What *Can* the Answer be?

4. Reciprocal Basis in *n* Dimensions and other Ramifications

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The previous articles of this series were:

1. Elementary vector analysis, August 1996.
2. Reciprocal basis and dual vectors, October 1996.
3. Reciprocal basis in two dimensions and other nice things, May 1997.

This final article in the series first addresses the problem of calculating reciprocal vectors in *n*-dimensions. The deeper definition of vectors (and other quantities such as tensors) in terms of the transformation properties under rotations is brought out. Some examples which generalise this notion to other kinds of transformations are given.

In this final part of this series we begin (as promised in part 3) with the problem of finding the reciprocal basis in n dimensions. With the help of the Levi-Civita symbol $\varepsilon_{ijkl\ldots}$ and the summation convention introduced in part 3, we are ready, at last, to find the basis (**A, B, C, D**, ...) reciprocal to a given basis set of vectors (**a, b, c, d**, ...) in an arbitrary number (n) of dimensions. It is most instructive to write down the answer in 2D and 3D (equations (7) and (1) respectively of part 3) in the notation just introduced. To avoid any confusion, let us use the symbols $p, q, r, s, \ldots$ for the indices occurring in the 'volume' in the denominator. In 2D,

$$A_i = V_2^{-1}\, \varepsilon_{ij}\, b_j, \quad B_j = V_2^{-1} \varepsilon_{ij}\, a_i \tag{1}$$

where $V_2 = \varepsilon_{pq}\, a_p\, b_q$. In 3D,

$$A_i = V_3^{-1}\, \varepsilon_{ijk}\, b_j c_k, \quad B_j = V_3^{-1} \varepsilon_{ijk}\, a_i\, c_k, \quad C_k = V_3^{-1} \varepsilon_{ijk}\, a_i\, b_j \tag{2}$$

where $V_3 = \varepsilon_{pqr}\, a_p\, b_q\, c_r$. It is now easy to guess that the answer in any dimension n is simply — and what else can it be! —

$$A_i = V_n^{-1}\, \varepsilon_{ijkl\ldots}\, b_j\, c_k\, d_l \ldots, \quad B_j = V_n^{-1}\, \varepsilon_{ijkl\ldots}\, a_i\, c_k\, d_l \ldots,$$
$$C_k = V_n^{-1}\, \varepsilon_{ijkl\ldots}\, a_i\, b_j\, d_l \ldots, \ldots \tag{3}$$

and so on down the line for each of the n vectors **A, B**, ... (for

Crystal Symmetry in n Dimensions

We mentioned in part 2 that the reciprocal basis is very useful, among other applications, in crystallography. The latter involves a fascinating branch of mathematics, the theory of discrete groups. The total number of 'crystallographic groups' (related to the kinds of crystalline symmetry possible) is 230 in 3D. The corresponding quantity in higher dimensions is of interest in group theory and certain applications of mathematical physics. It is 4783 in 4D, and increases very rapidly as n increases!

A_i, omit a_i on the right; for B_j, omit b_j; etc.) Here $V_n = \varepsilon_{pqrs\ldots} a_p\, b_q\, c_r\, d_s \ldots$ It is not difficult to verify that (3) is indeed the general solution sought. It satisfies the requirements $\mathbf{A}\cdot\mathbf{a}=\mathbf{B}\cdot\mathbf{b} \ldots = 1$, all the other scalar products such as $\mathbf{A}\cdot\mathbf{b}$, $\mathbf{A}\cdot\mathbf{c}$, …, $\mathbf{B}\cdot\mathbf{a}$, $\mathbf{B}\cdot\mathbf{c}$, … etc being equal to zero. You are now ready to begin the study of crystallography in n dimensions (see *Box*)!

The Gram Determinant

We noted before (7) in part 3 that in 2D, $(a_1b_2 - a_2b_1)^2 = a^2b^2 - (\mathbf{a}\cdot\mathbf{b})^2$. But this is the same as saying that

$$\begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix}^2 = \begin{vmatrix} a_1 & a_2 \\ b_1 & b_2 \end{vmatrix} \begin{vmatrix} a_1 & b_1 \\ a_2 & b_2 \end{vmatrix} = \begin{vmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} \end{vmatrix} \qquad (4)$$

Note how we have written the square on the LHS as the product of the determinant and its transpose. It is immediately clear that a similar relationship is valid in n dimensions as well! Thus

$$\begin{vmatrix} a_1 & a_2 & & a_n \\ b_1 & b_2 & & b_n \\ & & & \\ & & & \end{vmatrix} \begin{vmatrix} a_1 & b_2 & & \\ a_2 & b_2 & & \\ & \cdot & & \\ a_n & b_n & & \end{vmatrix} =$$

$$\begin{vmatrix} \mathbf{a}\cdot\mathbf{a} & \mathbf{a}\cdot\mathbf{b} & & \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & & \\ & & & \\ & & & \cdot \end{vmatrix} \qquad (5)$$

The *Cauchy-Schwarz inequality* is useful in establishing the Heisenberg uncertainty relation between two observables in quantum mechanics.

The determinant on the RHS, formed by taking the scalar products of the n vectors (**a**, **b**, **c**, ...) among themselves, is called the *Gram determinant* of that set of vectors. Denoting this by G_n, we have now found that $G_n = V_n^2$, V_n being the 'volume' of the (hyper-)parallelepiped formed by the n vectors **a**, **b**, ... As G_n is the square of a real number,

$$G_n \geq 0. \tag{6}$$

Moreover, G_n is *equal* to zero if and only if $V_n = 0$ — that is, if the hyperparallelepiped collapses to a lower dimensional object – in other words, when the vectors **a**, **b**, ... are not linearly independent of each other. For instance, if the vector **a** is in the plane formed by **b** and **c**, the volume **a** (**b**×**c**) becomes zero because the parallelepiped collapses into the plane of **b** and **c**.

Now, for any two vectors **a** and **b**, we know that

$$(\mathbf{a}\cdot\mathbf{a})(\mathbf{b}\cdot\mathbf{b}) - (\mathbf{a}\cdot\mathbf{b})^2 = a^2 b^2 (1-\cos^2\theta) \geq 0 \tag{7}$$

(where θ is the angle between **a** and **b**), because $|\cos\theta| \leq 1$ for any angle θ. The equality sign in (7) occurs if and only if **a** and **b** are collinear. When extended to any two vectors in a general 'linear vector space', (7) is known as the *Cauchy-Schwarz inequality*. This inequality is useful, for instance, in establishing the Heisenberg uncertainty relation between two observables in quantum mechanics. The relation (6) is thus a *generalization of the Cauchy-Schwarz inequality* to an arbitrary number (n) of vectors! The way we have derived it here brings out its geometrical interpretation.

What is a Vector?

Throughout this series of articles, I have used the terms 'scalar' and 'vector' without formal definition, in the 'common' or 'usual' sense familiar to us from high school: a scalar only has a numerical value, while a vector 'has both magnitude and direction'. This is not a very satisfactory definition even at high school! Direction with respect to what set of axes? If the answer is, "Some given, fixed set of axes," then why is it that this set is never specified right at the beginning of each book dealing with vectors? And how is it that the same equation, say $\mathbf{F} = m\mathbf{a}$, makes sense whether it is written down in Mumbai or Mogadishu, although it is unlikely that the orientation of the coordinate frames chosen in the two cases will be the same?

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The correct way to define scalars, vectors, tensors, etc. is via their *transformation properties under changes of coordinate frames*. Once this is done, any equation or relationship involving only those quantities whose transformation properties are specified is guaranteed to remain the same in form *(form-invariant)* for two users who choose different coordinate frames. (That is why books dealing with vector equations do not bother to specify any special set of axes right in the beginning !) Even this definition is not adequate. What *sort(s)* of coordinate transformations are we talking about?

The usual (high school!) scalars and vectors that we have considered are actually defined with respect to the set of *rotations* of the coordinate axes. The value of a scalar so defined(e.g., the distance of a point from the origin of coordinates) does not change at all under such a rotation. A vector comprises a set of numbers (components) that do change under a rotation of the coordinate axes - but they do so *in precisely the same manner as the coordinates of any point themselves change*. Tensors of higher rank $(2, 3, \ldots)$ are defined in an analogous manner; they have (slightly) more involved transformation properties. In technical terms : the scalars and vectors I have used so far (except for the general cases mentioned briefly in part 2 of the series) are 'scalars and vectors under the group of proper rotations in n-dimensional Euclidean space'. Now that we have become quite familiar with these quantities, the statement just made should be much easier to digest. As my whole aim has been to provide a simple, *heuristic* approach to some aspects of vector analysis, I have preferred to

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mention these technical subtleties at the end, rather than open the discussion with them. And I have glossed over many mathematical technicalities wherever these have not been directly relevant to the point being made. For instance, I stated earlier that the cross-product of two vectors is itself a vector in (Euclidean) 3D space. A mathematician would regard this as a loose statement, and accuse me (rightly) of confusing 2-forms in $\mathbf{R}^3$ with vector fields in $\mathbf{R}^3$! However, this subtlety can be ignored for our present purposes.

Extensions and Generalizations

The elementary concepts I have tried to describe in this series have wide-ranging extensions and generalizations, with remarkably diverse applications. I can only mention some of these here.

The *form invariance* of physical laws under changes from one coordinate frame to another is a cornerstone of all modern physics. In a vastly generalized and extended form it is, in fact, *the number one guiding principle* in all modern physics! (Examples include the general theory of relativity and quantum field theories describing the interactions of elementary particles, but we shall not go into this here.) This means that the laws of physics *must* be specified in terms of quantities whose transformation properties are prescribed — e.g., scalars, vectors, tensors, etc. — *quantities which carry their own dictionaries*, so to speak, so that different users related to each other by these transformations can simultaneously and unambiguously use the same laws. This is why we write the laws of Newtonian mechanics in terms of vectors, and not because 'each vector equation stands for three equations (one for each component), thus saving space in books'!

We can see immediately that it might be necessary and possible to have scalars, vectors,... (or their equivalents) under *other* sets of transformations than just rotations of the coordinate axes — and in spaces that are more complicated than the Euclidean spaces we have used. For instance, we believe that in regions where space-time is essentially 'flat' (*i.e.*, in the absence of very intense gravitational fields), the laws of physics are form-invariant under Lorentz transformations (which *include* rotations of the spatial coordinate axes), rather than just rotations of the axes. Moreover, the space-time geometry is not strictly Euclidean. We must therefore deal with scalars, vectors and other such objects defined with respect to the set (group) of Lorentz transformations in a non-Euclidean 4D space-time 'manifold'. In the presence of gravitational fields, this manifold itself becomes 'curved'. The set of transformations under which physical laws are required to remain form-invariant is now even more general. The distinction between vectors and their corresponding dual vectors is now non-trivial, and not just a matter of using oblique axes in a flat (Euclidean) space. To help keep this in mind, the indices are written as *superscripts* for vectors and *subscripts* for their dual counterparts. In tensor analysis, the traditional names for these quantities are *contravariant vectors* and *covariant vectors*. In mathematics, they are simply *vectors* and *co-vectors*, which is much better terminology.

In classical dynamics too, vectors and co-vectors play a crucial role. In the Lagrangian formalism, we describe a system in terms of a set of generalized coordinates and the corresponding generalized velocities. In the Hamiltonian formalism, the latter are replaced by generalized momenta. Roughly speaking, the shift from velocities to momenta corresponds to going from a vector space to its dual vector space. Pursuing this further, we arrive at the modern mathematical description of Hamiltonian dynamics, using differential geometry and topology. That is another story!

In quantum mechanics, as I have already mentioned in part 2, we describe a system by a 'state vector' or ket vector $|\psi\rangle$ in a so-called *'Hilbert space'*. (The corresponding dual is the bra vector $\langle\psi|$.) It turns out, however, that the multiplication of $|\psi\rangle$ by any complex number of the form $e^{i\theta}$ does not lead to a new state, so that $|\psi\rangle$ and $e^{i\theta}|\psi\rangle$ describe the same state. In terms of the corresponding bra vectors, this means that $\langle\psi|$ and $|\psi\rangle\ e^{-i\theta}$ are equivalent. Consequently, the appropriate vector space in quantum mechanics is a *projective* Hilbert space rather than the original Hilbert space itself, and the descriptor of a state is the object $|\psi\rangle\langle\psi|$ rather than the ket $|\psi\rangle$ or bra $\langle\psi|$ by itself. (In this combination, the factors $e^{i\theta}$ and $e^{-i\theta}$ cancel out each other.) By now, we can recognise an object like $|\psi\rangle\langle\psi|$; like **aA**, it is an *operator*. Its formal name in quantum mechanics is *density operator*. The most general descriptor of the state of a quantum mechanical system is its density operator ρ. The evolution of the system with time is governed by the so-called Liouville equation for $\partial\rho/\partial t$. This too, is another story !

These remarks are meant merely to give an idea of the generality of the concept of the reciprocal basis and dual vectors, and to whet your appetite.

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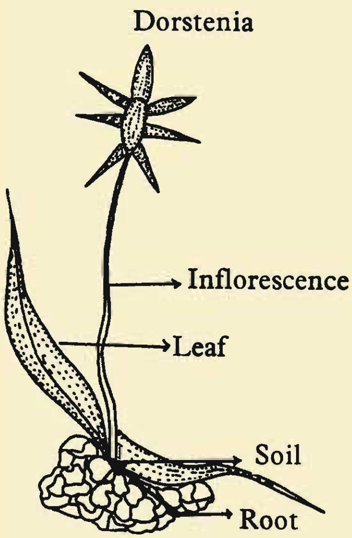
A Stemless Plant



Dorstenia barnimiana is a minute plant of the grasslands of Kenya. Dorstenia is a herbaceous genus often stemless in nature. This peculiar plant has leaves arising on long stalks directly from a perennial rhizome. It has an inflorescence consisting of a flattened receptacale surrounded by a tendril like projection.

Most species are found in tropical America and Africa, some in the middle East and India. It belong to the family Moraceae. It is used in India as a medicinal plant. The root of *D. contrajerrva* is a source of medicine. It is used as an antidote to snake-bite and as a stimulant and tonic in case of nervous-disability.

Useful plants of India. CSIR Publication. New Delhi, 1988.
The Wealth of India. CSIR Publication. New Delhi, 1988.

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