3 3d Vectors (I)

Now we introduce formalism in the easier case of 3d, which will lead to powerful, compact manipulations of vector algebra and calculus in 3d as well as counterparts in relativity.

Define an *orthonormal* basis set: $\{\hat{\mathbf{e}}_1, \hat{\mathbf{e}}_2, \hat{\mathbf{e}}_3\} = \{\hat{\mathbf{e}}_i\}$, where

$$\hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} .$$

introducing the **Kronecker delta**, δ_{ij}, i.e. the unit matrix in 3d.

Properties of the Kronecker Delta
Properties of δ_{ij}:

(i) $\delta_{ij} = \delta_{ji}$ (symmetric) .

(ii) The trace of δ_{ij}, $\sum_{i=1}^{3} \delta_{ii} = \delta_{11} + \delta_{22} + \delta_{33} = 3$. (NB: in 2d the answer = 2.)

(iii) $\sum_{j=1}^{3} \delta_{ij} A_j = A_i$ for the components of a column vector, A_i e.g. for $i = 1$: $\delta_{11}A_1 + \delta_{12}A_2 + \delta_{13}A_3 = A_1$.

(iv) $\sum_{j=1}^{3} \delta_{ij}\delta_{jk} = \delta_{ik}$. this expresses the square of the unit matrix is a unit matrix.

Vector Components
Consider vector $\mathbf{A}$:

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

We may extract components, using property (iii):

$$\mathbf{A} \cdot \hat{\mathbf{e}}_j = \sum_{i=1}^{3} A_i \, \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = \sum_{i=1}^{3} A_i \, \delta_{ij} = A_j .$$

Express the scalar product in terms of components, again using property (iii):

$$\begin{aligned} \mathbf{A} \cdot \mathbf{B} &= \sum_{i=1}^{3} A_i \hat{\mathbf{e}}_i \cdot \sum_{j=1}^{3} B_j \hat{\mathbf{e}}_j \\ &= \sum_{i=1}^{3} \sum_{j=1}^{3} A_i B_j \, \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j \\ &= \sum_{i=1}^{3} \sum_{j=1}^{3} A_i B_j \, \delta_{ij} \\ &= \sum_{i=1}^{3} A_i B_i . \end{aligned}$$

3.1 The Einstein Summation Convention

The summation signs are cumbersome and almost always unnecessary – an expression may almost always be interpreted unambiguously without them. The **Einstein Summation Convention** (ESC) is defined as:

(E1) Any suffix occurring **once** in a term of an equation may be chosen to take 3 values: 1, 2, 3. This is called a '**free**' index or suffix.

(E2) Any suffix occurring **twice** is **summed** from 1 to 3.

(E3) The same suffix cannot occur **more than twice**.

i.e. $A_i B_i C_i$ is undefined.

(E4) Occasionally override the convention by explicitly stating "no sum" over a particular index. **Very rare**.

Examples (compare with previous expressions):

(i) $\mathbf{A} = A_i \hat{\mathbf{e}}_i$ (i.e. sum over i.)

(ii) $\mathbf{A} \cdot \hat{\mathbf{e}}_j = A_i \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = A_i \delta_{ij} = A_j$.

(iii)

$$\begin{aligned} \mathbf{A} \cdot \mathbf{B} &= A_i \hat{\mathbf{e}}_i \cdot B_j \hat{\mathbf{e}}_j \quad \text{(note use of \textbf{different} suffixes)} \\ &= A_i B_j \, \hat{\mathbf{e}}_i \cdot \hat{\mathbf{e}}_j = A_i B_j \, \delta_{ij} = A_i B_i \ . \end{aligned}$$

(iv) $(\mathbf{A} \cdot \mathbf{B})\mathbf{C} = A_i B_i C_j \hat{\mathbf{e}}_j$.

(v) Sometimes we will find it is useful to reverse the logic in some of the above, inserting a Kronecker delta, i.e.

$$A_i = \delta_{ij} A_j \quad \text{and} \quad A_i B_i = A_i \delta_{ij} B_j \ ,$$

whose counterparts will also be useful in a relativistic context.

Notes:

(i) If a suffix is summed (i.e. occurs twice) then the choice of suffix is free (as in expression with summation sign):

$$A_i B_i = A_j B_j \quad \text{as in} \quad \sum_{i=1}^{3} A_i B_i = \sum_{j=1}^{3} A_j B_j \ . \tag{3.1}$$

(subject to constraint of suffix not occurring more than twice). The suffix i or j is called a **dummy suffix** in this case.

(ii) Until we involve **derivatives**, order of terms is irrelevant. Labelling of suffixes ties summed pairs together, e.g.:

$$(\mathbf{A} \cdot \mathbf{B})\mathbf{C} = A_i B_i C_j \hat{\mathbf{e}}_j = C_j A_i B_i \hat{\mathbf{e}}_j \quad \text{etc.}$$

Matrix Multiplication

For a matrix M (we use bold sans serif font for a matrix – corresponding to the use of bold for a vector, but italic for components, as for vectors), M_{ij} means the component of M in the ith row and jth column.

We may apply ESC to matrix multiplication. For example a matrix multiplying a column vector:

$$\mathbf{M}\cdot\mathbf{v} = \begin{pmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} \ .$$

Thus:

$$(\mathbf{M}\cdot\mathbf{v})_i = \sum_{j=1}^{3} M_{ij} v_j = M_{ij} v_j \quad (i = 1, 2, 3) \ .$$

Example: A rotation matrix, $\mathbf{R}(\theta)$, acting on vector $\mathbf{v}$ to provide the components, v'_i, in the rotated basis set:

$$v'_i = R_{ij} v_j \ .$$

4 Non-orthogonal 3d Vectors

A readily visualised example related to the mathematical aspects of the Minkowski metric is normal, Euclidean, space described by a non-orthogonal basis set. This is useful in describing crystals, whose axes are often not orthogonal (see Y2 QAS and Y3 Condensed Matter).

4.1 Non-orthogonal Basis

Consider a basis set $\{\mathbf{e}_i\}$, assumed to be linearly independent (i.e. not all lying in same plane) with

$$\mathbf{e}_i \cdot \mathbf{e}_j = g_{ij} \neq \delta_{ij} \ ,$$

where g_{ij} is the *metric tensor*, for reasons to be seen presently.

We may expand vectors in terms of this set to define components (the reason for the index being a superscript will emerge):

$$\mathbf{A} = A^i \mathbf{e}_i \ .$$

But:

$$\mathbf{e}_j \cdot \mathbf{A} = A^i \mathbf{e}_j \cdot \mathbf{e}_i = A^i g_{ji} \neq A^j \ ,$$

as $\delta_{ij} \neq g_{ij}$.

However we may define another set of vectors which can provide the components. These are the *reciprocal* (or *dual*) vectors, $\mathbf{e}^{*i}$ (the * is a convention – no relation to complex conjugation), obeying

$$\mathbf{e}^{*i} \cdot \mathbf{e}_j = \delta^i{}_j \ , \tag{4.1}$$

Such a set may be constructed in 3d as:

$$\mathbf{e}^{*1} = \frac{1}{\Omega}\mathbf{e}_2 \times \mathbf{e}_3 \quad \mathbf{e}^{*2} = \frac{1}{\Omega}\mathbf{e}_3 \times \mathbf{e}_1 \quad \mathbf{e}^{*3} = \frac{1}{\Omega}\mathbf{e}_1 \times \mathbf{e}_2 \ ,$$

where

$$\Omega = \mathbf{e}_1 \cdot (\mathbf{e}_2 \times \mathbf{e}_3) \ .$$

the geometric significance of Ω is the volume of the parallelepiped formed with edges $\mathbf{e}_j$, i.e. the volume of the unit cell in a crystal (an extra factor of 2π is often included there for reasons to do with Fourier transforms and diffraction). It is easy to check that this choice of $\{\mathbf{e}^{*i}\}$ satisfies Eq. (4.1), e.g.

$$\mathbf{e}^{*2} \cdot \mathbf{e}_1 = \frac{1}{\Omega}(\mathbf{e}_3 \times \mathbf{e}_1) \cdot \mathbf{e}_1 = 0 \ , \quad \mathbf{e}^{*1} \cdot \mathbf{e}_1 = \frac{1}{\Omega}(\mathbf{e}_2 \times \mathbf{e}_3) \cdot \mathbf{e}_1 = \frac{\Omega}{\Omega} = 1 \ .$$

We may use this to get A^i:

$$\mathbf{e}^{*j} \cdot \mathbf{A} = \mathbf{e}^{*j} \cdot A^i \mathbf{e}_i = \delta^j{}_i A^i = A^j \ .$$

(i) The set $\{\mathbf{e}_i\}$ are associated with **directions**; whereas $\{\mathbf{e}^{*i}\}$ are naturally associated with **planes** (as $\mathbf{e} \times \mathbf{e}$ is a **normal** to a plane (or vice versa: $\mathbf{e} \propto \mathbf{e}^* \times \mathbf{e}^*$, although this is tedious to show until later in module).

(ii) We do not need the $\mathbf{e} \times \mathbf{e}$ construction – can use (g^{-1}) to construct $\mathbf{e}^*$, albeit one needs to invert the 3d matrix. The above treatment is faster.

(iii) $\{\mathbf{e}^*\}$ are used in condensed matter physics – the **reciprocal lattice** – to label planes from which X-ray diffraction (e.g.) occurs, hence connection to Fourier transformation.

4.2 Covariant and Contravariant Components

But we may define another set of components for **A** by: (Note which set indicated by position of index)

$$\mathbf{A} = A_i \mathbf{e}^{*i} = A^i \mathbf{e}_i \tag{4.2}$$

reflecting two descriptions of the same intrinsic vector, **A**, with:

$$\mathbf{e}_j \cdot \mathbf{A} = A_i \mathbf{e}_j \cdot \mathbf{e}^{*i} = A_j \ .$$

To distinguish the components with indices up and down, they are called:

$$A_i \ : \ \textbf{covariant} \text{ components} \quad A^i \ : \ \textbf{contravariant} \text{ components} \ .$$

They are related via the metric tensor, using the two expressions for **A**, Eq. (4.2):

$$\begin{aligned} \mathbf{e}_i \cdot \mathbf{A} &= \mathbf{e}_i \cdot A_j \mathbf{e}^{*j} = A_i \\ &= \mathbf{e}_i \cdot A^j \mathbf{e}_j = g_{ij} A^j \qquad (4.3) \\ \Rightarrow \quad A_i &= g_{ij} A^j \ . \qquad (4.4) \end{aligned}$$

We may take the scalar product with the reciprocal lattice basis to deduce the form of the inverse metric tensor:

$$\begin{aligned} \mathbf{e}^{*i} \cdot \mathbf{A} &= \mathbf{e}^{*i} \cdot A^i \mathbf{e}_j = A^i \\ \text{(Defining } G^{ij}\text{)} \quad &= \mathbf{e}^{*i} \cdot A_j \mathbf{e}^{*j} = G^{ij} A_j \qquad (4.5) \\ \Rightarrow \quad A^i &= G^{ij} A_j \qquad (4.6) \\ \Rightarrow \quad g_{ki} A^i &= g_{ki} G^{ij} A_j \qquad (4.7) \\ \Rightarrow \quad A_k &= g_{ki} G^{ij} A_j \qquad (4.8) \\ \Rightarrow \quad g_{ki} G^{ij} &= \delta_k{}^j \qquad (4.9) \\ \Rightarrow \quad G^{ij} &= (g^{-1})^{ij} = g^{ij} \ , \qquad (4.10) \end{aligned}$$

where we have used the notation g^{ij} for brevity.

This also implies a relation between the two bases sets similar to that between the covariant and contravariant components:

$$\mathbf{A} = \begin{cases} A^i \mathbf{e}_i & = A_j g^{ji} \mathbf{e}_i = A_j \mathbf{e}^{*j} \\ A_j \mathbf{e}^{*j} & = A^i g_{ij} \mathbf{e}^{*j} \end{cases} \ .$$

i.e. we may interconvert the bases:

$$g^{ji} \mathbf{e}_i = \mathbf{e}^{*j} \quad \text{and} \quad g_{ji} \mathbf{e}^{*i} = \mathbf{e}_j \ .$$

Finally notice that the definition of the unit matrix to have one contravariant and one covariant index is consistent with

$$\delta_i{}^j A_j = A_i \ .$$

4.3 Scalar Products

$$
\begin{aligned}
\mathbf{A}\cdot\mathbf{B} &= A^i\mathbf{e}_i\cdot B^j\mathbf{e}_j \\
&= A^iB^j\,\mathbf{e}_i\cdot\mathbf{e}_j \\
&= A^iB^jg_{ij} \\
&= A_jB^j \quad \text{(absorbing } g \text{ into } A_i) \\
&= A^iB_i \quad \text{(absorbing } g \text{ into } B_i)
\end{aligned}
\tag{4.11}
$$

So the distinction between covariant and contravariant components may be regarded as a convention to absorb g_{ij}. If we retained g's everywhere we could work with only one or the other.

Scalar products have one set of covariant components and one set of contravariant.

We may use the scalar product to motivate the term "metric tensor" for g_{ij}. Use the modulus squared of the position vector:

$$\mathbf{r}\cdot\mathbf{r} = r^i\mathbf{e}_i\cdot r^j\mathbf{e}_j = r^ig_{ij}r^j \tag{4.12}$$

i.e. distance^2 from origin.