

# Linear Algebra

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## Abstract

This document is an instruction manual for the linear algebra portion of the course on Mathematical Methods.

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## 1 Introduction

A vector space is a place where you have things called vectors, and what you can do with them is to add them and stretch them. You also need to tell when some of them are equal. In order to tell who got added to whom, vectors are usually drawn as lines with an arrow at the tip, according to which the rule is: start at a tail, go to the head and if there is a vector to be added, put its tail there and continue. Of course, a lot of things are implicit in such an informal definition, such as that vectors can be moved around without essentially changing them, that there ought to be a single place called an origin where vectors get started off, and if they are just laying around and happen to cross, that doesn't count.

Addition is commutative, in the sense that you reach the same destination whichever order is followed, something called a parallelogram law. It is also assumed that stretching is related to addition, in the sense that  $2X = X + X$ , and so on for all the constructions related to integers, rational numbers, real factors and even going so far as complex numbers.

It is one thing to work up an axiomatic theory of something, like groups, or topologies, or vector spaces, or whatever. It is quite another to discover that all of those systems and indeed almost every theory that one can imagine, have very similar structural features, for which there is an applicable metatheory, sometimes called Universal Algebra. That higher level theory is based on the ideas of equivalence and order relations, classifying the functions mapping one set to another, and the generation of new structures via the intermediary of cartesian products. To appreciate this view of vector spaces, consider:

## 2 Axiomatic Viewpoint

### 2.1 Vector space axioms

A Vector Space is formed from two sets, the vectors and the scalars, which are their coefficients. Vectors form an abelian group with respect to addition, which is to say that sums are closed, associative, commutative, and that there are negatives and a zero.

The scalars comprise a field (supposedly commutative to avoid undue complications, and typically are either the real numbers or, when occasion demands, the complex numbers). That means, among other things, that 1 is a scalar, that scalars have reciprocals, that 0 is also a scalar, and that it is hard to tell the negative vectors from positive vectors with a negative coefficient.

The distributive laws, right and left, link vector addition with scalar multiplication. Even though there is a right distributive law, coefficients are always written on the left.

### 2.2 Order relations

Any subset of the vectors in a vector space, keeping the same coefficients, which is a vector space all by itself, is called a subspace. Of course, the coefficients could be changed too - to pass from a complex space to a real space, for instance - but that is a specialty which not usually considered to be a part of an introduction to vector space theory. Save closure, finding zero, and locating negatives, none of the other axioms depends on whether a subset is being considered or not. Checking all three requirements at once can be accomplished by considering closure under differences.

Vector subspaces are familiar enough: in three dimensions, just think of lines and planes. The important point is that in whatever vector space, the subspaces are ordered by inclusion. Moreover, there is a smallest subspace, containing just zero itself (the origin), which is contained in every other subspace. Apparently trivial, but still important for consistency, the whole space is not just a subspace, but it is the largest subspace, within which every other is contained.

Comparison between pairs of subspaces can be attempted, yet pairs are rarely arranged so that one is contained within the other. Instead, there is a largest subspace common to both, as well as a smallest subspace containing the two. The first of these is just the setwise intersection of the two, but the second requires some construction: it consists of all linear combinations of vectors in the two subsets; not just their union. Just keep on thinking of lines and planes.

It isn't just subspaces which have upper and lower bounds; mere subsets can be included in the hierarchy by looking for the smallest vector space containing a given subset, or the largest (if any) subspace which it contains. This is an idea which gives rise to bases: Start with any non-zero vector, and find the smallest vector space containing it. That will be the set of all its scalar multiples, or in short, a line passing through the vector (and evidently also passing through the origin) .

Supposing that there are some vectors still left in the full space, choose one of them, and repeat the process. But now we have to account for the first vector, so it is a good idea to find the smallest subspace containing both vectors, which is just the set of sums taken from the two subspaces. We might as well call that the sum of the two subspaces. Of course, there is some verifying involved, to ensure that everything is well done and consistent.

Maybe there are still vectors not accounted for; so start all over again, finding the smallest subspace containing all three vectors, and so on as long as the entire space hasn't been generated. If the process terminates, the chosen vectors are said to form a basis, whose dimension is the number of independent vectors which it contains (linear dependence means that one vector is a linear combination of others; equivalently, summing multiples of all of them, not all coefficients

being zero, still gives zero). The interesting thing is that the dimension always ends up the same, whatever sequence of vectors is chosen for the construction. It is not hard to prove; just replace the first basis by the second, one vector at a time, while substituting all the previous results in each new expression.

If the process of exhausting the supply of vectors never terminates, the space is not finite-dimensional, turning the search for bases into a much more intricate activity.

### 2.3 Functions

Pairing up elements in the style  $(x, f(x))$  so that there is never more than one  $f(x)$  for a given  $x$ , is what defines a function  $f$ . When the sets from which  $x$  and  $f(x)$  are chosen have structure, functions preserving the structure are usually set apart from more generic functions, and often have special properties themselves. For vector spaces, requiring linearity,

$$f(ax + by) = af(x) + bf(y),$$

does the job. However, it is easy to treat functions as though they were vectors, by saying

$$\begin{aligned} (af)(x) &= af(x), \\ (f + g)(x) &= f(x) + g(x), \end{aligned}$$

so that without further ado, we can regard all of the linear functions between a fixed pair of vector spaces  $U$  and  $V$  as forming another vector space. To give it a name, call it  $\text{Linear}(U,V)$ . From such humble beginnings, all sorts of different combinations of functions and vector spaces can be constructed.

Some of the possibilities are shown in the following diagram, Figure 1.

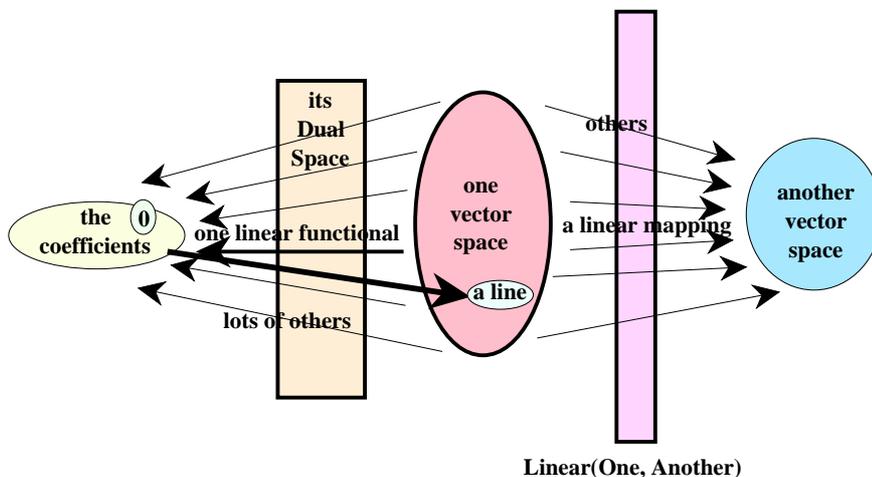


Figure 1: A schematic representation of different linear mappings.

Scalar valued functions of vectors are some of the easiest functions to define, which is appropriate considering their fundamental importance. The starting point is to recall the role of a basis – every

vector  $x$  is some linear combination of basis vectors  $\{v_i\}$ :

$$x = \sum a_i x_i,$$

whence the value of the linear function depends entirely on the values which it assigns to the basis:

$$f(x) = \sum a_i f(x_i),$$

It is a great temptation to make up a whole collection of new functions,  $\{g_i\}$ , each one charged with assigning its own basis vector the value 1, all the rest 0:

$$g_i(x_j) = \delta(i, j).$$

(here  $\delta$  would be Kronecker's delta). So doing, the function  $f$  would end up being represented by

$$f(x) = \sum f(x_i) g_i(x),$$

which in turn would make the  $g$ 's into a basis for scalar valued functions of vectors. This new space, of the same dimension as the old, is called its dual space. It is noteworthy that the dual of a dual reverts back to the original space, thanks to the fact that arguments can map their functions into values, all in a completely linear fashion.

Just because a space and its dual have the same dimension, they have to be practically identical. They both have bases, but it remains to be seen just how both bases could be drawn in the same picture the way vectors are usually visualized. First, though, it is convenient to discuss functions of several vectors, and then to make up biorthogonal bases.

### 3 Equivalence Relations

Presumably there are linear mappings between any pair of vector spaces; certainly the zero map always exists. If the spaces have different dimensions some discrepancies are bound to occur, because not even the basis vectors can be matched up one-to-one, much less all the rest of the vectors. One use of equivalence relations is to clarify the relationship between two spaces connected by a function, because the sets where the function takes a constant value are equivalence classes. General properties of equivalence relations are thereby transferred into general relationships among functions.

To begin with, all the counterimages of a linear mapping depend on the counterimage of zero. Suppose that  $f(r) = x$  and  $f(s) = x$  as well. Then

$$\begin{aligned} f(r - s) &= f(r) - f(s) \\ &= x - x \\ &= 0, \end{aligned}$$

placing the difference of any pair of elements with a common image amongst the elements which map into zero. That is enough to make the counterimage of zero, which is usually called the kernel of the mapping, into a vector space, and to make all the other equivalence classes differ from it by translation. As an example, think of orthogonal projection mapping space onto the x-y

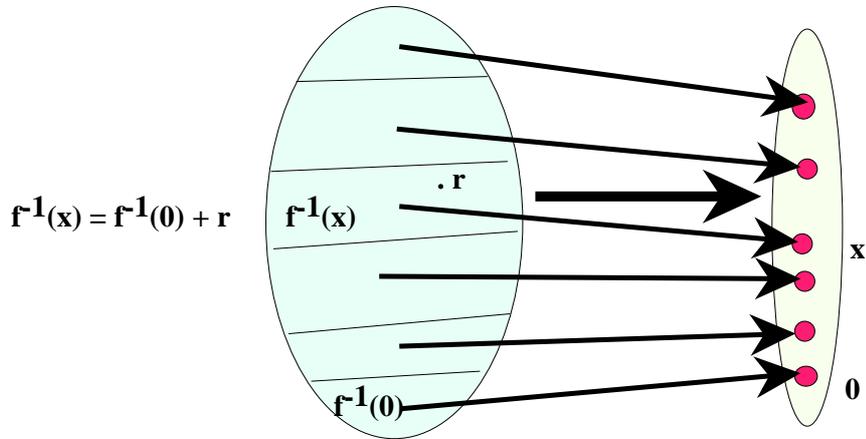


Figure 2: Equivalence relations is a linear mapping

plane. The z-axis is the kernel of the mapping whose translates are the vertical lines containing the counterprojections of any other point.

In passing, note that both the images and the counterimages of vector spaces are vector spaces, according to a linear mapping. As far as the vector spaces themselves are concerned, that is nothing but the definition of linear mapping. But it automatically carries over to all the subspaces as well, which is the useful part of the remark. Besides which, the multiplicity of counterimages is uniform everywhere, giving vector space theory an elegance which is not shared by all mathematical structures.

The functions in the dual space, unless they are zero, have to map onto a one-dimensional space because that is all there is. Each basis function maps its counterpart's multiples to the full coefficient space, leaving the space spanned by all the remaining basis vectors for its kernel. Altogether, the dual basis allocates each vector a line and a hyperplane omitting that line (but only because the basis was there already).

### 3.1 Cartesian products

To work with several things at once, it is easy enough just to make a list of them. This is the idea behind a cartesian product, although the name was originally associated with a list of distances of points from coordinate axes, collected for the purpose of doing geometry with algebra. It is one of the most straightforward ways of making something complicated by joining up a lot of simpler items.

Listing out the vectors of a basis is not quite the way cartesian products are usually found in a vector space, because the most familiar list enumerates the coefficients of the basis vectors instead. But the list could contain anything else, just so long as the nature of its contents is made clear.

A natural way to create operations on a list is to perform an operation relevant to its elements on every element simultaneously. For example, when it is a list of vectors, then sums and scalar

multiplication could be defined by:

$$\begin{aligned} a(x_1, x_2, \dots, x_n) &= (ax_1, ax_2, \dots, ax_n), \\ (x_1, x_2, \dots, x_n) + (y_1, y_2, \dots, y_n) &= (x_1 + y_1, x_2 + y_2, \dots, x_n + y_n). \end{aligned}$$

With such an understanding, a cartesian product of vector spaces is a new vector space. If the “vectors” in the product are taken from the one dimensional space of scalars, the result is still a vector space; in fact it is the canonical form of a vector space, with basis vectors

$$e_i = (0, 0, \dots, 1, \dots, 0),$$

and representation

$$x = \sum x_i e_i$$

and functions from the dual basis

$$g_j(x) = x_j$$

which simply read off the  $j^{\text{th}}$  scalar in the cartesian product list. Functions meeting this description are commonly called projections, serving to recover the original factors from which the cartesian product was constructed.

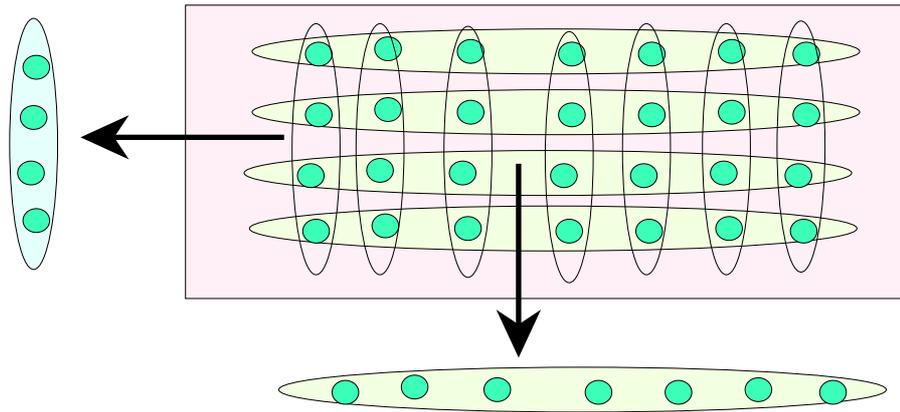


Figure 3: The Cartesian Product of Vector Spaces

### 3.2 Functions of cartesian products

Before cartesian products were mentioned, vector spaces already had a collection of attributes, such as bases, dual spaces, and the dual basis. Since cartesian products of vector spaces are vector spaces in their own right, curiosity would imply examine relationships between the product space and the factors. For example, the cartesian product of bases could be a basis for the cartesian product, but is it true that any basis for a cartesian product can be factored into a product of bases?

Just as there are cartesian products of sets, there should be cartesian products of functions. Directly interpreting such an idea, any product function applied to a cartesian product of arguments ought to produce a cartesian product of values.

However, there are less ambitious functions for product spaces than either of these two possibilities. Consider a scalar valued function of a pair of vectors which is linear separately for each term, rather than being required to be jointly linear:

$$\begin{aligned} f(ax + by, z) &= af(x, z) + bf(y, z) \\ f(x, ay + bz) &= af(x, y) + bf(x, z). \end{aligned}$$

The main difference is that we want either  $af(x, y) = f(ax, y)$  or  $af(x, y) = f(x, ay)$ , but not at all  $af(x, y) = f(ax, ay)$ , which it would have to be if  $(x, y)$  were a vector on which  $f$  were operating linearly. According to the modest definition, we would have  $f(ax, ay) = a^2f(x, y)$ .

### 3.3 Symmetric bilinear functions

Another traditional restriction concerns the symmetry of  $f$  with respect to exchanging its arguments. If the arguments matter but their order does not, it could be said that

$$f(x, y) = f(y, x).$$

In such a case only one of the linearity requirements would need to be given explicitly. Of course, such a switch supposes the that the same vector space is used for each argument.

Another possibility would be that changing the order would change the sign of the result. This assumption eventually leads to an axiomatic theory of determinants. But to stay with the symmetric alternative, the next step is to refer the function to a basis (for which a two dimensional space is sufficiently illustrative):

$$f(ae_1 + be_2, ce_1 + de_2) = acf(e_1, e_1) + adf(e_1, e_2) + bcf(e_2, e_1) + bdf(e_2, e_2).$$

This is nicely written as a matrix equation,

$$\begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} f(e_1, e_1) & f(e_1, e_2) \\ f(e_2, e_1) & f(e_2, e_2) \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}$$

showing how hard it is for linear algebra to escape from matrix notation. The central matrix is determined exclusively by the basis, and is symmetric because  $f$  was. Conversely, choosing the values of  $f$  just for the basis fixes its values everywhere else, and so uniquely defines the function. A plausible choice is the Kronecker delta, making  $f$  (the square of) Euclidean distance. Any other choice would be a metric matrix for some geometry, but this one gives the Euclidean metric. Interestingly, an antisymmetric matrix (from an antisymmetric  $f$ ) would imply a symplectic geometry with a symplectic metric.

What would be reasonable requirements for  $f$ , yet not depending on a basis? To always be positive for repeated arguments, and never zero except for a pair of zero vectors, seems to be adequate. As a consequence,

$$f(x - y, x - y) = f(x, x) + f(y, y) - 2f(x, y)$$

would have to be nonnegative. Dividing by  $\sqrt{f(x,x)f(y,y)}$ , which would not be zero if neither  $x$  nor  $y$  were, we need conditions for an expression of the form  $r + 1/r - s$  to be positive.

Note that  $r + 1/r$  has a minimum value of 2 at  $r = 1$ , for positive  $r$ , and a maximum at  $-1$ , for negative  $r$ . Thus a positive  $s$  could never exceed 2, nor a negative  $s$  ever fall below  $-2$ , which incidentally translates into a form of diagonal dominance for the metric matrix (if there were one).

It might also inspire the trigonometrically minded to make up an angle by writing

$$f(x, y) = \sqrt{f(x, x)}\sqrt{f(y, y)} \cos(\theta).$$

To pursue the idea of distance further, note that three of the four quantities in the expression for  $f(x - y, x - y)$  are positive, so that if it were necessary to add some positive quantity to the right hand side to make them all positive, an inequality would result:

$$|f(x - y, x - y)| \leq |f(x, x)| + |f(y, y)| + 2|f(x, y)|.$$

This inequality would take a more familiar form if the distance  $d(x, y)$  were defined as the positive root of  $d^2(x, y) = f(x - y, x - y)$ ,  $x - y$  were substituted for  $x$  in the inequality, and likewise  $y - z$  for  $y$ . The result,

$$d(x, z) \leq d(x, y) + d(y, z)$$

is the triangle inequality required to complete the axioms for a distance, which altogether read:

- distances are positive, zero only for coincident points,
- symmetric,
- and obey the triangle inequality.

This all sounds like deriving geometry from vector algebra, rather than the other way around.

Why do we go to so much trouble to make up this bilinear functional, especially since we already have the dual space and linear functionals to work with? For one thing, there are the connections with geometry - distances, projections and the cosines of angles. For another, it is less dependent on a basis, which is crucial for vector spaces which may not have bases, such as when their dimension is no longer finite, and which abound in quantum mechanics and its applications.

Here is an illustration of a basis  $i, j$  and its reciprocal basis,  $ii, jj$  which would have been a dual basis except that inner products work on two copies of the same vector space, rather than on the (space, dual) pair.

Note the difference between contravariant components which are the coefficients used in linear combinations (parallel projections on the dual basis), and covariant components, which result from perpendicular projection on the basis itself.

### 3.4 Antisymmetric multilinear functions

The contrasting property to symmetry is antisymmetry which, for a function of two interchangeable variables, would read:

$$f(x, y) = -f(y, x).$$

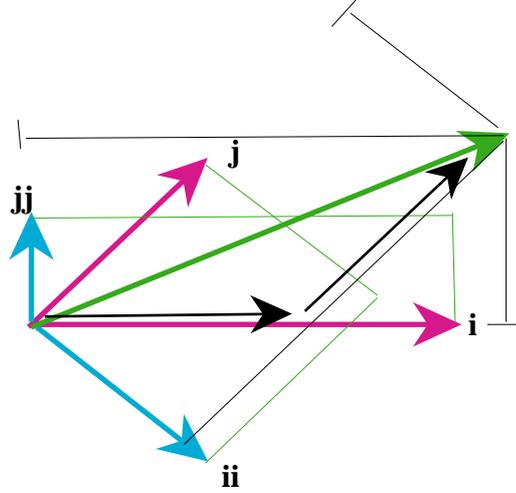


Figure 4: The Reciprocal Basis as a Dual Basis

Among the most visible changes would be the result  $f(x, x) = 0$ , with corresponding changes in its matrix representation with respect to a basis:

$$\begin{aligned} f(ae_1 + be_2, ce_1 + de_2) &= \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} f(e_1, e_1) & f(e_1, e_2) \\ f(e_2, e_1) & f(e_2, e_2) \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}, \\ &= \begin{bmatrix} a & b \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} c \\ d \end{bmatrix}, \end{aligned}$$

If the dimension of the space were larger, the dimension of the metric matrix would increase accordingly, although it would always be antisymmetric. The resulting geometry would be of a different kind, usually called *symplectic*, with interesting and characteristic properties of its own.

Alternating multilinear functions provide the abstract setting, based on linear algebra, within which to discuss objects such as determinants, minors, cofactors and a variety of vector products, which became well established in the applications of algebra long before the axiomatic point of view arose. Determinants, for which the number of arguments matches their dimension, are the outstanding example of the unifying approach, serving as a prototype for the study of the remainder of these functions. Its requirements are:

1.  $f$  is linear in each argument, the remaining arguments held constant,
2.  $f$  changes sign whenever a pair of arguments are exchanged,
3. the value assigned to a basis (with its vectors listed in order) is 1.

The third principle simply provides a normalization factor; if another function  $g$  follows the first two axioms but not the third, it will have the same value as  $f$ , but multiplied by  $g$  applied to the basis.

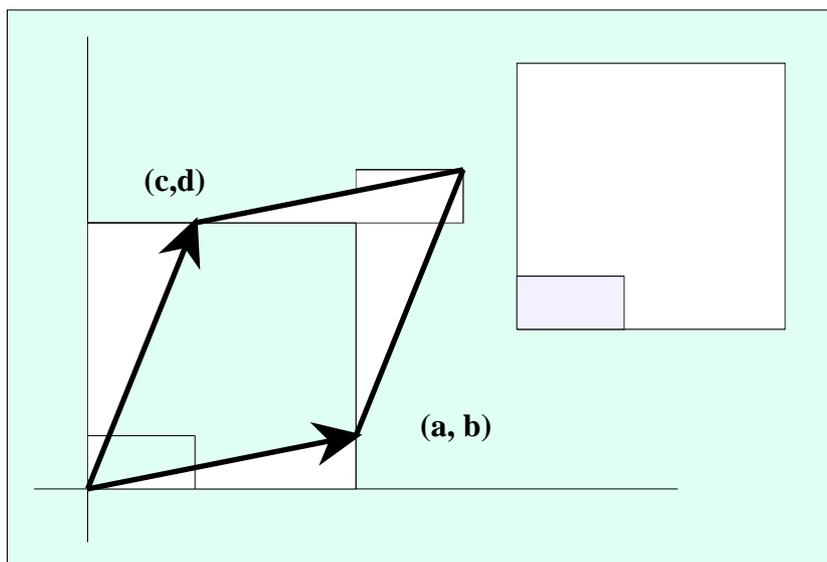


Figure 5: A Determinant referred to a Basis. The right triangles can be rearranged to show that the area of the parallelogram is  $(ad - bc)$ .

In two dimensions the formula above reduces to the familiar  $(ad - bc)$ ; in  $n$  dimensions, the same process obligingly yields the traditional signed sum of permuted products. It is only necessary to expand all the vectors according to a basis, usually the coordinate basis itself, change signs to put the basis vectors in order, and eliminate any terms with repetitions. The result is a sum over permutations,

$$|M| = \sum_{\text{permutations } \pi} \text{sign}(\pi) \prod_{i=1}^n m_{i\pi(i)},$$

where the traditional symbol  $|M|$  has been used for the determinant of the matrix  $M$ .

A less ambitious decomposition leads to Laplace's expansion; for example, write

$$|M| = \sum_{i=1}^n m_{i1} |e_i, X_2, X_3, \dots, X_n|.$$

Naturally, any column other than the first could have been chosen, at the cost of writing a messier formula.

Having applied the determinant formula to the summands, zeroes and ones will occur here and there because of the components of the constant vectors  $E_i$ . The resulting formulas can be simplified by observing that they refer to new determinants, gotten from the old by crossing out the first column and the  $i^{\text{th}}$  row of  $M$ . Those are the minors of  $|M|$ , say  $\mu_{i1}$ . In fuller generality, had the  $j^{\text{th}}$  column been used instead of the first,

$$|M| = \sum_{i=1}^n m_{ji} \mu_{ij},$$

and the transposition of the subscripts between  $m$  and  $\mu$  is quite correct.

In fact, if a wrong row of  $\mu$ 's were placed in this formula, it would describe a determinant in which a wrong column had been repeated twice; once where it belongs and once where the  $j^{\text{th}}$  column of  $M$  ought to have been. Far from being an annoying mistake, the substitution can be exploited to obtain the inverse of  $M$ . Under this interpretation,

$$\sum_{i=1}^n m_{ji} \text{sign}(i) \mu_{ik} = |M| \delta_{jk},$$

Signed minors are called *cofactors*, whilst the matrix of cofactors is called the *adjugate* of  $M$ , written  $M^A$ . Since these equations state that

$$MM^A = |M|I,$$

the inverse of  $M$  is

$$M^{-1} = \frac{1}{|M|} M^A$$

whenever its determinant is nonzero. Otherwise there is no inverse and the adjugate contains columns annihilated by  $M$ .

### 3.5 Using determinants

If an ordered set of edges is given the sign of its handedness, it is not so hard to associate determinants with the volume (or area, as the case may be) of the paralleliped whose edges are the columns of the determinant. Or its rows, for that matter. Multilinearity is a consequence of volume being base times height. Change of sign follows from changing the handedness of the edges, and a unit cube is always assigned unit volume. In fact, if the multilinearity is supposed to apply to negative (reversed direction) vectors as well as positive vectors (which it must, for arithmetic consistency), and repeating two arguments ("flatness") gives zero volume, then  $f(x - y, x - y) = 0$  implies  $f(x, y) + f(y, x) = 0$ , and the alternate attribute of  $f$  is a direct consequence.

The vanishing of a determinant is a good way to detect linear dependence; When one vector is a combination of the others, the altitude which it should carry is zero. Likewise, there should be some other vector perpendicular (measured by the inner product) to all the vectors of the determinant.

To see how nicely recourse to the axioms sometimes shortens proofs, consider the proposition that the determinant of a product is a product of determinants; at least when all the matrices are square and the determinant makes sense. Let  $P$  be one matrix,  $Q$  another, and consider the product  $PQ$ . Partition  $Q$  so that it is a row of columns, and note that, *as a function of  $Q$ ,*

$$|PQ| = |PX_1, PX_2, \dots, PX_n|$$

But,

$$\begin{aligned} |P(aX + bY), PX_2, \dots| &= |aPX + bPY, PX_2, \dots| \\ &= a|PX, PX_2, \dots| + b|PY, PX_2, \dots| \\ |\dots PX_i, \dots, PX_j, \dots| &= -|\dots PX_j, \dots, PX_i, \dots| \\ |Pe_1, Pe_2, \dots, Pe_n| &= |P|. \end{aligned}$$

Therefore,  $|PQ| = |P||Q|$ , whose vanishing, incidentally, requires that at least one factor vanish.

A longer calculation is required to show that the determinant of a matrix is the same as that of its transpose, but it does not have to be carried out in detail. Simply note that the axioms for a determinant could just as easily be stated in terms of rows as for columns, and that the only difference in the explicit formula could be expressed by writing  $m_{\pi(i)i}$  instead of  $m_{i\pi(i)}$ . Since permutations, by definition, are one-to-one and onto, the same sum results, signs and everything. Thus its rows and columns can be exchanged without altering the value of a determinant.

The vanishing of a determinant can be used to check for linear dependence even in the absence of an explicit basis. Suppose that the vectors are  $X_i$ ; make up a matrix  $M$  using them for columns, which will have to be rectangular. Whence there must be a vector  $X$ , expressing the linear dependence via  $MX = 0$ . The determinant

$$|M^T M| = \begin{bmatrix} (X_1, X_1) & (X_1, X_2) & \dots \\ (X_2, X_1) & (X_2, X_2) & \dots \\ \dots & \dots & \dots \end{bmatrix}$$

is called the Gram determinant (of the Gram matrix, naturally), can only be factored when  $M$  is square, but nevertheless always vanishes according to linear dependence or not. Note that it could be the metric matrix of the subspace of the  $X_i$ 's.

## 4 Mappings Between Vector Spaces

### 4.1 Mappings

In the domain of linear mappings from one vector space to another, the mappings to the one-dimensional space of scalar coefficients are especially important, and we have seen them in two forms: the vector space of all such functions, which is the dual space, and the collection of positive symmetric bilinear forms, which are usually called inner products, and written as  $(x, y)$ , without invoking any explicit function name. Functions of the dual space are often written in the same style,  $[x, y]$ , distinguished by square brackets rather than round parentheses. Curly brackets are reserved for sets, or lists of items.

Inner products serve to connect geometry to linear algebra, as a concept familiar from many introductory courses in engineering, physics, or even mathematics. The essential element of the relationship is the fact that bilinear functions with one fixed argument are linear functions of the other argument; just which one depends on the exact value of the constant argument. If that value is taken from the reciprocal basis, the result is a function from the dual basis, which establishes the connection between the two concepts.

When a fixed first argument makes the inner product work on basis vector columns, then reciprocal basis rows satisfy the Kronecker delta relationship needed for the dual basis. But if the reciprocal basis vectors are inserted into a matrix as rows, and the direct basis elements are placed in another matrix as columns, the mutual relationship just makes the matrices inverses of one another. That is where the reciprocal basis gets its name.

Passing on from mappings of all kinds from vector spaces and sets of vector spaces to the trivial vector space of scalar coefficients, the next important category of mappings consists of those from a vector space to itself; amongst all mappings, they enjoy the unique feature that they can be combined indefinitely since no other spaces ever have to be specified. Amongst other things, that means that mappings can be iterated, there are polynomials of mappings, and that there are such

things as fixed subspaces of mappings. Evidently finding a basis for a stable subspace is the key to finding the subspace itself; ever so much better if the basis itself is stable, which is the rationale for introducing eigenvectors.

Conducting efficient and reliable searches for eigenvectors is an important activity in the practical application of linear algebra, perhaps much more so than the other significant venture, which is the finding of matrix inverses. Over the years, the preferred schemes for finding eigenvectors have changed, both from changes in computing technology and as the result of theoretical investigations.

Before describing specific techniques, it is worth looking at some symmetry properties of matrices, because of the influence they have on the stable subspaces and the preferred bases associated with them. At the outset, there are two great categories of matrices, which have their own distinctive properties and areas of application. For physicists and engineers, normal matrices predominate, because of their relationship to such symmetry considerations as Newton's third law (action and reaction) or the passivity of electrical circuits. Those matrices have a complete orthonormal set of eigenvectors, with many nice estimates and limits for their eigenvalues.

Amongst normal matrices are those which are symmetric or hermitean, having only real eigenvalues, and even more specialized, those which are positive definite, having only positive eigenvalues.

The other great category consists of those matrices with positive matrix elements, which form a strict subset of those with non-negative elements. Those additional zeroes permit a great deal of limiting behavior which is not accessible to the positive matrices. Such matrices are of interest in probability theory, and in such fields of application as economics. The outstanding attribute of this category of matrices is the uniqueness of the largest eigenvalue, which are easily found by iteration, and the unique positive eigenvector associated with it.

## 4.2 Consequences of symmetry

First, a discussion of symmetry properties, which in turn relates to bases, dual bases, and transposes. This is required because we want to find relationships between self-mappings of a vector space and mappings such as the inner product, which have already been described. Each time something new is brought forth, its influence on all that has gone before needs to be considered.

### 4.2.1 transpose

If a bilinear form is altered by first mapping its left argument, the result is another bilinear form because of the linearity of matrix multiplication. To use a transient notation, suppose that  $((x, y)) = (x, My)$ . Because

$$((x, ay + bz)) = (x, M(ay + bz)) = (x, aMy + bMz) = a((x, y)) + b((x, y)),$$

the assertion is verified. But inner products are represented by projections from the reciprocal basis, or alternatively, vectors in the dual space, so this new function must be one of them, which prompts calling it the transposed function. Thus, by definition,  $M^T$  is the mapping of the dual space for which

$$(M^T x, y) = (x, My).$$

Because of the conventional representation of vectors as columns, and functions of the dual space as rows acting on the vectors by inner product, the use of the word transpose merely attests to the tradition of flipping rows to get columns and vice versa. In the fortunate circumstance that  $M$  is a

square matrix and  $M = M^T$ ,  $M$  is called symmetric. The Gram matrix fulfills this requirement, as did the matrix representation of a symmetric bilinear function. Another possibility is  $M = -M^T$ , making  $M$  antisymmetric.

#### 4.2.2 index raising and lowering

It is an interesting question, how to turn a matrix into its transpose, just using matrix operations. The simplest thing would be to write

$$M^T = (M^T M^{-1})M,$$

which is not an especially symmetric relationship, and of course supposes that  $M$  is invertible. Supposing further moment that  $M$ , as well as  $M^T$  had both square roots and inverses, we could have

$$M^T = (\sqrt{M})\sqrt{((M^T)^{-1})}^{-1}M\sqrt{(M^{-1})}\sqrt{(M^T)}$$

if we wanted it. At least  $g = \sqrt{M}\sqrt{((M^T)^{-1})}$  is ready for use at any time for writing  $M^T = g^{-1}Mg$ .

#### 4.2.3 left and right eigenvectors

Turning to the consequences of symmetry, in the technical sense of a symmetric matrix, the usual analysis observes that for left and right eigenvectors (writing vectors as columns means that rows are transposes of columns)

$$\begin{aligned} MX &= \lambda X \\ Y^T M &= \mu Y^T, \end{aligned}$$

so  $(Y^T M X)$  takes alternative values according to how the associative law is applied:

$$\lambda Y^T X = \mu Y^T X.$$

Accordingly, either  $\lambda = \mu$  or else  $Y^T X = 0$ , and the vectors are orthogonal. Complications arise when there are several linearly independent eigenvectors with a common eigenvalue, which happens when  $M$ 's fixed subspaces have higher dimension than 1, but it is all just a matter of going ahead and constructing a basis. Since we wouldn't want a zero vector for an eigenvector (trivial and uninteresting alternative) it could be supposed that left and right eigenvectors belonging to the same eigenvalue could be scaled to make  $Y^T X = 1$ .

This result holds for any matrix  $M$ , symmetric or not, and can be summarized by saying that if we make up two matrices, one a column of left eigenrows and the other a row of right eigencolumns, the two matrices are inverses. Or at least partial inverses, because we still don't know how many eigenvectors there actually are, and maybe there are not enough to complete a basis.

If  $M$  is itself a symmetric matrix, simply transposing the defining equation  $MX = \lambda X$  to get  $X^T M^T = X^T M = \lambda X^T$  shows that eigencolumns are eigenrows, keeping the same eigenvalue. Supposing there were enough eigenvectors to make a basis,  $B$ , a matrix of eigenvectors, would satisfy  $B^T = B^{-1}$ , a condition expressed by saying that  $B$  is *orthogonal*.

### 4.3 Canonical forms

Whether there is a sufficiency or insufficiency of eigenvectors eventually depends on cases, but some progress can be made by rewriting the defining equation as

$$(M - \lambda I)X = 0.$$

Were  $(M - \lambda I)$  invertible,  $X$  would have to be zero, which is not a desirable conclusion. For finite vector spaces, at least, there is a very simple numerical criterion for noninvertibility, namely

$$|M - \lambda I| = 0.$$

This determinant works out to be a polynomial of degree equal to the dimension of  $M$ ; usually called the *characteristic polynomial* of  $M$ . In practice, however, it is convenient to work with *monic* polynomials, which is the term applied to polynomials whose leading coefficient is  $+1$ . Consequently it would be preferable to use the definition

$$\chi(\lambda) = |\lambda I - M|.$$

Vanishing of the characteristic determinant is a requirement for the existence of an eigenvector. Conversely, if the determinant vanishes, the columns of  $M$  are dependent, whereupon the coefficients of the linear combination responsible generate a vector satisfying the eigenvalue equation. Therefore there must be at least one eigenvector for every number which is an eigenvalue; sometimes there are more if the equation has multiple roots.

Additionally, whatever the multiplicity of the roots of its characteristic equation, there always has to be at least one root, and so at least one eigenvector for whatever matrix. Such a definitive statement supposes that the coefficients of the matrix belong to an algebraically closed field; otherwise there may be no roots at all. Rotations in the real plane move all points save the origin; but their characteristic equation has only complex roots (unless the angle of rotation is zero and hence done by the identity matrix).

If all the roots are distinct, there have to be enough eigenvectors for a basis and a dual basis as well. Questions of insufficiency of eigenvectors hinge on the existence of multiple roots for the polynomial. Since slight alterations in the matrix elements could split the roots, it may be suspected that some sort of limiting process would account for matrices which lack their full complement of eigenvectors. Due to the wide variety of possible limits, however, some other approach to a general theory is preferable.

#### 4.3.1 characteristic polynomial

The invertibility of the matrix  $(\lambda I - M)$  merits further discussion. This particular inverse,  $(\lambda I - M)^{-1}$ , has a special name — the *resolvent* of  $M$ . But first things first: recalling the axiomatic definition of a determinant, calling the columns of  $M$   $M_i$ , and the coordinate vectors  $e_i$ , we have

$$\begin{aligned} |\lambda I - M| &= |\lambda e_1 - M_1, \lambda e_2 - M_2, \dots, \lambda e_n - M_n|. \\ &= |\lambda e_1, \lambda e_2, \dots, \lambda e_n| - \\ &\quad |M_1, \lambda e_2, \dots, \lambda e_n| - |\lambda e_1, M_2, \dots, \lambda e_n| - \dots - |\lambda e_1, \lambda e_2, \dots, M_n| + \\ &\quad |M_1, M_2, \dots, \lambda e_n| + \dots + |e_1, e_2, \dots, M_n| + \\ &\quad \dots \end{aligned}$$

$$\begin{aligned}
& \pm |M_1, M_2, \dots, M_n| \\
= & \lambda^n \\
& -\lambda^{n-1} \sum_{i=1}^n m_{ii} \\
& +\lambda^{n-2} \sum_{i=1}^n \sum_{j<i} \begin{vmatrix} m_{ii} & m_{ij} \\ m_{ji} & m_{jj} \end{vmatrix} \\
& -\lambda^{n-3} \sum_{i=1}^n \sum_{i<j} \sum_{i<j<k} \begin{vmatrix} m_{ii} & m_{ij} & m_{ik} \\ m_{ji} & m_{jj} & m_{jk} \\ m_{ki} & m_{kj} & m_{kk} \end{vmatrix} \\
& \dots \\
& \pm |M|.
\end{aligned}$$

This result exhibits  $\chi(\lambda)$  in terms of its coefficients, which are sums of diagonal minors, with orders corresponding to the power of  $\lambda$  which they multiply. They could be read out directly from the matrix, albeit while performing a greater or lesser quantity of arithmetic to get all the cofactors.

Noteworthy is the role of the negative of the *trace* (which is the sum of the diagonal elements) as the coefficient of the penultimate power of  $\lambda$ , and the determinant in the role of the constant term. If  $|M|$  vanishes,  $\lambda = 0$  is a root of  $\chi$ , and there is a vector for which  $MX = 0$ . Of course that prevents  $M$  from being invertible; an issue distinct from whether  $|M - \lambda I|$  vanishes.

#### 4.3.2 resolvent

Continuing on, it turns out that the resolvent can be calculated, in terms of the coefficients of the characteristic polynomial. Needing the adjugate of  $(\lambda I - M)$ , we start by knowing that it is a polynomial of degree  $n - 1$  in  $\lambda$  because that is the maximum dimension of the cofactors and thus the maximum number of  $\lambda$ s which could ever be multiplied together. Grouping the coefficients of  $\lambda^i$  together in a matrix called  $A_i$ , set

$$(\lambda I - M)^A = \sum_{i=0}^{n-1} \lambda^i A_i,$$

with a corresponding expansion of the characteristic polynomial

$$\chi(\lambda) = \sum_{i=0}^n c_i \lambda^i.$$

Then the equation

$$(\lambda I - M)(\lambda I - M)^A = \chi(\lambda)I$$

could be subjected to a series of transformations

$$(\lambda I - M) \sum_{i=0}^{n-1} \lambda^i A_i = \sum_{i=0}^n c_i \lambda^i I,$$

$$\sum_{i=0}^{n-1} \lambda^{i+1} A_i - \sum_{i=0}^{n-1} \lambda^i M A_i - \sum_{i=0}^n c_i \lambda^i I = O,$$

$$\sum_{i=0}^n \{A_{i-1} - M A_i - c_i I\} \lambda^i = O.$$

to get a result in which the matrix coefficient of each power of  $\lambda$  would have to vanish. That produces a chain of substitutions consisting of  $A_{i-1} = M A_i + c_i I$  (the missing  $A_{-1}$ , as well as the nonexistent  $A_n$  would both have to be  $O$ ).

$$\begin{aligned} A_{n-1} &= c_n I \\ A_{n-2} &= c_n M + c_{n-1} I \\ A_{n-3} &= c_n M^2 + c_{n-1} M + c_{n-2} I \\ &\dots \\ A_0 &= c_n M^{n-1} + c_{n-1} M^{n-2} + \dots + c_1 I \\ A_{-1} &= c_n M^n + c_{n-1} M^{n-1} + \dots + c_1 M + c_0 I \end{aligned}$$

Note that these equations are readily summarized in a single matrix equation,

$$\begin{bmatrix} O \\ A_0 \\ \dots \\ A_{n-3} \\ A_{n-2} \\ A_{n-1} \end{bmatrix} = \begin{bmatrix} c_0 & c_1 & c_2 & & c_{n-1} & c_n \\ c_1 & c_2 & c_3 & & c_n & \cdot \\ & & & \dots & & \\ c_{n-2} & c_{n-1} & c_n & & \cdot & \cdot \\ c_{n-1} & c_n & \cdot & & \cdot & \cdot \\ c_n & \cdot & \cdot & & \cdot & \cdot \end{bmatrix} \begin{bmatrix} I \\ M \\ \dots \\ M^{n-2} \\ M^{n-1} \\ M^n \end{bmatrix}.$$

Matrices of the strip antidiagonal form evident in this equation are called *Hankel matrices*; they occur frequently in such contexts as the moment problem or in fitting least squares approximations.

### 4.3.3 Cayley-Hamilton theorem

In fact,  $c_n = 1$ ; the last equation of the series, asserts that  $\chi(M) = O$ , a proposition generally known as the *Cayley-Hamilton Theorem*: a matrix satisfies its own characteristic equation.

If the factors of the characteristic polynomial are known, say by having evaluated the characteristic determinant and having found its roots, the matrix polynomial could be factored:

$$\chi(M) = (M - \lambda_1 I)(M - \lambda_2 I)(M - \lambda_3 I) \dots (M - \lambda_n I).$$

Grouping all but one of the factors, and equating the result to zero,

$$\begin{aligned} (M - \lambda_i I)g_i(M) &= 0 \\ M g_i(M) &= \lambda_i g_i(M), \end{aligned}$$

results in something which could be called an eigenmatrix of  $M$ ; in any event all its columns are eigenvectors for the eigenvalue  $\lambda_i$ , and of course, so are its rows.

If all the eigenvalues of  $M$  were distinct, there would only be one eigenvector for each eigenvalue, aside from a scalar multiplier. Therefore, using Dirac's bra and ket notation, and observing that

all the rows of  $g_i$  would be proportional, just as all the columns would have to manifest their dependence, one could deduce that  $g_i$  was proportional to

$$\frac{|i\rangle\langle i|}{\langle i|i\rangle}.$$

If a multiplication table were made up for such column-by-row products, the convenient denominator and the orthogonality of left and right eigenvectors would result in the table

$$\frac{|i\rangle\langle i||j\rangle\langle j|}{\langle i|i\rangle\langle j|j\rangle} = \delta_{ij} \frac{|i\rangle\langle i|}{\langle i|i\rangle},$$

containing orthogonal and idempotent matrices.

#### 4.3.4 Lagrange interpolation polynomials

By far the best approach to constructing such a table is to observe that the gee's are Lagrange interpolation polynomials without their normalization factor (which was provided by the inner product in the denominator in the column by row formulation), with which they ought to be given for the sake of greater consistency. Doing so, one gets

$$G_i(M) = \frac{\prod_{j \neq i}^n (M - \lambda_j I)}{\prod_{j \neq i}^n (\lambda_i - \lambda_j I)},$$

Once this detail is accommodated, the Gee's are equal to their own square, leaving a multiplication table resembling a unit matrix. The Lagrange polynomials intervene directly in the verification of the table, without having to look at the Gee's in detail, because they are completely defined by their values over a set of distinct points. Multiplying basis polynomials taking values of zero or unity leads to similar polynomials. If at least one of the two factors contributes a zero everywhere, the product must be the constant zero. That is just what happens when  $G_i$  contributes the factor which  $G_j$  was lacking to complete the characteristic polynomial.

On the other hand, if both factors take the value 1 in the same places, the product still takes the value 1, so the polynomial is the same, relative to the characteristic polynomial. It is even true that

$$I = \sum_{i=1}^n G_i$$

on account of having created an interpolation for the constant 1.

Not only can the constant function 1 be interpolated, but also the identity function  $f(x) = x$ , in the form

$$M = \sum \lambda_i G_i(M),$$

and even more generally results such as

$$\begin{aligned} f(M) &= \sum f(\lambda_i) G_i(M), \\ M^{-1} &= \sum \lambda_i^{-1} G_i(M), \quad [\lambda_i \text{ nonzero}]. \end{aligned}$$

The function formula even gives a mechanism for calculating square roots, at least for matrices with nonnegative eigenvalues. Such a quantity is required to map a matrix symmetrically into its transpose:

$$\sqrt{(M)} = \sum \sqrt{(\lambda_i)} G_i(M).$$

Note that failing to insist on positive roots of positive eigenvalues inevitably leads to a great multiplicity of square roots for any particular matrix, because of all the binary sign choices at non-zero roots.

### 4.3.5 confluent interpolation polynomials

Lest it seem that all these results are too good to be true, be assured of that; this form of Lagrange interpolation assumes that all points - that is, eigenvalues - are distinct. In the contrary case, confluent forms of the polynomials may be required; and even then, considerable discretion is required.

When there are multiple roots, they should be grouped together in factoring the characteristic polynomial. Suppose that  $m_i$  is the multiplicity of  $\lambda_i$  and that there are  $k$  distinct roots:

$$\chi(M) = (\lambda_1 I - M)^{m_1} (\lambda_2 I - M)^{m_2} (\lambda_3 I - M)^{m_3} \dots (\lambda_k I - M)^{m_k}.$$

This time the Gee's should be defined by

$$G_i = \prod_{j \neq i} \frac{(\lambda_j I - M)^{m_j}}{(\lambda_j - \lambda_i)^{m_i}}.$$

They should be accompanied by the additional polynomials

$$\begin{aligned} N_i^p &= \frac{1}{p!} (\lambda_i I - M)^p \prod_{j \neq i} \frac{(\lambda_j I - M)^{m_j}}{(\lambda_j - \lambda_i)^{m_i}} \\ &= \frac{1}{p!} (\lambda_i I - M)^p G_i(M). \end{aligned}$$

The factorial and reduced power attest their confluent origin, because these interpolating polynomials are specified by their values and  $p < n_i$  derivatives at each interpolation point  $\lambda_i$ . Note that  $G_i = N_i^0$ , and also that the superscript  $p$  in  $N_i^p$  is not quite an exponent, although it behaves like one.

Complications arise for the multiplication table for the  $N_i^p$  although it is still true that

$$N_i^p N_j^q = \begin{cases} O & i \neq j \\ O & i = j \quad p + q \geq m_i \end{cases}.$$

Consequently the  $G$ 's are still orthogonal idempotents, but they might not quite resolve the unit matrix. In principle, the remainder of the multiplication table could be worked out by calculating and evaluating the derivatives of the products to get the data required for the confluent interpolation.

Nevertheless their sum,

$$G = \sum_{i=1}^k G_i$$

by failing to vanish at any of the interpolation points, has no zeroes in common with any of the  $G_i$ , nor with the characteristic polynomial  $\chi(M)$ . That means that the greatest common denominator of  $G(M)$  and  $\chi(M)$  is the constant 1, thanks to which the Euclidean algorithm assures the existence of polynomials  $\sigma(\lambda)$  and  $\rho(\lambda)$  for which

$$\chi(\lambda)\rho(\lambda) + G(\lambda)\sigma(\lambda) = 1.$$

Recognizing that  $\chi(M) = O$  because of the Cayley-Hamilton theorem, the matrix version of the equation requires  $G(M)$  to be invertible given that

$$G(M)\sigma(M) = I.$$

In order to get the confluent version of Sylvester's formula, consider a Taylor's series for the function  $f$ , but written in the more complicated form

$$f(\lambda_i + \lambda - \lambda_i) = \sum_{n=0}^{\infty} \frac{f^{(n)}(\lambda_i)}{n!} (\lambda - \lambda_i)^n;$$

it has the immediate matrix counterpart

$$\begin{aligned} f(M) &= \sum_{n=0}^{\infty} \frac{f^{(n)}(\lambda_i)}{n!} (M - \lambda_i I)^n \\ &= f_{m_i}(M) + (M - \lambda_i I)^{s_i} t_{m_i}(M). \end{aligned}$$

where

$$\begin{aligned} f_{m_i}(M) &= \sum_{n=0}^{m_i} \frac{f^{(n)}(\lambda_i)}{n!} (M - \lambda_i I)^n \\ t_{m_i}(M) &= \sum_{n=s_i}^{\infty} \frac{f^{(n)}(\lambda_i)}{n!} (M - \lambda_i I)^{n-m_i} \end{aligned}$$

are respectively the head, and the tail with a common factor removed, of the Taylor's series based on each eigenvalue. This splitting foresees applying the sum of the Gees, combined with its inverse in the form of the unit matrix, to  $f(M)$ .

$$\begin{aligned} f(M) &= G^{-1} \sum_{i=1}^k G_i(M) f(M) \\ &= G^{-1} \sum (G_i(M) f_{m_i}(M) + G_i(M) (M - \lambda_i I)^{m_i} t_{m_i}(M)), \\ &= G^{-1} \sum_{\lambda_i} \left( \sum_{n=0}^{m_i-1} \frac{f^{(n)}(\lambda_i)}{n!} \prod_{\lambda_j \neq \lambda_i} \frac{(M - \lambda_j I)^{m_i}}{(\lambda_i - \lambda_j)^{m_i}} (M - \lambda_i I)^n \right) \\ &= G^{-1} \sum_{\lambda_i} \left( \sum_{n=0}^{m_i-1} f^{(n)}(\lambda_i) N_i^n \right) \end{aligned}$$

An inconvenient aspect of this formula is the presence of the factor  $G^{-1}$ , which compensates for the simple form of the basis polynomials  $N_i^p$ . Alternatively, a resolution of the identity could be used which would avoid having to find and use the overall factor  $G$ . Consider the identity

$$\frac{\chi(\lambda)}{\chi(\lambda)} = 1$$

in which the quotient  $1/\chi(\lambda)$  is first resolved into partial fractions, and then multiplied by the numerator  $\chi(\lambda)$  to get a sum of terms similar to the  $N_i^p$ . The difference between the formulations lies in relations between the basis polynomials and their dual basis. In one case, the use of powers complicates the dual, while in the other the dual is formed elegantly by just values and derivatives, but the basis no longer consists of simple power products.

#### 4.3.6 stable subspaces

Constructing interpolation polynomials based on the characteristic equation leads to a family of orthogonal idempotents resolving the identity. In the confluent case, there are supplementary nilpotent matrices which take up the slack left by the redundant eigenvectors. Since an idempotent satisfies the equation  $J^2 = J$  its eigenvalues can only be 0 or 1; similarly 0, can be the only eigenvalue of a matrix which satisfies  $N^p = O$ . That is the way to get a concise derivation of Sylvester's formula, without going through the steps of constructing a basis, which is the frame of reference likely to be required in applications.

Let  $M$  map a vector  $X$  to  $MX$ , which may or may not be parallel to  $X$ , depending on fortune. If it is not, map this new vector into  $MMX$ , and so on. Eventually the result has to be dependent on the foregoing vectors, because of the of the dimensionality.

The coefficients of the dependence can be transferred to the matrix powers (supposing, formally, that a zero power is the unit matrix), resulting in a polynomial in  $M$ :

$$\sum (a_i M^i) X = \varphi(M) X = 0$$

which annihilates  $X$ , although the precise coefficients could possibly differ according to the starting vector. To counter that alternative, note that  $M$  commutes with  $\varphi(M)$  so that there is a series of vanishing vectors,

$$\begin{aligned} \varphi(M) X &= 0, \\ \varphi(M) M X &= 0, \\ \varphi(M) M^2 X &= 0, \\ &\dots \quad \dots \end{aligned}$$

If they form a basis, then  $\varphi(M)$  can only annihilate all of them if it is zero, which is again the Cayley-Hamilton theorem. But the process is fairly haphazard — what if the original choice was already an eigenvector (consider using the unit matrix)? Or a member of some other stable subspace of less than the full dimension of the space?

Rather than trusting to luck, it would be possible to start with a basis consisting of vectors  $U_i$  comprising the columns of a matrix  $U$  to obtain a sequence of polynomials for which  $\varphi_i(M) U_i = O$ . Not knowing whether they have common factors, it would be necessary to say that

$$\prod_{i=1}^n \varphi_i(M) U = O$$

because there would be a factor in the product for every column which would annihilate it. The overall polynomial could possibly have degree  $n^2$ , the dimension of the space of matrices rather than the space of the vectors. Since we already know from the Cayley-Hamilton theorem that the characteristic polynomial with degree  $n$  does the job, there must be many common factors amongst the  $\varphi_i$ 's.

Just as in the case of repeated roots of the determinantal equation, there are messy cases to be accounted for when a polynomial of lesser degree suffices, or none of the starting vectors leads up to a full basis; as an extreme example, consider finding eigenvectors for the zero matrix or the unit matrix.

If the coefficient of  $I$  in  $\varphi(M)$  is not zero, implying that the vector chosen for the power search was a good choice, we could set  $I$  aside, assume its coefficient to be 1, and take  $M$  out of the remaining polynomial as a factor, to get

$$\text{inv}(M)M = I.$$

In other words, the inverse of a matrix could be calculated using the first few positive powers of the matrix.

This construction of the characteristic polynomial leaves the impression that the set of powers of a matrix is a vector space of the same dimension (or less) as the space on which the matrix itself operates. Of course the set of all linear mappings from a vector space to itself is another vector space, whose dimension would have to be the square of the original dimension. Polynomials in a single matrix constitute a subspace of  $\text{Linear}(V, V)$ ; one might speculate whether there could be another matrix, generating a second polynomial subspace, such that the entire set of linear mappings were expressible as polynomials in just those two variables.

#### 4.3.7 minimal polynomial

To understand the influence of repeated factors in the characteristic polynomial, it is worth considering whether their presence is essential for generating a zero matrix, in the sense of whether the product of the remaining factors is already zero, or it is not and the additional factor is required to realize the Cayley-Hamilton theorem. In other words, it could happen that there were other vanishing polynomials for the matrix  $M$ , say  $\phi(M) = O$  and  $\psi(M) = O$ . They could always be normalized to become monic. But, by long division, one of them, depending on their relative degrees, would be a multiple of the other with a remainder:

$$\phi(M) = \psi(M)\sigma(M) + \rho(M).$$

Since both  $\phi(M)$  and  $\psi(M)$  vanish, so must  $\rho(M)$ . The upshot of this is that there will always be a unique monic polynomial of least degree,  $\mu(M)$ , satisfied by any given matrix. Accordingly it would be called the minimal polynomial of the matrix, and ought to be used in place of the characteristic polynomial when discussing eigenmatrices.

Even so, the minimal polynomial may still have repeated roots, which means that there is a nontrivial chain of matrices, none of them zero, which map from one to another in sequence, and finally to zero. Their rows and columns must have the same property, which could be exploited in forming a basis and establishing a canonical form for the matrix.

## 4.4 Diagonal matrices

The eigenvectors of a matrix are expected to form a basis, something which is not always true but with exceptions which can be treated separately, or as limits. If we create a matrix  $U$  by writing a row of eigencolumns of  $M$ ,

$$U = [X_1, X_2, \dots, X_n],$$

then submatrix multiplication gives the immediate result

$$\begin{aligned} MU &= [MX_1, MX_2, \dots, MX_n], \\ &= [\lambda_1 X_1, \lambda_2 X_2, \dots, \lambda_n X_n], \\ &= [X_1, X_2, \dots, X_n] \begin{bmatrix} \lambda_1 & 0 & 0 & 0 & \dots \\ 0 & \lambda_2 & 0 & 0 & \dots \\ 0 & 0 & \lambda_3 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \\ &= U\Lambda, \end{aligned}$$

where  $\Lambda$  is a matrix full of zeroes except for its main diagonal, whose elements may also be zero, but usually are not. Such a matrix is called a *diagonal matrix*, satisfying the relationship  $MU = U\Lambda$ ; such an equation is possible because the scalars  $\lambda_i$  commute with the  $X_i$ 's, even when the  $M$ 's refuse.

Since  $U$  is a square matrix, it too is a mapping - one which transforms unit vectors into its columns - thereby making them into a basis of eigenvectors. Its inverse,  $V$ , goes in the other direction; from previous remarks, it can be described as a column of row eigenvectors, for which  $VM = \Lambda V$ . Using  $V$ , changing bases for  $M$  leads to

$$VMU = \Lambda,$$

a process which is called diagonalizing  $M$ . From this it is apparent that the eigenvectors comprise the preferred basis for a matrix, although in reality we have to work with a reciprocal pair of bases, one for vectors and the other for components.

## 4.5 Commuting matrices

As an application for diagonalization and the diagonal form, consider the question of discovering which matrices  $N$  commute with a given matrix  $M$ :

$$MN = NM.$$

Choosing the preferred basis,

$$\begin{aligned} VMUVNU &= VNUVMU \\ \Lambda K &= K\Lambda, \end{aligned}$$

after introducing  $K = VNU$ . In more explicit detail,

$$\begin{bmatrix} \lambda_1 & \cdot & \cdot & \cdot \\ \cdot & \lambda_2 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} k_{11} & k_{12} & \cdot & \cdot \\ k_{21} & k_{22} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix} = \begin{bmatrix} k_{11} & k_{12} & \cdot & \cdot \\ k_{21} & k_{22} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} \lambda_1 & \cdot & \cdot & \cdot \\ \cdot & \lambda_2 & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

in general summarized by the relations involving the individual matrix elements,

$$(\lambda_i - \lambda_j)k_{ij} = 0.$$

Once again, distinct eigenvalues yield a clearcut conclusion, whereas multiple eigenvalues require further analysis. The conclusion is:  $K$  is diagonal too, but in the presence of multiplicity, some further adjustment, resolved by a modified basis, may be necessary to manifest both matrices in that form.

The conclusion which we seem to have is that matrices commute only when one is a function of the other, or better yet, are common functions of a third matrix which has distinct eigenvalues. Which function, exacty? It is a polynomial whose degree is no higher than the dimension of the matrix, but to find out which one, the eigenvalues with which the Lagrange interpolation polynomials operate have to be taken over to the maclaurin basis to discern the coefficients of the polynomial.

The result also casts some doubt upon whether we know how to find the square root of a matrix; so far we really only know how to get square roots which commute with the matrix; there may still be others.

Another curiosity: the exponential of a matrix is just a polynomial, even though the exponential is an infinite series; the same observation holds for sines, cosines, and whatever other function. The infinite series still plays a role; it is one way to calculate the appropriate function of the eigenvalues before inverting the lagrange interpolation to get the polynomial.

## 4.6 Anticommuting matrices

A variant on commutation of matrices is anticommutation. As before, consider  $M$  and  $N$  as two matrices for which

$$MN = -NM,$$

with  $X$  an eigenvector for  $M$  whereby  $MX = \lambda X$ . Then

$$\begin{aligned} MNX &= -NMX \\ M(NX) &= (-\lambda)(NX). \end{aligned}$$

Either  $N$  is singular,  $\lambda$  is zero (making  $M$  singular), or  $(NX)$  is another eigenvalue belonging to  $-\lambda$ . Evidently the relationship is a mutual one,  $M$  mapping eigenvectors of  $N$  into new ones with reversed eigenvalue sign. We need to consider four regions: vectors annihilated by  $M$ , vectors annihilated by  $N$ , the vectors with positive eigenvalue associated with  $M$ , and those with negative eigenvalues, conjugated from the first group by  $N$ .

Setting up the explicit format of the previous section and repeating the derivation leads to the conclusion that

$$(\lambda_i + \lambda_j)k_{ij} = 0.$$

Various schematic representations of the situation are possible, but are probably best summarized by saying that  $M$  and  $N$  have the respective forms:

$$\left[ \begin{array}{cc|cc} A & \cdot & \cdot & \cdot \\ \cdot & -A & \cdot & \cdot \\ \hline \cdot & \cdot & F & \cdot \\ \cdot & \cdot & \cdot & \cdot \end{array} \right] \quad \left[ \begin{array}{cc|cc} \cdot & B & \cdot & \cdot \\ B & \cdot & \cdot & \cdot \\ \hline \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & G \end{array} \right]$$

The  $F$  and  $G$  parts can be discarded except for singularity (but then the dimension of  $M$  and  $N$  must be even), leaving the general impression that anticommuting matrices can be brought to a form with one of them diagonal, the other antidiagonal, and both with their nonzero eigenvalues arranged in negative pairs.

## 4.7 Fourier pairs

The anticommutativity condition can be extended in different directions. One is to look for more and more pairs which anticommute. That would lead to such things as quaternions, Dirac matrices, and similar artifacts. Another is to take some other numerical factor, writing  $MN = \omega NM$ . Then there is a new alternative:  $\omega$  would have to be a root of unity if  $M$  and  $N$  generated cycles of each others eigenvectors, or else one of the matrices would have to be singular to terminate the chain of eigenvectors, each with different eigenvalues. Or, finally, the space might not be finite dimensional.

Amongst all the possibilities, there is one which has an interesting symmetry. Suppose  $\omega$  is the  $n$ th root of unity with smallest nonzero argument for  $n$ -dimensional matrices  $M$  and  $N$ . Then following the same reasoning as before, these matrices could be brought to the associated forms  $W$  and  $S$ ,

$$W = \begin{bmatrix} 1 & \cdot & \cdot & \dots & \cdot \\ \cdot & \omega & \cdot & \dots & \cdot \\ \cdot & \cdot & \omega^2 & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \omega^{n-1} \end{bmatrix}$$

$$S = \begin{bmatrix} \cdot & 1 & \cdot & \dots & \cdot \\ \cdot & \cdot & 1 & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot \\ \cdot & \cdot & \cdot & \dots & \cdot \\ 1 & \cdot & \cdot & \dots & \cdot \end{bmatrix}$$

so any general matrix could be written in the form

$$A = \sum a_{ij} W^i S^j,$$

which is a Finite Fourier Series decomposition of  $A$ , in a manner of speaking.

## 4.8 Equivalent matrices

It takes eigenvectors and eigenvalues to define a matrix. We have seen that the condition of having a common eigenvector set depends on whether two matrices commute or not. One could equally wonder whether there is an analogous relationship for matrices which have common sets of eigenvalues? Since the eigenvectors define a basis, the question is essentially one of how to recognize pairs of matrices whose only difference lies in the coordinate system in which they are defined. Suppose that  $M$  and  $N$  are two square matrices, and that  $O$  defines a mapping between vector spaces (not necessarily the same one), in which case  $M$  and  $N$  could even have different dimensions.

$O$

$$\begin{array}{ccc}
\text{Space 1} & \longrightarrow & \text{Space 2} \\
M \downarrow & & \downarrow N \\
\text{Space 1} & \longrightarrow & \text{Space 2} \\
& & O
\end{array}$$

The required relationship is that

$$ON = MO.$$

with the further relationship

$$N = O^{-1}MO$$

whenever  $O$  is invertible. This is the usual representation for the new matrix after a change of basis.

So far it is just a question that  $M$  and  $N$  produce the same results, independently of the stage at which  $O$  is introduced, and nothing has been said about eigenvalues. Nevertheless note that if  $NX = \lambda X$ , we would have  $O(NX) = \lambda(OX)$  whilst  $(ON)X = M(OX)$  (indicating a use of the associative law by introducing parentheses). Altogether,  $M(OX) = \lambda(OX)$ , so that  $M$  and  $N$  can be expected to have matched eigenvectors with the same eigenvalue unless a singularity of  $O$  intervenes. To that extent,  $M$  and  $N$  have the same eigenvalues.

To observe the correspondence of the whole set of eigenvalues, suppose that  $U$  diagonalizes  $M$  to  $\Lambda$  and that  $V$  diagonalizes  $N$  to  $K$ :

$$\begin{aligned}
MU &= U\Lambda, \\
NV &= VK,
\end{aligned}$$

and that the eigenvalues correspond. They don't have to match in order, but they should have the same multiplicities. There is then a permutation of the diagonal elements of  $K$  to get the diagonal elements of  $\Lambda$ . This could be remedied by introducing a permutation matrix, but it is just as well to take advantage of the ambiguity in defining  $U$  and  $V$ , that their columns can be arranged in the order that we want, to make sure that the corresponding eigenvalues were listed in the same order since the beginning. That would make  $K = \Lambda$ , so

$$\begin{aligned}
M &= U\Lambda U^{-1} = (UV^{-1})(V\Lambda U^{-1}), \\
N &= V\Lambda V^{-1} = (V\Lambda U^{-1})(UV^{-1}).
\end{aligned}$$

Of course,  $\Lambda$  could be inserted elsewhere in a similar product and other variants may exist. The essential point is that there is a pair of matrices  $A$  and  $B$  such that  $M = AB$ ,  $N = BA$ . The existence of such a factorization could be taken as a test of whether  $M$  and  $N$  have a common set of eigenvalues. Furthermore,  $A$  and  $B$  play the role of  $O$  in the previous discussion because

$$MA = (AB)A = A(BA) = AN,$$

and similarly in the other direction.

## 4.9 Gerschgorin's disks

In the business of working with eigenvalues, it is useful to know how large or how small they can become. Likely as not to be negative, smallness is often a matter of absolute value, a zero eigenvalue implying singularity, while relative smallness of some eigenvalues relative to others could imply near singularity (if they were all tiny, it would likely be that the matrix was small overall). A good, general purpose upper bound for the absolute value arises from taking absolute values of the terms in the equation for a component of an eigenvector; if  $MX = \lambda X$ ,

$$\begin{aligned}\lambda x_i &= \sum_j m_{ij} x_j, \\ |\lambda| |x_i| &\leq \sum_j |m_{ij}| |x_j|.\end{aligned}$$

Not all the components are zero; furthermore there those for which  $|x_i|$  is larger than for any other; let  $I$  be the index of one of them. Then

$$|\lambda| \leq \sum_j |m_{Ij}| \frac{|x_j|}{|x_I|}.$$

Every one of these quotients is less than 1, so the inequality can only be enhanced by dropping them and using 1 instead, with the result

$$|\lambda| \leq \sum_j |m_{Ij}|.$$

Quite reasonable; although a matrix is a collection of numbers, products in which they are involved can't get much larger than the factors permit, nor can a sum of such products ever surpass  $n$  (the dimension) times the largest summand, a conclusion already evident in this inequality.

Changing the derivation slightly, moving the diagonal term of the sum over to the left hand side of the equation before taking absolute values, tells how far an eigenvalue may deviate from its diagonal element, even when the eigenvalues are complex.

$$|\lambda - m_{II}| \leq \sum_{j \neq I} |m_{Ij}|.$$

The resulting disks are Gerschgorin disks, so called in honor of the source of their inspiration. Since it is not always obvious from inspection which was the largest component of the eigenvector, all the disks have to be considered, with the assurance that the eigenvalue lies under at least one of them (no reason for them not to intersect, particularly if diagonal elements are equal or close to one another). Continuity arguments (multiply the off-diagonal elements by a factor and vary it from zero to one) require each isolated group of disks to have their quota of eigenvalues.

The derivation works as well for rows as for columns, providing a practical choice of the row sum or the column sum of absolute values, whichever gives the smaller disk. What doesn't matter in the presence of symmetry can still be useful in other contexts.

Finding an eigenvalue at the center of a Gerschgorin disk is possible, but less likely in the presence of additional elements in the same row or column. To find an eigenvalue on the rim of one of the disks requires a degree of cooperation, since all products of matrix elements by their

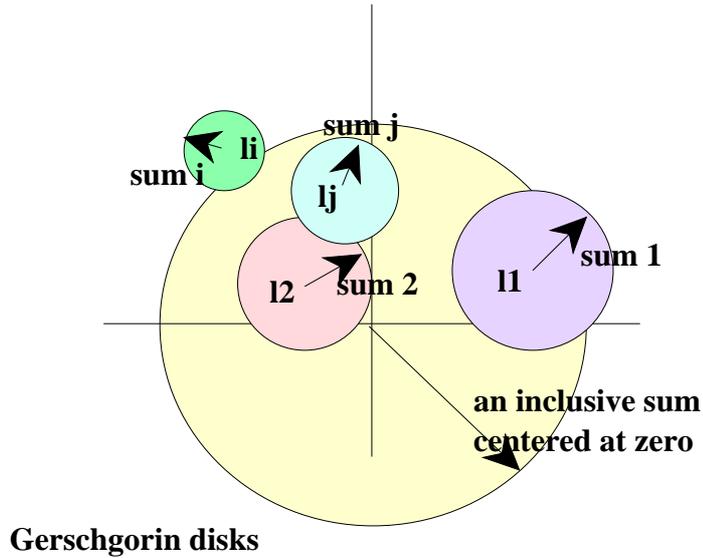


Figure 6: some Gerschgorin disks

matching component need a consistent sign to avoid discrepancies between the absolute value and the actual summand. Furthermore all those quotients replaced by ones must actually be ones, requiring the absolute values of all components of the eigenvector to be equal. In turn all row sums, using the sign convention established by the principal row, have to coincide. Under those conditions the eigenvalue lies on the rim, and all disks intersect at that point. The configuration is typical of stochastic matrices.

#### 4.10 Variational principle

A good way to visualize a matrix is to use it to define a conic - that is, a second degree surface - of the corresponding dimension. Given a symmetric matrix  $M$ , the conic could be defined as the contour for the value  $c$  of the function  $f(X) = (X, MX) = c$ . Another representation would be to chose vectors of unit length (for which  $(X, X) = 1$ ), graphing the values of  $f$ . Taking this point of view, and looking for stationary values of  $f$ ,  $X$  could be modified slightly by adding  $\varepsilon E$ , to obtain

$$\frac{(X + \varepsilon E, M(X + \varepsilon E))}{(X + \varepsilon E, X + \varepsilon E)}.$$

The denominator compensates for the change in length of  $X$ ; alternatively a Lagrange multiplier could have been used. Using the bilinearity and symmetry of of the inner product, we get

$$\begin{aligned} \text{numerator} &= (X, MX) + 2\varepsilon(X, ME) + \varepsilon^2(E, ME), \\ \text{denominator} &= (X, X) + 2\varepsilon(X, E) + \varepsilon^2(E, E). \end{aligned}$$

Dividing numerator and denominator by  $(X, X)$ , approximating  $1/(1 + \varepsilon)$  by  $(1 - \varepsilon)$ , and extracting the term proportional to  $\varepsilon$ , one gets

$$(E, MX) - (E, (X, MX)X),$$

which is supposed to vanish irrespective of E. If the bilinear form is positive definite, that can only happen when

$$MX = (X, MX)X,$$

which is to say, when  $X$  is an eigenvector and  $(X, MX)$  is its eigenvalue.

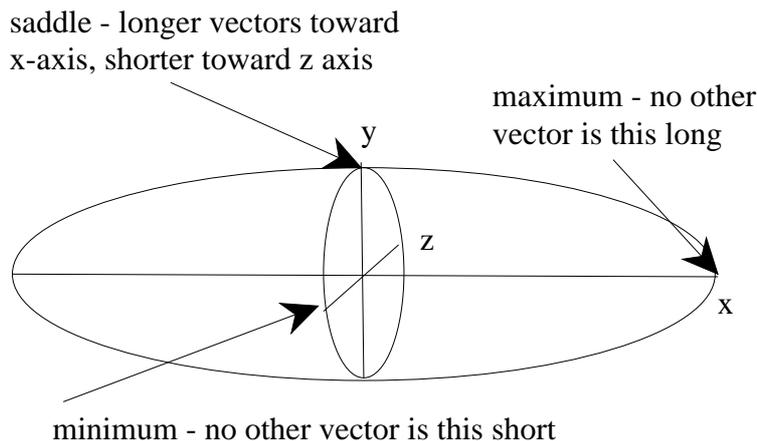


Figure 7: The Ellipsoid Defined by a Quadratic Form

These ideas have been expressed in a variety of ways. For example, the Courant Minimax Principle maximizes the quadratic form within a lower dimensional subspace, then minimizes for all such subspaces. To appreciate this in the figure at left, intersect the ellipsoid with planes and find the semimajor axis in each plane. Then choose the smallest of them all. That will get the one along the y-axis, not the x-axis, because the latter is not the longest axis in any ellipse at all.

The symmetry of  $M$  is not really a requirement, and the form  $(X, M Y)$  could be examined relative to independent variations of  $X$  and  $Y$ . The result would be separate equations for left and right eigenvectors, with the practical difficulty that the normalization by  $(X, X)$  would change to  $(X, Y)$  without a guarantee that the product would not vanish even when  $X$  and  $Y$  were non-zero. That possibility is excluded for normal matrices, but can readily occur whenever the Jordan normal form describes  $M$ ; in fact it characterizes nontrivial Jordan decomposition. Also note that we have been using calculus arguments in an algebraic environment, which may not always be such a good idea; for integer matrices, say.

#### 4.11 Avoided level crossings

In applications, there is not only a requirement for eigenvalues and eigenvectors of matrices; beyond that it is often required to have the eigenvalues of combinations of matrices, such as their sums or products. These quantities are evidently related to those of the constituents, but not always in a way which is easily seen. It is still possible to work out some guidelines.

Consider two matrices  $A$  and  $B$ , normal if you will, and their convex linear combination, by which we mean,  $C = (pA + (1 - p)B)$  for a parameter  $p$  varying between zero and one. If the two matrices commute there is no problem: there is a coordinate system in which they are simultaneously diagonal, the eigenvalues  $a_i$  and  $b_i$  can be listed in order so that we know which pair attach to the same eigenvector, and the new eigenvalues are

$$c_i = pa_i + (1 - p)b_i.$$

Of course, indexed order is not necessarily numerical order, so there could be some values of  $p$  for which  $c_i(p) = c_j(p)$ , a degeneracy which is always interesting and sometimes causes numerical problems.

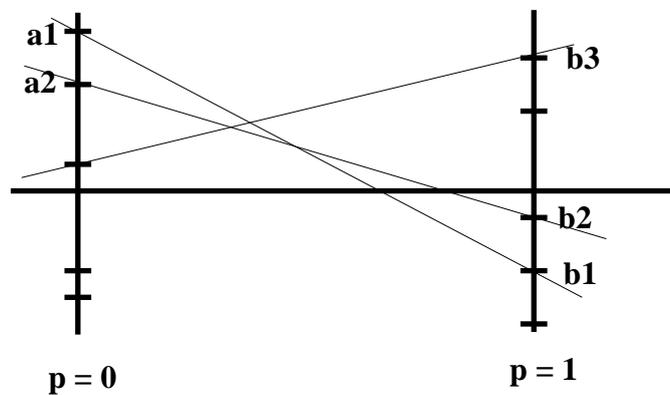


Figure 8: Eigenvalue crossing for common eigenvectors.

If  $A$  and  $B$  are changed ever so little, they may no longer commute, changing this picture, although the indexing scheme may still persist. For some insight into what may happen, consider that  $A$  is a  $2 \times 2$  diagonal matrix with eigenvalues 1 and -1, and that  $B$  is skewdiagonal, but symmetric with 1's in the corners, so that its eigenvalues are also 1 and -1. We are therefore interested in the  $2 \times 2$  matrix

$$\begin{bmatrix} 1 - p & p \\ p & p - 1 \end{bmatrix}$$

whose characteristic equation is

$$\begin{vmatrix} 1 - p - \lambda & p \\ p & p - 1 - \lambda \end{vmatrix}$$

or

$$2\left(p - \frac{1}{2}\right)^2 - \lambda^2 = \frac{1}{2},$$

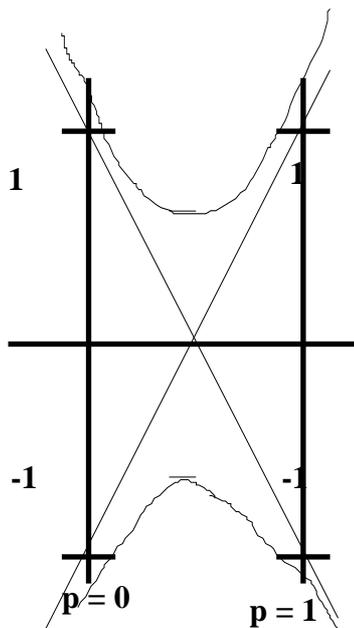


Figure 9: Eigenvalue crossing for differently oriented eigenvectors

which is the equation of a hyperbola opening upwards and downwards, with vertex at  $(0, 1/2)$  and approaching the x-axis no closer than  $1/\sqrt{2}$ . The lines of the previous diagram are now asymptotes, but the interpolating lines no longer cross and the energy levels keep their places, so to speak. That is the content of the “no crossing rule” which specifies that this is a general proposition so the eigenvalues will retain their relative order even when the two matrices do not commute. Unless some common eigenvectors still remain, that is.

#### 4.12 Perturbation

Continuing to speculate on the eigenvectors and eigenvalues of a sum of two matrices, consider the case where the second is small relative to the first, perhaps on account of multiplying it by a small parameter. Maybe a small change of coordinates, depending on the same parameter, could account for the changed matrix; suppose then that

$$(I - \varepsilon P)A(I + \varepsilon P) = A + \varepsilon B,$$

with the intention of disregarding anything multiplying  $\varepsilon^2$ . First,

$$A + \varepsilon(AP - PA) + \dots = A + \varepsilon B,$$

so the task becomes solving for the commutator  $AP - PA = B$ , which is a special case of a more general first order (not linear) equation involving an unknown  $P$  and given matrices  $A$  and  $B$ , or even  $A$ ,  $B$ , and  $C$  (instead of the second  $A$ ).

As usual, the first step is to diagonalize  $A$ , but it is reasonable to suppose that that has already been done, since it is only a question of the coordinate system. Once that is done, and the equation reduced to components, we find

$$\lambda_i p_{ij} - p_{ij} \lambda_j = b_{ij},$$

or for reference,

$$p_{ij} = \frac{b_{ij}}{(\lambda_i - \lambda_j)}.$$

As always, a problem arises when  $\lambda_i = \lambda_j$ , which is traditionally resolved by making still further preparations, namely choosing coordinates for which  $b_{ij}$  vanishes, avoiding the necessity of division by zero - just leave that part of the equation alone. The new eigenvectors can now be read off from the columns of  $I + \varepsilon P$  and the rows of  $I - \varepsilon P$ .

Not only is degeneracy an obstacle to this derivation, there is the implicit assumption that  $B$  has no diagonal elements, avoiding  $(\lambda_i - \lambda_i)$  as a divisor. Consequently this procedure cannot change the eigenvalues of  $A$ , just its eigenvectors. If it is necessary to change the eigenvalues of  $A$  as well, that has to be done independently of applying the operator  $P$ . Why is such a subterfuge necessary? Because

$$(I - \varepsilon P)(I + \varepsilon P) = I - \varepsilon^2 P,$$

making the transformation orthogonal to first order. That is a rotation, which will not change the lengths of semiaxes of an ellipsoid, which are eigenvalues.

This whole scheme is sometimes called Primas' method.

### 4.13 Matrices as vectors

Before leaving the subject of mappings, recall that  $\text{Linear}(\text{Space}, \text{Space})$  is a vector space itself, for it ought to have a basis, inner products, a bilinear functional, a dual, and so on. A Fourier Pair has already been exhibited as such a basis, at least for any matrix with a complete set of eigenvectors. The basis which is most directly connected with  $\text{Linear}(\text{Space}, \text{Space})$  is the collection of matrices  $e_{ij}$ , all of whose matrix elements are zero except for the one at the intersection of the  $i^{\text{th}}$  row and  $j^{\text{th}}$  column. The rule of multiplication is

$$e_{ij}e_{kl} = \delta(j, k)e_{il},$$

The expansion of a matrix in this basis is just

$$M = \sum m_{ij}e_{ij}.$$

The trace of a matrix is the sum of its diagonal elements, and is the coefficient of  $(-\lambda)^{n-1}$  in its characteristic polynomial. Consider the bilinear mapping of two matrices to the scalar coefficients,

$$[M, N] = \text{Trace}(MN).$$

It suffices to define a dual space, whilst the use of a transpose,

$$(M, N) = [M^T, N],$$

not only provides a positive definite inner product, but tells us that

$$(M, M) = \sum m_{ij}^2$$

which is eucliden length, squared, for a vector which is just a list of all the matrix elements. Another interpretation is that theis inner product is just the Gram Matrix of the columns of  $M$ , and that two matrices are orthogonal to one another if  $Trace(M^T N) = 0$ .

Why isn't the determinant of a matrix product a candidate for an inner product? Because it is not bilinear. Are other inner products feasible? Consider  $Trace(M^T Q N)$  for a positive definite matrix  $Q$ , but that is just like introducing a metric matrix into the ordinary inner product for vectors.

How do we get a basis for matrices compatible with the eigenvector basis for vectors? Consider the column-by-row products (column i)(row j); their multiplication table is similar to the multiplication table for standard vectors; the trace relationships are also verifiable.

How do we get a basis for matrices consisting of monomials  $M^i N^j$  when  $M$  and  $N$  don't commute and so  $MN$  isn't  $NM$  and  $MNM$  isn't  $M^2 N$ , and so on? Evidently it is sufficient to know how to rewrite  $NM$ , even though the calculation could be tedious. The best thing is to let the eigenvectors speak for themselves, which they do through the diagonalizing matrices and the column by row idempotents.

Suppose that  $M$  has a family of idempotents  $G_i$  which are column by row products of eigenvectors, and that  $N$  has a similar family  $H_i$ . That leaves us with four bases which can be collected into matrices:  $U$  whose columns are the eigenvectors of  $M$ ,  $U^{-1}$  whose rows are also eigenvectors of  $M$ ; similarly  $V$  and  $V^{-1}$  for  $N$ . All the column eigenvectors of  $N$  are linear combinations of column eigenvectors of  $M$  since  $V = U U^{-1} V (U^{-1} V)$  stands to the right since the matrix product wants to combine columns of  $U$  to get  $V$ ). That means that the products  $G_i H_j$  form a basis for square matrices, since they are just multiples of a column eigenvector of  $M$  by a row eigenvector of  $N$ , and columns by row already created bases, both for  $M$  and for  $N$ , just as they do in the standard basis. Also,  $U^{-1} = U^{-1} V V^{-1}$ , making a particular row eigenvector of  $M$  satisfy  $e_i U^{-1} = (e_i U^{-1} V) V^{-1}$ .

The point of this exercise is that  $M$  and  $N$ , as well as any other matrix, can be written in this mixed basis; in that form their powers and products can then be calculated in terms of the matrix  $U V^{-1}$  and its relatives.

If we truly believe everything we have said, then we ought to find

$$Q = \sum Trace(G_i H_j, Q) G_i H_j.$$

#### 4.14 Confluence

Consider the fate of a Vandermonde determinant when two of its columns coincide, for example when  $a$  and  $b$  were nearly equal.

$$\begin{vmatrix} 1 & 1 & 1 & 1 & 1 \\ x & a & b & c & d \\ x^2 & a^2 & b^2 & c^2 & d^2 \\ x^3 & a^3 & b^3 & c^3 & d^3 \\ f(x) & f(a) & f(b) & f(c) & f(d) \end{vmatrix} = 0.$$

Starting from the determinant, we could subtract the  $a$  column from the  $b$  column,

$$\begin{vmatrix} 1 & 1 & 0 & 1 & 1 \\ x & a & b - a & c & d \\ x^2 & a^2 & b^2 - a^2 & c^2 & d^2 \\ x^3 & a^3 & b^3 - a^3 & c^3 & d^3 \\ f(x) & f(a) & f(b) - f(a) & f(c) & f(d) \end{vmatrix} = 0.$$

and to save writing all the steps one by one, observe that  $(b - a)$  is now a common factor of all the terms in the third column except for the last which would leave  $(f(b) - f(a))/(b - a)$  and a determinant whose nearness to zero depends on this factor. That suggests discarding the factor and recognizing a derivative. The result is called the confluent form of the Vandermonde determinant, leading to Hermite interpolation when used for that purpose. It is not excluded that several pairs of points coalesce, it just means using more derivatives as well as values at all those points. If three points condense, the second derivative can also be extracted from the assemblage, and so on for as many clusters as might appear.

A similar limiting process recommends itself when the characteristic equation of a polynomial has multiple roots, because the spectral decomposition of the matrix is essentially a Lagrange interpolation over the eigenvalues. Derivatives ought to begin to make their appearance.

To see how this works, pick out a simple  $2 \times 2$  matrix, such as

$$\begin{bmatrix} 1 & 1 \\ \varepsilon^2 & 1 \end{bmatrix}.$$

whose characteristic equation is

$$((\lambda - 1)^2 - \varepsilon^2) = 0,$$

with roots  $1 + \varepsilon$  and  $1 - \varepsilon$ . Consequently, if  $\varepsilon$  were near zero, there would be an approximate degeneracy.

Two matrices of eigenvectors, left and right, are,

$$2\varepsilon U^{-1} = \begin{bmatrix} \varepsilon & 1 \\ \varepsilon & -1 \end{bmatrix}, U = \begin{bmatrix} 1 & 1 \\ \varepsilon & -\varepsilon \end{bmatrix}.$$

from which it appears that there is only one eigenvector when  $\varepsilon = 0$ , and that that left eigenvector would be orthogonal to the only right eigenvector, precluding its normalization to unit projection.

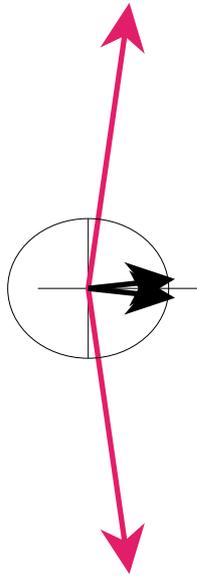


Figure 10: Confluence of eigenvectors in the Jordan Normal Form, showing how the left eigenvector becomes orthogonal to its own right eigenvector.

## 5 Band Matrices

A band matrix is one for which elements far from the diagonal are zero; distance is usually required to be uniform in the sense that the remoteness of the farthest nonzero element must always be the same. That closer elements are zero does not materially affect the behavior of such a matrix, but deciding whether a border element is zero can be a delicate numerical problem. The band need not be centered, a configuration which would be an automatic consequence of its forming part of a symmetric matrix.

### 5.1 Band matrices

Band matrices arise from a variety of sources; for example from discretizing a linear ordinary differential equation, from the classical equations of motion of a string of masses coupled by Hooke's law springs, or the study of the electrical characteristics of a lumped transmission line, the quantum mechanical study of pi electrons in linear organic molecules, and quite a goodly assortment of other places. For numerical analyses, straightforward procedures will reduce a matrix to band form, following which one of a variety of iterative procedures can be set in motion.

Diagonalizing a band matrix is particularly interesting for theoretical purposes because the procedure can be transformed into solving a recursion relation using supplementary matrices no larger than the width of the band, no matter how large to starting matrix. To see how it can all

be done, imagine a tridiagonal matrix  $A$  (band width three, centered) of the form

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdot & \cdot & \cdot & \cdot & \cdot \\ a_{21} & a_{22} & a_{23} & \cdot & \cdot & \cdot & \cdot \\ \cdot & a_{32} & a_{33} & a_{34} & \cdot & \cdot & \cdot \\ \cdot & \cdot & a_{43} & a_{44} & a_{45} & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}.$$

with its eigenvalue equation  $AX = \lambda X$ . For any one component the equation would read

$$a_{i,i-1}x_{i-1} + a_{i,i}x_i + a_{i,i+1}x_{i+1} = \lambda x_i,$$

which could be rearranged to the form

$$a_{i,i+1}x_{i+1} = (\lambda - a_{i,i})x_i - a_{i,i-1}x_{i-1},$$

and recognized as the first half of a  $2 \times 2$  matrix equation, whose second half consists of the tautology  $x_i = x_i$ :

$$\begin{bmatrix} x_{i+1} \\ x_i \end{bmatrix} = \begin{bmatrix} \frac{\lambda - a_{i,i}}{a_{i,i+1}} & -\frac{a_{i,i-1}}{a_{i,i+1}} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix}.$$

For ease of reference, suppose that this equation says  $MY_{i+1} = Y_i$ . Any high-indexed component can be derived from one with a lower index by successive substitution, which translates into calculating a product of  $2 \times 2$  matrices. There is always the question of how to start and stop, which in turn depends on some alternative structures for the matrix  $A$ . The extreme skewdiagonal corners could be non-zero without violating the bandwidth hypothesis if the system described by the matrix were cyclical, in which case it would be supposed that some power of  $M$  were the unit matrix.

Otherwise fictitious components  $x_0$  and  $x_{n+1}$  could be introduced, obligated to vanish, and the overall symmetry of  $A$  preserved by inserting arbitrary corner elements, for example ones which would preserve the integrity of the diagonal in which they sit.

Several conclusions can be drawn at once. The matrix  $M$  ought to be defined and invertible. Its definition supposes nonzero  $a_{i,i+1}$ , so the righthand edge of the band must be intact. For it to be invertible, its determinant  $a_{i,i-1}/a_{i,i+1}$  ought not vanish, placing a similar requirement on the left hand edge. Once those two conditions are realized, all possible consecutive pairs of components can be deduced from any single one of them, for example, a terminal pair.

The next observation is: whenever two consecutive components are zero, all components vanish, contrary to the assumption of non-zero eigenvectors. In applications to vibrating strings, places where the displacement vanishes at all times are called nodes, implying that nodes contain no more than a single particle.

A different matrix  $M_i$  would arise from each row of  $A$ , not excluding that some of them might be numerically equal if  $A$  had some similar rows. In fact, that is one of the most interesting cases, since it would imply a physical problem derived from connecting a series of similar units. The eigenvalue of  $A$  is a parameter in these matrices, resulting in matrix elements which were polynomials in the eigenvalue after a series of  $M$ 's were multiplied together. To give  $M$  or its products a name, they are often called a transfer matrices, because they relate components in one place to those in another. Nor should it be surprising to find the characteristic polynomial of  $A$  amongst the matrix elements

of an all-encompassing transfer matrix running from one of the string to the other. Depending on the context from which  $A$  arose, its eigenvalues (the roots of the characteristic equation) would be frequencies (squares of frequencies, actually), decay rates, energy levels, or whatever.

Ease in calculating transfer matrices would reduce the labor calculating components of eigenvectors, especially that part relating the extreme components which reveals the characteristic polynomial. Calculation with matrices often reduces to diagonalizing them to get their eigenvector basis, creating an entirely new eigenvalue problem for the matrix  $M$  instead of the matrix  $A$ , namely finding  $Y$  for which  $MY = \mu Y$ . Once done, we end up writing the components of  $X$  as linear combinations of the eigenvectors of  $Y$ . Because of the likelihood that  $A$  has something to do with vibrations, eigenvectors of  $M$  are called waves, its eigenvalues wave numbers, and its characteristic polynomial a dispersion relation. That is because it influences how fast a wave of a given frequency travels, and the fact that they usually don't all travel at the same speed.

Although it is theoretically possible to bring any symmetric matrix to tridiagonal form (for general matrices it is called a hessenberg form, which only has to be banded on one side of the diagonal), there are advantages in not doing so if there is a polydiagonal form with appreciable regularity. That would happen from the beginning if the matrix resulted from discretizing a higher order (than second) differential equation or maybe from studying the vibration of a chain of coupled masses with long range coupling.

The principal differences between tridiagonal and polydiagonal matrices lie in the maximum width of a node, and in the complexity of the dispersion relation, which would be a polynomial of ever increasing degree. And of course, the number of waves - basis vectors for the transfer matrix - grows with the width of the band. The components of the eigenvectors of a tridiagonal  $A$  form a Sturm sequence, but wider bands begin to allow a certain number of coincident roots - related to the thicker nodes - which complicate discussions of the separation of frequencies, which bespeaks a possibility for degeneracy which is absent from tridiagonal matrices.

Since tridiagonal matrices already show most of the characteristics of polydiagonal matrices, but with  $2 \times 2$  matrices  $M_i$ , studying their properties is a good place to begin. To avoid working with fractions, the previous matrix elements can be assigned some letters, to obtain

$$\begin{bmatrix} x_{i+1} \\ x_i \end{bmatrix} = \begin{bmatrix} a\lambda - b & -c \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix}$$

Observing that

$$\begin{bmatrix} 1 & 0 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x_{i+1} \\ x_i \end{bmatrix} = \begin{bmatrix} a\lambda - b & -c \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_{i+1} \\ x_{i+1} - x_i \end{bmatrix}$$

it is easy enough to transform the equation into

$$\begin{bmatrix} x_{i+1} \\ x_{i+1} - x_i \end{bmatrix} = \begin{bmatrix} a\lambda - b - c & -c \\ a\lambda - b - c - 1 & 0 \end{bmatrix} \begin{bmatrix} x_i \\ x_i - x_{i-1} \end{bmatrix}.$$

The point of this exercise is to use a vector consisting of displacements and an approximation to their derivatives, and to show that the sequence of such vectors is generated the same way as before, albeit with a different matrix, whose characteristic equation has to be the same because of the similarity transformation.

The original form might as well be retained, along with the characteristic equation for the wave number,

$$\begin{vmatrix} a\lambda - b - \mu & -c \\ 1 & -\mu \end{vmatrix} = 0,$$

or

$$\mu^2 - \mu(a\lambda - b) + c = 0.$$

There is advantage to dividing the characteristic equation by the nonzero  $\mu\sqrt{c}$  ( $M$  must be invertible, so no root is zero;  $c$  cannot vanish) and writing

$$\frac{\mu}{\sqrt{c}} + \frac{\sqrt{c}}{\mu} = a\lambda - b.$$

The advantage lies in seeing the dispersion relation immediately, but also presenting the lefthand side as  $\cosh(t)$ , permissible if  $\mu/\sqrt{c} = \exp(t)/2$ . Should this series of substitutions seem somewhat contrived, bear in mind that we really want to raise  $M$  to powers, and that multiplying logarithms is a good way to do that. Not to be overlooked is that  $c$  would be 1 if the two bands of  $A$  were equal, and that balancing powers of  $\mu$  against their reciprocals to get hyperbolic cosines eventually depends of the form of the bands in a polydiagonal  $A$ .

Calling the two roots of the characteristic equation  $\mu+$  and  $\mu-$ , the (unnormalized) matrices of eigenvector rows and eigenvector columns are

$$U^{-1} = \begin{bmatrix} \mu+ & -c \\ \mu- & -c \end{bmatrix}$$

$$U = \begin{bmatrix} \mu+ & \mu- \\ 1 & 1 \end{bmatrix}.$$

With eigenrows and eigencolumns, the spectral decomposition is immediate:

$$M = \frac{\mu+}{\langle +|+ \rangle} |+\rangle \langle +| + \frac{\mu-}{\langle -|- \rangle} |-\rangle \langle -|$$

## 5.2 Sturm sequences

The matrix elements of each transfer matrix are polynomials with respect to the eigenvalue  $\lambda$ , beginning with the basic matrix whose 11 element is of the first degree in  $\lambda$ , which is absent from the remaining elements. Multiplying transfer matrices raises the degree of the matrix elements, the 11 element always retaining the highest degree - the sum of the degrees of the factors - when the matrices have the form we are using. Boundary conditions eventually dictate that some combination of matrix elements gives zero, which means the vanishment of a polynomial whose degree is the length of the string, whose expression is evidently the characteristic equation of  $A$ .

If the boundary condition is independent of the length of the string, there is a series of characteristic equations, each having a similar structure yet differing by the degree of the polynomial involved. Moreover, the peculiar structure of the matrix  $M$ , arising from the tautology which was incorporated in its definition, interlaces the polynomials used at each stage. It is worth seeing how this is done, in the simple case where the boundary condition is that there be a terminal node.

$$M_{i+1} = \begin{bmatrix} a\lambda - b & -c \\ 1 & 0 \end{bmatrix} \begin{bmatrix} P_{11}^i & P_{12}^i \\ P_{21}^i & P_{22}^i \end{bmatrix}$$

$$= \begin{bmatrix} (a\lambda - b)P_{11}^i & (a\lambda - b)P_{21}^i \\ P_{11}^i & P_{12}^i \end{bmatrix}$$

If the initial vector were  $(1, 0)$ , implying  $x_1 = 0, x_2 = 1$  (any factor will do), and the final vector were  $(0, 1)$  implying that  $x_{i+1}$  were also zero, then the 11 element of  $M_{i+1}$  would vanish, or

$$(a\lambda - b)P_{11}^i - cP_{21}^i = 0,$$

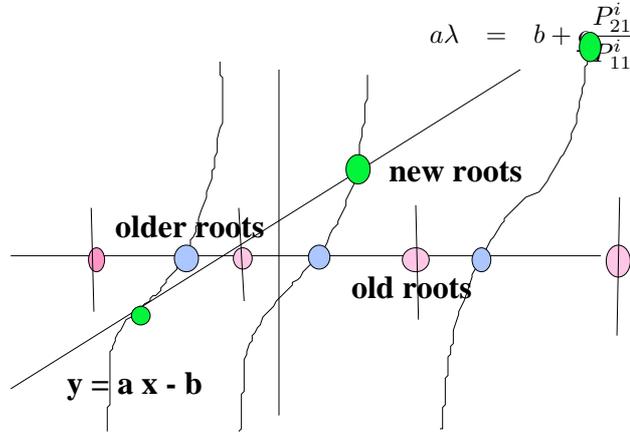


Figure 11: Interleaving of eigenvalues

The new roots lie on a line determined by the diagonal element of  $A$  with slope likewise determined by  $A$  - the ratio of its diagonal to off-diagonal elements. The roots also lie on the quotient of two polynomials; the zeroes of the denominator are just the roots of the next smaller  $A$ , the roots of the numerator are those of the second previous  $A$ . Not both polynomials have roots in the same place because of the limit on the maximal thickness of a node. Thus zeros and poles of the quotient alternate, and the new roots lie between the poles so they are also separated. Thus all roots are distinct, and interleaved; this is called a Sturm sequence.

There are interesting details in the graph which has been sketched. The derivative of the quotient is nonzero and always has a consistent sign, making it monotone within the panels delimited by its poles. Consequently the intersecting line crosses the quotient just once in each panel, assuring the interleaving of roots and keeping them real. The root cause of all this is the sign-symmetry of the matrix  $A$ ; were it sign-antisymmetric, roots would have to run along in conjugate pairs. In fact, the interleaving property was already proved on more general grounds by Ledermann, so that we mainly have a more graphic presentation of the result.

The value where the line crosses the axis is the diagonal element of the bordering matrix, which will not be an eigenvalue although it will necessarily sit between some pair of old roots. It acts as a center of readjustment, crowding new eigenvalues toward the edges of the panels defined by the old eigenvalues while distancing them from still older eigenvalues. Eventually there will be very little change in eigenvalues far from that diagonal element since the line will intersect the quotient near its asymptotes, but finally one of the new eigenvalues will lie outside the range established previously.

### 5.3 A uniform treatment for 2x2 matrices

The foregoing discussion is related to the Riactti transformation for differential equations, wherein a linear system is converted into a nonlinear system (actually, a second order system) by introducing

a quotient of the linear solutions. The quotient would also be the basis for a continued fraction exposition of the properties of the solutions of the recursion equation, but nowadays matrix theory is more familiar than continued fraction theory which is why it is used instead.

Nevertheless, the graph of the quotient which figures in the development just outlined is very reminiscent of the graph of the tangent of a multiple angle, leading to the question: why not use the angle itself? This would be analogous to using the Prüfer transformation from differential equation theory, and is not so far from the appearance of hyperbolic cosines in the dispersion relation.

### 5.3.1 quaternions versus elementary matrices

The best way to get this point of view, and at the same time give the whole topic of  $2 \times 2$  matrices an elegant formulation, is to use quaternions. Starting from the natural basis for  $2 \times 2$  matrices,

$$\begin{aligned} \mathbf{e}_{11} &= \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \\ \mathbf{e}_{12} &= \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \\ \mathbf{e}_{21} &= \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \\ \mathbf{e}_{22} &= \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}. \end{aligned}$$

whose rule of multiplication is  $\mathbf{e}_{ij}\mathbf{e}_{kl} = \delta_{jk}\mathbf{e}_{il}$ , quaternion-like matrices can be defined by

$$\begin{aligned} \mathbf{1} &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \\ \mathbf{i} &= \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \\ \mathbf{j} &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \\ \mathbf{k} &= \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \end{aligned}$$

In detail,

$$\mathbf{1} = \mathbf{e}_{11} + \mathbf{e}_{22}, \mathbf{i} = \mathbf{e}_{12} - \mathbf{e}_{21}, \mathbf{j} = \mathbf{e}_{12} + \mathbf{e}_{21}, \mathbf{k} = \mathbf{e}_{11} - \mathbf{e}_{22},$$

all built from sums and differences, thereby retaining real matrices. Like quaternions, these matrices anticommute (except for the identity), so the difference is that only one square is  $-\mathbf{1}$ , the others are  $+\mathbf{1}$ . Because of that, exponentials will follow Euler's formula by using either trigonometric or hyperbolic functions according to the sign.

The multiplication table is

	<b>1</b>	<b>i</b>	<b>j</b>	<b>k</b>
<b>1</b>	<b>1</b>	<b>i</b>	<b>j</b>	<b>k</b>
<b>i</b>	<b>i</b>	<b>-1</b>	<b>k</b>	<b>-j</b>
<b>j</b>	<b>j</b>	<b>-k</b>	<b>1</b>	<b>-i</b>
<b>k</b>	<b>k</b>	<b>j</b>	<b>i</b>	<b>1</b>

The usual way of performing algebraic operations on these matrices is to write a sum such as  $a\mathbf{1} + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$  in the form  $s + \mathbf{v}$ , where  $s = a\mathbf{1}$  and  $\mathbf{v}$  is the rest of the sum. Doing that allows writing

$$(s + \mathbf{u})(t + \mathbf{v}) = st + s\mathbf{v} + t\mathbf{u} + (\mathbf{u}\cdot\mathbf{v}) + (\mathbf{u} \times \mathbf{v}), \quad (1)$$

particular interest attaching to the case where  $s$  and  $t$  are zero, leaving the product of two vectors to take the form of a scalar plus a vector. However, the inner (or dot) product is not the usual one, rather one with a Minkowski type metric:

$$\begin{aligned} (\mathbf{u} \cdot \mathbf{v}) &= -u_1v_1 + u_2v_2 + u_3v_3, \\ &= \begin{bmatrix} u_1 & u_2 & u_3 \end{bmatrix} \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix}. \end{aligned}$$

Since the inner product for a Minkowski metric can be positive, negative, or zero, taking it for the square of a norm requires considering the sign, unless an imaginary norm is acceptable. So to define the norm of a vector, use the absolute value of the metric, by setting

$$|\mathbf{v}| = \sqrt{\text{abs}((\mathbf{v}, \mathbf{v}))},$$

note that it can vanish for a nonzero vector, and never forget the possible influence of the bypassed sign.

In turn the vector product differs slightly from its cartesian version. It is

$$\begin{aligned} \mathbf{u} \times \mathbf{v} &= (u_3v_2 - u_2v_3)\mathbf{i} + (u_3v_1 - u_1v_3)\mathbf{j} + (u_1v_2 - u_2v_1)\mathbf{k}. \\ &= - \begin{vmatrix} u_2 & u_3 \\ v_2 & v_3 \end{vmatrix} \mathbf{i} + \begin{vmatrix} u_3 & u_1 \\ v_3 & v_1 \end{vmatrix} \mathbf{j} + \begin{vmatrix} u_1 & u_2 \\ v_1 & v_2 \end{vmatrix} \mathbf{k} \\ &= \begin{vmatrix} -\mathbf{i} & \mathbf{j} & \mathbf{k} \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix} \end{aligned}$$

The latter formula, almost traditional, abuses determinantal notation. But this particular formula never implies any multiplication of quaternions, so it works out well enough, although differing from the classical formula in the sign of the term associated with  $\mathbf{i}$ .

### 5.3.2 quaternion inverse

The easiest way to get the inverse of a full quaternion  $a\mathbf{1} + \mathbf{v}$  is to go back to its representation by elementary matrices, in the  $2 \times 2$  form

$$a\mathbf{1} + b\mathbf{i} + c\mathbf{j} + d\mathbf{k} \rightarrow \begin{bmatrix} a + d & b + c \\ -b + c & a - d \end{bmatrix}.$$

The determinant,  $(a + d)(a - d) - (c + b)(c - b) = a^2 - d^2 + b^2 - c^2$ , which is  $a^2 - (\mathbf{v}, \mathbf{v})$ , could be considered to be a candidate for the square of the norm of a full quaternion, in contrast to the norm of a mere vector. Under that assumption, the formula for the inverse of a  $2 \times 2$  matrix gives the inverse quaternion

$$\frac{1}{(a^2 - |\mathbf{u}|^2)} \begin{bmatrix} a - d & -b - c \\ b - c & a + d \end{bmatrix} \rightarrow \frac{1}{(a^2 - |\mathbf{u}|^2)} (a\mathbf{1} - b\mathbf{i} - c\mathbf{j} - d\mathbf{k}).$$

which is almost the formula for inverting Hamilton's authentic quaternions, except for the way the norm is calculated.

Nevertheless, the difference is important, because null quaternions exist, just as well as null vectors, and they cannot be invertible. Hamilton's quaternions are invertible unless zero. Not only do they constitute a field, albeit noncommutative; they lie amongst the very few examples of algebraically and topologically complete infinite fields. The objects which we have just defined are not quaternions according to Hamilton's definition; neither are Hamilton's own quaternions taken with complex coefficients (look at  $(\mathbf{i} - i\mathbf{j})^2$ , which vanishes).

At least we have a quantity which decides the invertibility of a quaternion such as  $a\mathbf{1} + \mathbf{v}$ , multiplicative for being a determinant, and consistent with the definition of the vector norm relative to a sign choice.

$$\|a\mathbf{1} + \mathbf{v}\|^2 = a^2 - (\mathbf{v}, \mathbf{v})$$

### 5.3.3 null vectors

There are null vectors in the Minkowski metric, which is to say, nonzero vectors with zero norm. What would a null vector look like? Consider  $\sqrt{2}\mathbf{i} + \mathbf{j} + \mathbf{k}$ .

$$\begin{bmatrix} 1 & 1 + \sqrt{2} \\ 1 - \sqrt{2} & -1, \end{bmatrix}$$

whose trace and determinant are both zero, yet it is not the zero matrix. It has to have the Jordan normal form with eigenvalue zero. Those are generally the null vectors; by satisfying  $\mathbf{u}^2 = \mathbf{0}$ , they are their own eigenvectors, and manifestly nilpotent.

### 5.3.4 vector inverse

Since the square of a vector is not only a scalar, but the square of its Minkowski norm, it follows that it once divided by that norm, it is its own inverse, or that a unit vector is involutory. That is almost true, since the square of the vector can be negative; in that case the square root of the absolute value should be taken, and a minus sign should be appended to the inverse.

### 5.3.5 square roots

The unit quaternions are square roots of either unity or of minus one. Are there any others? According to Eq. 1, to get a root of unity needs

$$\begin{aligned} (s + \mathbf{u})^2 &= s^2 + 2s\mathbf{u} + (\mathbf{u}, \mathbf{u}) \\ &= \mathbf{1}, \end{aligned}$$

leading to two mutually exclusive alternatives

$$\begin{aligned} s^2 &= \mathbf{1} & \mathbf{u} &= \mathbf{0} \\ (\mathbf{u}, \mathbf{u}) &= \mathbf{1} & s &= 0. \end{aligned}$$

Besides the two expected scalar roots, any vector of unit norm fills the bill, infinitely many in all. A second glance at the derivation shows that any vector, the square of whose norm is  $-1$  (such as  $\mathbf{i}$ ) is a root of  $-\mathbf{1}$ , but that there are no (real) scalar roots.

As for square roots in general, the square root of any scalar follows the same line of reasoning with the exception that everything is scaled by the positive square root of the scalar when it has one. The general requirement for

$$s + \mathbf{u} = \sqrt{(t\mathbf{1} + \mathbf{v})}$$

would be

$$\begin{aligned} (s + \mathbf{u})^2 &= s^2 + 2s\mathbf{u} + (\mathbf{u}\cdot\mathbf{u}) \\ &= t\mathbf{1} + \mathbf{v}, \end{aligned}$$

which would require in succession

$$\begin{aligned} \mathbf{u} &= \frac{\mathbf{v}}{2s} \\ s^2 + \frac{(\mathbf{v}\cdot\mathbf{v})}{4s^2} &= t \\ s^2 &= \frac{1}{2}(t \pm \sqrt{t^2 - (\mathbf{v}\cdot\mathbf{v})}) \end{aligned}$$

If  $s$  were 0 then  $\mathbf{v}$  would have to be zero, and only a scalar could have a vector square root. But non-vector quaternions can have quaternion roots, of which there would appear to be exactly four possible values for  $s$ , not all necessarily real. For example,  $\sqrt{\mathbf{i}} = \pm(\mathbf{1} + \mathbf{i})/\sqrt{2}$ .

### 5.3.6 quaternionic eigenvectors

To find an eigenvector with respect to quaternion multiplication, consider that  $\mathbf{1}$  commutes with all quaternions, so adding or subtracting a scalar will only add or subtract from any eigenvalue, leaving the task of diagonalizing the vector part of the quaternion. In turn, a scalar factor of the vector will only multiply the eigenvalues by that factor, so the real task is finding eigenvectors of unit vectors - those of norm 1 or norm  $-1$  (and those of norm 0, for completeness). The eigenvalues of unit vectors had better be  $\pm 1$ , those of norm  $-1$  had better be  $\pm i$ , and those of the null vectors, 0.

Unit vector or not, we have two expressions, according to sign

$$\begin{aligned} \mathbf{v}(\mathbf{v} + |\mathbf{v}|\mathbf{1}) &= |\mathbf{v}|^2\mathbf{1} + |\mathbf{v}|\mathbf{v} \\ &= |\mathbf{v}|(\mathbf{v} + |\mathbf{v}|\mathbf{1}) \\ \mathbf{v}(\mathbf{v} - |\mathbf{v}|\mathbf{1}) &= |\mathbf{v}|^2\mathbf{1} - |\mathbf{v}|\mathbf{v} \\ &= -|\mathbf{v}|(\mathbf{v} - |\mathbf{v}|\mathbf{1}). \end{aligned}$$

In other words, its norm is  $\mathbf{v}$ 's eigenvalue, with associated eigenvector given by the formula.

Although these formulae give eigenmatrices, the matrices are singular, containing each eigencolumn twice, each eigenrow twice. It would be nice to get one of each, and both in the same matrix. Try

$$\begin{aligned} \mathbf{v}(\mathbf{v} + |\mathbf{v}|\mathbf{k}) &= |\mathbf{v}|^2\mathbf{1} + |\mathbf{v}|\mathbf{v}\mathbf{k} \\ &= \mathbf{v}|\mathbf{v}|\mathbf{k} + |\mathbf{v}|\mathbf{k}|\mathbf{v}|\mathbf{k} \\ &= (\mathbf{v} + |\mathbf{v}|\mathbf{k})(|\mathbf{v}|\mathbf{k}), \end{aligned}$$

and it works.

### 5.3.7 vector exponential

All this introduction may look tedious, but its reward is to be found in the elegance and beauty of the exponential of a vector, defined according to the traditional power series.

$$\begin{aligned}
 \exp(\mathbf{v}) &= \mathbf{1} + \mathbf{v} + \frac{1}{2!}\mathbf{v}^2 + \frac{1}{3!}\mathbf{v}^3 + \dots \\
 &= [\mathbf{1} + \frac{1}{2!}(\mathbf{v} \cdot \mathbf{v}) + \frac{1}{4!}(\mathbf{v} \cdot \mathbf{v})^2 + \dots] + \\
 &\quad \frac{\mathbf{v}}{\sqrt{(\mathbf{v} \cdot \mathbf{v})}} [\sqrt{(\mathbf{v} \cdot \mathbf{v})} + \frac{1}{3!}\sqrt{(\mathbf{v} \cdot \mathbf{v})}^3 + \dots] \\
 &= \mathbf{1} \cosh(\sqrt{(\mathbf{v} \cdot \mathbf{v})}) + \frac{\mathbf{v}}{\sqrt{(\mathbf{v} \cdot \mathbf{v})}} \sinh(\sqrt{(\mathbf{v} \cdot \mathbf{v})}), \\
 &= \mathbf{1} \cosh(|\mathbf{v}|) + \frac{\mathbf{v}}{|\mathbf{v}|} \sinh(|\mathbf{v}|)
 \end{aligned}$$

generalizing Euler's formula. The exponential of a quaternion is not much more complicated, since any scalar which could be added would commute with the quaternion, so its exponential could just be set aside as a multiplying scalar factor. How much to set aside in the general case depends on satisfying the identity  $\cosh^2(x) - \sinh^2(x) = 1$ , but in general there is much to be said in favor of working with vectors of unit norm and treating norms separately.

So, where is all that beauty? In great part, it lies in the law of exponents. Notice that the angle,  $\sqrt{(\mathbf{v} \cdot \mathbf{v})}$ , is the norm of  $\mathbf{v}$ , and that imaginary quantities can be avoided by using trigonometric functions, such as should be done in association with the quaternion  $\mathbf{i}$ .

Consider, for unit vectors  $\mathbf{u}$  and  $\mathbf{v}$ ,

$$\begin{aligned}
 \exp(\alpha\mathbf{u}) \exp(\beta\mathbf{v}) &= (\mathbf{1} \cosh(\alpha) + \mathbf{u} \sinh(\alpha))(\mathbf{1} \cosh(\beta) + \mathbf{v} \sinh(\beta)) \\
 &= \mathbf{1}(\cosh(\alpha) \cosh(\beta) + \sinh(\alpha) \sinh(\beta)(\mathbf{u} \cdot \mathbf{v})) + \\
 &\quad \mathbf{u} \sinh(\alpha) \cosh(\beta) + \mathbf{v} \cosh(\alpha) \sinh(\beta) + \\
 &\quad (\mathbf{u} \times \mathbf{v}) \sinh(\alpha) \sinh(\beta),
 \end{aligned}$$

and the prospects for seeing this as

$$\exp(\gamma\mathbf{w}) = \mathbf{1} \cosh(\gamma) + \mathbf{w} \sinh(\gamma).$$

Just define a new angle,  $\cosh(\theta) = (\mathbf{u} \cdot \mathbf{v})$ ; then copy the two parts of the previous result:

$$\begin{aligned}
 \cosh(\gamma) &= \cosh(\alpha) \cosh(\beta) + \sinh(\alpha) \sinh(\beta) \cosh(\theta), \\
 \mathbf{w} &= \mathbf{u} \sinh(\alpha) \cosh(\beta) + \mathbf{v} \cosh(\alpha) \sinh(\beta) + \\
 &\quad (\mathbf{u} \times \mathbf{v}) \sinh(\alpha) \sinh(\beta).
 \end{aligned}$$

Somewhere between trivial and formidable, the definition begins by ascertaining the angle  $|\gamma|$  using a formula reminiscent of the spherical law of cosines, but in actuality the variant relevant to a two-sheeted hyperboloid of revolution. Once that much is known, the vector  $\mathbf{w}$  is defined in terms of known quantities, for which it can be said that it lies off the plane of  $\mathbf{u}$  and  $\mathbf{v}$  unless they lie on a line, in which case  $\mathbf{w}$  falls on the same line giving a much more familiar law of exponents. By the antisymmetry of the cross product, when the order of the factors is reversed,  $\mathbf{w}$  moves to the other side of the  $\mathbf{u} - \mathbf{v}$  plane.

### 5.3.8 relation to complex numbers

This collection of arithmetic curiosities can be summarized by referring to the original objective in introducing quaternions, to be able to rotate vectors. Rotating implies angles, and suggests polar coordinates. In the familiar environment of complex numbers, the norm is the radius and the argument is the angle measured from the real axis. Real and imaginary refer to cartesian coordinates. The following table draws analogies between complex numbers, Hamilton's quaternions, and the  $2 \times 2$  matrices.

concept	complex	quaternion	$2 \times 2$ matrix
number	$z = x + iy$	$\mathbf{q} = a\mathbf{1} + b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$	$m = \begin{bmatrix} p & r \\ s & t \end{bmatrix}$
real part	$x$	$a$	$\begin{bmatrix} \frac{p+t}{2} & 0 \\ 0 & \frac{p+t}{2} \end{bmatrix}$
remaining part	$y$	$b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$	$\begin{bmatrix} \frac{p-t}{2} & r \\ s & -\frac{p-t}{2} \end{bmatrix}$
conjugate	$z^* = x - iy$	$\mathbf{q}^* = a\mathbf{1} - b\mathbf{i} - c\mathbf{j} - d\mathbf{k}$	$\dots$
adjugate	$\dots$	$b\mathbf{i} + c\mathbf{j} + d\mathbf{k}$	$\begin{bmatrix} t & -r \\ -s & p \end{bmatrix}$
squared norm	$ z ^2 = x^2 + y^2$	$\ \mathbf{q}\ ^2 = a^2 + b^2 + c^2 + d^2$	$\det(m) = pt - rs$
angle	$\phi = \arctan \frac{y}{x}$	$\cosh(\phi) = \frac{ \mathbf{u} }{a}$	$\cosh(\phi) = \frac{1}{2}\text{trace}(m)$
inverse	$\frac{x-iy}{x^2+y^2}$	$\frac{\mathbf{q}^*}{\ \mathbf{q}\ ^2}$	$\frac{1}{pt-rs} \begin{bmatrix} t & -r \\ -s & p \end{bmatrix}$
polar form	$ z  \exp(i\phi)$	$\ \mathbf{q}\  \exp(\mathbf{u}\phi)$	

## 6 Applications to String Vibrations

To illustrate the quaternion representation, a series of examples from the theory of electrical transmission lines, or equivalently, the small vibrations of a classical string, can show both some mathematical techniques and illustrate diverse properties of these systems.

### 6.1 Description of the physical problem

Suppose that there is an indexed system of particles, each bound to a position of repose by an elastic spring obeying Hooke's law while its excursions from equilibrium follow Newton's law:

$$m_i \frac{d^2 x_i}{dt^2} = -k_i x_i.$$

Subscripting all three, displacements from rest, masses, and elastic constants, implies that in full generality, every particle has its own characteristics and environment. The solutions to differential equations such as these are well known to be sines and cosines, or phased cosines, or even complex exponentials taken up in real combinations.

An easy way of letting some of these particles be influenced by their neighbors is to suppose the existence of additional elastic springs whereby the displacement of one particle from its equilibrium exerts a force on some other particle - in the direction of the displacement, in contrast to the force felt from a particle's own displacement, which urges it back to whence it came. If the influence extends to neighboring particles and no farther, a collection of differential equations describing the motion would be

$$m_i \frac{d^2 x_i}{dt^2} = k_{i-1} x_{i-1} - (k_{i-1} + k_i + k_{i+1}) x_i + k_{i+1} x_{i+1}.$$

In these equations, signs have been chosen so that the symbols themselves represent positive quantities. The middle terms are negative because all springs restrain a moved particle if the others are fixed at their origins.

The system can be placed in a more agreeable form by transformations which can either be made at the outset, or incorporated later by suitable matrix transformations, but the present interest is in the matrix, not the physics. Suffice it to say that multiplying by square roots of masses solves the immediate problem (or just suppose they all equal one gram, or adjust the unit of time to compensate) and get on with the differential equation which still lets the elastic constants vary. There is a vector of coordinates and a matrix of elastic constants satisfying the differential equation

$$\frac{d^2}{dt^2} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \dots \end{bmatrix} = \begin{bmatrix} \frac{k_{11}}{m_1} & \frac{k_{12}}{\sqrt{m_1}\sqrt{m_2}} & \cdot & \cdot & \cdot \\ \frac{k_{21}}{\sqrt{m_2}\sqrt{m_1}} & \frac{k_{22}}{m_2} & \frac{k_{23}}{\sqrt{m_2}\sqrt{m_3}} & \cdot & \cdot \\ \cdot & \frac{k_{32}}{\sqrt{m_3}\sqrt{m_2}} & \frac{k_{33}}{m_3} & \frac{k_{34}}{\sqrt{m_3}\sqrt{m_4}} & \cdot \\ \cdot & \cdot & \frac{k_{32}}{\sqrt{m_3}\sqrt{m_2}} & \frac{k_{11}}{m_1} & \frac{k_{12}}{\sqrt{m_1}\sqrt{m_2}} \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \dots \end{bmatrix}$$

### 6.2 Solving the vibration equations

Without going too deeply into differential equation theory, one way to solve the equation is to diagonalize the matrix of coefficients, which can be done by a constant transformation that is

invisible to the second derivative, once again solving differential equations in a single variable, setting out initial conditions, and transforming back to the coupled equations. Each eigenvector, which is called a normal mode, has its own time dependence, that of the overall system is their sum. An alternative would be to postulate exponential solutions, note that the second derivative multiplies the left hand vector by the square of the frequency, and treat discovering the frequencies as an eigenvalue problem. Either route requires diagonalizing the tridiagonal matrix of coefficients.

Using matrix algebra, and assuming that matrix calculus differs from scalar calculus mostly through the necessity to maintain the order of factors in a product and to write inverses where they belong instead of quotients, it is easy to describe the solution to forced motion once it is assumed that free motion is governed by the matrix exponential solution to a system of second order equations with constant coefficients.

### 6.2.1 solving inhomogeneous equations

First, consider a system inhomogeneous equations written in matrix form:

$$\frac{dZ}{dt} = RZ + F$$

$Z$  could be a vector, but all the linearly independent solutions of the system can be treated simultaneously by gathering them up into a matrix as columns. In that case the forcing terms  $F$  should be spread out into a matrix as well.

Now suppose that  $Z = UV$  and recall the rule for differentiating a product:

$$\frac{dUV}{dt} = \frac{dU}{dt}V + U\frac{dV}{dt},$$

whereupon

$$\frac{dU}{dt}V + U\frac{dV}{dt} = RUV + F.$$

If the homogeneous equation

$$\frac{dU}{dt} = RU,$$

has already been solved, especially from the unit matrix as an initial condition, its terms would drop out of the equation, leaving

$$\begin{aligned} U\frac{dV}{dt} &= F, \\ \frac{dV}{dt} &= U^{-1}F, \end{aligned}$$

At this stage, the right hand side of the equation is a completely known matrix of functions, characterizing the solution as a quadrature:

$$V(t) = V(0) + \int_0^t U^{-1}(\sigma)F(\sigma)d\sigma,$$

and the entire solution by:

$$Z(t) = U(t)Z(0) + \int_0^t U(t)U^{-1}(\sigma)F(\sigma)d\sigma,$$

### 6.2.2 solving second order equations

A second order version of the inhomogeneous system which has just been solved, suitable for a chain of particles, would read

$$M \frac{d^2 X}{dt^2} = -KX + F.$$

It should be turned into a pair of first order systems by inventing momenta (mass times velocity), but splitting the mass coefficient in the interests of having a symmetrical dynamical matrix to diagonalize later on:

$$\begin{aligned} \sqrt{(M)} \frac{dX}{dt} &= \sqrt{(M)}^{-1} P \\ \sqrt{(M)}^{-1} \frac{dP}{dt} &= -\sqrt{(M)}^{-1} K \sqrt{(M)}^{-1} \sqrt{(M)} X + \sqrt{(M)}^{-1} F. \end{aligned}$$

For the sake of not writing so many mass radicals, weighted coordinates and momenta could be introduced, and the elastic matrix replaced by a dynamical matrix. The forcing term might as well be adjusted too. So define:

$$\begin{aligned} \xi &= \sqrt{(M)} X \\ \pi &= \sqrt{(M)}^{-1} P \\ \kappa &= \sqrt{(M)}^{-1} K \sqrt{(M)}^{-1} \\ f &= \sqrt{(M)}^{-1} F \end{aligned}$$

to have the pair of systems of equations summarized in one matrix equation,

$$\frac{d}{dt} \begin{bmatrix} \pi \\ \xi \end{bmatrix} = \begin{bmatrix} 0 & -\kappa \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \pi \\ \xi \end{bmatrix} + \begin{bmatrix} f \\ 0 \end{bmatrix}$$

The coefficient matrix is a matrix of constants, so the solution of the homogeneous equation is a matrix exponential. Furthermore, since

$$\begin{bmatrix} 0 & -\kappa \\ 1 & 0 \end{bmatrix}^2 = \begin{bmatrix} -\kappa & 0 \\ 0 & -\kappa \end{bmatrix},$$

there is an Euler's formula

$$\begin{aligned} \exp\left(\begin{bmatrix} 0 & -\kappa \\ 1 & 0 \end{bmatrix} t\right) &= \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \cos(\sqrt{\kappa} t) + \begin{bmatrix} 0 & -\kappa \\ 1 & 0 \end{bmatrix} \sqrt{\kappa}^{-1} \sin(\sqrt{\kappa} t) \\ &= \begin{bmatrix} \cos(\sqrt{\kappa} t) & -\sqrt{\kappa} \sin(\sqrt{\kappa} t) \\ \sqrt{\kappa}^{-1} \sin(\sqrt{\kappa} t) & \cos(\sqrt{\kappa} t) \end{bmatrix}. \end{aligned}$$

Note that since  $\kappa$  is a matrix, it could only invite misunderstandings to write  $1/\sqrt{\kappa}$  instead of  $\sqrt{\kappa}^{-1}$  in these formulas.

Turning at last to the inhomogeneous term, the overall solution is

$$\begin{aligned} \begin{bmatrix} \pi(t) \\ \xi(t) \end{bmatrix} &= \begin{bmatrix} \cos(\sqrt{\kappa} t) & -\sqrt{\kappa} \sin(\sqrt{\kappa} t) \\ \sqrt{\kappa}^{-1} \sin(\sqrt{\kappa} t) & \cos(\sqrt{\kappa} t) \end{bmatrix} \begin{bmatrix} \pi(0) \\ \xi(0) \end{bmatrix} \\ &+ \int_0^t \begin{bmatrix} \cos(\sqrt{\kappa}(t-\sigma)) & -\sqrt{\kappa} \sin(\sqrt{\kappa}(t-\sigma)) \\ \sqrt{\kappa}^{-1} \sin(\sqrt{\kappa}(t-\sigma)) & \cos(\sqrt{\kappa}(t-\sigma)) \end{bmatrix} \begin{bmatrix} f(\sigma) \\ 0 \end{bmatrix} d\sigma. \end{aligned}$$

The integral, which makes a sine or cosine transform of the forcing function, has various interpretations, one of which is that it reduces all the accumulated forces to equivalent initial conditions which then modify the stated initial conditions propagate the result up to time  $t$ . The forcing function can be a pulse, a function of limited duration, or a permanent influence. Supposing the latter to be a harmonic force, say a sine or cosine itself, the phenomenon of resonance makes its appearance. Assuming that  $\kappa$  were diagonal, there would be a series of scalar (really, 2x2) equations saying (putting  $\sqrt{\kappa} = \omega_0$  and  $f = \sin(\omega t)$ )

$$\begin{aligned}\xi(t) &= \text{initialvalue} + \frac{1}{\omega_0} \int_0^t \sin(\omega_0(t - \sigma)) \sin(\omega\sigma) d\sigma \\ &= \text{initialvalue} + \frac{1}{2\omega_0} \int_0^t (\cos(\omega_0 t - (\omega_0 - \omega)\sigma) - \cos(\omega_0 t - (\omega_0 + \omega)\sigma)) d\sigma \\ &= \text{initialvalue} + \left[ \frac{\sin(\omega_0 t - (\omega_0 - \omega)\sigma)}{2\omega_0(\omega_0 - \omega)} + \frac{\sin(\omega_0 t - (\omega_0 + \omega)\sigma)}{2\omega_0(\omega_0 + \omega)} \right]_0^t\end{aligned}$$

Given that  $\omega_0$  is (the square root of) an eigenvalue, and that its provenance from a square root could endow it with either sign, one of the two terms will have a zero denominator whenever the forcing frequency coincides with  $\omega_0$ . No doubt physicists and engineers first became aware of eigenvalues on account of this circumstance. Although the denominator could be zero, that does not mean that the amplitude is immediately infinite, only that it will build up without limit. The integral with  $\omega = \omega_0$  has a constant integrand, and the amplitude will build linearly at first, giving the zero denominator time to take effect.

In practice, a mechanical system would have friction, which would render  $\omega_0$  complex, so resonances could be large without becoming infinite. Equivalently, the exciting force could be damped, with an implicit complex  $\omega$ , so the excitation would never last long enough to build up to an extreme amplitude.

## 7 A Variety of String Vibration Examples

There are some standard layouts which give various insights into the vibrations of a string, some of which will be discussed as examples.

1. uniform string with fixed ends,
2. uniform string with unrestrained ends,
3. two half-strings joined in the middle,
4. two half-strings with an impedance-matching joint,
5. a diatomic string - one with two masses alternating heavy, light,
6. a string with a point defect, say a discrepant mass,
7. a string with an insert larger than a point, of a different material,
8. a whip, with mass continuously varying from one end to the other.
9. a disordered string, whose masses and elastic constants are chosen at random from a probability distribution.

### 7.1 Uniform strings

The tridiagonal matrix for the vibrations of a uniform string consisting of particles of mass  $m$  connected by springs of elastic constant  $k$ , none of whose particles is bound in place (all the oscillations are due to the influence of the particles on one another) would have the form

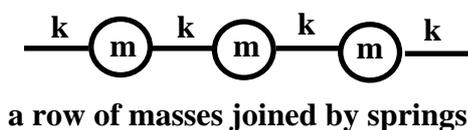


Figure 12: a row of identical masses connected by identical springs

$$A = \frac{k}{m} \begin{bmatrix} -2 & 1 & . & . & . & . \\ 1 & -2 & 1 & . & . & . \\ . & 1 & -2 & 1 & . & . \\ . & . & 1 & -2 & 1 & . \\ . & . & . & . & . & . \end{bmatrix}.$$

### 7.1.1 eigenvalues and eigenvectors

The equations for the wave matrices would all have the form

$$\begin{bmatrix} x_{i+1} \\ x_i \end{bmatrix} = \begin{bmatrix} \frac{m\lambda}{k} - 2 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix},$$

whose characteristic equation, or dispersion relation, could be written in one of the other of two forms, the first favoring trigonometry and the second, half-angles:

$$\begin{aligned} \mu^2 - \mu\left(\frac{m\lambda}{k} - 2\right) + 1 &= 0, \\ \left(\sqrt{\mu} + \frac{1}{\sqrt{\mu}}\right)^2 &= \frac{m\lambda}{k}. \end{aligned}$$

Matrices of (unnormalized) row and column eigenvectors are as before,

$$\begin{aligned} (\text{rows}) &= \begin{bmatrix} \mu_+ & -1 \\ \mu_- & -1 \end{bmatrix} \\ (\text{columns}) &= \begin{bmatrix} \mu_+ & \mu_- \\ 1 & 1 \end{bmatrix} \end{aligned}$$

making Sylverster's theorem read:

$$f(M) = \frac{f(\mu_+)}{(\mu_+^2 - 1)} \begin{bmatrix} \mu_+ \\ 1 \end{bmatrix} \begin{bmatrix} \mu_+ & -1 \end{bmatrix} + \frac{f(\mu_-)}{(\mu_-^2 - 1)} \begin{bmatrix} \mu_- \\ 1 \end{bmatrix} \begin{bmatrix} \mu_- & -1 \end{bmatrix}$$

### 7.1.2 Tchebycheff polynomials

This expression simplifies drastically when  $\mu$  is written as an exponential,  $\mu = \exp(\varphi)$ , and it is supposed that  $f$  is an  $n^{\text{th}}$  power:

$$\begin{aligned} M^n &= \frac{\exp(n\varphi_+)}{\exp(2\varphi_+) - 1} \begin{bmatrix} \exp(\varphi_+) \\ 1 \end{bmatrix} \begin{bmatrix} \exp(\varphi_+) & -1 \end{bmatrix} + \\ &\quad \frac{\exp(n\varphi_-)}{\exp(2\varphi_-) - 1} \begin{bmatrix} \exp(\varphi_-) \\ 1 \end{bmatrix} \begin{bmatrix} \exp(\varphi_-) & -1 \end{bmatrix}, \\ &= \frac{1}{\exp(2\varphi_+) - 1} \begin{bmatrix} \exp((n+2)\varphi_+) & \exp((n+1)\varphi_+) \\ \exp((n+1)\varphi_+) & \exp(n\varphi_+) \end{bmatrix} + \\ &\quad \frac{1}{\exp(2\varphi_-) - 1} \begin{bmatrix} \exp((n+2)\varphi_-) & \exp((n+1)\varphi_-) \\ \exp((n+1)\varphi_-) & \exp(n\varphi_-) \end{bmatrix} \end{aligned}$$

Still further simplification awaits: First take exponential factors out of the denominators

$$\begin{aligned} M^n &= \frac{1}{\exp(\varphi_+) - \exp(-\varphi_+)} \begin{bmatrix} \exp((n+1)\varphi_+) & -\exp(n\varphi_+) \\ \exp(n\varphi_+) & -\exp((n-1)\varphi_+) \end{bmatrix} + \\ &\quad \frac{1}{\exp(\varphi_-) - \exp(-\varphi_-)} \begin{bmatrix} \exp((n+1)\varphi_-) & -\exp(n\varphi_-) \\ \exp(n\varphi_-) & -\exp((n-1)\varphi_-) \end{bmatrix} \end{aligned}$$

and then recognize that the  $\mu$ 's are reciprocals, so their logarithms are negatives. The matrix  $M^n$  is accordingly a function of a single angle and with common denominators the sum becomes a difference:

$$M^n = \frac{1}{\sinh(\varphi)} \begin{bmatrix} \sinh((n+1)\varphi) & -\sinh(n\varphi) \\ \sinh(n\varphi) & -\sinh((n-1)\varphi) \end{bmatrix}$$

Moreover, the matrix elements, with the participation of the obstreperous denominators, are nothing other than Tchebycheff polynomials of the second kind (with imaginary argument),

$$U_n(\cos(\varphi)) = \frac{\sin((n+1)\varphi)}{\sin(\varphi)},$$

the denominator  $\sin(\varphi)$  generally serving to make derivatives turn out right.

$$M^n = \begin{bmatrix} U_n(\cos(\varphi)) & -U_{n-1}(\cos(\varphi)) \\ U_{n-1}(\cos(\varphi)) & -U_{n-2}(\cos(\varphi)) \end{bmatrix}$$

Some patience with trigonometric identities will confirm  $M^m M^n = M^{m+n}$ , which must be so because of the context in which it occurs.

Slight additional trigonometrical transformation (writing s and c for sinh and cosh to fit the formula onto the page) produces

$$\begin{aligned} M^n &= \frac{1}{\sinh(\varphi)} \begin{bmatrix} \sinh((n+1)\varphi) & -\sinh(n\varphi) \\ \sinh(n\varphi) & -\sinh((n-1)\varphi) \end{bmatrix} \\ &= \frac{1}{\sinh(\varphi)} \begin{bmatrix} s(n\varphi)c(\varphi) + c(n\varphi)s(\varphi) & -\sinh(n\varphi) \\ \sinh(n\varphi) & -s(n\varphi)c(\varphi) + c(n\varphi)s(\varphi) \end{bmatrix} \\ &= \cosh(n\varphi) \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{\sinh(n\varphi)}{\sinh(\varphi)} \begin{bmatrix} \cosh(\varphi) & -1 \\ 1 & -\cosh(\varphi) \end{bmatrix} \\ &= \exp \left( n\varphi \begin{bmatrix} \cosh(\varphi) & -1 \\ 1 & -\cosh(\varphi) \end{bmatrix} \right). \end{aligned}$$

The algebra of the wave matrices having been attended to, the determination of the eigenvalues of the dynamical matrix depends on choosing appropriate boundary conditions for a relationship such as

$$X_n = M^n X_1.$$

### 7.1.3 boundary conditions and the spectrum

An expedient, and sometimes physically appropriate, condition is to suppose that the string closes upon itself, treating the first particle as though it were an  $(n+1)^{st}$  particle; the cyclic boundary condition would require a unit matrix:

$$M^n = I.$$

Two of the four requirements on the matrix elements of  $M^n$  are identical but all four are consistent:

$$\begin{aligned} U_{n-1}(\cosh(\varphi)) &= 0, \\ \frac{\sinh(n\varphi)}{\sinh(\varphi)} &= 0, \\ \varphi &= i \frac{k\pi}{n}. \end{aligned}$$

With such values of  $\varphi$  ( $\varphi = 0$  being excluded),  $\mu = \exp(i\frac{k\pi}{n})$ , leaving

$$\lambda = \frac{4k}{m} \cos(2\frac{k\pi}{2n})$$

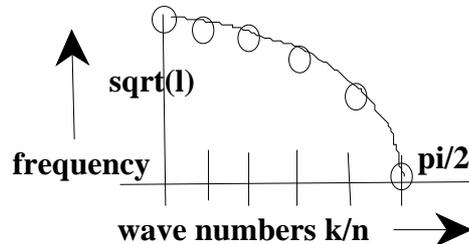


Figure 13: the dispersion relation for a uniform string

To check whether this is credible, suppose there is only one single particle. Then no shift is needed,  $n = 1$ , and  $M$  ought to be the unit matrix. So  $\lambda = 0$ , there is no restoring force, and the result is correct. If there were two particles,  $\lambda = 0$  persists, but for  $k = 1$ ,  $\lambda = 2k/m$  is also possible, appropriate to having a pair of springs to connect the particles.

Altogether there are many other ways of assigning boundary conditions to a string. which can be broadly subclassified into boundary values and boundary conditions. A boundary value specifies the value of a component, such as making it zero to signify that the particle is constrained so that it cannot move. A boundary condition specifies a linear combination of components, and would be realized as a row vector whose inner product with a wave vector would vanish, for instance. The two kinds of condition mostly state the same information in two different ways. Whatever their form, an expression relating elements of the wave matrix must vanish, producing a polynomial equation which is the characteristic polynomial of the dynamical matrix. Since the arguments of the polynomial are built from wave numbers, the characteristic equation is a dispersion relation.

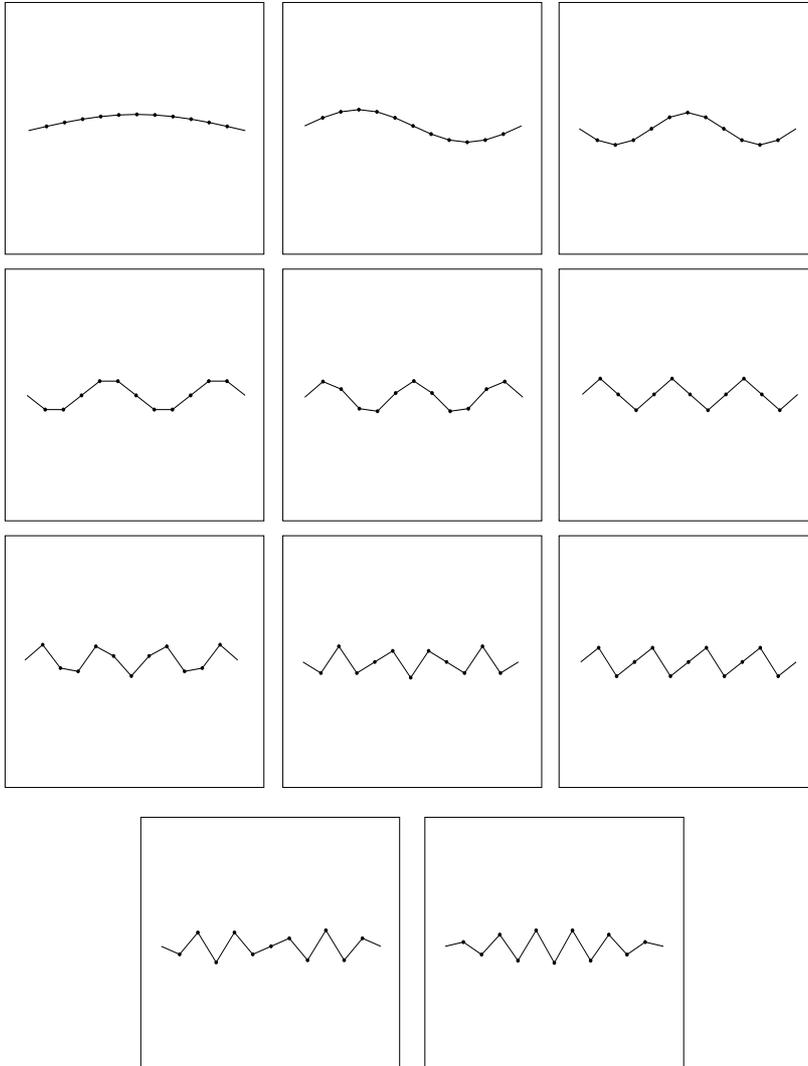


Figure 14: Normal modes of a uniform chain of eleven particles with with fixed ends. The amplitude distribution of the displacements of the particles is sinusoidal, each normal mode displaying one additional node as its frequency increases. The only nodes for the lowest frequency are the points of restraint, each particle having approximately the same displacement as its neighbors. Nodes for the highest frequency lie between adjacent particles, each of which keeps as great a distance from its neighbor as possible.

## 7.2 Joining dissimilar strings

Solving a uniform string with wave matrices requires powers of a single wave matrix, which turns out to be a convenient combination of Tchebycheff polynomials. Mixing wave matrices for nonuniform strings is more complicated algebraically, not only because the wave matrices don't commute, but also because the wave matrix at the joint is slightly different. To start with a simple example, consider two dissimilar strings joined together.

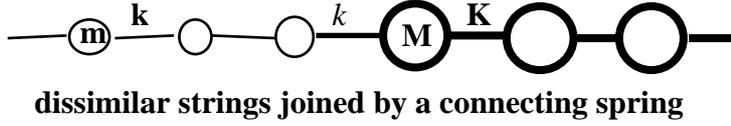


Figure 15: two strings spliced by a single connecting spring

The dynamical matrix would look like:

$$A = \begin{bmatrix} \cdots & \cdot & \cdots \\ \cdots & \frac{k}{m} & \frac{-2k}{m} & \frac{k}{m} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cdot & \frac{k}{m} & \frac{-2k}{m} & \frac{k}{m} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cdot & \cdot & \frac{k}{m} & \frac{-k-kk}{m} & \frac{kk}{\sqrt{(mM)}} & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cdot & \cdot & \cdot & \frac{kk}{\sqrt{(mM)}} & \frac{-kk-K}{M} & \frac{K}{M} & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cdot & \cdot & \cdot & \cdot & \frac{K}{M} & \frac{-2K}{M} & \frac{K}{M} & \cdot & \cdot & \cdots \\ \cdots & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{K}{M} & \frac{-2K}{M} & \frac{K}{M} & \cdot & \cdots \\ \cdots & \cdot & \cdots \end{bmatrix}$$

with two lines of recursion differing from those in the main body of the matrix. They only affect the wave matrix in the respect that its 12 element is no longer  $-1$ , but something else. In terms of masses  $m$  and  $M$ , with elastic constants  $k$ ,  $K$ , and an intermediate  $k'$ , we need

$$\begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{a}{c} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{c}{b} \\ 1 & 0 \end{bmatrix}$$

in terms of their eigenvalues and eigenvectors (or else to endure the algebra resulting from using them in their crude form).

A first observation is that the two new wave matrices are probably not unimodular (determinant 1), an essential requirement for the derivation of the uniform chain just given, but easily remedied by division of the whole matrix by the square root of their determinant. The result is

$$\sqrt{\frac{c}{a}} \begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{a}{c} \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} \frac{\lambda+a+c}{\sqrt{(ac)}} & -\sqrt{\frac{a}{c}} \\ \sqrt{\frac{c}{a}} & 0 \end{bmatrix},$$

with dispersion relation

$$(-\mu) \frac{\lambda + a + c}{\sqrt{ac}} - \mu + 1 = 0;$$

as before, it can be rewritten

$$2 \cosh(\varphi) = \frac{\lambda + a + c}{\sqrt{ac}};$$

the half-angle formula could even be extracted with a little initiative. However, the eigenvector matrices change over into

$$\begin{aligned} (\text{rows}) &= \begin{bmatrix} \mu_+ & -\sqrt{\frac{a}{c}} \\ \mu_- & -\sqrt{\frac{a}{c}} \end{bmatrix} \\ (\text{columns}) &= \begin{bmatrix} \sqrt{\frac{a}{c}}\mu_+ & \sqrt{\frac{a}{c}}\mu_- \\ 1 & 1 \end{bmatrix} \end{aligned}$$

leaving a normalization factor of  $(\mu^2 - 1)\sqrt{a/c}$  for Sylvester's theorem, which is not only a numerical multiple of the previous normalizer, but one which is the same for both eigenvalues. Moreover the projectors themselves will behave consistently, with the net result that the Tchebycheff polynomials will have some numerical factors, and the angle of their argument will be slightly different.

In the end it is necessary to calculate

$$\begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{a}{c} \\ 1 & 0 \end{bmatrix}^M \begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{c}{b} \\ 1 & 0 \end{bmatrix}^N,$$

for  $M$  particles of one type and  $N$  of the other. Even before working out the details, it is not hard to foresee the results. If the element  $c$  in the dynamical matrix were zero, there would be two independent chains which would follow the guidelines already worked out for uniform chains, which means two cosinusoidal spectra with sinusoidal eigenvectors, although the exact nature of their boundary conditions would have to be worked out. To first order, the perturbation  $c$  should not change the eigenvalues, but would result in a slight adjustment to the eigenvectors, in magnitude depending on the relation of eigenvalue difference to matrix elements. Mainly, the waves could no longer be zero in each other's domains, as they would have been before.

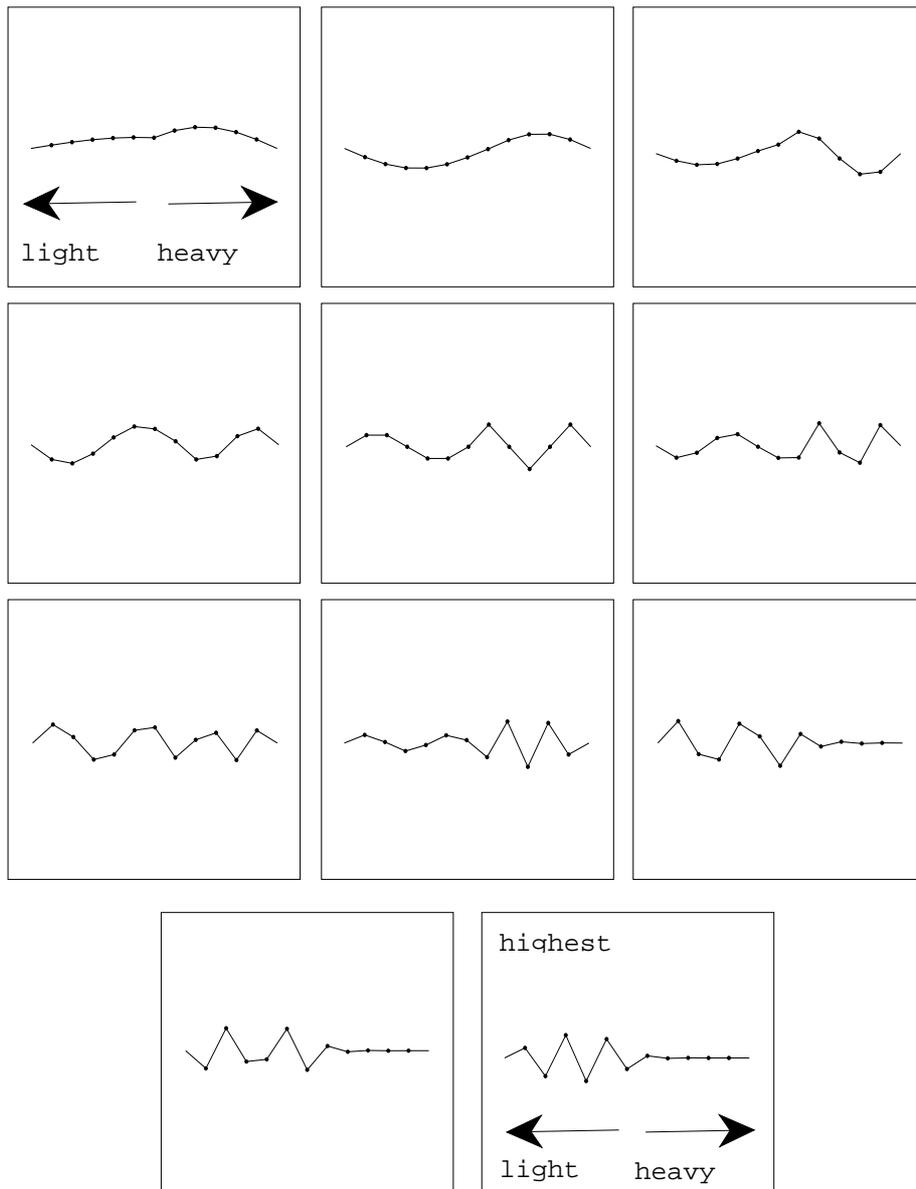


Figure 16: Normal modes of a split chain of eleven particles with with fixed ends and two different masses.

### 7.3 Point defect

The dynamical matrix would look like:

$$A = \begin{bmatrix} \cdots & \cdot & \cdots \\ \cdots & \frac{k}{m} & \frac{-2k}{m} & \frac{k}{m} & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cdot & \frac{k}{m} & \frac{-2k}{m} & \frac{k}{m} & \cdot & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cdot & \cdot & \frac{k}{m} & \frac{-k-kk}{m} & \frac{kk}{\sqrt{(mM)}} & \cdot & \cdot & \cdot & \cdots \\ \cdots & \cdot & \cdot & \cdot & \frac{kk}{\sqrt{(mM)}} & \frac{-kk-K}{M} & \frac{K}{M} & \cdot & \cdot & \cdots \\ \cdots & \cdot & \cdot & \cdot & \cdot & \frac{K}{M} & \frac{-2K}{M} & \frac{K}{M} & \cdot & \cdots \\ \cdots & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{K}{M} & \frac{-2K}{M} & \frac{K}{M} & \cdots \\ \cdots & \cdot & \cdots \end{bmatrix}$$

with two lines of recursion differing from those in the main body of the matrix. They only affect the wave matrix in the respect that its 12 element is no longer  $-1$ , but something else. In terms of masses  $m$  and  $M$ , with elastic constants  $k$ ,  $K$ , and an intermediate  $k'$ , we need

$$\begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{a}{c} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{c}{b} \\ 1 & 0 \end{bmatrix}$$

in terms of their eigenvalues and eigenvectors (or else to endure the algebra resulting from using them in their crude form).

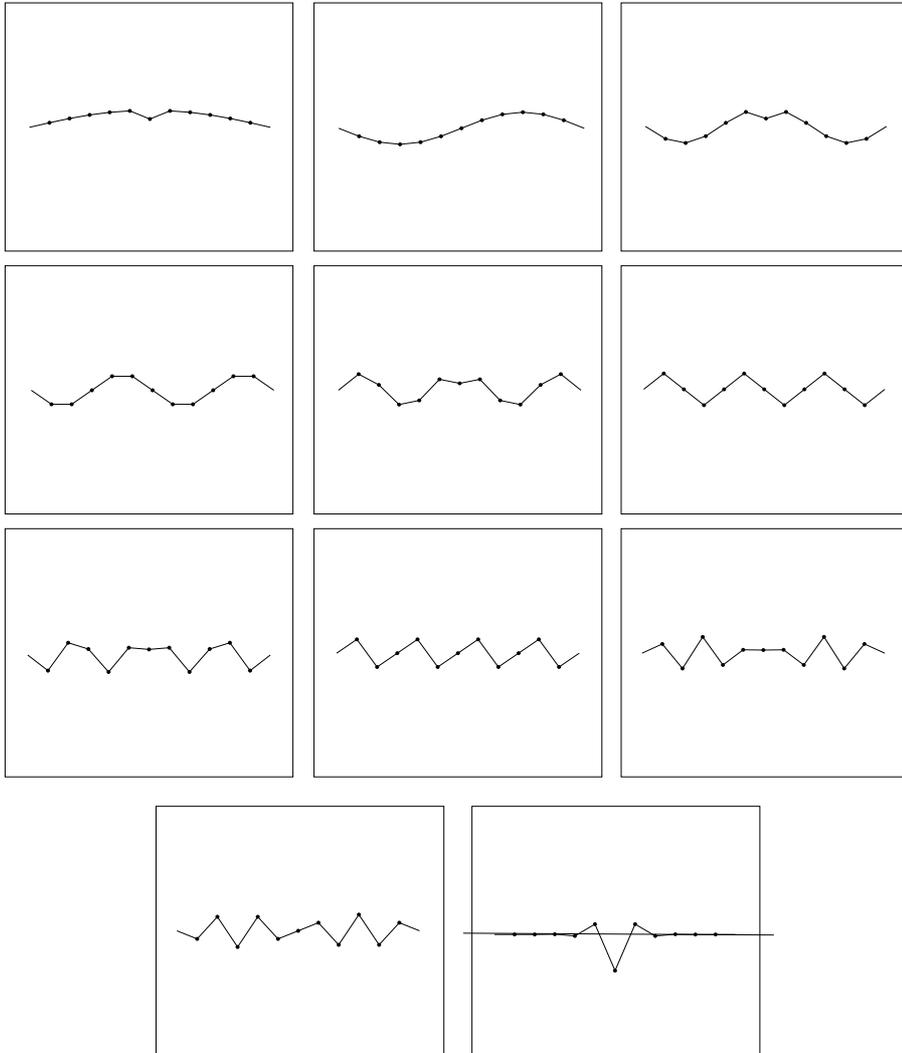


Figure 17: Normal modes of a chain of eleven particles with with fixed ends and a point defect consisting of a variant mass.

## 7.4 Diatomic string

In a diatomic chain, two different kinds of particles are supposed, but they alternate with one another rather than having similar particles grouped together in sequence. The effect remains the interaction of one group with the other, but now that they are interspersed, the consideration has to be the even numbered particles competing with the odd numbered particles.

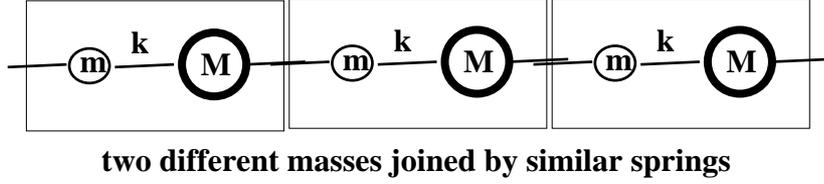


Figure 18: heavy and light particles alternate

The dynamical matrix would look like:

$$A = \begin{bmatrix} \frac{-2k}{m} & \frac{k}{\sqrt{Mm}} & \cdot & \cdot & \cdot & \cdot \\ \frac{k}{\sqrt{mM}} & \frac{-2k}{M} & \frac{k}{\sqrt{Mm}} & \cdot & \cdot & \cdot \\ \cdot & \frac{k}{\sqrt{Mm}} & \frac{-2k}{m} & \frac{k}{\sqrt{mM}} & \cdot & \cdot \\ \cdot & \cdot & \frac{k}{\sqrt{mM}} & \frac{-2k}{M} & \frac{k}{\sqrt{mM}} & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}.$$

Introducing a mass ratio  $\rho = \sqrt{M/m}$  and writing the common factor  $k/\sqrt{Mm}$  outside the matrix gives the dynamical matrix a better appearance:

$$A = \frac{k}{\sqrt{Mm}} \begin{bmatrix} -2\rho & 1 & \cdot & \cdot & \cdot & \cdot \\ 1 & \frac{-2}{\rho} & 1 & \cdot & \cdot & \cdot \\ \cdot & 1 & -2\rho & 1 & \cdot & \cdot \\ \cdot & \cdot & 1 & \frac{-2}{\rho} & 1 & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}.$$

Mathematically, what could be done is to combine a consecutive pair into a single unit cell by multiplying their wave matrices, and then raising this product to a power. Depending on whether the chain is of even or odd length overall, a single wave matrix may have to be incorporated to finish off the full chain. Although the dispersion relation for a single cell has to be more complicated, the advantage of constant wave numbers irrespective of the number of unit cells remains.

The eigenvalue equation for this matrix gives even and odd recursion equations,

$$\begin{aligned} x_{i-1} - \frac{2}{\rho}x_i + x_{i+1} &= \frac{\sqrt{Mm}}{k}\lambda x_i && \text{even, light mass} \\ x_{i-1} - 2\rho x_i + x_{i+1} &= \frac{\sqrt{Mm}}{k}\lambda x_i && \text{odd, heavy mass} \end{aligned}$$

Note that the geometric mean of the masses is a factor of  $\lambda$  in both equations. To avoid square roots, introduce

$$\omega^2 = \frac{\sqrt{(Mm)}}{k} \lambda$$

and two wave matrices,

$$\begin{aligned} \begin{bmatrix} \omega^2 + \frac{2}{\rho} & -1 \\ 1 & 0 \end{bmatrix} & \quad \text{even, light mass} \\ \begin{bmatrix} \omega^2 + 2\rho & -1 \\ 1 & 0 \end{bmatrix} & \quad \text{odd, heavy mass} \end{aligned}$$

Individually, they define dispersion relations similar to those for the uniform chain, but here it is necessary to evaluate their alternating products, taking into account that they do not commute unless  $\rho = 1$ .

$$\begin{bmatrix} \omega^2 + \frac{2}{\rho} & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \omega^2 + 2\rho & -1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} (\omega^2 + \frac{2}{\rho})(\omega^2 + 2\rho) - 1 & -(\omega^2 + \frac{2}{\rho}) \\ \omega^2 + 2\rho & -1 \end{bmatrix}.$$

By symmetry, changing the order of the product would exchange the skewdiagonal elements. Recalling that  $AB$  has the same eigenvalues as  $BA$ , the dispersion relation is the same for either product, namely

$$(\omega^2 + \frac{2}{\rho})(\omega^2 + 2\rho) - 1 - \mu)(-1 - \mu) + (\omega^2 + \frac{2}{\rho})(\omega^2 + 2\rho) = 0$$

Introduce more abbreviations,

$$\begin{aligned} \nu &= \mu + 1 \\ \Omega &= (\omega^2 + \frac{2}{\rho})(\omega^2 + 2\rho) \end{aligned}$$

to get the sequence

$$\begin{aligned} (\Omega - \nu)(-\nu) + \Omega &= 0 \\ \Omega\nu + \nu^2 + \Omega &= 0 \\ \Omega(\nu - 1) &= \nu^2 \\ \Omega &= \frac{\nu^2}{\nu - 1} \\ &= \frac{(\mu + 1)^2}{\mu} \\ &= \mu + 2 + \frac{1}{\mu} \\ &= 4 \cosh^2(\varphi). \end{aligned}$$

So the calculation of  $\Omega$  goes pretty much as usual. To get  $\omega$  out of  $\Omega$  is the interesting part; to simplify formulas still further, define  $\alpha = \rho + 1/\rho$ .

$$\Omega = \omega^4 + 2\omega^2\alpha + 4$$

$$\begin{aligned}\omega^2 &= \frac{-2\alpha \pm \sqrt{(4\alpha^2 - 4(4 - \Omega))}}{2} \\ &= -\alpha \pm \sqrt{(\alpha^2 + 4 \sinh^2(\varphi))}\end{aligned}$$

$$\begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{a}{c} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \frac{\lambda+a+c}{c} & -\frac{c}{b} \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} \frac{\lambda+a+c}{c} & \frac{\lambda+a+c}{c} - \frac{c}{b} \frac{\lambda+a+c}{c} & -\frac{c}{b} \\ 1 & 1 & -\frac{c}{b} \end{bmatrix}$$

What really counts is whether  $\sinh(\varphi)$  has to be imaginary or complex, which is best seen by yet another reformulation of the dispersion relation.

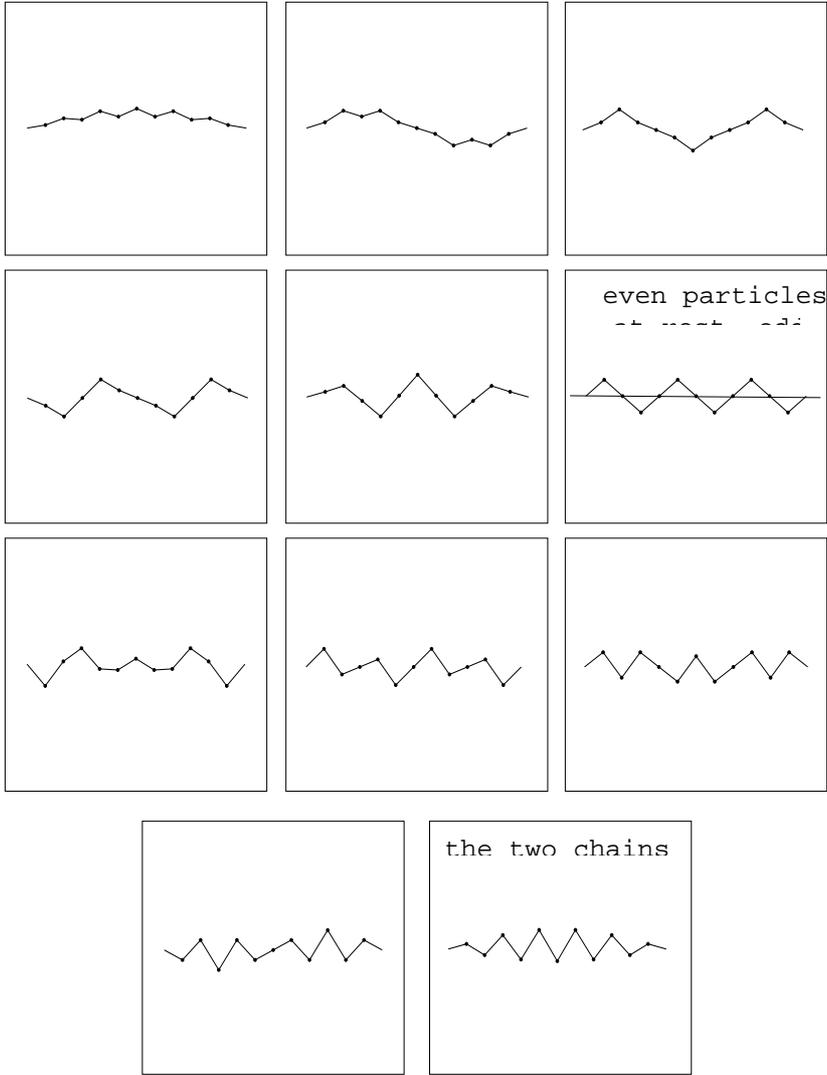


Figure 19: heavy and light particles alternate

## 7.5 Tapered string

The dynamical matrix would look like:

$$A = \begin{bmatrix} \frac{k_1}{m_1} & \frac{k_2}{\sqrt{m_1}\sqrt{m_2}} & \cdot & \cdot & \cdot \\ \frac{k_2}{\sqrt{m_2}\sqrt{m_1}} & \frac{k_3}{m_2} & \frac{k_4}{\sqrt{m_2}\sqrt{m_3}} & \cdot & \cdot \\ \cdot & \frac{k_3}{\sqrt{m_3}\sqrt{m_2}} & \frac{k_4}{m_3} & \frac{k_5}{\sqrt{m_3}\sqrt{m_4}} & \cdot \\ \cdot & \cdot & \frac{k_4}{\sqrt{m_4}\sqrt{m_3}} & \frac{k_5}{m_4} & \frac{k_6}{\sqrt{m_4}\sqrt{m_5}} \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix}$$

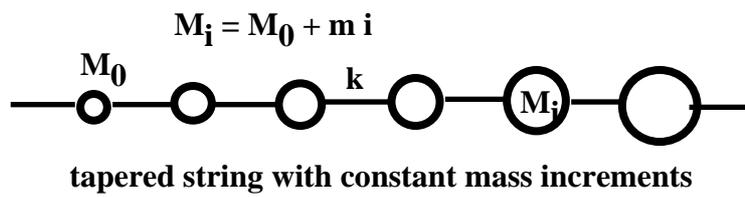


Figure 20: A tapered string with a constant mass increment running to the right.

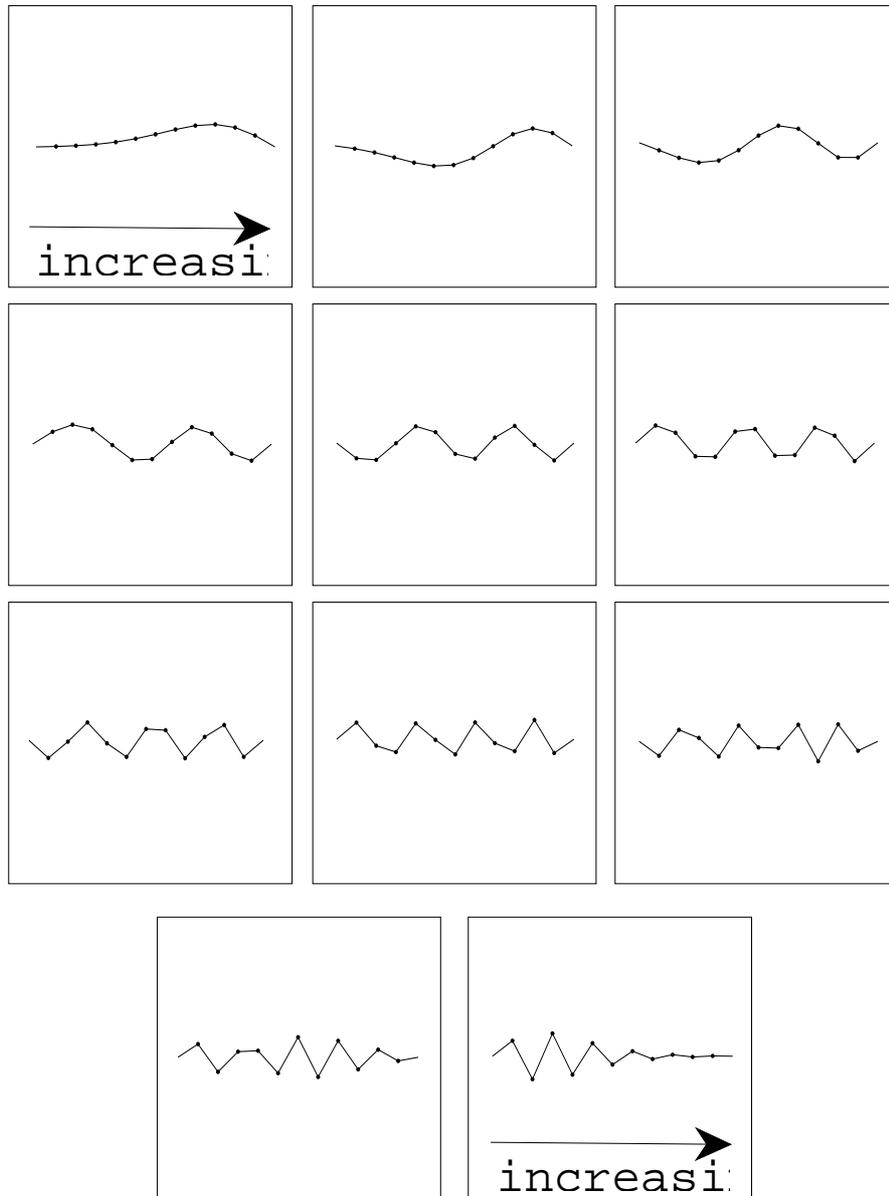


Figure 21: A tapered string with a constant mass increment running to the right.

## 7.6 Second neighbor influences

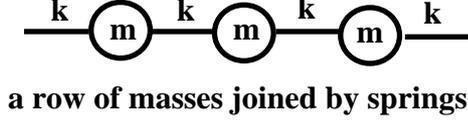


Figure 22: a row of identical masses with identical springs connecting neighbors and another set of springs connecting second neighbors

$$A = \frac{k}{m} \begin{bmatrix} \dots & \cdot & \dots \\ \dots & y & 1 & -2(1+y) & 1 & y & \cdot & \cdot & \cdot & \dots \\ \dots & \cdot & y & 1 & -2(1+y) & 1 & y & \cdot & \cdot & \dots \\ \dots & \cdot & \cdot & y & 1 & -2(1+y) & 1 & y & \cdot & \dots \\ \dots & \cdot & \dots \end{bmatrix}.$$

The component by component equations for the eigenvectors of a pentadiagonal matrix would have the form

$$ax_{i-2} + bx_{i-1} + cx_i + bx_{i+1} + ax_{i+2} = \lambda x_i$$

which would turn into recursion relations by writing

$$x_{i+2} = -\alpha x_{i+1} + (\lambda - \beta)x_i - \alpha x_{i-1} - x_{i-2},$$

and finally an equation with a wave matrix

$$\begin{bmatrix} x_{i+2} \\ x_{i+1} \\ x_i \\ x_{i-1} \end{bmatrix} = \begin{bmatrix} -\alpha & (\lambda - \beta) & -\alpha & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_{i+1} \\ x_i \\ x_{i-1} \\ x_{i-2} \end{bmatrix}.$$

The characteristic equation for the wave matrix reads

$$\mu^4 + \alpha\mu^3 + (\lambda - \beta)\mu^2 + \alpha\mu + 1 = 0$$

which in turn is a quadratic equation for  $c = \mu + 1/\mu = 2 \cosh(\phi)$ .

$$c^2 + \alpha c + (\lambda - \beta) = 0$$

## 8 Block Matrices

Matrices sometimes have a structure in which some submatrix is repeated over and over, usually reappearing in the form of different multiples. For example, the product of a column by a row is a rectangular matrix, in which all the rows are proportional, just as the columns are likewise proportional. When the repetition of one matrix is guided by another, the result is sometimes called a Kronecker product of the two matrices, and at other times a tensor product. For example, given matrices  $P$  and  $Q$ ,

$$P = \begin{bmatrix} a & b \\ c & d \end{bmatrix}, \quad Q = \begin{bmatrix} A & B \\ C & D \end{bmatrix},$$

their Kronecker product  $P \otimes Q$  would be defined by

$$\begin{aligned} P \otimes Q &= \begin{bmatrix} aQ & bQ \\ cQ & dQ \end{bmatrix} \\ &= \begin{bmatrix} a \begin{bmatrix} A & B \\ C & D \end{bmatrix} & b \begin{bmatrix} A & B \\ C & D \end{bmatrix} \\ c \begin{bmatrix} A & B \\ C & D \end{bmatrix} & d \begin{bmatrix} A & B \\ C & D \end{bmatrix} \end{bmatrix} \\ &= \begin{bmatrix} aA & aB & bA & bB \\ aC & aD & bC & bD \\ cA & cB & dA & dB \\ cC & cD & dC & dD \end{bmatrix}. \end{aligned}$$

In complete generality, give  $P \otimes Q$  four indices in the form of two pairs, and set

$$[P \otimes Q]_{ij,kl} = P_{ik}Q_{jl}$$

These indices are to be run out in lexicographic order, which means that  $P \otimes Q$  is not the same thing as  $Q \otimes P$ , although it is equivalent by a change of basis which permutes the indices.

$$\begin{bmatrix} aA & aB & bA & bB \\ aC & aD & bC & bD \\ cA & cB & dA & dB \\ cC & cD & dC & dD \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} aA & bA & aB & bB \\ cA & dA & cB & dB \\ aC & bC & aD & bD \\ cC & dC & cD & dD \end{bmatrix}$$

Calculation with Kronecker products is facilitated by verifying all the algebraic rules, such as distributivity or associativity, which they obey, thereafter using them automatically. Let  $I$  stand for a unit matrix,  $O$  zero matrices of the appropriate size and shape,  $P$ ,  $Q$  and  $R$  generic matrices. As needed,  $\alpha$  and  $\beta$  could be scalar factors. Then

$$\begin{aligned} I \otimes I &= I \\ O \otimes P &= O \\ P \otimes O &= O \\ (P + Q) \otimes R &= P \otimes R + Q \otimes R \\ R \otimes (P + Q) &= R \otimes P + R \otimes Q \\ (\alpha P) \otimes (\beta Q) &= (\alpha\beta)(P \otimes Q) \\ (P_1 P_2) \otimes (Q_1 Q_2) &= (P_1 Q_1) \otimes (P_2 Q_2) \\ (P \otimes Q) \otimes R &= P \otimes (Q \otimes R). \end{aligned}$$

Apparently a Kronecker product resembles a cartesian product, in the sense that the factors combine fairly independently when it comes to mingling the Kronecker product with other operations such as linear combination or matrix multiplication. Some further results are useful; if the factors are invertible,

$$P^{-1} \otimes Q^{-1} = (P \otimes Q)^{-1},$$

wherein it should be noted that the order of the factors is preserved.

If there are eigenvectors  $PX = \lambda X$  and  $QY = \mu Y$ ,

$$(P \otimes Q)(X \otimes Y) = (\lambda\mu)(X \otimes Y),$$

This means that the Kronecker product has all possible products of eigenvalues associated with all possible Kronecker products of eigenvectors, due regard being given to the possibility of Jordan normal forms, and with similar results whenever they occur. Beyond that, under the same assumptions,

$$\begin{aligned} (P \otimes I + I \otimes Q)(X \otimes Y) &= (\lambda + \mu)(X \otimes Y), \\ (P \otimes I - I \otimes Q)(X \otimes Y) &= (\lambda - \mu)(X \otimes Y), \end{aligned}$$

which provides a matrix with all the possible sums, or all the possible differences, of the eigenvalues of two given matrices as its own eigenvalues. Checking whether the second combination were singular would tell immediately whether a pair of matrices had common eigenvalues.

## 9 Symmetry

Symmetry arises when a system looks the same in different coordinate systems; for example, the spherical symmetry of a central potential. Symmetry does not require that motion in a symmetrical system has to be symmetric, only that similar motion follows out from similar initial conditions. For example, the nodal patterns in the vibration of an isotropic square membrane do not have to have square symmetry. But it is true that for every normal mode of a given frequency, there is another, rotated from the first, with that very same frequency; similarly for reflected modes.

The mathematical description of symmetry is that the dynamical matrix  $A$  has a change of basis  $S$  for which  $SA = AS$  (an equivalence) which could of course also be written as

$$S^{-1}AS = A.$$

### 9.1 Wave symmetry

#### 9.1.1 $2 \times 2$ wave matrices

Consider the  $2 \times 2$  wave matrices

$$\begin{bmatrix} x_{i+1} \\ x_i \end{bmatrix} = \begin{bmatrix} a & b \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix}.$$

If the direction of indexing is reversed, that can be described by a matrix

$$\begin{bmatrix} x_{i+1} \\ x_i \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_{i+1} \\ x_i \end{bmatrix},$$

so the whole sequence could be reversed by writing

$$\begin{aligned} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_{i+1} \\ x_i \end{bmatrix} &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a & b \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix}, \\ \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix} &= \begin{bmatrix} 0 & 1 \\ b & a \end{bmatrix} \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix} \\ &= \begin{bmatrix} 0 & 1 \\ b & a \end{bmatrix} \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix} \\ &= \frac{-1}{b} \begin{bmatrix} 0 & 1 \\ b & a \end{bmatrix} \begin{bmatrix} x_i \\ x_{i-1} \end{bmatrix} \end{aligned}$$

In the case  $b = -1$ , which was true in the wave matrix for a uniform chain, the same wave matrix serves for either direction. However,  $b = -1$  makes the wave matrix unimodular, so that its eigenvalues occur in reciprocal pairs, and their logarithms, the wave numbers, are negatives of one another. In other words, similar waves propagate in opposite directions.

#### 9.1.2 $4 \times 4$ wave matrices

A similar result applies to the  $4 \times 4$  wave matrix of uniform second neighbor interactions,

$$\begin{bmatrix} x_{i+2} \\ x_{i+1} \\ x_i \\ x_{i-1} \end{bmatrix} = \begin{bmatrix} a & b & c & d \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} x_{i+1} \\ x_i \\ x_{i-1} \\ x_{i-2} \end{bmatrix}.$$

The sequence of indices is reversed by the self-inverse

$$R = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix},$$

so

$$\begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a & b & c & d \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ d & c & b & a \end{bmatrix},$$

while

$$\begin{bmatrix} a & b & c & d \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}^{-1} = \frac{1}{d} \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & -a & -b & -c \end{bmatrix}.$$

This time it is  $d$  which should be  $-1$ , although  $d = 1$  is also a possibility. Then it is also required that  $a = c$ , so the recursion relation

$$x_{i+2} + ax_{i+1} + bx_i + cx_{i-1} + dx_{i-2} = \lambda x_i$$

has to be symmetric with respect to reversing the order of the indices.

The characteristic equation of a  $4 \times 4$  wave matrix reads

$$\begin{vmatrix} a - \mu & b & c & d \\ 1 & -\mu & 0 & 0 \\ 0 & 1 & -\mu & 0 \\ 0 & 0 & 1 & -\mu \end{vmatrix} = 0$$

Laplace expansion by the first row gives

$$(a - \mu)(-\mu)^3 - b(-\mu)^2 + c(-\mu) - d = 0$$

Thus  $d$  is the determinant, the product of all the roots, and should be  $+1$ . Putting the other symmetry condition,  $a = c$ ,

$$\begin{aligned} (-\mu)^4 + a(-\mu)^3 - b(-\mu)^2 + a(-\mu) - d &= 0 \\ \mu^4 - a\mu^3 - b\mu^2 - a\mu + 1 &= 0 \\ (\mu^2 + \frac{1}{\mu^2}) - a(\mu + \frac{1}{\mu}) - b &= 0 \\ (\mu + \frac{1}{\mu})^2 - a(\mu + \frac{1}{\mu}) - (b + 2) &= 0 \end{aligned}$$

As before, the roots occur in reciprocal pairs, as they should when a matrix is equivalent to its inverse.

## 9.2 Dynamical matrix symmetry

What we have worked out are the consequences for the wave matrix of a reflective symmetry. Rather than leaving the wave matrices unchanged, it turns them into their inverses. It is the dynamical matrix which should be unchanged. Let

$$R = \begin{bmatrix} \dots & \cdot & \dots \\ \dots & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \dots \\ \dots & \cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \dots \\ \dots & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \dots \\ \dots & \cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & \cdot & \dots \end{bmatrix}$$

$$A = \begin{bmatrix} \dots & \cdot & \dots \\ \dots & -2 & 1 & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & 1 & -2 & 1 & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & \cdot & 1 & -2 & 1 & \cdot & \cdot & \cdot & \dots \\ \dots & \cdot & \cdot & 1 & -2 & 1 & \cdot & \cdot & \dots \\ \dots & \cdot & \cdot & \cdot & 1 & -2 & 1 & \cdot & \dots \\ \dots & \cdot & \cdot & \cdot & \cdot & 1 & -2 & \cdot & \dots \\ \dots & \cdot & \dots \end{bmatrix}$$

Then  $RA = AR$ , every element is reflected across the center of the matrix, and remains unchanged. That means for all eigenvectors  $X$ ,

$$\begin{aligned} AX &= \lambda X \\ A(RX) &= R(AX) \\ &= R(\lambda X) \\ &= \lambda(RX). \end{aligned}$$

Thus either  $RX = \theta X$  and  $X$  is an eigenvector of  $R$  (when two matrices commute, they have common eigenvectors) or else  $X$  and  $RX$  are two linearly independent eigenvectors belonging to the same eigenvalue of  $A$ . Of course, it might also happen that  $RX = 0$ . Here,  $R^2 = I$ , so  $RX \neq 0$ . Neither is it possible to go on finding still more eigenvectors belonging to the common eigenvalue.

In other words symmetry

$$RA = AR$$

implies degeneracy

$$AX = \lambda X \Rightarrow ARX = \lambda RX.$$

Conversely, an appeal to Sylvester's theorem shows that forming linear combinations of degenerate eigenvectors should commute with  $A$  and so should induce a symmetry. Clearly the size and number of degenerate subspaces depends on the action of  $R$ , and it is evidently a mutual relationship.

Continuing to think of the dynamical matrix for the vibrations of a string, the influence of reflective symmetry is that for every normal mode, the reflection has to be another normal mode.

That doesn't actually produce nodes of different shape; because  $R^2 = I$ , its eigenvalues are  $\pm 1$ , making normal modes either even (and hence unchanged) or odd with respect to reflection. In general, half the sum and half the difference of any mode and its reflection would be eigenvectors of the reflection.

Cyclic chains have another symmetry, which is shifting from one particle to the next:

$$S = \begin{bmatrix} \dots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & 1 & 0 & \cdot & \cdot & \cdot & \cdot & \dots \\ \dots & \cdot & 1 & 0 & \cdot & \cdot & \cdot & \dots \\ \dots & \cdot & \cdot & 1 & 0 & \cdot & \cdot & \dots \\ \dots & \cdot & \cdot & \cdot & 1 & 0 & \cdot & \dots \\ \dots & \cdot & \cdot & \cdot & \cdot & 1 & 0 & \dots \\ \dots & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \dots \end{bmatrix}$$

because  $SA = AS$ . In fact,  $A$  is a function of  $S$ , given that

$$A = S^{-1} - 2I + S$$

That means the cyclic shift of any normal mode has to be another normal mode of the same frequency. The relationship is less obvious than the one resulting from reflection, because  $S$  has complex eigenvalues and eigenvectors. Recall that when diagonalizable matrices commute we have to find a set of *mutual* eigenvectors so that both will be diagonal in the same coordinate system. The symmetry shows up through the use of sines and cosines to describe the normal modes rather than complex exponentials. As the situation is usually described, the normal modes are standing waves rather than travelling waves.

Altogether the cyclic string has two symmetries,  $R$  and  $S$ , and they don't commute with one another:  $RS = S^{-1}R$ . This lack of commutation obliges  $A$  to have multiple eigenvalues, because of the difficulty in finding vectors which are simultaneously eigenvectors of  $A$ ,  $R$ , and  $S$ . The condition of degeneracy is sufficient, but for particular combinations there could be still further degeneracies which were not based on the shifting of the eigenvectors of one of the matrices by the others.

### 9.3 Groups

A collection of symmetries has the important property of forming a group. That is, if  $AS = SA$  and  $AT = TA$ , then

$$\begin{aligned} A(ST) &= (AS)T \\ &= (SA)T \\ &= S(AT) \\ &= S(TA) \\ &= (ST)A \end{aligned}$$

This derivation is pretty detailed, but such meticulous attention to detail is usual when working with the axiomatics of groups. Its conclusion is that the product of two matrices which commute with a third also commutes with the third, which is the closure requirement in the definition of a group.

Altogether, the definition of a group requires a collection of objects and a binary operation, called multiplication for the sake of argument, which associates a third element with a given pair. The postulates for group multiplication are

**closure** multiplication is defined for all pairs,

**associativity** multiplication is associative:  $a(bc) = (ab)c$ ,

**left identity** there is an element  $e$  for which  $ea = a$ , whatever  $a$ ,

**left inverse** for every  $a$ , there is a  $b$  satisfying  $ba = e$ .

As usual with concise mathematical statements, some reassurance often improves understanding. For example, insisting on one identity does not of itself preclude there being others; however that is the one which should be used in applying the fourth postulate.

If the statement of the postulates appears a little strange, that is because they are usually given in both a strong form and a weak form. The advantage of the weak form, with *left* identities, *left* inverses (the handedness does have to be the same), and no mention of uniqueness, is that there is less to verify while recognizing a group. But there is sufficient information present to show that uniqueness holds, that the identity and inverses work from both sides, useful relationships such as  $(ab)^{-1} = b^{-1}a^{-1}$  or  $(a^{-1})^{-1} = a$ , and that equations are always solvable.

This latter property, that  $ax = b$  has the unique solution  $x = a^{-1}b$ , is probably the one most responsible for the importance of the group concept.

Groups are excellent objects to which to apply the mathematical theory of structures, so it is convenient to recognize subgroups, factor groups, and product groups.

## 9.4 Subgroups

A subgroup is simply a subset of a group which is also a group. Since a subgroup necessarily contains the identity and its own inverses, and the associative law is already known for all possible triple products including those which might come from a prospective subgroup, the only doubt of consequence in verifying a subgroup lies in checking closure. That would be the normal sequence, locating the identity, finding inverses and examining products; but sometimes a proof can be shortened by simply applying the criterion that a subset is a subgroup if it contains all quotients.

The reasoning is that if  $x = y$  in  $xy^{-1}$ , it will turn up  $xx^{-1} = e$ , giving a check for the identity. Once  $e$  is there, putting  $e$  and  $x$  in the test runs through the inverses because  $ex^{-1} = x^{-1}$ . Finally pairing  $x$  and  $y^{-1}$  locates all the products due to  $x(y^{-1})^{-1} = xy$ , which was what was intended from the beginning. So this tricky wording allows a three-stage procedure to be described by one single algorithm. Note that it is not very practical when applied to a group table because it won't work without knowing what the inverses are. But later on, when complicated groups have been constructed with the help of algebraic formulas, including an extra inverse in a calculation could be preferable to checking all the special cases.

Subgroups are ordered by inclusion, so that the full group is the maximum subgroup, the unit class of the identity the minimum subgroup. The intersection of two subgroups is their lower bound, but the least upper bound is a more complicated matter; it is usually larger than their union. It also has to contain all their finite products, but that is actually sufficient; the resulting assemblage is called a hull, and can even be formed for subsets which are not subgroups. The smallest subgroup containing a given element, or specified set of elements, is often useful, and contains at least their powers and inverses.

## 9.5 Mappings and equivalence

Mappings between groups which conserve their group products are called homomorphisms, with a full range of adjectives to distinguish self-maps, surjective and injective maps. Each mapping defines an equivalence relation, compatible to a greater or lesser extent with the group multiplication. Sometimes the equivalence classes themselves are groups, multiplication having been defined setwise rather than pointwise.

Finally there are different kinds of multiplication which can be defined for cartesian products, still satisfying the requirement that projections are homomorphisms. The study of their existence and properties would complete the structure theory.

Not all equivalence relations in a group correspond to homomorphisms. Those which do are called congruence relations. The two basic equivalence relations, whose equivalence classes are the cosets, are defined with respect to a subgroup,  $H$  say.

$$\begin{aligned}x \equiv y &\Leftrightarrow xy^{-1} \in H \quad [\text{left coset}] \\x \equiv y &\Leftrightarrow x^{-1}y \in H \quad [\text{right coset}]\end{aligned}$$

In words, two elements are equivalent whenever they are common multiples of elements taken from a subgroup. The idea is that a subgroup should be seen as the identity element by a mapping which is unwilling to distinguish between its members. What we want is that  $ax \equiv ay$  whenever  $x \equiv y$ , say. To get rid of whatever  $a$  we should test  $(ay)^{-1}(ax)$ .

For what should we test? We want  $x \equiv x$ , so  $e$  should be one of the quotients. We need  $x \equiv y \Leftrightarrow y \equiv x$ , so we should always have  $xy^{-1}$  along with  $yx^{-1}$ , so quotients should always be paired with their inverses. Finally, the transitive law requires products, so all the requirements for a subgroup have been specified without saying which subgroup. Any will do, so there are cosets for all subgroups, left or right according to the handedness of the group multiplication required.

To get a congruence relation, and equivalence irrespective of the factor being replaced, a subgroup is required whose left cosets are the same as its right cosets; such a subgroup is called a normal subgroup. Its cosets are then congruence classes, the subgroup itself is the counterimage of the identity subgroup with respect to a homomorphism.

Homomorphic images of subgroups are subgroups. So are homomorphic counterimages.

Equivalence relations can be ordered by inclusion of their equivalence classes. Upper and lower bounds of cosets of the same handedness follow from the ordering of their defining subgroups; between handednesses the structures are called double cosets.

There is still another important equivalence relation, whose equivalence classes are simply called classes.

$$x \equiv y \Leftrightarrow \exists a \ni ax = ya.$$

It is the same relationship. applied internally to a group and its own group multiplication that characterizes equivalence in terms of mappings and commutative diagrams.

Because group multiplication is always invertible, multiplication by a fixed factor permutes the group elements; that is to say, if  $ax = ay$  it follows that  $x = y$ . For that reason, any group can be regarded as a group of permutations. If the permutations were written as matrices, that would also exhibit the group as a collection of matrices, with matrix multiplication as the group operation. But there is another approach which is capable of characterizing all the possible sets of matrices homomorphic to a given group.

## 9.6 Convolution algebra

Consider a collection of mappings from a group, regarded as a point set, to the complex numbers. Actually, any field would do, but choosing the complex numbers gives results of wide and common applicability. Such a collection of mappings is reminiscent of the dual space for a vector space and it will be seen that the theories follow quite similar lines. It always seems to be advantageous to work with the functions of a point set in place of the set itself.

Characteristic functions of subsets follow the definition:

$$\delta(S; x) = \begin{cases} 1 & x \in S \\ 0 & \text{otherwise} \end{cases}$$

Amongst the characteristic functions, those of the unit classes constitute a basis because any function  $f(x)$  can be written

$$f(x) = \sum_{g \in G} f(g) \delta(g; x).$$

Linear combinations and products of functions are to be defined as usual,

$$\begin{aligned} (\alpha f + \beta g)(x) &= \alpha f(x) + \beta g(x), \\ (fg)(x) &= f(x)g(x). \end{aligned}$$

So far nothing remarkable has been produced, but the influence of group multiplication has not yet been felt. That results from defining the convolution of two functions,

$$f * g(x) = \sum_{ab=x} f(a)g(b).$$

It results that  $f * g$  is not necessarily commutative, but that it is bilinearly distributive and associative.

## 9.7 Matrix representation

There are now two ways to get a matrix representation of a the group multiplication, according to whether the characteristic functions are used as left factors or as right factors for a convolution. In each case, the other factor is expanded in a basis as though it were a vector. For the left regular representation,

$$\begin{aligned} (\delta_g * f)(x) &= \sum_{ab=x} \delta(g; a) f(b), \\ &= \sum_a \delta(g; a) f(a^{-1}x), \\ &= f(g^{-1}x). \end{aligned}$$

So far, this is just a representation by permutations, as would be seen by specializing to characteristic functions.

Consider that a representation is given, a set of matrices  $\Gamma = \{D(e), D(a), \dots\}$  for which  $D(a)D(b) = D(ab)$ , and look at the matrix elements  $d_{ij}(a)$ . These are complex valued functions of the group elements and thereby subject to the preceding formula:

$$\begin{aligned} (\delta_a * d_{ij})(x) &= d_{ij}(a^{-1}x), \\ &= \sum_k d_{ik}(a^{-1})d_{kj}(x). \end{aligned}$$

for fixed  $a$  and function argument  $x$ .

We need to know whether the matrices of  $\Gamma$  are diagonal or not and if not, to what extent. Recall that matrices commute when they have common eigenvectors, and hence can be chosen to be diagonal, all of them at once. If any matrix but a multiple of the identity commutes with all the matrices of  $\Gamma$ , and that multiple can be diagonalized with two different eigenvalues, all the matrices of  $\Gamma$  must follow suit.

Therefore, if all of  $\Gamma$  cannot be placed in the form of diagonal blocks by some choice of coordinates, the matrix which commutes with all of them must be a multiple of the identity, a result which is known as Schur's first lemma. His second lemma relates to the possibility of forming an equivalence between two different matrix representations  $\Gamma^1$  and  $\Gamma^2$ . Give the matrices identifying superscripts and suppose a matrix  $V$  for which, whatever group element,

$$VD^1(x) = D^2(x)V.$$

If the dimensions are discrepant,  $V$  will be rectangular; suppose there are more columns than rows, reversing the indices in the contrary case. There must be some columns which are linear combinations of others, and therefore a column  $X$  expressing this dependence via  $VX = 0$ .

On the other hand, if  $V$  is not zero, there will be a row such that  $T^T V$  is non-zero; it just needs a 1 in a strategic place to take advantage of one of  $V$ 's non-zero elements.

Finally, consider that neither  $D^1(a)$  nor  $D^2(a)$  are singular (we really wouldn't want to consider a set of zero matrices a representation) because  $D(a)^{-1} = D(a^{-1})$  and every group element has an inverse.

Therefore  $D^1$  cannot map a non-zero vector into zero, so  $T^T VD^1(a)$  is nonzero, contradicting the vanishing of  $D^2(a)VX$ . So  $V$  would have to vanish in its entirety, which is the statement of Schur's second lemma.

There is a little more to be said because  $V$  could be square, leaving the existence of  $X$  in question. If there were such an  $X$ ,  $V$  would still be singular and would need to vanish, leading to the same conclusion. If, on the contrary,  $V$  were invertible, the representations  $\Gamma^1$  and  $\Gamma^2$  would have to be equivalent so the only possibility for inequivalent representations, even of the same dimension, would be  $V = 0$ .

In summary, a representation is irreducible when there is no choice of basis where all its matrices are simultaneously partitioned into diagonal nonzero blocks. Of course, some of the individual matrices, such as the identity matrix representing the identity element, may well be reduced; but not all of them in the same way at once. If only the zero equivalence can connect two representations, they are inequivalent, and if they are both the same representation, only a multiple of the identity can connect them.

Averaging over a group yields a plentiful supply of equivalences, depending upon what is averaged. Define  $V$ , for any matrix  $Q$  compatible with the two dimensions,

$$V(Q) = \frac{1}{|G|} \sum_{g \in G} D^2(g^{-1})QD^1(g),$$

and follow out the following derivation, step by step:

$$\begin{aligned}
V(Q) D^1(a) &= \left( \frac{1}{|G|} \sum_{g \in G} D^2(g^{-1}) Q D^1(g) \right) D^1(a), \\
&= \frac{1}{|G|} \sum_{g \in G} D^2(g^{-1}) Q (D^1(g) D^1(a)), \\
&= \frac{1}{|G|} \sum_{g \in G} D^2(g^{-1}) Q D^1(ga), \\
&= \frac{1}{|G|} \sum_{ga \in G} D^2(a(ga)^{-1}) Q D^1(ga), \\
&= \frac{1}{|G|} \sum_{ga \in G} (D^2(a) D^2((ga)^{-1})) Q D^1(ga), \\
&= D^2(a) \left( \frac{1}{|G|} \sum_{ga \in G} D^2((ga)^{-1}) Q D^1(ga) \right), \\
&= D^2(a) V(Q),
\end{aligned}$$

Dividing the sum by the order of the group was really unnecessary, but it will be convenient later on. For example, if  $Q = I$  and the same representation is used both times, the result will be  $V(I) = I$ . According to Schur's lemma, after adorning  $V$  with superscripts to trace its definition and inventing a sort of generic Kronecker delta for matrices,

$$V^{\alpha\beta}(I) = \Delta(\alpha, \beta).$$

Expressed in terms of matrix elements ( $\delta(k, \ell)$  is the matrix element of  $I$ ),

$$\frac{1}{|G|} \sum_{g \in G} d_{ik}^{\alpha}(g^{-1}) d_{\ell j}^{\beta}(g) = \delta(\alpha, \beta) \delta(i, k) \delta(\ell, j),$$

which expresses the biorthonormality of two vector sets, possibly bases, for the group's function space, or convolution algebra. The sets have  $\dim(\Gamma^{\alpha})^2$  elements for each irreducible representation, placing an upper limit on the number of irreducible representations (which can never exceed  $|G|$ ) and their dimensions (which can never exceed  $\sqrt{|G|}$ ). Evidently high dimensional representations come at the price of finding fewer of them.

## 9.8 Characters

The basis relations for group functions can be rearranged by taking traces of the matrix elements, and noticing that traces are invariant under change of basis. On the one hand, traces are invariants of equivalences so the result will not depend on changing to an equivalent representation. On the other, the same is true for internal equivalences of the group, making traces functions of classes, not merely of individual group elements. The trace is a function for which the classes are equivalence classes.

The trace-valued group function is called a character for its representation, defined by

$$\chi^\alpha(g) = \sum_{i=1}^{\dim(\Gamma)} d_{ii}^\alpha(g).$$

Especially note that  $\chi^\alpha(e) = \dim(\Gamma^\alpha)$ . On taking the appropriate sums in the biorthogonality relations,

$$\frac{1}{|G|} \sum_{g \in G} \chi^\alpha(g^{-1}) \chi^\beta(g) = \delta(\alpha, \beta).$$

Because of the constancy over classes, the result is also a biorthogonality relation for class space. Call a typical class  $C_i$ , observe that the set of inverses of class members is another class (maybe the same one), and average within classes (where the number of elements in class  $C_i$  is  $|C_i|$ ) to get

$$\frac{1}{|G|} \sum_{C_i} |C_i| \chi^\alpha(C_i^{-1}) \chi^\beta(C_i) = \delta(\alpha, \beta).$$

There is now a new function space, mapping classes to complex numbers, for which the characters of the irreducible representations form a biorthonormal set, which would mean that the number of inequivalent irreducible representations cannot exceed the number of classes.

As remarked, characters are not only insensitive to equivalences arising within the group, but to external influences as well. That all equivalent representations have the same character allows their characterization, which was undoubtedly the origin of the term. Beyond that, if a representation is reducible, the biorthonormality of characters permits finding out which irreducible representations are in the blocks. For a representation  $\Gamma = \{D(g)\}$ ,

$$\begin{aligned} \chi(g) &= \sum \chi_\alpha(g) \\ &= \sum' n_\alpha \chi_\alpha(g), \end{aligned}$$

the prime implying a sum over inequivalent representations and  $n_\alpha$  counting the multiplicity of each irreducible representation.

$$\frac{1}{|G|} \sum_G \chi(g^{-1}) \chi(g) = \sum n_\alpha^2$$

For the sum to be exactly 1 would be indicative that the representation was irreducible. As a further result, note that the trace of an element in a permutation representation is the number of fixed points for that particular element. The regular representation is a permutation representation for which only the identity fixes any points - all of them. Therefore

$$\chi^{\text{regular}}(g) = \begin{cases} |G| & g = e \\ 0 & \text{otherwise} \end{cases}$$

For whatever representation, the trace of the identity is its dimension, so  $\chi^\alpha(e) = \dim(\Gamma^\alpha) = d_\alpha$ ; in comparison with the regular representation, for which all traces except the identity vanish, the other traces do not matter. So

$$\frac{1}{|G|} \sum_G \chi^{\text{regular}}(g^{-1}) \chi^\alpha(g) = d_\alpha$$

and each irreducible representation present is repeated its own dimensionality number of times. The important thing here is that it doesn't matter how an irreducible representation was manufactured, working with the space of complex valued group functions guarantees its place in the regular representation, and the sum of the squares of all their dimensions adds up to the order of the group.

At the same time, because the regular representation contains an equivalent of any irreducible representation at all, their characters have to be present among the complex valued class functions. The only obstacle to knowing that the number of irreducible representations is equal to the number of classes would be to show that the characteristic function of a class was a linear combination of characters. Pretty much by definition, the reverse is true, characters are linear combinations of characteristic functions of classes.

We already know that the characteristic functions of points are linear combinations of matrix elements; if

$$f(g) = \sum_{\alpha i j} c_{\alpha i j} d_{i j}^{\alpha}(g),$$

taking inner products with dual basis elements gives

$$\begin{aligned} (f(g), d_{i j}^{\alpha}(z)) &= c_{i j}^{\alpha}, \\ f(g) &= \sum_{\alpha i j} (f(g), d_{i j}^{\alpha}(z)) d_{i j}^{\alpha}(z) \\ \delta(g; z) &= \sum_{\alpha i j} d_{i j}^{\alpha}(z^{-1}) d_{i j}^{\alpha}(g) \end{aligned}$$

The sum of products of matrix elements is either zero or one; but that was the conclusion from Schur's lemmas.

Next, consider that a class arises from finding conjugates from within the group: elements for which  $xs = sy$  for all  $s$ . So sums over a class just average these conjugacies:  $s(x + y + z + \dots) = (x + y + z + \dots)s$ . Representationwise here is a matrix commuting with an irreducible representation, so

$$\sum_{\text{class}} d_{i j}^{\alpha}(g) = \lambda^{\alpha} \delta(j; k),$$

$\lambda^{\alpha}$  being the multiplier of the identity in the  $\alpha^{\text{th}}$  irreducible representation.

$$\begin{aligned} \delta(\text{class}; z) &= \sum_{\alpha i j} \sum_{\text{class}} \lambda^{\alpha} \delta(j; k), \\ &= \sum_{\alpha} \lambda^{\alpha} \chi^{\alpha}(z) \end{aligned}$$

which makes the characteristic function of a class a linear combination of characters, and the characters indeed form a basis for all complex valued class functions. So we now know that the number of irreducible representations equals the number of classes, and is not just limited by their number.

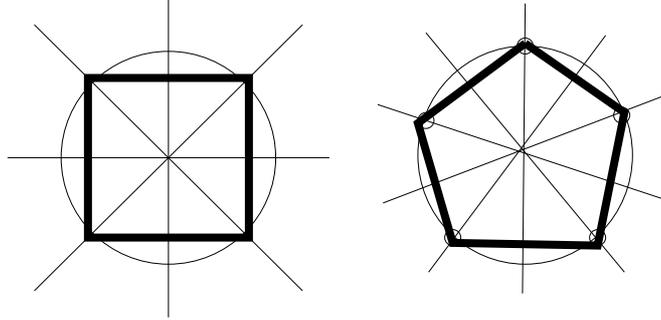


Figure 23: Reflections fall into one or two classes according to the parity of the n-gon.

## 9.9 Symmetry of a regular polygon

Having introduced the study of symmetry by using the example of a cyclic chain, which has both shift and reflection symmetry, we could finish by examining the symmetry group, its irreducible representations, and their effect on the dynamical matrix. If the particles were located at the vertices of a regular polygon, the symmetry group could be interpreted as the set of rotations and reflections of that geometric figure.

Symmetry of an n-gon has two generators, a rotation  $S$  for which  $S^n = I$ , and a reflection  $R$  for which  $R^2 = I$ , for which  $RS = S^{-1}R$ . Groups are often defined by listing a set of generators and a set of relations, three in this case. The full group table is supposed to be deduced from this information, but that is not always possible, for reasons which lead deeply into the theory of recursive functions. Fortunately the table for the symmetry of polygons is easily calculated, resulting there are only  $2n$  symmetries, of the form  $S^i R^j$ ,  $0 \leq i < n$ ,  $0 \leq j < 2$  with the rule of multiplication

$$(S^i R^j)(S^k R^\ell) = S^{(i-k) \pmod n} R^{(j+\ell) \pmod 2}.$$

The symmetry group of a plane n-gon is called a dihedral group of order  $n$ ,  $D_n$ , in contrast to a cyclic group of order  $n$ ,  $C_n$ . The latter contains only the powers of a single generator, whereas a dihedral group incorporates a reflection besides.

If  $n$  has divisors, both cyclic and dihedral groups contain subgroups whose orders are the divisors, generated by the powers of  $S$  complementary to the divisor. Thus both  $D_2$  generated by  $R$  and  $S^3$ , and  $D_3$ , generated by  $R$  and  $S^2$  are subgroups of  $D_6$ .

In addition, any of the products  $S^k R$  generate subgroups of order 2, since  $S^k R S^k R = S^{k-k} R^2 = I$ . The generators of these subgroups are reflections, and come in two forms. If  $n$  is even, reflections in lines passing through opposite vertices are not the same as reflections in perpendicular bisectors

of opposite edges. In fact, the vertex splitting reflections constitute a class, the edge-splitting reflections another.

On the other hand, when  $n$  is odd, reflections bisect one vertex angle and one opposite edge each, so there is no distinction and all the reflections make up one single class.

The subgroups mentioned are all there are. Each defines a family of cosets, but only the cyclic subgroups are normal.

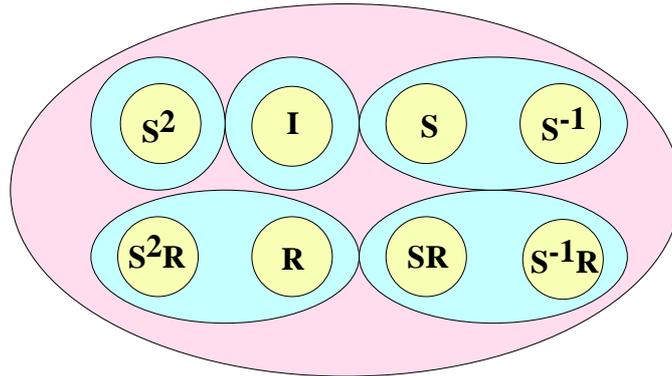


Figure 24: the symmetry group of a 4-gon (square) has five classes

In enumerating the classes, we have just seen that the reflections form either one single class or two distinct classes, according to the parity of the  $n$ -gon. Since all the rotations commute, the size of one of their classes depends on the reflections, which map rotations into their inverses. Therefore, again according to parity, there are  $(n + 2)/2$  or  $(n + 1)/2$  classes of rotations. When  $n$  is even,  $S^{n/2} = (S^{n/2})^{-1}$ , so it and  $I$  each sit in a single class, for a total of 2. The other  $n - 2$  rotations pair up in  $n/2 - 1$  classes, for the total stated. When  $n$  is odd, only the identity is self-conjugate, so the prospective number of classes is reduced by 1.

If the  $n$ -gon is a plane figure, we already have a matrix representation with  $2 \times 2$  matrices:

$$D(S) = \begin{bmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{bmatrix},$$

$$D(R) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

Irreducible representations for the symmetry of a square can be read off from the following table

	$I$	$S$	$S^2$	$S^3$	$R$	$SR$	$S^2R$	$S^3R$
	1	1	1	1	1	1	1	1
	1	1	1	1	-1	-1	-1	-1
	1	-1	1	-1	1	-1	1	-1
	1	-1	1	-1	-1	1	-1	1
	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

and characters from a similar table

$I$	$S$	$S^2$	$SR$	$S^2R$
1	1	1	1	1
1	1	1	-1	-1
1	-1	1	-1	1
1	1	1	1	-1
2	0	-2	0	0

## 10 Affine and Projective Algebra

Formalizing geometry by introducing coordinate systems and using linear algebra captures only a part of the material traditionally regarded as geometry. The missing part has much to do with matters of scale; beyond that, the selection of an origin as a point of reference runs contrary to all the independence of position and orientation which characterizes geometrical reasoning.

Two different, but nevertheless related, concepts recapture geometry within a framework of linear algebra. Including translations along with the linear transformations, and especially rotations, leads to the concept of an affine space, at the price of working in a nonlinear environment. Projections not only eliminate the nonlinearity; they offer the additional advantages of scaling and inversion - reflections in spheres.

### 10.1 Affine space

The semidirect product of groups was known to crystallographers and others as the way to describe the symmetry group of a lattice, long before the idea was taken up by mathematicians in the 1950's. The concept arises from combining lattice symmetry expressed by the addition of translation vectors with point symmetry implemented using matrices rotating or reflecting the vectors displacing unit cells.

Written in terms of components, a typical formula  $X' = MX + P$  would read

$$\begin{aligned} \begin{bmatrix} x' \\ y' \end{bmatrix} &= \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} + \begin{bmatrix} p \\ q \end{bmatrix} \\ &= \begin{bmatrix} ax + by + p \\ cx + dy + q \end{bmatrix}. \end{aligned}$$

Such a mapping of a vector space is called an affine transformation, to distinguish it from a linear transformation; note that

$$\begin{aligned} M(\alpha X + \beta Y) + P &= M\alpha X + M\beta Y + P \\ &\neq \alpha(MX + P) + \beta(MY + P), \end{aligned}$$

so that  $P$  appears only once in the result and it isn't scaled at all. Although the mapping isn't linear, it is certainly useful, which invites the study of its properties.

One of them is the rule of composition. Suppose that we regard the pair  $(M, P)$  as the cartesian product of two functions, and apply two such pairs in succession to a vector  $X$ , and take due note of the confusion arising from using parentheses to define a compound function on the one hand, and their normal use to group terms within an algebraic expression. Then

$$\begin{aligned} ((M, P)(M', P'))(X) &= (M, P)((M'P')(X)) \\ &= (M, P)(M'X + P') \\ &= MM'X + MP' + P \\ &= (MM', MP' + P)(X), \end{aligned}$$

which is the rule of composition for the two mappings.

## 10.2 Projective space

The projective viewpoint would regard the defining equation  $X' = MX + P$  as a fragment of a partitioned matrix equation:

$$\begin{bmatrix} \xi' \\ \eta' \\ \zeta' \end{bmatrix} = \left[ \begin{array}{cc|c} a & b & p \\ c & d & q \\ 0 & 0 & 1 \end{array} \right] \begin{bmatrix} \xi \\ \eta \\ \zeta \end{bmatrix}.$$

The componentwise equations,

$$\begin{aligned} \xi' &= a\xi + b\eta + p\zeta \\ \eta' &= c\xi + d\eta + q\zeta \\ \zeta' &= 0\xi + 0\eta + 1\zeta \end{aligned}$$

could be reconciled with the earlier equations by introducing the mapping

$$\begin{aligned} x &= \frac{\xi}{\zeta} \\ y &= \frac{\eta}{\zeta} \end{aligned}$$

Projective geometry is more comprehensive than affine geometry because there is no reason to restrict the transformation matrix to be upper triangular. If the more elaborate matrix

$$\left[ \begin{array}{cc|c} a & b & p \\ c & d & q \\ r & s & w \end{array} \right]$$

were used, the projective transformation would read

$$\begin{aligned} x' &= \frac{ax + by + p}{rx + sy + w} \\ y' &= \frac{cx + dy + q}{rx + sy + w}. \end{aligned}$$

A special case would include uniform dilation

$$\begin{aligned} x' &= \lambda x \\ y' &= \lambda y. \end{aligned}$$

Generally speaking, a linear transformation of  $n$  coordinates can be mapped into a projective transformation of  $(n - 1)$  coordinates, and conversely a nonlinear transformation of  $n$  coordinates having the projective form can be mapped into a linear transformation of  $n + 1$  coordinates. In neither case is the transformation one-to-one, since all multiples of a vector have a common projective image, just as the counterimage of a projection has to include all multiples of any one of its points.

### 10.3 Mappings of a line

Related to the question of discovering and describing linear and projective mappings is the related question of whether mappings are invertible or not. That depends to a certain extent on how the function is described - that is, whether it is a polynomial, rational fraction, or specified in some much more general context. In general calculus, if a set of functions  $y_i(x_1, x_2, \dots, x_n)$  have derivatives, the differential relationships

$$\begin{aligned} dy_1 &= \frac{\partial y_1}{\partial x_1} dx_1 + \frac{\partial y_1}{\partial x_2} dx_2 + \dots + \frac{\partial y_1}{\partial x_n} dx_n \\ dy_2 &= \frac{\partial y_2}{\partial x_1} dx_1 + \frac{\partial y_2}{\partial x_2} dx_2 + \dots + \frac{\partial y_2}{\partial x_n} dx_n \\ &\dots \\ dy_n &= \frac{\partial y_n}{\partial x_1} dx_1 + \frac{\partial y_n}{\partial x_2} dx_2 + \dots + \frac{\partial y_n}{\partial x_n} dx_n \end{aligned}$$

have a matrix formulation

$$\begin{bmatrix} dy_1 \\ dy_2 \\ \dots \\ dy_n \end{bmatrix} = \begin{bmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \dots & \frac{\partial y_1}{\partial x_n} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \dots & \frac{\partial y_2}{\partial x_n} \\ \dots & \dots & \dots & \dots \\ \frac{\partial y_n}{\partial x_1} & \frac{\partial y_n}{\partial x_2} & \dots & \frac{\partial y_n}{\partial x_n} \end{bmatrix} \begin{bmatrix} dx_1 \\ dx_2 \\ \dots \\ dx_n \end{bmatrix}$$

in which the matrix could be called a Jacobian matrix in analogy to the well-known Jacobian determinant. Actually there is a similar set of equations, using the transposed Jacobian matrix, relating partial derivatives with respect to one set of variables to those with respect to another. In either event, the nonvanishing of the Jacobian determinant is the criterion for local invertibility of the set of mappings. Less commonly discussed is whether the Jacobian matrix has eigenvalues and eigenvectors, although it would seem that they could surely provide further information concerning the local nature of the mapping.

Such general criteria provide only local information, although conclusions could be drawn from the nonsingularity of the Jacobian determinant over entire regions. Suppose, however, that the variables are related in a more implicit form, by the vanishing of a series of polynomial equations, and that to confine the discussion to the simplest case, that just the variables  $x$  and  $y$  are so related. Then the coefficients of powers of  $y$  could be gathered together to make up a polynomial in  $y$  whose roots would imply that several combinations of  $x$  and constant coefficients producing the same value for  $y$ . To avoid that eventuality, no powers of  $y$  should occur - just  $y$  itself and terms independent of  $y$ .

By symmetry, the same could be said of  $x$ . Only the meagre possibility

$$axy + bx + cy + d = 0 \tag{2}$$

remains, which could be rendered explicit in either one of the two forms

$$\begin{aligned} x &= -\frac{cy + d}{ay + b} \\ y &= -\frac{bx + d}{ax + c} \end{aligned}$$

Both of these expressions look like one-dimensional projective transformations of an affine plane; if they were written in matrix form there would result

$$\begin{aligned} \begin{bmatrix} x \\ 1 \end{bmatrix} &= \begin{bmatrix} -c & -d \\ a & b \end{bmatrix} \begin{bmatrix} y \\ 1 \end{bmatrix} \\ \begin{bmatrix} y \\ 1 \end{bmatrix} &= \begin{bmatrix} -b & -d \\ a & c \end{bmatrix} \begin{bmatrix} x \\ 1 \end{bmatrix} \end{aligned}$$

This matrix form, while not unique, reveals the convenience of a nonvanishing determinant  $ad - bc$ ; otherwise  $x$  would have a value independent of  $y$  and conversely. Neither would yield the single valued mapping we are looking for.

The matrices, except for the determinantal factor and the placement of some signs, are inverses, forerunning the observation that functional composites follow the rules of matrix multiplication. Since a quotient is involved, or otherwise stated, the original equation is homogeneous with respect to the coefficients, multiplying the matrices by a factor could give them a unit determinant, so the transformation can always be represented by unimodular matrices. To ensure the validity of matrix multiplication for their representation, the coefficients should always be arranged as shown, not reversed. In fact, it is worth looking at the substitution in detail, paying attention to the direction of the mapping, the direction of composition, and the placement of the coefficients in the matrix. If it were given, following the representation of  $x$  as a function of  $y$ , a sequence of two mappings,

$$\begin{aligned} x &= \frac{-cy - d}{ay + b} \\ w &= \frac{-Cx - D}{Ax + B} \end{aligned}$$

then substitution would say

$$\begin{aligned} w &= \frac{-C \left( \frac{-cy - d}{ay + b} \right) - D}{A \left( \frac{-cy - d}{ay + b} \right) + B} \\ &= \frac{-C(-cy - d) - D(ay + b)}{A(-cy - d) + B(ay + b)} \\ &= \frac{(Cc - Da)y - (cD - Db)}{(-Ac + Ba)y + (Ad + Bb)} \end{aligned}$$

which would correspond to a matrix product

$$\begin{bmatrix} -C & -D \\ A & B \end{bmatrix} \begin{bmatrix} -c & -d \\ a & b \end{bmatrix} = \begin{bmatrix} Cc - Da & -(Cd - Db) \\ -Ac + Ba & Ad + Bb \end{bmatrix}$$

The conclusion of this line of analysis is that under very general conditions — namely implicit representation by coefficients of a vanishing polynomial — the only invertible mapping of a line into itself is a projective transformation. Note that projective transformations are slightly more general than affine transformations (but only slightly) because projection from a linear space envisions not just one affine transformation, but even a quotient of two of them.

## 10.4 The cross ratio

There is a rather complicated quotient of quotients, called the cross ratio, which is an invariant of projective transformations, whose discovery apparently dates back to Pappus during the last stages of greek antiquity. One way to obtain his result is the following:

### 10.4.1 matrix interpretation

Consider the projective line as an image of a two-dimensional linear algebra plane, and observe that determinants are multiplicative for linear transformations. Take a  $2 \times 2$  matrix  $P$  containing the two columns of a basis and a transformation  $M$ . Then  $|MP| = |M||P|$ , so  $|P|$  is not an invariant. But take another basis matrix  $Q$  for which  $|MQ| = |M||Q|$ . Then the quotient  $|P|/|Q|$  is invariant, although its terms are not.

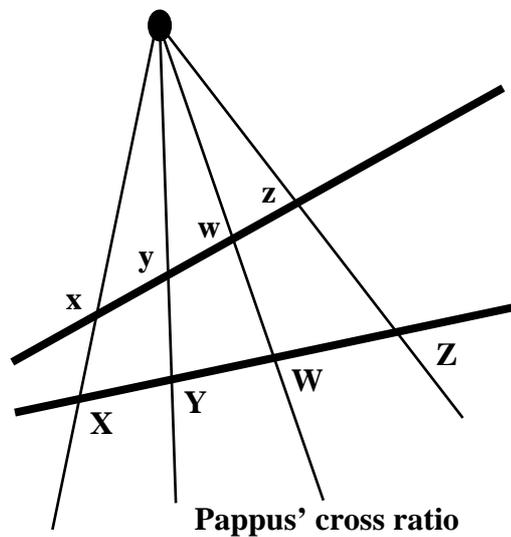


Figure 25: Pappus' construction for the invariance of the cross ratio. It would take a more cartesian form if the projection point were moved to the origin and one of the lines were  $y = 1$ . As a scheme for mapping lines, this is not a projection of a plane to a line; however it *is* a 1:1 mapping of one line to another.

Carrying the result over to the projective line, write the matrices in projective form

$$P = \begin{bmatrix} xs & yt \\ s & t \end{bmatrix}, \quad Q = \begin{bmatrix} wu & zv \\ u & v \end{bmatrix},$$

and calculate the determinants. Note that  $w, x, y, z$  are the values of points on the projective line, whereas  $s, t, v, u$  are the multipliers lost by the projection. We have

$$\frac{|P|}{|Q|} = \frac{(x-y)st}{(w-z)uv}$$

Although this quotient is invariant enough, the multipliers would normally be unknown. Choosing more vectors and dividing once again would only create more multipliers, but the same multipliers can be kept by just rearranging the four vectors in the two bases. There are twenty four possibilities, the permutations of four objects, but only some of them produce the cancellation which would free the points from the multipliers.

The nice symmetry of the formula shows how to get the cancellation; note that each difference is multiplied by the product of its two multipliers. Making up a product of four multipliers in two different ways would allow cancelling the unknown factors while retaining the differences in the points themselves.

So make up two new matrices,

$$R = \begin{bmatrix} xs & zv \\ s & v \end{bmatrix}, \quad S = \begin{bmatrix} wu & yt \\ u & t \end{bmatrix}.$$

The combination which we actually want is

$$\begin{aligned} \frac{|PQ|}{|RS|} &= \frac{(x-y)st(w-z)uv}{(x-z)sv(w-y)ut} \\ &= \frac{(x-y)(w-z)}{(x-z)(w-y)} \\ &= \left(\frac{x-y}{x-z}\right) / \left(\frac{w-y}{w-z}\right), \end{aligned}$$

which is the quotient of quotients of distances from the customary formula to be found in all textbooks.

#### 10.4.2 relative distance interpretation

The derivation of the cross ratio given in the last subsection was based on determinants in the plane, according to which it is really a result about areas, likewise in the plane. The drawing for Pappus's construction also uses a plane, although only as a device to illustrate a one-to-one reversible mapping between two lines gotten by drawing lines out from a focus, to see where they intersect a couple of lines.

Confined to the interior of a line, the invariance of the cross ratio tells something about trying to locate a point by specifying its relative distance from a pair of reference points. Under an affine transformation, which would be a combination of dilation and translation, that ought to suffice. By projective transformation, where the dilation is not uniform, it is the ratio of ratios which is invariant. In other words, if it is  $\rho$  times as far from  $w$  to  $x$  as it is from  $w$  to  $y$ , and it is  $\sigma$  times as far from  $z$  to  $x$  as it is from  $z$  to  $y$  (all of this being taken with due regard for sign), then the ratio of  $\sigma$  to  $\rho$  will always be the same, even when  $\rho$  and  $\sigma$  are not.

To give this a still more concrete interpretation, suppose that  $w$  is the midpoint between  $x$  and  $y$ . It probably isn't still the midpoint after projection, although if two points were halfway between, they would have to move together. Trisectors of an interval,  $w$  and  $z$  with ratios of 2 : 1 and 1 : 2 probably won't map into trisectors either, but the quotient 4 would have to be respected. And so on.

To summarize a long series of special cases, observe that although a cross ratio is unaffected by whatever projective transformation, its particular value still depends on the four points chosen. It

is a reasonable question, given the cross ratio and three of the points, to ask for the fourth. Put

$$\sigma = \frac{w - z}{w - y}$$

to get, for cross ratio  $\phi$ ,

$$\begin{aligned}\phi &= \frac{(x - y)(w - z)}{(x - z)(w - y)} \\ x &= \frac{\phi z - y\sigma}{\phi - \sigma}\end{aligned}$$

The invariance of the cross ratio can be used much less explicitly. Suppose that it is desired to map points  $x_1, x_2, x_3$  into points  $y_1, y_2, y_3$ , and to find the consequences for other points. Note that for whatever value of  $\phi$  arising from  $x, x_1, x_2, x_3$ , there is always a  $y$  determined by the same  $\phi$  and further values  $y_1, y_2, y_3$ . Using that common value of the cross ratio and unknown points  $x$  and  $y$ , we get

$$\begin{aligned}\phi &= \frac{(x - x_1)(x_3 - x_2)}{(x - x_2)(x_3 - x_1)} \\ \phi &= \frac{(y - y_1)(y_3 - y_2)}{(y - y_2)(y_3 - y_1)},\end{aligned}$$

so the equation for the mapping would be

$$\frac{(x - x_1)(x_3 - x_2)}{(x - x_2)(x_3 - x_1)} = \frac{(y - y_1)(y_3 - y_2)}{(y - y_2)(y_3 - y_1)}. \quad (3)$$

It can be checked by substitution and, if necessary, the use of l'Hopital's rule.

Since Eq. 3 has the form prescribed in Eq. 2, it should be possible to obtain it directly by using Lagrange interpolation polynomials on Eq. 2, bearing in mind that a cartesian product of the polynomial bases

### 10.4.3 the six values of the permuted cross ratio

It should be realized that any number at all, including infinity and negative numbers, could be a cross ratio, similar to the observation that any positive number could be the radius of a circle. It is just that a cross ratio is the invariant for projections, whereas radius is the invariant for rotations in another kind of space.

It is of combinatorial interest to recognize that the ordering of the points in the definition of the cross ratio is likely to change its value, although any of the  $4! = 24$  orderings is just as useful as any other. As it works out, the simultaneous exchange of both members of two pairs (the permutation  $(ij)(kl)$ ) fixes the cross ratio. As they generate a normal subgroup of order four of the tetrahedral group, there are six equivalence classes of alternative values for the cross ratio itself.

coset	alternativevalue
fourgroup	$\phi$
fourgroup	$1 - \phi$
fourgroup	$1/\phi$
fourgroup	$1/(1 - \phi)$
fourgroup	$(\phi - 1)/\phi$
fourgroup	$\phi/(\phi - 1)$

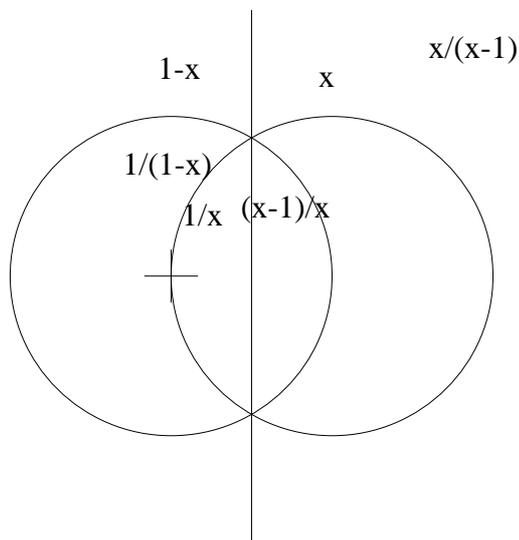


Figure 26: Six regions in the complex plane intermapped by permuting the arguments of a cross ratio.

These mappings should constitute, as a group of mappings, the symmetry group of a triangle, generated by the reflections  $1 - \phi$  and  $1/\phi$ . The triangle group has subgroups, from which particular values of  $\phi$  might be fixed; for example, if  $\phi = 1/\phi$ , then  $\phi = 1$  would only be associated with 0, 1, and  $\infty$ , three rather than six alternatives. The other choice,  $\phi = -1$  has the orbit  $-1, 2, 1/2$ , also containing three points.

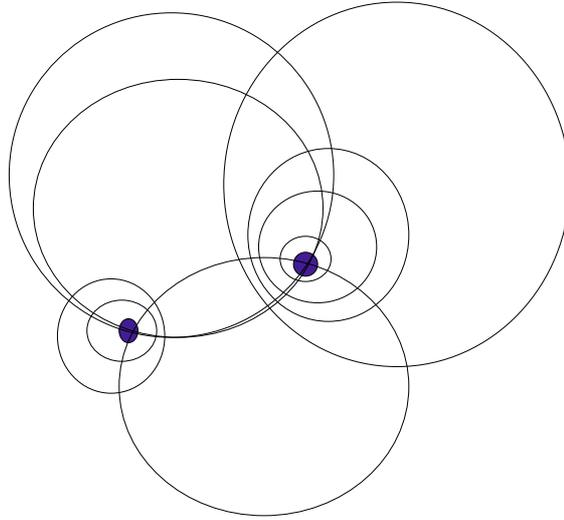
Another reduced set of values results from  $1/(1 - \phi) = \phi$ , which leads to  $\phi^2 - \phi + 1 = 0$ , or  $\phi = (1 \pm i\sqrt{3})/2$ , complex cube roots of unity, two of which comprise the orbit of this symmetry.

#### 10.4.4 points of high cross-ratio symmetry

As compositions of mappings go, the cross ratio commutes with simultaneous projective transformations on each of its arguments. Additionally it commutes with the normal subgroup of simultaneous pair permutation (plus the identity). In the distance interpretation, comparing ratios of distances between one pair of points to another, it is insensitive to exchanging the *from* points for the *to* points.

The additional symmetries get special names:

name	symmetry	ratios
harmonic ratio		1
anharmonic ratio		-1
equianharmonic ratio		$\omega$



**elliptic and hyperbolic orbits**

Figure 27: Elliptic trajectories run around circles surrounding one of the fixed points. Hyperbolic trajectories run along circular arcs connecting the two fixed points, away from one towards the other. Parabolic trajectories arise when the two fixed points coalesce, in which case the two families of orbits look the same, just rotated  $90^\circ$ .

## 10.5 Fixed points for projective mappings

A fixed point should satisfy the equation (assuming  $ad - bc = 1$ )

$$\begin{aligned} x &= \frac{ax + b}{cx + d} \\ &= \frac{(a - d) \pm \sqrt{((d + a)^2 - 1)}}{2c}. \end{aligned}$$

These fixed points are not the eigenvalues of the matrix of the mapping, but rather its eigenvectors. Although the eigenvalues are not directly evident, they still enter into the dynamics of the mapping.

Given their representation as unimodular matrices, the transformations follow an Euler formula with a unit vector and angle of hyperbolic rotation. If the angle is real, the fixed points are real, describing motion from one real fixed point toward the other; if it is imaginary there is no real fixed point. Which of the two cases depends on the size of  $a + d$ .

Of course, for a complex line, there are always fixed points. If the fixed points were zero and infinity, the hyperbolic mappings would be contractions or dilations. If the eigenvalue were imaginary, the elliptic mappings would be rotations about the origin. In either case they could be raised to integer, or even rational or real powers, sweeping out either radial arcs or circular arcs, which could be considered as trajectories of the mapping.

For other pairs of fixed points, the trajectories would be the images of circles (radii, and straight lines in general, are circles through infinity), and so themselves circles positioned with respect to the fixed points. Elliptical orbits encircle the fixed points, hyperbolic orbits ooze from the vicinity of one fixed point toward the vicinity of the other, again along circular arcs.

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