is given by \( \vec{F} = x\hat{i} + y\hat{j} \). Verify Divergence theorem for a cylinder of radius 2 and height 5. The origin of the coordinate system is at the centre of the base of the cylinder and z-axis along the axis.

**Solution :**

The problem is obvious simple in cylindrical coordinates. The divergence of the field vector can be easily seen to be \( 3(x^2 + y^2)^{\frac{1}{2}} = 3\rho^2 \). Recalling that the volume element is \( \rho \, d\rho \, d\theta \, dx \), the integral is

\[
\int \text{div} \vec{F} \, dV = \int 3\rho^2 \, dV = 3 \int_0^2 \int_0^{2\pi} \rho^2 \, d\rho \, d\theta \int_0^5 \, dz = 120\pi
\]

In order to calculate the surface integral, we first observe that the end faces have their normals along \( \pm \hat{k} \). Since the field does not have any \( z \)-component, the contribution to surface integral from the end faces is zero. We will calculate the contribution to the surface integral from the curved surface.

Using the coordinate transformation to cylindrical

\[ x = \rho \cos \theta \quad y = \rho \sin \theta \]

and
Using these

\[
\hat{i} = \hat{\rho} \cos \theta - \hat{\theta} \sin \theta \\
\hat{j} = \hat{\rho} \sin \theta + \hat{\theta} \cos \theta \\
\hat{k} = \hat{k}
\]

The area element on the curved surface is \( R \) \( d\theta dx \hat{\rho} \), where \( R \) is the radius. Thus the surface integral is

\[
\int F \cdot dS = R^2 \int_0^{2\pi} (\cos^4 \theta + \sin^4 \theta) d\theta \int_0^5 dx
\]

\[
= \left( \frac{3\pi}{2} \right) \cdot 5 = 120\pi
\]

where we have used \( \int_0^{2\pi} \sin^4 \theta d\theta = \int_0^{2\pi} \cos^4 \theta d\theta = 3\pi/4 \).

**Exercise 8**

In the Exercise following Example 13, we had seen that surface integral of the vector field \( \vec{V} = 2\hat{\rho} - 3\hat{\rho} \hat{\theta} + z\hat{\rho} \hat{k} \) through the surface of a cylinder of radius 1 and height 2 is \( 2\pi \sqrt{3} \). Re-confirm the same result using divergence theorem.

**Example 20**

A hemispherical bowl of radius 1 lies with its base on the x-y plane and the origin at the centre of the circular base. Calculate the surface integral of the vector field \( \vec{F} = x^2 \hat{i} + y^2 \hat{j} + z^3 \hat{k} \) in the hemisphere and verify the divergence theorem.

**Solution**:

The divergence of \( \vec{F} \) is easily calculated

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

\[
= \frac{\partial x^2}{\partial x} + \frac{\partial y^2}{\partial y} + \frac{\partial z^3}{\partial z}
\]

\[
= 2x + 2y + 3z^2
\]

where \( \rho \) is the distance from origin. The volume integral over the hemisphere is conveniently calculated in spherical polar using the volume element \( \rho^2 \sin \theta d\theta d\phi d\rho \). Since it is a hemisphere with \( z = 0 \) as the base, the range of \( \theta \) is \( 0 \) to \( \pi/2 \).
\[ \nabla \cdot \vec{F} \, dV = 3 \int r^2 \, dV = 3 \int_0^1 r^4 \, dr \int_0^{\pi/2} \sin \theta \, d\theta \int_0^{2\pi} d\phi \]

\[ = 3 \times \frac{1}{5} \times 1 \times 2\pi = \frac{6\pi}{5} \]

The surface integrals are calculated conveniently in spherical polar. There is no contribution to the flux from the base because the outward normal points in the \(-z\) direction but the z-component of the field is zero because the base of the hemisphere is \(z = 0\).

In order to calculate the flux from the curved face we need to express the force field and the unit vectors in spherical polar coordinates. Using the transformation properties given earlier and observing that we only require the radial component of the vector field since the area element is radially directed. Using \(R^2 \sin \theta \, d\theta \, d\phi\) as the area element, a bit of laborious algebra gives

\[ \vec{F} \cdot d\vec{S} = R^5 \int_0^{\pi/2} \sin^5 \theta \, d\theta \int_0^{2\pi} \cos^4 \phi \, d\phi + R^5 \int_0^{\pi/2} \sin^5 \theta \, d\theta \int_0^{2\pi} \sin^4 \phi \, d\phi \]

\[ + R^5 \int_0^{\pi/2} \cos^4 \theta \sin \theta \, d\theta \int_0^{2\pi} d\phi \]

Using \(\int_0^{\pi/2} \sin^5 \theta \, d\theta = \frac{8}{15}\) and \(\int_0^{2\pi} \cos^4 \phi \, d\phi = \frac{3\pi}{4}\), the above integral can be seen to give the correct result.

**Recap**

In this lecture you have learnt the following

- Gradint of a scalar function was defined. Gradient is a scalar function.

- The magnitude of the gradient is equal to the maximum rate of change of the scalar field and its direction is along the direction of greatest change in the scalar function.

- The net outward flux from a volume element around a point is a measure of the divergence of the vector field at that point.

- We derived the divergence theorem which shows that the volume integral of the divergence of a vector function over any volume is equal to the outward flux through a surface which encloses this volume.

- Divergence was calculated for functions in different coordinate systems and divergence theorem was verified.