Lecture 3: Vector Spaces and Orthonormal Bases *RHB, 7.1.0, 7.1.1, 6.4*

3. 1. Review of vector spaces RHB 7.1.0

Let V denote a vector space. Then vectors in V obey the following rules for addition and multiplication by scalars

$$\begin{aligned} \underline{a} + \underline{b} \in V \quad &\text{if} \quad \underline{a}, \underline{b} \in V \\ \alpha \underline{a} \in V \quad &\text{if} \quad \underline{a} \in V \\ \alpha(\underline{a} + \underline{b}) &= \alpha \underline{a} + \alpha \underline{b} \\ (\alpha + \beta)\underline{a} &= \alpha \underline{a} + \beta \underline{a} \end{aligned}$$

and the space should contain a zero vector $\underline{0}$.

Of course as we have seen, vectors in $I\!R^3$ (usual 3 dimesnional real space) obey these axioms. Other simple examples are a plane through the origin which forms a two dimensional space and a line through the origin which forms a one dimensional space.

3. 2. Linear Independence

Consider two vectors $\underline{A}$ and $\underline{B}$ in a plane through the origin and the equation:–

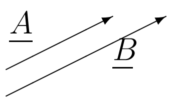
$$\boxed{\alpha \underline{A} + \beta \underline{B} = 0} \, .$$

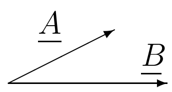
If this is satisfied for *non-trivial* α and β (*i.e.* at least one of α and β are *non-zero*), then $\underline{A}$ and $\underline{B}$ are **linearly dependent**.

$$i.e. \ \underline{B} = -\frac{\alpha}{\beta} \underline{A} \, .$$

Clearly $\underline{A}$ and $\underline{B}$ are **collinear** (either parallel or anti-parallel).
If this equation can be satisfied *only* for $\alpha = \beta = 0$, then $\underline{A}$ and $\underline{B}$ are **linearly independent**, and obviously *not collinear* (*i.e.* no λ can be found such that $\underline{B} = \lambda \underline{A}$).

Linearly Dependent **Linearly Independent**





Notes

(i) If $\underline{A}$, $\underline{B}$ are linearly independent any vector $\underline{r}$ in the plane may be written uniquely as a linear combination

$$\underline{r} = a\underline{A} + b\underline{B}$$

(ii) We say $\underline{A}$, $\underline{B}$ span the plane or $\underline{A}$, $\underline{B}$ form a basis for the plane

(iii) We call (a, b) a representation of $\underline{r}$ in the basis formed by $\underline{A}$, $\underline{B}$ and a, b are the components of $\underline{r}$ in this basis.

In 3 dimensions the definition of linear dependence of two vectors remains the same. Three vectors are linearly dependent if we can find non-trivial α, β, γ (at least one non-zero) such that

$$\boxed{\alpha \underline{A} + \beta \underline{B} + \gamma \underline{C} = 0}$$

otherwise $\underline{A}, \underline{B}, \underline{C}$ are linearly independent (no one is a linear combination of the other two).

Notes

(i) If $\underline{A}$, $\underline{B}$ and $\underline{C}$ are linearly independent they span $\mathbb{R}^3$ and form a basis *i.e.* for any vector $\underline{r}$ we can find scalars a, b, c such that

$$\underline{r} \;=\; a\underline{A} + b\underline{B} + c\underline{C}\ .$$

(ii) The **triple** of numbers (a, b, c) is the **representation** of $\underline{r}$ in this basis; a, b, c are components of $\underline{r}$ in this basis.

(iii) The geometrical interpretation of linear dependence in three dimensions is that

$$\boxed{\text{three linearly dependent vectors} \Leftrightarrow \text{three coplanar vectors}}$$

To see this note that if $\alpha \underline{A} + \beta \underline{B} + \gamma \underline{C} = 0$ then

$$\begin{array}{ll} \alpha \neq 0 & \alpha \underline{A} \cdot (\underline{B} \times \underline{C}) = 0 \Rightarrow \underline{A}, \underline{B}, \underline{C} \quad \text{are coplanar} \\ \alpha = 0 & \text{then } \underline{B} \text{ is collinear with } \underline{C} \text{ and } \underline{A}, \underline{B}, \underline{C} \text{ are coplanar} \end{array}$$

Arbitrary dimensions

One can consider vector spaces of arbitrary dimension *e.g.* in quantum mechanics one requires an infinite dimensional vector space. An arbitrary number of vectors are linearly dependent if we can find non-trivial $\alpha, \beta, \gamma, \delta \ldots$ such that $\boxed{\alpha \underline{A} + \beta \underline{B} + \gamma \underline{C} + \delta \underline{D} \cdots = 0}$

For a space of dimension n one can find at most n linearly independent vectors.

3. 3. Reciprocal basis

If $\underline{L}, \underline{M}, \underline{N}$ form a basis for $\mathbb{R}^3$ then the components of an arbitrary vector

$$\underline{r} \;=\; l\underline{L} + m\underline{M} + n\underline{N}\ .$$

can be found using

$$l = \underline{r} \cdot \underline{L}^* \quad m = \underline{r} \cdot \underline{M}^* \quad n = \underline{r} \cdot \underline{N}^*$$

where the reciprocal basis vectors $\underline{L}^*$, $\underline{M}^*$, $\underline{N}^*$ are defined by

$$\underline{L}^* = \frac{\underline{M} \times \underline{N}}{\underline{L} \cdot (\underline{M} \times \underline{N})} \quad \underline{M}^* = \frac{\underline{N} \times \underline{L}}{\underline{M} \cdot (\underline{N} \times \underline{L})} \quad \underline{N}^* = \frac{\underline{L} \times \underline{M}}{\underline{N} \cdot (\underline{L} \times \underline{M})}$$

You should verify this by substitution. Question 2.5 and 2.6 explore reciprocal vectors further. They are of prime importance in crystallography, for example in describing the positions of sites on a non-cubic lattice (see Physics 2 Properties of Matter course).

3. 4. Scalar Product

Consider the scalar product of $\underline{r} = l\underline{L}+m\underline{M}+n\underline{N}$ with a different vector $\underline{s} = l'\underline{L}+m'\underline{M}+n'\underline{N}$:

$$\begin{aligned}\underline{r}\cdot\underline{s} &= ll'L^2 + mm'M^2 + nn'N^2 + (ml'+lm')\underline{L}\cdot\underline{M} \\ &\quad +(ln'+nl')\underline{L}\cdot\underline{N} + (mn'+nm')\underline{M}\cdot\underline{N}\ .\end{aligned}$$

For a general basis comprising $\underline{L}$, $\underline{M}$ and $\underline{N}$, this is very clumsy. It simplifies if the basis vectors are

- of *unit length* ($L^2 = M^2 = N^2 = 1$) and
- *mutually orthogonal* ($\underline{L}\cdot\underline{M} = \underline{L}\cdot\underline{N} = \underline{M}\cdot\underline{N} = 0$),

then

$$\underline{r}\cdot\underline{s} = ll' + mm' + nn'.$$

and the components are easily obtained

$$l = \underline{r}\cdot\underline{L} \quad m = \underline{r}\cdot\underline{M} \quad n = \underline{r}\cdot\underline{N}$$

Such a basis, in which the basis vectors are *orthogonal* and *normalised* (of unit length) is called an **orthonormal** basis.

This is a very special type of basis that is *self-reciprocal i.e.* $\underline{L}^* = \underline{L}$, $\underline{M}^* = \underline{M}$, $\underline{N}^* = \underline{N}$

3. 5. Standard orthonormal basis: Cartesian basis

A common convention that you should already have encountered refers to the 3 directions of the orthonormal basis vectors as the x, y and z-axes, the basis vectors being denoted by either $\underline{i}$, $\underline{j}$ and $\underline{k}$ or $\underline{e}_x$, $\underline{e}_y$ and $\underline{e}_z$.

In the 'xyz' notation the components of a vector $\underline{A}$ are A_x, A_y, A_z, and a vector is written in terms of the basis vectors as

$$\underline{A} = A_x\,\underline{i} + A_y\,\underline{j} + A_z\,\underline{k} \quad \text{or} \quad \underline{A} = A_x\,\underline{e}_x + A_y\,\underline{e}_y + A_z\,\underline{e}_z\ .$$

Also note that in this basis, the basis vectors themselves are represented by

$$\underline{i} = \underline{e}_x = (1,0,0) \quad \underline{j} = \underline{e}_y = (0,1,0) \quad \underline{k} = \underline{e}_z = (0,0,1)$$

3. 6. Suffix or Index notation

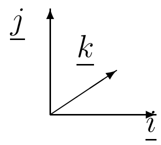
A more systematic labelling of orthonormal basis vectors for $I\!R^3$ is by $\underline{e}_1$, $\underline{e}_2$ and $\underline{e}_3$. i.e. instead of $\underline{i}$ we write $\underline{e}_1$, instead of $\underline{j}$ we write $\underline{e}_2$, instead of $\underline{k}$ we write $\underline{e}_3$. Then

$$\left.\begin{array}{l}\underline{e}_1\cdot\underline{e}_1 = \underline{e}_2\cdot\underline{e}_2 = \underline{e}_3\cdot\underline{e}_3 = 1; \\ \underline{e}_1\cdot\underline{e}_2 = \underline{e}_2\cdot\underline{e}_3 = \underline{e}_3\cdot\underline{e}_1 = 0.\end{array}\right\} \quad \#$$

Similarly the components of any vector $\underline{A}$ in are 3-d space are denoted by A_1, A_2 and A_3

This scheme is known as the **suffix** notation. Its great advantages over 'xyz' notation are that it clearly generalises easily to any number of dimensions and greatly simplifies manipulations and the verification of various identities (see later in the course).

Old Notation | **New Notation**



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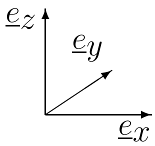

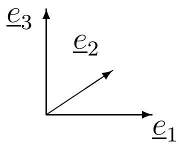

$\underline{r} = x\underline{i} + y\underline{j} + z\underline{k}$ $\quad$ $\underline{r} = x\underline{e}_x + y\underline{e}_y + z\underline{e}_z$ $\quad$ $\underline{r} = x_1\underline{e}_1 + x_2\underline{e}_2 + x_3\underline{e}_3$

Thus any vector $\underline{A}$ is written as

$$\underline{A} = A_1\,\underline{e}_1 + A_2\,\underline{e}_2 + A_3\,\underline{e}_3 = \sum_{i=1}^{3} A_i\,\underline{e}_i\,.$$

$$\boxed{\text{The final summation will often be abbreviated to } \underline{A} = \sum_i A_i\,\underline{e}_i\,.}$$

Notes

(i) The numbers A_i are called the **(Cartesian) components** (or representation) of $\underline{A}$ with respect to the $\underline{e}_i$ basis.

(ii) We may write $\underline{A} = \sum_{i=1}^{3} A_i\,\underline{e}_i = \sum_{j=1}^{3} A_j\,\underline{e}_j = \sum_{\alpha=1}^{3} A_\alpha\,\underline{e}_\alpha$ where i, j and α are known as summation or 'dummy' indices.

(iii) The components are obtained by using orthonormality properties (#):

$$\underline{A}\cdot\underline{e}_1 = (A_1\underline{e}_1 + A_2\underline{e}_2 + A_3\underline{e}_3)\cdot\underline{e}_1 = A_1$$

$$\boxed{A_1 \text{ is the projection of } \underline{A} \text{ in the direction of } \underline{e}_1.}$$

Similarly for the components A_2 and A_3. So in general we may write

$$\underline{A}\cdot\underline{e}_i = A_i \quad \text{or sometimes} \quad (\underline{A})_i$$

where in this equation i is a 'free' index and may take values $i = 1, 2, 3$.

(iv) $\boxed{\text{In terms of these components, the scalar product takes on the form:} - \ \underline{A}\cdot\underline{B} = \sum_{i=1}^{3} A_i\,B_i\,.}$