Module 1A - Calculus

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Contents

Objectives: Review the basic calculus concepts to be used in future modules.

Prerequisite Knowledge: High-school calculus, algebra
Prerequisite Modules: N/A

Difficulty: Easy

Summary: This module summarizes key calculus concepts that will be used in subsequent modules in physics of food systems, optimization, numerical methods, and food applications.

1 Theory

1.1 Vectors, Products and Norms

In this work, boldface symbols imply vectors or tensors. A fixed Cartesian coordinate system will be used throughout this monograph. The unit vectors for such a system are given by the (fixed) mutually orthogonal triad (e_1, e_2, e_3). For the inner product of two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ we have in three dimensions

$$\boldsymbol{u} \cdot \boldsymbol{v} = \sum_{i=1}^{3} u_i v_i = u_1 v_1 + u_2 v_2 + u_3 v_3 = ||u|| ||v|| \cos\theta, \tag{1.1}$$

where

$$||\boldsymbol{u}|| = \sqrt{u_1^2 + u_2^2 + u_3^2}, \tag{1.2}$$

represents the Euclidean norm in R^3 and θ is the angle between them. We recall that a norm has three main characteristics for any two bounded vectors $\boldsymbol{u}$ and $\boldsymbol{v}$ ($||\boldsymbol{u}|| < \infty$ and $||\boldsymbol{v}|| < \infty$):

- $||\boldsymbol{u}|| \geq 0$, $||\boldsymbol{u}|| = 0$ if and only if $\boldsymbol{u} = 0$,
- $||\boldsymbol{u} + \boldsymbol{v}|| ||\boldsymbol{u}|| + ||\boldsymbol{v}||$ and
- $||\gamma \boldsymbol{u}|| = |\gamma| ||\boldsymbol{u}||$, where γ is a scalar.

Two vectors are said to be orthogonal if $\boldsymbol{u} \cdot \boldsymbol{v} = 0$. The cross (vector) product of two vectors is

$$\boldsymbol{u} \times \boldsymbol{v} = -\boldsymbol{v} \times \boldsymbol{u} = \begin{vmatrix} e_1 & e_2 & e_3 \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix} = \|\boldsymbol{u}\| \|\boldsymbol{v}\| \sin\theta \boldsymbol{n} \tag{1.3}$$

where $\boldsymbol{n}$ is the unit normal to the plane formed by the vectors $\boldsymbol{u}$ and $\boldsymbol{v}$.

The temporal differentiation of a vector-valued function is given by

$$\frac{d}{dt} u(t) = \frac{du_1(t)}{dt} e_1 + \frac{du_2(t)}{dt} e_2 + \frac{du_3(t)}{dt} e_3 = \dot{u}_1 e_1 + \dot{u}_2 e_2 + \dot{u}_3 e_3 \tag{1.4}$$

The spatial gradient of a scalar-valued function (a dilation to a vector) is given by

$$\nabla_x \phi = \left(\frac{\partial \phi}{\partial x_1} e_1 + \frac{\partial \phi}{\partial x_2} e_2 + \frac{\partial \phi}{\partial x_3} e_3 \right) \tag{1.5}$$

The gradient of a vector-valued function is a direct extension of the preceding definition. For example, $\nabla_x \boldsymbol{u}$ has components of $\frac{\partial u_i}{\partial x_j}$. The divergence of a vector (a contraction to a scalar) is defined by

$$\nabla_x \cdot \boldsymbol{u} = \left(e_1 \frac{\partial}{\partial x_1} + e_2 \frac{\partial}{\partial x_2} + e_3 \frac{\partial}{\partial x_3} \right) \cdot (u_1 e_1 + u_2 e_2 + u_3 e_3) = \left(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3} \right). \tag{1.6}$$

The curl of a vector is defined as:

$$\nabla_x \times \boldsymbol{u} = \begin{vmatrix} e_1 & e_2 & e_3 \\ \frac{\partial}{\partial x_1} & \frac{\partial}{\partial x_2} & \frac{\partial}{\partial x_3} \\ u_1 & u_2 & u_3 \end{vmatrix} \tag{1.7}$$

The triple product of three vectors is

$$\boldsymbol{w} \cdot (\boldsymbol{u} \times \boldsymbol{v}) = \left(\begin{vmatrix} w_1 & w_2 & w_3 \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix} \right) = (\boldsymbol{w} \times \boldsymbol{u}) \cdot \boldsymbol{v} \tag{1.8}$$

This represents the volume of a parallelpiped formed by the three vectors.

1.2 Integral Transformations

The divergence of a vector-valued function (a contraction to a scalar-valued function) is defined by

$$\nabla_x \cdot \boldsymbol{u} = \sum_{i=1}^{N} u_{i,i} \tag{1.9}$$

whereas for a second order tensor (a contraction to a vector):

$$\nabla_x \cdot A \text{ has components of } \sum_{j=1}^{N} A_{ij,j}. \tag{1.10}$$

The gradient of a vector (a dilation to a second order tensor) is:

$$\nabla_x \boldsymbol{u} \text{ has components of } u_{i,j}, \tag{1.11}$$

whereas for a second order tensor (a dilation to a third order tensor):

$$\nabla_x \boldsymbol{A} \text{ has components of } A_{ij,k}. \tag{1.12}$$

The gradient of a scalar (a dilation to a vector):

$$\nabla_x \phi \text{ has components of } \phi_{,i}. \tag{1.13}$$

The scalar product of two second order tensors, for example the gradients of first order vectors, is defined as

$$\nabla_x \boldsymbol{v} : \nabla_x \boldsymbol{u} = \underbrace{\frac{\partial v_i}{\partial x_j} \frac{\partial u_i}{\partial x_j}}_{\text{in Cartesian bases}} \stackrel{\text{def}}{=} v_{i,j} u_{i,j} \quad i,j = 1,2,3, \tag{1.14}$$

where $\partial u_i / \partial x_j, \partial v_i / \partial x_j$ are partial derivatives of u_i and v_i, and where u_i, v_i are the Cartesian components of $\boldsymbol{u}$ and $\boldsymbol{v}$ and

$$\nabla_x \boldsymbol{u} \cdot \boldsymbol{n} \text{ has components of } \underbrace{u_{i,j} n_j}_{\text{in Cartesian bases}}, \quad i,j = 1,2,3. \tag{1.15}$$

For a scalar, we have

$$\int_\Omega \nabla_x \phi d\Omega = \int_{\partial\Omega} \phi \boldsymbol{n} dA \qquad \int_\Omega \phi_{,i} d\Omega = \int_{\partial\Omega} \phi n_i dA \tag{1.16}$$

and for a vector

$$\int_\Omega \nabla_x \boldsymbol{u} d\Omega = \int_{\theta\Omega} \boldsymbol{u} \otimes \boldsymbol{n} dA \qquad \int_\Omega u_{i,j} d\Omega = \int_{\partial\Omega} u_i n_j dA \tag{1.17}$$

The divergence theorem for vectors is

$$\int_\Omega \nabla_x \cdot \boldsymbol{u} d\Omega = \int_{\partial\Omega} \boldsymbol{u} \cdot \boldsymbol{n} dA \qquad \int_\Omega u_{i,i} d\Omega = \int_{\partial\Omega} u_i n_i dA \tag{1.18}$$

and analogously for a tensor $\boldsymbol{B}$

$$\int_\Omega \nabla_x \cdot \boldsymbol{B} d\Omega = \int_{\partial\Omega} \boldsymbol{B} \cdot \boldsymbol{n} dA \qquad \int_\Omega B_{ij,j} d\Omega = \int_{\partial\Omega} B_{ij} n_j dA \tag{1.19}$$

where n is the outward normal to the bounding surface. These standard operations arise throughout the analysis. A generalization of these last results is

$$\int_\Omega \nabla_x * \boldsymbol{B} d\Omega = \int_{\partial\Omega} \boldsymbol{n} * \boldsymbol{B} dA \tag{1.20}$$

where, when $* = \cdot$, we have the divergence theorem and when $* = \times$ we have the "cross-product" theorem.[1] For proofs, see Chandrasekharaiah and Debnath [47] or Malvern [45].

[1] Also, we have the point-wise product rule:

$$\frac{d}{dt}(\boldsymbol{a} * \boldsymbol{b}) = \frac{d\boldsymbol{a}}{dt} * \boldsymbol{b} + \boldsymbol{a} * \frac{d\boldsymbol{a}}{dt}$$

2 Example

Two example problems are given below:

1. Vectors $\boldsymbol{v}$ and $\boldsymbol{u}$ are defined as $\boldsymbol{v} = [2, 3, 6]$ and $\boldsymbol{u} = [-3, 4, 0]$. The magnitude of $\boldsymbol{v}$ is:

$$||\boldsymbol{v}|| = \sqrt{2^2 + 3^2 + 6^2} = \sqrt{49} = 7 \tag{2.1}$$

The dot product P is

$$P = \boldsymbol{v} \cdot \boldsymbol{u} = 2 \cdot (-3) + 3 \cdot (4) + 6 \cdot 0 = -6 + 12 + 0 = 6 \tag{2.2}$$

The angle between $\boldsymbol{v}$ and $\boldsymbol{u}$ is calculated using the relation $\boldsymbol{v} \cdot \boldsymbol{u} = ||\boldsymbol{v}||||\boldsymbol{u}|| \cos\theta$:

$$cos\theta = \frac{\boldsymbol{v} \cdot \boldsymbol{u}}{||\boldsymbol{v}||||\boldsymbol{u}||} = \frac{6}{7 \cdot 5} = \frac{6}{35} \tag{2.3}$$

Then, the angle is:

$$\theta = \cos^{-1}(\frac{6}{35}) = 1.40\ rad \tag{2.4}$$

The cross product, $\boldsymbol{v} \times \boldsymbol{u}$ is:

$$\boldsymbol{v} \times \boldsymbol{u} = \begin{vmatrix} e_1 & e_2 & e_3 \\ 2 & 3 & 6 \\ -3 & 4 & 0 \end{vmatrix} = \big(3 \cdot\ 0 - 6 \cdot\ 4, 6\,(-3) - 2 \cdot\ 0, 2 \cdot\ 4 - 3\,(-3)\big) = \big(-24, -18, 17\big) \tag{2.5}$$

2. We can evaluate the following integral:

$$F(r) = \frac{1}{\pi R^2} \int_0^R U_o \Big(1 - \frac{r}{R}\Big)^m 2\pi r dr \tag{2.6}$$

where U_o, R, m are constants.

$$\frac{2\pi U_o}{\pi R^2} \int_0^R U_o \left(1 - \frac{r}{R}\right)^m r dr \tag{2.7}$$

Using u-substitution:

$$u = 1 - \frac{r}{R}, \quad du = -\frac{1}{R} dr \to dr = -R du \tag{2.8}$$

$$F(r) = \frac{2U_o}{R^2} \int_{u_1}^{u_2} u^m (1 - u) \cdot -R du \tag{2.9}$$

$$u_2 = 1 - \frac{R}{R} = 0, \quad u_1 = 1 - 0 = 1 \tag{2.10}$$

$$@U_o \int_1^0 u^m (u - 1) du = 2U_o \int_1^0 (u^{m+1} - u^m) du \tag{2.11}$$

$$2U_o \left[\frac{u^{m+2}}{m+2} - \frac{u^{m+1}}{m+1}\right]_1^0 \tag{2.12}$$

$$F(r) = \frac{2U_o}{(m+1)(m+2)} \tag{2.13}$$

3 Assignment

CALCULUS REVIEW (100 POINTS)

In this assignment, you will be reviewing the basics concepts of calculus. *The typical report format will not be required for this assignment, and unless otherwise specified, either hand-written or typed information is acceptable.* If you use Matlab or another language for simplifying answers or evaluating specific numbers, clearly set up the equations before showing your numerical results. Correct answers without supporting work will be penalized, and incorrect answers without supporting work will receive zero credit.

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1. Defining the two vectors **A** and **B** such that $|\mathbf{A}| = 23.0$ and makes an angle of 17° with respect to the horizontal (x -axis); and $|\mathbf{B}| = 31.0$ and tilts 45° counterclockwise from the vertical (y-axis). Each vector lies in the xy -plane.

   - (a) Graph these two vectors on an x, y coordinate system.
   - (b) Resolve each vector into components.
   - (c) Find their sum $\mathbf{R} = \mathbf{A} + \mathbf{B}$.
   - (d) Find their scalar product $P = \mathbf{A} \cdot \mathbf{B}$.
   - (e) Find their cross product $\mathbf{C} = \mathbf{A} \times \mathbf{B}$
   - (f) If instead you do each operation in (c), (d) and (e) in reverse order ($eg, \mathbf{R} = \mathbf{B} + \mathbf{A}$), will you get the same answer? Identify any differences.
   - (g) If one has the components of the two vectors, one can calculate the cross product as a determinant:

     $$\mathbf{A} \times \mathbf{B} = \begin{vmatrix} e_1 & e_2 & e_3 \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix}$$

     From the component form of **A** and **B** found in Problem 1b, calculate $\mathbf{A} \times \mathbf{B}$ by taking the determinant of the matrix. Do you get the same answer as Problem 1e ?

2. In a parallelepiped, three of the edges are formed by three non coplanar vectors originating from one vertex. The volume of such a figure can be calculated as the absolute value of the the so-called 'triple-scalar product' defined as $\mathbf{A} \cdot (\mathbf{B} \times \mathbf{C})$ for three vectors $\mathbf{A}, \mathbf{B}, \mathbf{C}$.

   Suppose that one has the vectors $\boldsymbol{u} = 4.0\hat{\imath} + 2.0\hat{\jmath} + 1.0\hat{k}$ $\boldsymbol{v} = 5.0\hat{\imath} + 8.0\hat{\jmath} + 0.5\hat{k}$ and $\mathbf{w} = 3.0\hat{\jmath} + 12.0\hat{k}$ that define a parallelepiped. Calculate the volume of this parallelepiped.

3. Calculate the integral

   $$\int_0^1 9Y^2 x^9 dx \tag{3.1}$$

   where Y is a constant.

4. Calculate the gradient of the function of 3 variables,

   $$f(x, y, z) = x^4 y^5 + K e^{yz} \tag{3.2}$$

   where K is a constant.

5. Consider a region R in the first quadrant of the x-y plane, bounded by the function $y = 4 - \frac{1}{2}x^4$.Express the area A as a double integral.

6. Consider a curve A parametrized by

$$\boldsymbol{r}(t) = < t^2, 2t^3, \sqrt{4t} > \tag{3.3}$$

   where $t \in (0, 1)$

   - (a) Calculate the tangent vector $\frac{d\boldsymbol{r}}{dt}$
   - (b) Calculate the length of the tangent vector.

7. Consider a fluid flow in 2D. The fluid velocity is given as $\boldsymbol{u} = (2x - y, 3xy)$, in knots. Calculate the divergence and the curl of the velocity field. Include units.

4 Solution

The assignment solution is encoded in Matlab below.

1. P1

```
%(ab)
A_mag = 23; % A magnitude
B_mag = 31; % B magnitude
A_ang = 17; % A angle
B_ang = 135; % B angle

Ax = linspace(0,A_mag*cosd(17),1000);
Ay = sqrt((Ax./cosd(17)).^2-Ax.^2);

Bx = linspace(-B_mag*cosd(45),0,1000);
By = sqrt((Bx./cosd(135)).^2-Bx.^2);


plot(Ax,Ay)
hold on
plot(Bx,By)
axis equal
legend('A','B')

%(c)
SumP = [Ax+Bx;Ay+By];
R = SumP(:,1000); %take the tip of the vectors from the discretized points


%(d)
P1 = Ax(1000)*Bx(1)+Ay(1000)*By(1);
%alternatively
P2 = A_mag*B_mag*cosd(B_ang-A_ang);

%(e)
C = A_mag*B_mag*sind(B_ang-A_ang);

%(f)
Answer to (e) would yield a different direction but the same magnitude
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2. P2

```
u = [4,2,1]; v = [5,8,0.5]; w = [0,3,12];

V = dot(u,cross(v,w));
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3. P3

   Answer: $(9/10Y^2x^{10})_0^1 = 9/10Y^2$

4. P4

   Answer: $\nabla \cdot f =< 4x^3y^5, 5x^4y^4 + Kze^{yz}, Kye^{yz} >$

5. P5

   Answer: $A = \int_0^{2\sqrt{2}} \int_0^4 (4 - \frac{1}{2}x^4)dydx$

6. P6

   Answer:

   - (a) $dr/dt = < 2t, 6t^2, 1/\sqrt{t} >$
   - (b) magnitude $= \sqrt{4t^2 + 36t^4 + 1/t}$

7. P7

   Answer:

   - $\nabla \cdot u = 2 + 3x \rightarrow divergence$
   - $\nabla \times u = (0, 0, 3y + 1) \rightarrow curl$

5 References

1. Zohdi, T. I. and Wriggers, P. (Book, 2005, 2008) Introduction to computational micromechanics.
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