

Vector calculus and numerical mathematics

Worksheet 1

Problem 1: Vectors

The position vectors of the four corners of a regular tetrahedron (e.g., a methane molecule CH_4) are given as

$$\mathbf{r}_1 = \begin{pmatrix} x_1 \\ 0 \\ z_1 \end{pmatrix}, \quad \mathbf{r}_{2,3} = \begin{pmatrix} x_2 \\ \pm y_2 \\ z_1 \end{pmatrix}, \quad \mathbf{r}_4 = \begin{pmatrix} 0 \\ 0 \\ \ell \end{pmatrix} \quad (\ell = 1.087 \text{ \AA}, \quad x_1 > 0).$$

- Given that $\ell, x_1 > 0$, what are the signs of the constants x_2 and z_1 ?
- Utilizing the tetrahedral symmetry, find the values of x_1 , x_2 , y_2 , and z_1 .
- Find side length a and bond angle θ of a CH_4 molecule.

Problem 2: Vector product

Writing $\mathbf{a} = a_1\mathbf{u}_1 + a_2\mathbf{u}_2 + a_3\mathbf{u}_3$ and $\mathbf{b} = b_1\mathbf{u}_1 + b_2\mathbf{u}_2 + b_3\mathbf{u}_3$, show that

$$\mathbf{a} \times \mathbf{b} \equiv \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} \times \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} a_2b_3 - a_3b_2 \\ a_3b_1 - a_1b_3 \\ a_1b_2 - a_2b_1 \end{pmatrix}.$$

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Worksheet 2

Problem 1: Vectors of velocity and acceleration

The motion of a particle is described by the vector function

$$\mathbf{r}(t) \equiv \begin{pmatrix} x(t) \\ y(t) \\ z(t) \end{pmatrix} = \begin{pmatrix} R \cos(\frac{1}{2}\alpha t^2) \\ R \sin(\frac{1}{2}\alpha t^2) \\ 0 \end{pmatrix},$$

representing the position vector \mathbf{r} of the particle as a function of time t .

- What are the physical dimensions (m, s, kg, etc.) of the two constant parameters R and α ?
- What is the geometrical shape of this particle's orbit ?
By geometrical intuition, find the cartesian coordinates of unit vectors $\mathcal{T}(t)$ tangential and $\mathcal{N}(t)$ normal to the orbit at the time t . Are these vectors defined uniquely ?
- Find the velocity vector $\mathbf{v}(t)$ of the particle at the time t .
- Find the acceleration vector $\mathbf{a}(t)$ of the particle at the time t .
What are the tangential and the normal components of $\mathbf{a}(t)$?
Discuss the force $\mathbf{F}(t)$ acting on the particle, according to Newton's law $\mathbf{F} = m\mathbf{a}$.

Problem 2: Scalar field

A rectangular metal plate covers the region $\{-a \leq x \leq a, 0 \leq y \leq b\}$ on the xy -plane, with two given lengths a and b . As a model for the temperature distribution on the plate, consider the function

$$T(x, y) = T_0 \frac{y}{y + c(a^2 - x^2)(b - y)} \quad (T_0, c = \frac{1}{\ell^2} > 0). \quad (1)$$

- Choosing $a = b = \ell = 1\text{m}$ and $T_0 = 50^\circ\text{C}$, find the temperature $T(x, y)$ at the point $(x|y) = (-0.3\text{m} | 0.7\text{m})$ on the plate.
- Show that $T(x, y)$ is constant on each one of the four edges of the plate.
- Draw a contour plot of $T(x, y)$.
- Evaluating partial derivatives, find the gradient of the 2D scalar field $T(x, y)$,

$$\mathbf{G}_T(x, y) \equiv \nabla T(x, y) = \begin{pmatrix} T_x(x, y) \\ T_y(x, y) \end{pmatrix}.$$

Evaluate the vector $\mathbf{G}_T(x, y)$ for $(x, y) = (0.3a, 0.5b)$, $(0.5a, 0.5b)$, and $(0.8a, 0.5b)$. Enter these vectors as arrows at the corresponding positions in the contour plot.

Problem 3: Surface integral

Consider the 2D scalar field (with constants a, b, c),

$$f(x, y) = c - ax^2 - by^2.$$

- (a) Sketch the triangle Ω with the corners $A(-2|0)$, $B(1|3)$ and $C(1|-3)$ in the xy -plane.
- (b) Evaluate the surface integral

$$\int_{\Omega} d^2r f(\mathbf{r}).$$

Problem 4

- (a) Evaluate the 2D surface integral $\int_{\Sigma} d^2r f(\mathbf{r})$ of the scalar field

$$f(x, y) = ax - by$$

(with constants $a, b > 0$) over the domain

$$\Sigma = \left\{ (x, y) \in \mathbb{R}^2 \mid 0 \leq x \leq 1, \quad 0 \leq y \leq 1 - x \right\}.$$

- (b) Find the volume $V = \int_{\Omega} d^3r 1$ of the 3D region

$$\Omega = \left\{ (x, y, z) \in \mathbb{R}^3 \mid (x, y) \in \Sigma, \quad 0 \leq z \leq f(x, y) \right\}.$$

Problem 5

Let $\Omega \subset \mathbb{R}^2$ be the triangle with corners $A(4|0)$, $B(4|3)$, and $C(0|1)$ in the xy -plane.

- (a) Evaluate the surface integral

$$\int_{\Omega} d^2r f(x, y)$$

for the (linear!) function $f(x, y) = ax + by$, where $a, b \in \mathbb{R}$ are constant numbers. To find the proper integration limits, first sketch the triangle Ω in the xy -plane.

- (b) To check your result, mark in your sketch the points $P_i(x_i|y_i)$ with the coordinates

$$(x_1|y_1) = (1|1), \quad (x_2|y_2) = \left(\frac{7}{2}|\frac{1}{2}\right), \quad (x_3|y_3) = (3|2),$$

and evaluate the function values $f(x_i, y_i)$ for $i \in \{1, 2, 3\}$. Why can we expect that

$$\int_{\Omega} d^2r f(x, y) \approx A_{\Omega} \cdot \frac{1}{3} \sum_{i=1}^3 f(x_i, y_i),$$

where A_{Ω} is the area of the triangle Ω ?

- (c) In terms of the position vectors \mathbf{r}_A , \mathbf{r}_B , and \mathbf{r}_C of its corners, the position vector \mathbf{r}_M of the triangle's center of mass M is given by the vector sum $\mathbf{r}_M = \frac{1}{3}(\mathbf{r}_A + \mathbf{r}_B + \mathbf{r}_C)$, with coordinates x_M and y_M . Compare the value of the integral $\int_{\Omega} d^2r f(x, y)$ with

$$A_{\Omega} \cdot f(x_M, y_M).$$

- (d) Repeat parts (a), (b), and (c) for the quadratic function $f(x, y) = ax^2 + bxy + cy^2$.
Hint: You might need the binomic formula $(a + b)^3 = a^3 + 3a^2b + 3ab^2 + b^3$.

Problem 6

In the xy -plane, we consider the region

$$\Omega = \left\{ (x, y) \in \mathbb{R}^2 \mid 0 \leq y \leq 4 - x^2, \quad |x| \leq 2 \right\}.$$

- (a) Draw a sketch of Ω . By elementary integration, find the area A_{Ω} of Ω .
(b) Evaluate the surface integral

$$\int_{\Omega} d^2r f(\mathbf{r})$$

for the function $f(x, y) = x^2 + y^2$.

- (c) What is the average value $\langle f(\mathbf{r}) \rangle_{\mathbf{r} \in \Omega}$ of this function in Ω ?
(d) **Bonus:** Find the minimum and maximum values of $f(\mathbf{r})$ for $\mathbf{r} \in \Omega$ without performing any calculation. Hint: Make a rough sketch of the 3D-plot of f !

Problem 7

In 3D xyz -space, we consider the volume region ($\frac{1}{8}$ of a sphere with radius a !)

$$\Omega = \left\{ (x, y, z) \mid x, y, z \geq 0 \quad \text{and} \quad x^2 + y^2 + z^2 \leq a^2 \right\}.$$

Evaluate the volume integrals $\int_{\Omega} d^3r f(\mathbf{r})$ for the following scalar fields.

- (a) $f(x, y, z) = xz$.
(b) $f(x, y, z) = xyz$.