Unit VIII
Matrices, Eigenvalues and Eigenvectors

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In this unit, we will investigate some of the techniques appropriate to matrix usage in physics. We will concentrate on two particular operations: the inversion of matrices, and the discovery of eigenvalues and eigenvectors.

The theoretical analysis of a system often proceeds naturally in one direction, starting with a model of the system, and producing predictions for experimental data. Almost invariably, there are undetermined parameters in the model, which must be determined by experiment. Naturally, the understanding of these undetermined parameters will be of great interest, so we need to have methods of going back from the experimental data to the basic parameters. The connection between these two arenas is not uncommonly made through a matrix. So, to be able to interpret data, one must be able to invert the conversion matrix. An example of this is given in Koonin's book *Computational Physics* in section 5.4, where experimental high energy electron scattering data is used to deduce the charge distribution of a nucleus. While we will not actually work through this example, I encourage you to glance at it to get some idea of a real application.

First, however, we should refamiliarize ourselves with simple matrix multiplication, and then we will move on to a practical method of inversion.

Guidebook Entry VIII.1: Matrix Multiplication

Recall that the multiplication of two matrices proceeds that mixes the rows and columns. In particular, for a 2x2 pair of matrices, the product is given by

$$\begin{bmatrix} \alpha & \beta \\ \gamma & \delta \end{bmatrix} \times \begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} \alpha a + \beta c & \alpha b + \beta d \\ \gamma a + \delta c & \gamma b + \delta d \end{bmatrix}.$$

Make a spreadsheet that multiplies two arbitrary 2x2 matrices. For format, you should do something like the following: allocate cells A1:B2 for the first matrix, A4:B5 for the second matrix, and A7:B8 for the product matrix.

Check your sheet by verifying the product

$$\begin{bmatrix} 1 & -2 \\ -4 & 1 \end{bmatrix} \times \begin{bmatrix} 1 & 2 \\ 4 & 2 \end{bmatrix} = \begin{bmatrix} -7 & -2 \\ 0 & -6 \end{bmatrix}$$

In the next activity, you will use your multiplication techniques to do some inversion of one of these matrices. The technique we will use is more applicable to large matrices, but we will do this on this minimal matrix first.

Guidebook Entry VIII.2: Inverting a 2x2 Matrix

The textbook technique usually encountered for inverting matrices involves adjoints and cofactors [Cramer's Rule]--useful for proving some general results, but computationally expensive for actual calculations. Instead, we will use a method known as the Gauss-Jordan method. Let us say we wish to invert a matrix A. In other words, we want to find the matrix A^{-1} such that

$$A^{-1} A = I$$

where I is the identity matrix. It is difficult to guess this, but it is not difficult to get to the identity matrix step by step by a series of matrix multiplications, so that we will have

$$T_3(T_2(T_1(A))) = I$$

so that we will ultimately find

$$T_3T_2T_1 = A^{-1}.$$

Let's try this out on a real example. Consider the matrix we saw above of

$$\begin{bmatrix} 1 & 2 \\ 4 & 2 \end{bmatrix}.$$

Multiply this on the left by the matrix

$$T_1 = \begin{bmatrix} -1 & 1 \\ 0 & 1 \end{bmatrix}.$$

What is your result?

You should have effectively replaced the first row with the second row minus the first row. Check to see that this is true.

This has now placed a zero in the upper right element, a good step toward creating the identity matrix. With our result above, how can you combine the top and bottom rows in a way that allows you to replace the bottom row now with a new row that has a zero in the left position?

How can you write that operation as a matrix (T_2)?

Multiply the intermediate result above by this matrix, and make sure that your result agrees with your multiplication by hand.

You should now have a matrix that is purely diagonal, although not yet the identity matrix. Show that you can produce the identity matrix by multipling by another diagonal matrix.

What is that matrix (T_3) for your example?

Calculate the matrix $T_3T_2T_1$ and then show by direct multiplication that this is the inverse of our original matrix.

Now, write a spreadsheet that attempts this inversion automatically for an arbitrary 2x2 matrix. To do this, I suggest you make your sheet as follows. Place two multiplying routines side by side. The left one starts out multiplying the original matrix [A] from the left, the right one multiplying the identity matrix from the left. Now make the left multiplicand [T_1] for the left multiplication such that it produces a result with a zero in the upper left corner. You should be able to do this such that the sheet will do it automatically for any starting matrix. Use this T_1 matrix also as the left multiplicand of the identity matrix. Then cut and past the multiplying routines down immediately below the originals (leave a space to keep things pretty). In each case, the new right hand multiplicand is the result from the multiplication immediately above. You should be able to generate the correct T matrices based on the values in certain cells of the various results.

Once you think you have this working, test it on several matrices by directly multiplying the resulting inverses by the original matrices. Give some examples below.

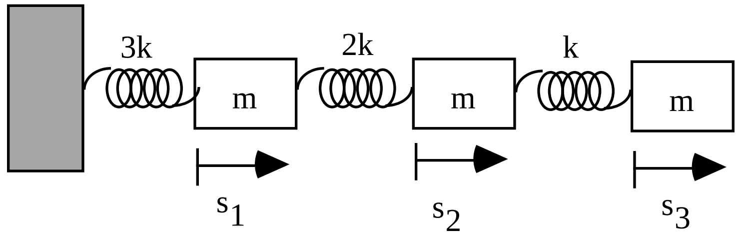
In a homework problem, you will extend this method to 3x3 matrices. In this case, you simply need to systematically work through the off-diagonal elements getting each to turn to zero one at a time. With seven multiplications, you should have your inverse.

Now let's turn to the eigenvalue problem. This turns up often in physics, most familiarly in complex oscillating systems (searching for normal modes) and in quantum mechanics in the matrix format.

Let's look at a real problem, which is developed in Acton's book *Numerical Methods that Work* in the beginning of Chapter 8.

Guidebook Entry VIII.3: Coupled Oscillations

Imagine that we have three identical objects connected in series by a set of springs as shown:



Show that that can be described by the differential equations

$$-\frac{m}{k}\frac{d^2 s_1}{dt^2} = 5s_1 - 2s_2$$
$$-\frac{m}{k}\frac{d^2 s_2}{dt^2} = -2s_1 + 3s_2 - s_3$$
$$-\frac{m}{k}\frac{d^2 s_3}{dt^2} = -s_2 + s_3.$$

The usual game played here is to assume normal mode solutions, that is, each object is oscillating sinusoidally, all at the same frequency. The solutions then can be written as

$$s_i = A_i \cos \omega t.$$

If we define a new version of the frequency as

$$x = \frac{\omega^2 m}{k}$$

show that the solution to these simultaneous differential equations becomes solution to the following equations:

$$xA_1 = 5A_1 - 2A_2$$
$$xA_2 = -2A_1 + 3A_2 - A_3$$

$$xA_3 = -A_2 + A_3$$

Show that this can also be written as the matrix equation

$$\begin{bmatrix} 5-x & -2 & 0 \\ -2 & 3-x & -1 \\ 0 & -1 & 1-x \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}.$$

If this were an equation with scalars, we would say that one of the two multiplicands must be non-invertable, that is, zero. Matrices are a bit more interesting. They may not have an inverse and still be non-zero. This affords us the opportunity to have some interesting solutions here. We know that a matrix can't be inverted if its determinant is zero. So, what we can do is find the determinant of this matrix, solve for the x values that make this go to zero, and we have found the normal mode solutions. These are also called eigenvalue solutions, or eigensolutions, which comes from the German word for "same." The appropriateness of this terminology is clearer if we rewrite the matrix equation as

$$\begin{bmatrix} 5 & -2 & 0 \\ -2 & 3 & -1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix} = x \begin{bmatrix} A_1 \\ A_2 \\ A_3 \end{bmatrix}$$

where the vector is called an eigenvector, and x is the characteristic value, or eigenvalue.

Let's use Mathematica to investigate the solutions to this a bit. First, let's enter the matrix. To do this, you simply enter the numbers as a list of lists:

a={{5-x,-2,0},{-2,3-x,-1},{0,-1,1-x}}

Taking the determinant is no more complicated than

Det[a]

which should give you a cubic polynomial in x. This suggests there are three zeroes, which agrees nicely with the number of degrees of freedom of our oscillating system. At this point, you may wish to solve for the eigenvalues analytically using

Solve[%==0,x],

where the % refers to the output line immediately above, which must be then placed into the form of an equation, hence the ==0. In case you have some intervening outputs, you can always refer to output line 23 as %23. Try using Solve, and describe your results.

You may want to get actual numbers, which you can do with N[%], as we have used before.

If you are just interested in numerical values for these roots, you may find it easier to first plot the determinant:

Plot[%,{x,-10.10}]

to see where the zeros might be, and then close in on them individually by making a good estimate of their location in the command

FindRoot[%==0,{x,0}]

where here I am guessing there is a root near x = 0. Do this, and sketch the curve, and find all three roots.

Now let's see how smart Mathematica can be. Re-enter a new matrix, the matrix that we actually want to find the eigenvalues of:

b={{5,-2,0},{-1,3,-1},{0,-1,1}}.

Let Mathematica do the hard work and find the eigenvalues:

Eigenvalues[N[b]]

and the eigenvectors:

Eigenvectors[N[b]].

The use of the N forces the matrix to be interpreted numerically, which then gives real numbers as a result. How do the eigenvalues compare with the values you got earlier?