**Introduction to Linear Algebra**

Linear algebra is crucial for chemists as it provides the mathematical framework for understanding and describing various chemical phenomena. For example, it is used in quantum chemistry to solve Schrödinger's equation, model molecular orbitals, and analyze atomic interactions. In spectroscopy, linear algebra helps process and interpret large data sets, such as from NMR or IR spectroscopy. It also plays a key role in molecular modeling, where vector and matrix operations are used to understand molecular geometry, predict reaction outcomes, and simulate chemical processes.

# 1 Scalars

Most of the computational operations rely on the manipulations of numbers one at a time. This is what we defined as **scalars**. One of the most common examples of scalars is temperature, and we can manipulate scalars using functions,

$$t_C = f(t_F) = \frac{5}{9}\left(t_F - 32\right). \tag{1}$$

In the majority of the text books, scalars are denoted by lower-case letters, for example $t_C$ or $x$. It is important to remember that scalars are continuous real-valued and commonly defined as,

$$x \in \mathbb{R}, \tag{2}$$

where $\in$ means "in" and $\mathbb{R}$ are the real numbers set.

Scalars numbers have the possible operations,

- addition, $x + y$
- multiplication $xy$
- division $\frac{x}{y}$
- exponentiation $x^y$

In programming, scalars are implemented as tensors that only contain a single element, and slicing operations are prohibited.

# 2 Vectors

In the hierarchy of tensors, vectors are the first structure that has a single dimension, meaning they are $1^{\text{st}}$ oder tensors. From the computational perspective, vectors are considered a fixed-length array of scalars, commonly assumed to be vertically,

$$\mathbf{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}, \tag{3}$$

where $x_i \in \mathbb{R}$, and $d$ is the number of items in $\mathbf{x}$. Vectors are also represented as arrows with a direction and an angle (I personally not fan of this notation).

## 2.1 Unitary vectors

In physics, it is common to represent vectors in terms of unitary vectors,

$$\mathbf{u} = u_x\,\mathbf{i} + u_y\,\mathbf{j} + u_z\,\mathbf{k}, \tag{4}$$

where

$$\mathbf{i} = \begin{bmatrix}1\\0\\0\end{bmatrix} \mathbf{j} = \begin{bmatrix}0\\1\\0\end{bmatrix} \mathbf{k} = \begin{bmatrix}0\\0\\1\end{bmatrix}. \tag{5}$$

Here we present some of the most common operations for vectors.

## 2.2 Scalar multiplication

The operation between a scalar and a vector is called scalar multiplication. In scalar multiplication, each component of the vector is multiplied by the scalar, resulting in a new vector that points in the same (or opposite) direction but with a scaled magnitude.

$$c\,\mathbf{x} = \begin{bmatrix}cx_0\\\vdots\\cx_d\end{bmatrix}, \tag{6}$$

where $cx_i$ is the multiplication of each entry of $\mathbf{x}$ by the scalar $c$.

## 2.3 Addition

The addition of vectors involves adding corresponding components of two vectors to produce a new vector,

$$\mathbf{x} + \mathbf{y} = \begin{bmatrix}x_0\\\vdots\\x_d\end{bmatrix} + \begin{bmatrix}y_0\\\vdots\\y_d\end{bmatrix} = \begin{bmatrix}x_0 + y_0\\\vdots\\x_d + y_d\end{bmatrix} \tag{7}$$

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We can combine scalar multiplication and addition of two vectors to compose the subtraction of two vectors, $\mathbf{x} - \mathbf{y} = \mathbf{x} + (-1)\,\mathbf{y}$.

The sum of two vectors using the physics notation, is defined as,

$$\mathbf{u} \pm \mathbf{v} = (u_x \pm v_x)\,\mathbf{i} + (u_y \pm v_y)\,\mathbf{j} + (u_z \pm v_z)\,\mathbf{k}\,. \tag{8}$$

## 2.4 Division

Division of vectors is not defined in the same straightforward way as addition, subtraction, or scalar multiplication. Unlike scalars, vectors don't have a direct division operation. However, there are some related concepts, i) scalar division and ii) element-wise division. For scalar division, we can use Eq. 6, where the scalar is defined as $\frac{1}{c}$, making the operation for each element of $\mathbf{x}$, $\frac{x_i}{c}$.

In programming, the division between two vectors is the element-wise division,

$$\mathbf{x}\,/\,\mathbf{y} = \begin{bmatrix} \frac{x_0}{y_0} \\ \vdots \\ \frac{x_d}{y_d} \end{bmatrix}, \tag{9}$$

where each element of the new vector is the division of elements of the two vectors.

One must be careful with element-wise operations as they are only valid for vectors with the same number of elements.

## 2.5 Dot product

The dot product, also known as the *scalar product*, is an operation that takes two vectors and returns a scalar. It measures the extent to which two vectors point in the same direction. The scalar product is defined as,

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^\top \mathbf{v} = \|u\| \|v\| \cos(\theta), \tag{10}$$

where $\|u\|$ is the norm of the vector $\mathbf{u}$ and, $\theta$ is the angle between both vectors. $\mathbf{u}^\top$ is the transpose of the vector $\mathbf{u}$, which means a *row vector*,

$$\mathbf{x}^\top = [x_0, \cdots, \mathbf{x}_d]. \tag{11}$$

The norm, magnitude or length of a vector is defined as

$$\| \mathbf{u} \| = \sqrt{x_0^2 + x_1^2 + \cdots + x_d^2} = \left( \sum_{i=0}^{d} x_i^2 \right)^{\frac{1}{2}}. \tag{12}$$

**Exercise**:
Compute, $\| \mathbf{u} + \mathbf{v} \|$ for $\mathbf{u} = [2, -1, 3]$ and $\mathbf{v} = [-1, 1, -1]$.

**Exercise**:
What is the dot product of $\mathbf{i} \cdot \mathbf{i}$ and $\mathbf{i} \cdot \mathbf{j}$?

**Exercise**:
What is the dot product of $\mathbf{u} \cdot \mathbf{v}$ for For, $\mathbf{u} = u_x\,\mathbf{i} + u_y\,\mathbf{j} + u_z\,\mathbf{k}$ and $\mathbf{v} = v_x\,\mathbf{i} + v_y\,\mathbf{j} + v_z\,\mathbf{k}$?

A more general definition of the dot product for $d$-dimensional vectors is,

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u}^\top \mathbf{v} = \sum_{i=1}^{d} u_i v_i. \tag{13}$$

**Exercise**:
What is the value of $\theta$ between $\mathbf{u} = \mathbf{i} + 3\,\mathbf{j} - \mathbf{k}$ and $\mathbf{v} = \mathbf{j} - \mathbf{k}$?

## 2.6 Cross product

The cross product, also known as *vector product* is an operation between two vectors that results in a new vector perpendicular to both original vectors. It is defined as,

$$\mathbf{u} \times \mathbf{v} = \|u\|\|v\|\mathbf{c}\sin(\theta), \tag{14}$$

where $\mathbf{c}$ is a unit vector perpendicular to the plane form by $\mathbf{u}$ and $\mathbf{v}$. We can find $\mathbf{c}$ using the following equations,

$$\begin{aligned} \mathbf{u}^\top \mathbf{c} &= 0 & (15)\\ \mathbf{v}^\top \mathbf{c} &= 0 & (16)\\ \mathbf{c}^\top \mathbf{c} &= 1, & (17) \end{aligned}$$

in matrix notation we get,

$$\begin{aligned} u_x c_x + u_y c_y + u_z c_z &= 0 & (18)\\ v_x c_x + v_y c_y + v_z c_z &= 0 & (19)\\ c_x c_x + c_y c_y + c_z c_z &= 1. & (20) \end{aligned}$$

We will see later in the course that these non-linear equations can be solved using optimization methods.

For three dimensional vectors and using unitary vectors, the cross product is defined as,

$$\mathbf{u} \times \mathbf{v} = (u_y v_z - u_z v_y)\,\mathbf{i} + (u_z v_x - v_x v_z)\,\mathbf{j} + (u_x v_y - u_y v_x)\,\mathbf{k}\,. \tag{21}$$

Commonly, you will find that,

$$\mathbf{u} \times \mathbf{v} = \underbrace{\begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ u_x & u_y & u_z \\ v_x & v_y & v_z \end{vmatrix}}_{determinant} = (u_y v_z - u_z v_y)\,\mathbf{i} + (u_z v_x - v_x v_z)\,\mathbf{j} + (u_x v_y - u_y v_x)\,\mathbf{k}\,. \tag{22}$$

**Exercise**:
What is the value of $\mathbf{u} \cdot (\mathbf{v} \times \mathbf{w})$? For each vector you can consider the physics notation.

# 3 Matrices