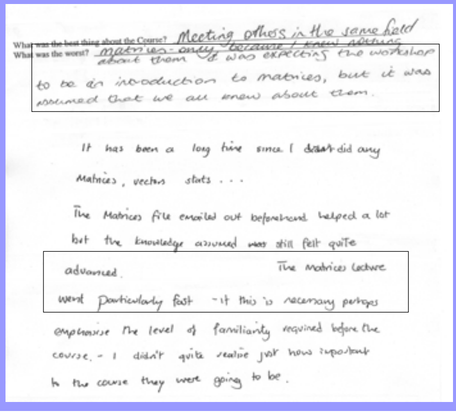
Matrices


What was the best thing about the Course? Meeting others in the same field

What was the worst? matrices - only because I knew nothing about them & was expecting the workshop to be an introduction to matrices, but it was assumed that we all knew about them.

It has been a long time since I ~~dealt~~ did any Matrices, vectors stats . . .

The Matrices file emailed out beforehand helped a lot but the knowledge assumed ~~was~~ still felt quite advanced. The Matrices lecture went particularly fast - if this is necessary perhaps emphasise the level of familiarity required before the course. - I didn't quite realise just how important in the course they were going to be.

Matrices

Don't Panic

Get a good book

Computing Methods in Crystallography. ed J.S. Rollett, Pergamon Press, 1965

Mathematical Methods in Crystallography and Materials Science, E. Prince, Springer-Verlag, 1994

Matrices

These *can* be your friend.

If you need to convert something more complex than a single number into something else, matrices will do it for you.

Some Examples

Imagine that you have a structure in $P2_1/c$ which is related to a similar structure published in $P2_1/n$.

A matrix transformation may enable you to put them on a common axial system, thus facilitating comparisons

The transformation will generate new indices for the reflections and new coordinates and adps for the atoms

Some Examples

If a crystal is randomly orientated on a fibre on a diffractometer, the orientation of the unit cell axes with respect to the diffractometer axes can be represented by an *orientation matrix*. This matrix can be used to compute the direction of the diffracted beam for a given index, and setting angles of the diffractometer.

The Elements of a Matrix

The old coordinates *x* are transformed into the new ones *y*

$$\begin{matrix} y_1 \\ y_2 \\ y_3 \end{matrix} = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} . \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix}$$

Matrix Tranposition

In matrix transposition, the elements which originally formed the rows are use to construct columns.

A matrix with a few long rows becomes a matrix with lots of short rows.

$$\begin{matrix} a & b & c & d & e \\ f & g & h & i & j \end{matrix} \Rightarrow \begin{matrix} a & f \\ b & g \\ c & h \\ d & i \\ e & j \end{matrix}$$

A square matrix stays a square matrix.

Symmetric Matrices

The numbers above the leading diagonal are the same as the corresponding ones below.

$$\begin{matrix} y_1 \\ y_2 \\ y_3 \end{matrix} = \begin{matrix} a_{11} & \boxed{a_{21}} & \boxed{a_{31}} \\ \boxed{a_{21}} & a_{22} & \boxed{a_{32}} \\ \boxed{a_{31}} & \boxed{a_{32}} & a_{33} \end{matrix} . \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix}$$

Matrix Multiplication

- It's easy to get wrong by hand, but worth mastering.
- There are several ways of remembering how to do it properly.
- The following method is pinched from a website.

Matrix Multiplication Demo

matmult.htm

Matrix Division

In ordinary algebra, division can be written as:

$a = b/c$ or $a = c^{-1}.b$

c^{-1} is the *inverse* of c, and is undefined if c=0

In matrix algebra, this is always written as:

$A = C^{-1}.B$

C^{-1} is the inverse of C.

It is undefined if the *determinant of C* is zero.

Calculating C^{-1} is best left to computers.

Orthogonal Matrices

Orthogonal matrices are common in physical science.

One important property is that when they are applied to an object, they do not change its shape.

They can be interpreted as a rotation/inversion about an axis.

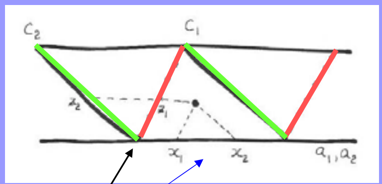
The sum of the squares of the elements in every row and column is unity.

$$\begin{matrix} a_2 \\ b_2 \\ c_2 \end{matrix} = \begin{matrix} Cos & Sin & 0 \\ -Sin & Cos & 0 \\ 0 & 0 & 1 \end{matrix} . \begin{matrix} a_1 \\ b_1 \\ c_1 \end{matrix}$$

The inverse is equal to the transpose

Example

Consider converting data collected in $P2_1/c$ to $P2_1/n$



$a_{new} = a_{old}$

$c_{new} = c_{old} - a_{old}$

$$\begin{matrix} a_2 \\ b_2 \\ c_2 \end{matrix} = \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{matrix} . \begin{matrix} a_1 \\ b_1 \\ c_1 \end{matrix}$$

Note something weird has happened to the *x* coordinate

Determinants

- The determinant of a matrix is a single number.
- All the information contained in the matrix is condensed into this number, which can thus be used as a measure of the information content.
- There is always a potential problem of rounding errors.

Computing a Determinant

Form the sum of the products of each red triplet

$$\begin{matrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{matrix} \qquad \begin{matrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{matrix} \qquad \begin{matrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{matrix}$$

Computing a Determinant

Form the sum of the products of each green triplet

Determinant = red sum – green sum

$$\begin{matrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{matrix} \qquad \begin{matrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{matrix} \qquad \begin{matrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{matrix}$$

Computing a Minor

The minor corresponding to the green element is the determinant of the black elements

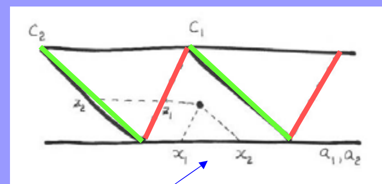
$$\begin{matrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{matrix} \qquad \begin{matrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{matrix}$$

$M_{11} = (1 \times 1)-(0 \times 0) = 1$

$M_{32} = (1 \times 0)-(1 \times 1) = -1$

An Example Revisited

Consider converting data collected in $P2_1/c$ to $P2_1/n$



$a_{new} = a_{old}$

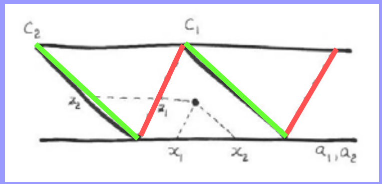
$c_{new} = c_{old} - a_{old}$

$$\begin{matrix} a_2 \\ b_2 \\ c_2 \end{matrix} = \begin{matrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -1 & 0 & 1 \end{matrix} . \begin{matrix} a_1 \\ b_1 \\ c_1 \end{matrix}$$

Note something weird has happened to the *x* coordinate

An Example Revisited

If the reflection indices are transformed by $h_2 = A.\,h_1$,
Then the coordinates are transformed by $x_2 = [A^{-1}]^T.x_1$



$x_{new} = x_{old}$

$z_{new} = z_{old} + z_{old}$

$$\begin{matrix} x_2 \\ y_2 \\ z_2 \end{matrix} = \begin{matrix} 1 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{matrix} . \begin{matrix} x_1 \\ y_1 \\ z_1 \end{matrix}$$

An Example Revisited

If the reflection indices are transformed by:

$h_2 = A.\,h_1,$

Then the coordinates are transformed by:

$x_2 = [A^{-1}]^T.x_1$

And the adps are transformed by:

$U_2 = A.U.A^T$

Eigenvalues

These are not an invention of the devil.

Often, some physical event or process can be represented as a matrix (or a tensor, which looks much the same).

$$\begin{matrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{matrix} . \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix} = \begin{matrix} y_1 \\ y_2 \\ y_3 \end{matrix}$$

Eigenvalues

The determinant is a single number which measures the total information content of a matrix

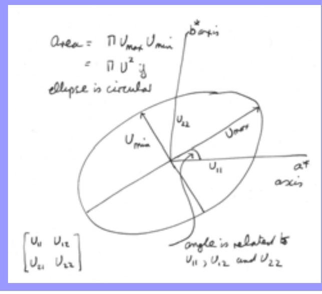
The eigenvalues are a small number of values which tell you about the principal components of this information.

Extracting eigenvalues is often called Principal Component Analysis.

Eigenvalues

The maths is messy, and best left to a computer.

For a 2x2 tensor, the interpretation is quite easily visualised.



Eigenvalues

An anisotropic adp is a symmetric 3x3 tensor, and reflects the uncertainty of an atom’s location about its mean position.

The nature of the atomic displacement is not immediately evident from the adp itself.

This 3x3 tensor can be *diagonalised*,which means finding its eigenvalues.

Eigenvalues & Vectors

We have sneakily introduced eigenvectors. These go with the eigenvalues.

The 3x3 adp represents a 3D ellipsoid. It can be rotated in space so that its 3 principal axes point along the space coordinate axes.

The length of each principal axis is an eigenvalue of the original tensor.

The 3D rotation needed to see this is the matrix of eigenvectors.

Eigenvalues & Vectors

Diagonalising it helps reveal its physical properties.

The matrix *V* of eigenvectors tells us how we must rotate the adp to see the principal components.

$$\begin{matrix} u_{11} & u_{21} & u_{31} \\ u_{21} & u_{22} & u_{32} \\ u_{31} & u_{32} & u_{33} \end{matrix} = V . \begin{matrix} u_1 & 0 & 0 \\ 0 & u_2 & 0 \\ 0 & 0 & u_3 \end{matrix} . V'$$

Eigenvalues & Vectors

This technique can be applied to other problems cases. Very small eigenvalues indicate that the problem is less complex than we thought (lower dimensionality), or that we don’t have enough information to properly resolve the problem.