Mathematics for chemical engineers

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10. Introduction to Vector Analysis

Obsah

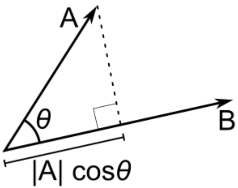
Scalar product

Vector space $(V, +, \cdot)$ ... the set V, on which two operations are defined: addition $(+)$ and multiplication by a real number $(\cdot)$. These operations fulfill eight axioms (commutativity, asociativity, distributivity, zero and an opposite element with respect to addition and a unitary element with respect to multiplication by a real number).

Scalar product: $a = (a_1, a_2, \ldots, a_n) \in \mathbb{R}^n$, $b = (b_1, b_2, \ldots, B_n) \in \mathbb{R}^n$,

$$\Longrightarrow \quad a \cdot b = \sum_{i=1}^{n} a_i b_i \,,$$

in $\mathbb{R}^2$



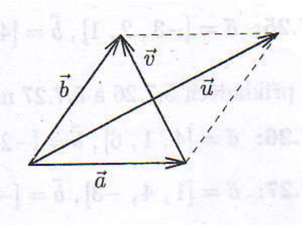
$||b|| \cdot \cos\alpha$ ... the orthogonal projection of the vector b in the direction of the vector a,

$a \cdot b = ||a|| \cdot ||b|| \cdot \cos\alpha$

Properties of the scalar product

$$\begin{aligned} a\cdot b &= b\cdot a \\ a\cdot(b+c) &= a\cdot b + c\cdot d \\ (\alpha\, a)\cdot(\beta\, b) &= (\alpha\,\beta)\, a\cdot b \\ a\cdot b = 0 &\iff a=0 \,\vee\, b=0 \,\vee\, \underbrace{a\perp b}_{\cos\frac{\pi}{2}=0} \end{aligned}$$

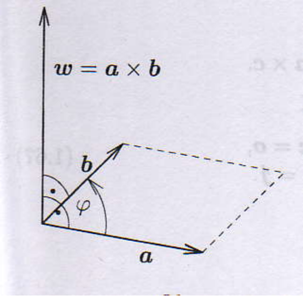
Example Prove that the diagonals in rhombus are perpendicular one to another one.



Two adjacent sides of the rhombus can be regarded as two vectors a, b. The vectors a, b are linearly independent and $||a|| = ||b|| \neq 0$. If also the diagonals of the rhombus are considred as vectors u and v, we have $u = a+b$, $u \neq 0$, $v = b-a$, $v \neq 0$. Then $u\cdot v = (a+b)\cdot(b-a) = -||a||^2 + ||b||^2 = 0$, i.e., the vectors u and v are perpendicular.

Vector product

The vector product is defined only for vectors in $\mathbb{R}^3$, i. e., $a \in \mathbb{R}^3,\ b \in \mathbb{R}^3$. Let $\vec{i} = (1,0,0),\ \vec{j} = (0,1,0),\ \vec{k} = (0,0,1)$. Then



$$w = a \times b = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} =$$

$$= \vec{i} \cdot \begin{vmatrix} a_2 & a_3 \\ b_2 & b_3 \end{vmatrix} - \vec{j} \cdot \begin{vmatrix} a_1 & a_3 \\ b_1 & b_3 \end{vmatrix} + \vec{k} \cdot \begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix} =$$

$$= (a_2 b_3 - a_3 b_2, -a_1 b_3 + a_3 b_1, a_1 b_2 - a_2 b_1) \in \mathbb{R}^3.$$

The area of the parallelogram (φ is the smaller of angles that vectors grip)

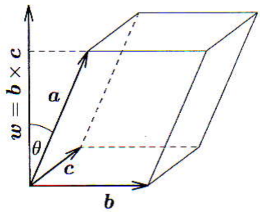
$$|a \times b| = ||a|| \cdot ||b|| \cdot \sin\varphi\,.$$

Properties of the vector product

$$
\begin{aligned}
a \times b &= -b \times a \\
a \times b = 0 &\iff a = 0 \vee b = 0 \vee a \parallel b \\
a \times (b + c) &= a \times b + a \times c \\
(\alpha a) \times b &= \alpha (a \times b) \\
a \times b &= ||a|| \cdot ||b|| \cdot \sin\alpha \cdot n, \quad \text{where } \alpha \in \langle 0, \pi \rangle
\end{aligned}
$$

$n \ldots$ the unit normal vector, i.e., the unit vector perpendicular to the plane defined by vectors a and b.

Remark



Mixed product

$$a \cdot (b \times c)\,.$$

$V = |a \cdot (b \times c)|$ ... volume of the parallelogram determined by vectors a, b, c

Directional derivative

Let $f = f(x_1, x_2, \ldots, x_n)$ is a function of n variables, point $X_0 \in D(f)$ and $\overrightarrow{a} = (a_1, a_2, \ldots, a_n) \in \mathbb{R}^n$ with the norm $||\overrightarrow{a}|| = 1$. Then the limit

$$\lim_{t \to 0} \frac{f(X_0 + ta) - f(X_0)}{t},$$

if it exists, is called the derivative of the function f in the point X_0 in the direction of the vector $\overrightarrow{a}$. It is denoted as $D_a f(X_0)$.

Remark

- Derivative of f in the direction of the vector $\overrightarrow{a}$ describes the rate of climb or descent values of the function f in the direction of the vector $\overrightarrow{a}$.
- For a function of two variables the partial derivative $\dfrac{\partial f}{\partial x}$ is the derivative in the direction of the vector $\overrightarrow{e}_1 = (1, 0)$ and the partial derivative $\dfrac{\partial f}{\partial y}$ the derivative in the direction of the vector $\overrightarrow{e}_2 = (0, 1)$. Prove it.

Gradient

Let $f(X) = f(x_1, x_2, \ldots, x_n)$ is a function of n variables, $X_0 \in D(f)$. The vector of the first partial derivatives of the function f evaluated at the point X_0 is called gradient of the function f at the point X_0,

$$\mathrm{grad} f(X_0) = \left(\frac{\partial f(x_1, \ldots, x_n)}{\partial x_1}, \frac{\partial f(x_1, x_2, \ldots, x_n)}{\partial x_2}, \ldots, \frac{\partial f(x_1, x_2, \ldots, x_n)}{\partial x_n} \right) \Big|_{X_0},$$

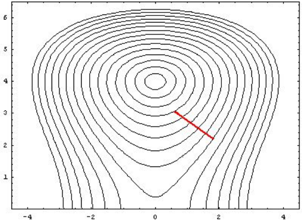
The gradient of the function f at the point X_0 is also denoted as $\nabla f(X_0)$, where ∇ is the differential operator "nabla".

Theorem Let f be differentiable at the point X_0 and let the vector $\overrightarrow{a} \in \mathbb{R}^n$ have the unit length: $||\overrightarrow{a}|| = 1$. Then

$$D_a f(X_0)\, \underbrace{\nabla f(X_0) \cdot \overrightarrow{a}}_{\text{scalar product}} = ||\nabla f(X_0)|| \cdot ||\overrightarrow{a}|| \cdot \cos\varphi\,. \tag{1}$$

From the equation (1) it can be seen that $D_a f(X_0)$ will be the greatest for $\varphi = 0$, i. e., $\overrightarrow{a}$ will be the unit vector corresponding to the gradient: $\overrightarrow{a} := \dfrac{\nabla f(X_0)}{||\nabla f(X_0)||}$, i.e., the gradient is the vector, which "heads" in the direction of the greatest growth of the function values.

Remark For $f : \mathbb{R}^2 \to \mathbb{R}$ is the gradient always orthogonal to the level sets.



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Example Compute the derivative of the function $f(x,y) = x^2y - xy^2$ in the direction $\vec{a}$ at the point $(1,2)$; $\vec{a}$ is the unit vector corresponding to the vector $v = (3,4)$.

Solution $||v|| = 5 \;\Rightarrow\; a = \dfrac{1}{5}(3,4)$, f is continuous, differentiable function,

$$\nabla f(x,y) = \mathrm{grad}\, f(x,y) = \left(\frac{\partial f}{\partial x}(x,y), \frac{\partial f}{\partial y}(x,y)\right) = (2xy - y^2, x^2 - 2xy)\,,$$

$$D_a f(1,2) = \nabla f(1,2)\cdot a = (0,-3)\cdot\frac{1}{5}(3,4) = -\frac{12}{5}\,.$$

Example Compute the derivative of the function f in the direction of the vector $a = (1,0)$ at the point $(1,0)$, $f(x,y) = x\sqrt{y}$.

Solution f is continuous but at the point $(1,0)$ is not differentiable. We have to calculate the derivative at this point by the definition.

$$D_a f(1,0) = \lim_{t\to 0}\frac{f(x+ta) - f(x)}{t} = \lim_{t\to 0}\frac{f(1+t,0) - f(1,0)}{t} = 0\,.$$

Example $f(x,y,z) = x^2 + x\ln z - y^3$. Compute $\nabla f(1,2,\mathrm{e})$.

Solution:

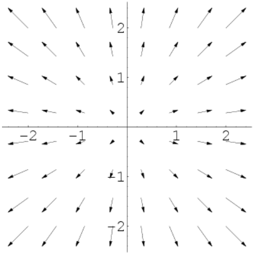
$$\nabla f(x,y,z) = (2x + \ln z, -3y^2, \frac{x}{z}), \quad \nabla f(1,2,\mathrm{e}) = (3,-12,\frac{1}{\mathrm{e}})\,.$$

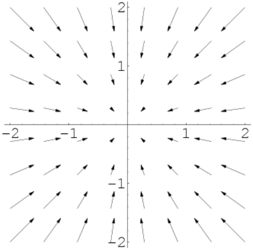
Divergence

Divergence and curl are two vector operators with properties derived from observations of the behavior of the vector field of liquid or gas.

We can imagine the divergence of the vector field so that the vector field F gives velocity to the fluid flow. As the flow rate increases, the fluid expands away from the beginning. In this case the divergence of the vector field is positive (Fig. Left) $\operatorname{div} F > 0$.

If the vector field represents fluid which flows so that it compresses into the beginning, the divergence of the vector field is negative $\operatorname{div} F < 0$, fluid compression occurs (Fig. right).





$F := F(x, y)$ ... two-dimensional velocity vector field
$F := F(x, y, z)$ ... vector velocity field in three-dimensional space

The divergence of the vector field measures the expansion or compression of the vector field at that point, but does not indicate the direction in which the expansion or compression is going on $\Longrightarrow$ the divergence is a scalar

$$F : \mathbb{R}^3 \longrightarrow \mathbb{R}^3, \quad F = (F_1, F_2, F_3), \quad \mathrm{div}\, F = \frac{\partial F_1}{\partial x} + \frac{\partial F_2}{\partial y} + \frac{\partial F_3}{\partial z}$$

Notation:

$$\nabla \ \dots \text{ operator nabla } \dots \quad \nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right).$$

Then the divergence is the scalar product of the vectors ∇ and F,

$$\nabla \cdot F = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right) \cdot (F_1, F_2, F_3) = \frac{\partial}{\partial x} F_1 + \frac{\partial}{\partial y} F_2 + \frac{\partial}{\partial z} F_3$$

★ Examples

Example 1. $F(x,y,z) = (-y, xy, z) \implies \operatorname{div} F = 0 + x + 1 = x + 1$

Example 2. $F(x,y,z) = (x,y,z) \implies \operatorname{div} F = 1 + 1 + 1 = 3 \ldots$ positive constant.In this case the divergence is independent on the choice of the point (x,y,z). The fluid expands.

Example 3. Let us compute the divergence of the vector field

$$F(x,y,z) = \frac{(x,y,z)}{(x^2+y^2+z^2)^{3/2}}, \qquad (x,y,z) \neq (0,0,0).$$

Solution $\operatorname{div} F(x,y,z) =$

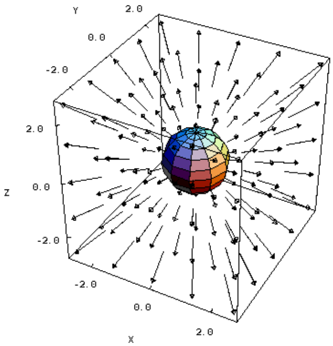
$$= \frac{\partial}{x}\frac{x}{(x^2+y^2+z^2)^{3/2}} + \frac{\partial}{y}\frac{y}{(x^2+y^2+z^2)^{3/2}} + \frac{\partial}{z}\frac{z}{(x^2+y^2+z^2)^{3/2}}$$

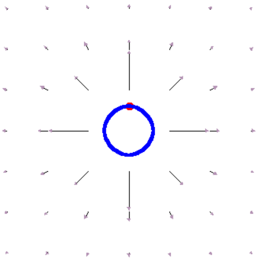
$$= \frac{(x^2+y^2+z^2) - 3x^2}{(x^2+y^2+z^2)^{5/2}} + \frac{(x^2+y^2+z^2) - 3y^2}{(x^2+y^2+z^2)^{5/2}} + \frac{(x^2+y^2+z^2) - 3z^2}{(x^2+y^2+z^2)^{5/2}}$$

$$= \frac{3(x^2+y^2+z^2) - 3(x^2+y^2+z^2)}{(x^2+y^2+z^2)^{5/2}} = 0$$

So if we are not at the origin, the flow is not expanding nor contracting, $\operatorname{div} F = 0$.

Let us sink a small ball mounted at the origin into the liquid and consider the vector field from Example 2. The fluid flows away from the ball. Because the vector field has a positive divergence everywhere, the flow of the vector field will be away from the ball, even if we move the ball from the origin.
In the left figure, there is the vector velocity field in three-dimensional space from Example 2, on the right, there is the two-dimensional vector field from Example 4.





★ Dependence on the dimension

Example 4. Two-dimensional version of the vector field from Example 3.

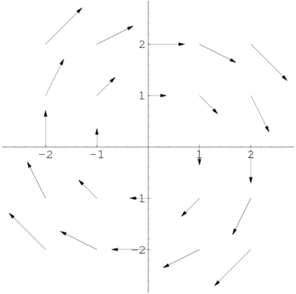
$$F(x,y) = \frac{(x,y)}{(x^2+y^2)^{3/2}}, \qquad (x,y) \neq (0,0)$$

$$\begin{aligned}
\operatorname{div} F(x,y) &= \frac{\partial}{x}\frac{x}{(x^2+y^2)^{3/2}} + \frac{\partial}{y}\frac{y}{(x^2+y^2)^{3/2}} \\
&= \frac{(x^2+y^2)-3x^2}{(x^2+y^2)^{5/2}} + \frac{(x^2+y^2)-3y^2}{(x^2+y^2)^{5/2}} \\
&= \frac{2(x^2+y^2)-3(x^2+y^2)}{(x^2+y^2)^{5/2}} = \frac{-1}{(x^2+y^2)^{3/2}} < 0
\end{aligned}$$

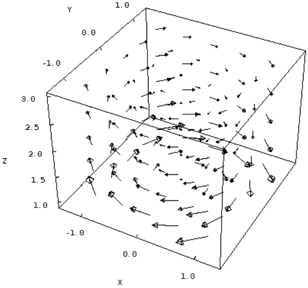
Everywhere except at the origin we have $\operatorname{div} F(x,y) < 0$. The fluid is compressed, although it flows "out". As a result of fluid flow, if we put the circle to the flowing fluid, the fluid flows into the circle faster than from the circle.

Rotation

The notion of the vector operator curl is based on the idea how liquid or gas can rotate (circulate).



curl of 2-dimensional vector field



curl of 3-dimensional vector field

F ... a vector field that represents the flow of fluid

Place a small ball into the liquid and fixed the center of the ball $\Longrightarrow$ the ball can rotate in any direction around its center, but can not move. This rotation measures $\mathrm{curl}\, F$ of the vector field F at the center of the (small) ball ... microscopic rotation (circulation) of the vector field F. Operator curl is a vector, $\mathrm{curl}\, F \in \mathbb{R}^3$, that points along the axis of the rotation and its orientation is determined according to the right-hand rule.

$$\mathrm{curl}\, \mathbf{F} = \nabla \times \mathbf{F} = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right) \times (F_1, F_2, F_3) =$$

$$= \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_1 & F_2 & F_3 \end{vmatrix} = \mathbf{i} \begin{vmatrix} \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ F_2 & F_3 \end{vmatrix} - \mathbf{j} \begin{vmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial z} \\ F_1 & F_3 \end{vmatrix} + \mathbf{k} \begin{vmatrix} \frac{\partial}{\partial x} & \frac{\partial}{\partial y} \\ F_1 & F_2 \end{vmatrix} =$$

$$\left(\frac{\partial F_3}{\partial y} - \frac{\partial F_2}{\partial z}\right)\mathbf{i} - \left(\frac{\partial F_3}{\partial x} - \frac{\partial F_1}{\partial z}\right)\mathbf{j} + \left(\frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y}\right)\mathbf{k},$$

where $\mathbf{i} = (1,0,0), \mathbf{j} = (0,1,0), \mathbf{k} = (0,0,1)$ are the unit vectors in the direction of the coordinate axes.

★ Examples

Example $F(x,y,z) = (-y, xy, z)$. Compute $\operatorname{curl} F$.

$$\operatorname{curl} F = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ -y & xy & y \end{vmatrix} = \mathbf{i}(0-0) - \mathbf{j}(0-0) + \mathbf{k}(y+1) = (0,0,y+1)\,.$$

Example $F(x,y,z) = (y, x^2, -z)$. Compute $\operatorname{curl} F$.

$$\operatorname{curl} F = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ y & x^2 & -z \end{vmatrix} = \mathbf{i}(0-0) - \mathbf{j}(0-0) + \mathbf{k}(2x-1) = (0,0,2x-1)\,.$$

Notation:

$$\operatorname{curl} F = \nabla \times F\,, \quad F = (F_1, F_2, F_3) \in \mathbb{R}^3, \quad \operatorname{curl} F \in \mathbb{R}^3$$

Macroscopic rotation

Microscopic rotation – a small ball thrown into the liquid with the center fixed, so the small ball can rotate in all directions around its center, but can not move

Macroscopic rotation – if we release the center of the ball then the ball starts to spin in circles carried by fluid flow. The macroscopic rotation can not be easily calculated as a $\mathrm{curl} F$.

Example $F(x, y, z) = (-y, x, 0)$ ... rotation around the axis z. In this case we can imagine the macroscopic rotation as the rotation of the (free) ball in the fluid in the plane $z = 0$. Attention!!! The macroscopic rotation is not $\mathrm{curl} F$ of the vector field F. To be able to measure $\mathrm{curl} F$, we have to fix the center of the ball. Verify that $\mathrm{curl}\, F = (0, 0, 2)$.

Example $F(x, y, z) = \dfrac{(-y, x, 0)}{x^2 + y^2}$, $\quad (x, y) \neq (0.0)$.

We distinguish two cases: Along circles $x^2 + y^2 = constant \implies$ we get the previous example, a macroscopic rotation around z axis. For a general point that does not lie on the axis z we obtain $\mathrm{curl}\, F = (0, 0, 0)$. Verify.

Green's Theorem

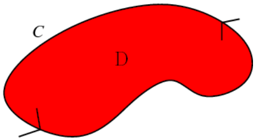
$\mathcal{C}$ ... oriented, simple, **closed** curve $\Longrightarrow$

curve integral $\displaystyle\int_{\mathcal{C}} F\mathrm{d}s$ represents rotation F "around"the curve $\mathcal{C}$.

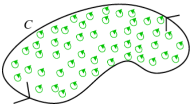
For example if F represents water flow velocity field, this integral shows how large tendency has water to circulate along a path in the direction of the orientation of $\mathcal{C}$.

Green's Theorem ... transforms the calculation of the curve integral over a closed curve $\mathcal{C}$ to the calculation of the double integral over the interior of $\mathcal{C}$. But what we will integrate over the interior of $\mathcal{C}$ to obtain the same result as we would integrate over a closed curve $\mathcal{C}$?

Green's Theorem shows the relationship between the microscopic rotations along a closed path $\mathcal{C}$ and the sum of microscopic rotations inside $\mathcal{C}$



Macroscopic circulation of the vector field F along $\mathcal{C}$



Sum of microscopic circulations of the vector field F inside $\mathcal{C}$

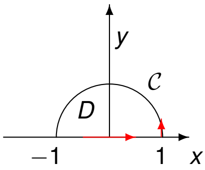
$$\int_{\mathcal{C}} F \, \mathrm{d}s = \iint_D \underbrace{\text{microscopic circulation } F}_{\mathrm{curl} F \cdot \mathbf{k}} \, \mathrm{d}A$$

D ... the domain "inside" the closed curve $\mathcal{C}$,
$\mathbf{k}$ ... the unit vector in the direction of the axis z,
$\mathrm{curl}\, F \cdot \mathbf{k}$ ... $z-$component of the operator $\mathrm{curl}\, F$

Green's Theorem Let $\mathcal{C}$ be positively oriented simple closed curve, and D be the "interior" of the closed curve $\mathcal{C}$. Then

$$\int_{\mathcal{C}} F\,\mathrm{d}s = \iint_D (\mathrm{rot}\,F)\cdot \mathbf{k}\,\mathrm{d}A = \iint_D \left(\frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y}\right)\mathrm{d}A\,.$$

Example Compute $\displaystyle\int_{\mathcal{C}} y^2\mathrm{d}x + 3xy\mathrm{d}y$, where $\mathcal{C}$ is positively oriented boundary of the upper semicircle D.



$$F(x,y) = (y^2, 3xy)$$

Using the double integral: integrand

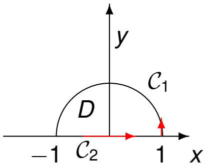
$$\frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y} = 3y - 2y = y$$

domain D: $-1 \le x \le 1, \quad 0 \le y \le \sqrt{1-x^2}$

$$\int_{\mathcal{C}} y^2 \mathrm{d}x + 3xy\mathrm{d}y = \iint_D (\mathrm{rot}\, F) \cdot \mathbf{k}\, \mathrm{d}A = \iint_D y \mathrm{d}A =$$
$$= \int_{-1}^{1} \left(\int_0^{\sqrt{1-x^2}} y \mathrm{d}y \right) \mathrm{d}x = \frac{1}{2} \int_{-1}^{1} (1 - x^2) \mathrm{d}x = \frac{2}{3} .$$

Alternative calculation: curve integral:

$\mathcal{I} = \int_{\mathcal{C}} y^2 \mathrm{d}x + 3xy\mathrm{d}y$, $\mathcal{C}$ is positively oriented border of the upper semicircle D.



Parametrization $\mathcal{C}_1$: $r = 1,\ t \in \langle 0, \pi \rangle$,
$x = \cos t,\ y = \sin t$, $\mathrm{d}x = -\sin t\mathrm{d}t,\ \mathrm{d}y = \cos t\mathrm{d}t$

Parametrization $\mathcal{C}_2$: $t \in \langle -1, 1 \rangle$,
$x = t,\ y = 0$, $\mathrm{d}x = \mathrm{d}t,\ \mathrm{d}y = 0$

$$\mathcal{I} = \int_{\mathcal{C}_1} y^2 \mathrm{d}x + 3xy\mathrm{d}y + \int_{\mathcal{C}_2} y^2 \mathrm{d}x + 3xy\mathrm{d}y = \int_0^{\pi} (-\sin^3 t + 3\cos t \sin t)\mathrm{d}t + \int_{-1}^{1} 0\mathrm{d}t =$$

$$= \int_0^{\pi} \sin t\,(-\sin^2 t + 3\cos t)\mathrm{d}t = -\int_0^{\pi} \sin t(1-\cos^3 t)\mathrm{d}t + 3\int_0^{\pi} \sin t \cos t\mathrm{d}t$$

$$-\int \sin t\,(1-\cos^2 t)\mathrm{d}t = \left| \begin{array}{rcl} \cos t & = & u \\ -\sin t\mathrm{d}t & = & \mathrm{d}u \end{array} \right| = \int (1-u^2)\mathrm{d}u = 1 - \frac{1}{3}\cos^3 t$$

$$\int \sin t \cos t\mathrm{d}t = \left| \begin{array}{rcl} \cos t & = & u \\ -\sin t\mathrm{d}t & = & \mathrm{d}u \end{array} \right| = -\int u\mathrm{d}u = -\frac{1}{2}\cos^2 t$$

$$\mathcal{I} = \left[1 - \frac{1}{3}\cos^3 t\right]_0^{\pi} - \frac{1}{2}\left[\cos^2 t\right]_0^{\pi} = \frac{2}{3}\,.$$

Exercise Using Green's Theorem, compute (draw the curve)

$$\int_{\mathcal{C}} (\sqrt{x} - y)\,\mathrm{d}x + \left(\frac{1}{1+y^2} + x\right)\,\mathrm{d}y\,,$$

where he curve $\mathcal{C}$ is a union of the part of the parabola $y^2 = x$ between the points $A = (0;0)$ and $B = (1;1)$ and a line segment AB. The curve is positively oriented.

Remark Path independence for curve integrals: Let $F = (F_1, F_2, F_3)$ be a vector field on simply connected domain $G \subset \mathbb{R}^3$, $\mathcal{C}$ be a closed curve. Then the curve integral of the vector field

$\int_{\mathcal{C}} F \mathrm{d}s$ is path independent, i.e., the vector field F is conservative (potential) on G

$$\Longleftrightarrow$$

$$\frac{\partial F_1}{\partial y} = \frac{\partial F_2}{\partial x}, \quad \frac{\partial F_1}{\partial z} = \frac{\partial F_3}{\partial x}, \frac{\partial F_2}{\partial z} = \frac{\partial F_3}{\partial y},$$

$$\Longleftrightarrow$$

$$\operatorname{curl} F = 0\,.$$

Remark Integral definition of divergence – it concerns the surface integral and we will not deal with it here.

Remark Chemical interpretation of divergence:
$\operatorname{div} v(P)$, where the vector field v is the concentration gradient, represents the quantity of the chemical substance, which in a neighborhood of point P will be added by diffusion or arises by a chemical reaction $(\operatorname{div} v(P) < 0)$ or from the neighborhood of the point P disappears $(\operatorname{div} v(P) > 0)$.

Definition The point P, in which $\operatorname{div} v(P) > 0$ (expansion) is called a source of the vector field v. The point P, in which $\operatorname{div} v(P) < 0$ (compression) is called a sink of the vector field v.

Remark The vector field v on the domain G is called solenoidal (or divergenceless) $\iff$

$$\operatorname{div} v(P) = 0 \quad \forall P \in G,$$

i.e. in G, there are no sources, nor sinks.

Remark If $v(x, y, z)$ is a velocity field in fluid then in hydrodynamics we call the condition

$$\operatorname{div} v = 0$$

the continuity equation for incompressible fluids.

Definition Let the vector field $v(x, y, z)$ on the domain G be the velocity field of a flowing fluid. Then $\operatorname{curl} v$ represents the tendency of particles at the point (x, y, z) to rotate about the axis that points in the direction of $\operatorname{curl} v$. If

$$\operatorname{curl} v(x, y, z) = 0 \quad \forall (x, y, z) \in G,$$

then the fluid is called irrotational.

When to apply the Green's Theorem?

Green's Theorem allows us to calculate the line integral of the vector field as a double integral:

$$\int_C F \mathrm{d}s = \iint_D \left(\frac{\partial F_2}{\partial x} - \frac{\partial F_1}{\partial y} \right) \mathrm{d}x\mathrm{d}y \,,$$

where $D \subset \mathbb{R}^2$, $C = \partial D$ is a positively oriented closed curve.

Equivalently: $F(x,y) = (P(x,y), Q(x,y))$, $P : D \longrightarrow \mathbb{R}$, $Q : D \longrightarrow \mathbb{R}$, ∂D is a closed curve ,

$$\int_{\partial D} P\mathrm{d}x + Q\mathrm{d}y = \iint_D \left(\frac{\partial Q}{\partial x} - \frac{\partial P}{\partial y} \right) \mathrm{d}x\mathrm{d}y \,.$$

Remark: If F is a conservative (potential) vector field, ∂D is a positively oriented closed curve, then

$$\int_{\partial D} F \mathrm{d}s = 0 \,.$$

2nd order differential operations

Let $f(x,y,z)$ be a scalar field, $f : \mathbb{R}^3 \longrightarrow \mathbb{R}$, $f \in C^2(G)$, and $a(x,y,z)$ be a vector field, $a \in C^2(G)$. We already know differential operations of the first order:

$$\nabla f = \operatorname{grad} f\,, \quad \nabla \cdot a = \operatorname{div} a\,, \quad \nabla \times a = \operatorname{curl} a\,.$$

Applying ∇ again we obtain second derivatives for a scalar or a vector field.

- $\operatorname{div} \operatorname{grad} f$

$$\operatorname{div} \operatorname{grad} f = \nabla \cdot \nabla f = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z}\right)\left(\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial z}{\partial z}\right) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

Let us set

$$\triangle f = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$

$\triangle$ ... Laplace operator, Laplacian

The following notation is also in use

$$\triangle = \underbrace{\nabla \cdot \nabla}_{\text{dot product}} = \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

Laplace's equation, Poisson's equation

Laplace's equation is a second-order partial differential equation named after Pierre-Simon Laplace who first studied its properties. This is often written as:

$$\triangle u = 0, \quad \text{or} \quad \nabla^2 u = 0$$

where $\triangle = \nabla^2$ is the Laplace's operator and u is a scalar function. Laplace's equation and Poisson's equation are the simplest examples of elliptic partial differential equations. The general theory of solutions to Laplace's equation is known as potential theory. The solutions of Laplace's equation are the harmonic functions, which are important in many fields of science.

$$\triangle u = g \neq 0 \quad \text{Poisson's equation}$$

- div rot a

$$\operatorname{div}\operatorname{rot} a = \nabla\cdot(\nabla\times a) = \nabla\cdot\left(\frac{\partial a_3}{\partial y}-\frac{\partial a_2}{\partial z},\frac{\partial a_1}{\partial z}-\frac{\partial a_3}{\partial x},\frac{\partial a_2}{\partial x}-\frac{\partial a_1}{\partial y}\right) =$$

$$\frac{\partial^2 a_3}{\partial x\partial y}-\frac{\partial^2 a_2}{\partial x\partial z}+\frac{\partial^2 a_1}{\partial y\partial z}-\frac{\partial^2 a_3}{\partial x\partial y}+\frac{\partial^2 a_2}{\partial x\partial z}-\frac{\partial^2 a_1}{\partial y\partial z}=0$$

$$\Longrightarrow \qquad \operatorname{div}\operatorname{rot} a = 0\,.$$

Exercise Simplify $\operatorname{rot}(\operatorname{rot} a)$.

- rot grad f, $\quad f \in C^2(G)$

$$\text{rot grad } f = \nabla \times \nabla f = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ \dfrac{\partial f}{\partial x} & \dfrac{\partial f}{\partial y} & \dfrac{\partial f}{\partial z} \end{vmatrix} =$$

$$\mathbf{i}\left(\frac{\partial^2 f}{\partial y \partial z} - \frac{\partial^2 f}{\partial z \partial y}\right) - \mathbf{j}\left(\frac{\partial^2 f}{\partial x \partial z} - \frac{\partial^2 f}{\partial x \partial z}\right) + \mathbf{k}\left(\frac{\partial^2 f}{\partial y \partial z} - \frac{\partial^2 f}{\partial z \partial y}\right) = 0.$$

Hence,

$$\text{rot grad } f = 0\,.$$

Remark If we consider $(\nabla \times \nabla) f \ldots$

$$\nabla \times \nabla = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \\ \dfrac{\partial}{\partial x} & \dfrac{\partial}{\partial y} & \dfrac{\partial}{\partial z} \end{vmatrix} = 0, \quad \text{i.e.,} \quad (\nabla \times \nabla) f = 0 \cdot f = 0$$

Gauss-Ostrogradsky's theorem

Theorem Gauss-Ostrogradsky's

Let $\Omega \subset \mathbb{R}^2$ be a compact domain with a Lipschitz boundary Γ, $u \in H^1(\Omega)$. Then

$$\int_\Omega \frac{\partial u}{\partial x_i} \mathrm{d}x = \int_\Gamma u \, n_i \mathrm{d}S \,, \quad i = 1, 2,$$

where $n = (n_1, n_2)$ is the unit outer normal to the boundary Γ .

The theorem says that the double integral over the domain Ω (= the inside of the closed positively oriented curve Γ) is equal to the line integral over the boundary Γ.

In the theorem, let us set $u := v \cdot w$. We obtain

$$\int_\Omega \left(\frac{\partial v}{\partial x_i} w + \frac{\partial w}{\partial x_i} v \right) \mathrm{d}x = \int_\Gamma v \cdot w \cdot n_i \mathrm{d}S \,, \quad i = 1, 2, \quad v, w \in C^1(\Omega), \ \Omega \subset \mathbb{R}^2 \,.$$

1. Green's formula

$$\int_\Omega \frac{\partial v}{\partial x_i} w \mathrm{d}x = \int_\Gamma v \cdot w \cdot n_i \, \mathrm{d}S - \int_\Omega \frac{\partial w}{\partial x_i} v \mathrm{d}x \,, \ i = 1, 2, \ v, w \in C^1(\Omega), \ \Omega \subset \mathbb{R}^2 \,.$$

The 1st Green's formula in components:

$$\int_\Omega \frac{\partial v}{\partial x_1} w \mathrm{d}x = \int_\Gamma v \cdot w \cdot n_1 \, \mathrm{d}S - \int_\Omega \frac{\partial w}{\partial x_1} v \mathrm{d}x \tag{2}$$

$$\int_\Omega \frac{\partial v}{\partial x_2} w \mathrm{d}x = \int_\Gamma v \cdot w \cdot n_2 \, \mathrm{d}S - \int_\Omega \frac{\partial w}{\partial x_2} v \mathrm{d}x \tag{3}$$

We substitute in the equation (2) $w := \frac{\partial w}{\partial x_1}$ and in the equation (3) $w := \frac{\partial w}{\partial x_2}$. Hence,

$$\int_\Omega \frac{\partial v}{\partial x_1} \frac{\partial w}{\partial x_1} \mathrm{d}x = \int_\Gamma v \cdot \frac{\partial w}{\partial x_1} \cdot n_1 \, \mathrm{d}S - \int_\Omega \frac{\partial^2 w}{\partial x_1^2} v \mathrm{d}x \tag{4}$$

$$\int_\Omega \frac{\partial v}{\partial x_2} \frac{\partial w}{\partial x_2} \mathrm{d}x = \int_\Gamma v \cdot \frac{\partial w}{\partial x_2} \cdot n_2 \, \mathrm{d}S - \int_\Omega \frac{\partial^2 w}{\partial x_2^2} v \mathrm{d}x \tag{5}$$

Now, we add equations (4) and (5) and obtain

$$\int_\Omega \left(\frac{\partial v}{\partial x_1} \frac{\partial w}{\partial x_1} + \frac{\partial v}{\partial x_2} \frac{\partial w}{\partial x_2} \right) \mathrm{d}x =$$

$$\int_\Gamma v \cdot \left(\frac{\partial w}{\partial x_1} \cdot n_1 + \frac{\partial w}{\partial x_2} \cdot n_2 \right) \mathrm{d}S - \int_\Omega \left(\frac{\partial^2 w}{\partial x_1^2} + \frac{\partial^2 w}{\partial x_2^2} \right) v \mathrm{d}x,$$

i.e.,

$$\int_\Omega \mathrm{grad}\ v \cdot \mathrm{grad}\ w \mathrm{d}x = \int_\Gamma v\ \mathrm{grad}\ w \cdot n \mathrm{d}S - \int_\Omega \triangle\ w \cdot v \mathrm{d}x\,,$$

equivalently

$$\int_\Omega \nabla v\ \nabla w \mathrm{d}x = \int_\Gamma v\ \frac{\partial w}{\partial n} \mathrm{d}S - \int_\Omega \triangle w\ v \mathrm{d}x\,.$$

Finally we obtain 2nd Green's formula:

$$-\int_\Omega \triangle w\ v \mathrm{d}x = -\int_\Gamma v\ \frac{\partial w}{\partial n} \mathrm{d}S + \int_\Omega \nabla v\ \nabla w \mathrm{d}x\,.$$

★ Divergence theorem (Gauss–Green–Ostrogradsky's theorem)

Definition (generalized surface) The surface $S \subset \mathbb{R}^n (n \geq 2)$ is called a generalized $(n-1)-$surface if S is the finite union of smooth $(n-2)-$surfaces, $(n-3)-$surfaces, $\ldots$, $2-$surfaces, smooth curves and points.

Theorem (Gauss–Green–Ostrogradsky's) Let Ω be a bounded, connected opened set in $\mathbb{R}^n$, $n \geq 2$, with the boundary $\partial\Omega$ that is a generalized $(n-1)-$surface. Let all functions (scalars or vectors) integrated be (for simplicity) continuous together with their needed derivatives on $\overline{\Omega}$. We denote $\vec{\nu}$ a unit vector of outer normal to Ω in points $\partial\Omega$, in which it exists.

For $f : \overline{\Omega} \subset \mathbb{R}^n \to \mathbb{R}$, and for $\vec{T} : \overline{\Omega} \subset \mathbb{R}^n \to \mathbb{R}^n$, respectively, it holds

- Gauss–Green–Ostrogradsky's theorem for $k \in \{1, \ldots, n\}$:

$$\int_{\Omega} \frac{\partial f}{\partial x_k} \mathrm{d}x = \int_{\partial\Omega} f \nu_k \mathrm{d}S.$$

- Divergence theorem:

$$\int_{\Omega} \operatorname{div} \vec{T} \mathrm{d}x = \int_{\partial\Omega} \vec{T} \cdot \vec{\nu} \mathrm{d}S.$$

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