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## Linear Algebra

### Introduction

Useful for converting between various coordinate systems. In crystallography, this includes:

- × Laboratory coordinates (beam axis? which direction points to the sky?)
- × Reciprocal coordinates (which reflections should I see on the detector?)  
(e.g. the  $2\bar{1}0$  reflection.)
- × Miller indices
- × Fractional coordinates  
(screw axis involves a translation of 0.25 on the  $a$  axis).
- × Real space coordinates (terminal amine is at  $(13, -5, 6)$  Ångströms in unit cell).
- × Detector panel coordinates (to describe a panel tilted  $45^\circ$  with respect to the beam.)

Assumption of knowledge: I have chosen to assume the same knowledge base as I had before starting my PhD.

I could manipulate vectors, with dot / cross products.

I knew matrices formed a closed, self-consistent group but I did not know they described coordinate systems. I knew how to manually add, multiply, invert matrices and multiply a vector by a matrix (these can be easily looked up). Ask me if you need filling in. This should be suitable for those from a biologically-focused background (like me).

Writing this in code: I will adapt to your working environment and help with specific examples.

### Matrices describe coordinate systems.

$$\begin{pmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{pmatrix}$$

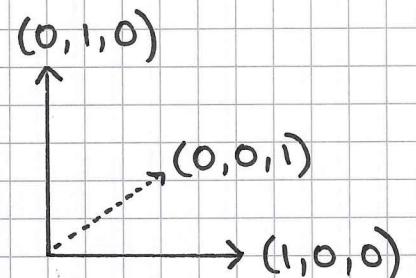
↑      ↑      ↑  
each column is a basis vector.

→ This matrix can describe a three-dimensional space if the three basis vectors are linearly independent, i.e. no one vector can be described as a combination of the other two.

For example,  $(x_0, x_1, x_2)$  and  $(y_0, y_1, y_2)$  could describe the horizontal and vertical directions in the plane of a detector panel, and  $(z_0, z_1, z_2)$  would be the cross-product, i.e. normal to the plane of the detector.

### Identity matrix

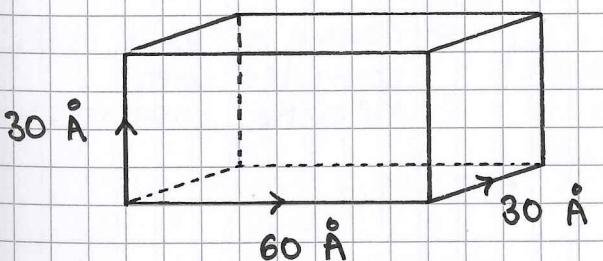
$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Rightarrow$$



- × Equivalent of 1 in real numbers (unity).

It is up to the convention of a program to relate the identity matrix to some real-world basis, and needs to be self-consistent. Make a note of it!

### Describe an orthogonal system.



$$\Rightarrow \begin{pmatrix} 60 & 0 & 0 \\ 0 & 30 & 0 \\ 0 & 0 & 30 \end{pmatrix}$$

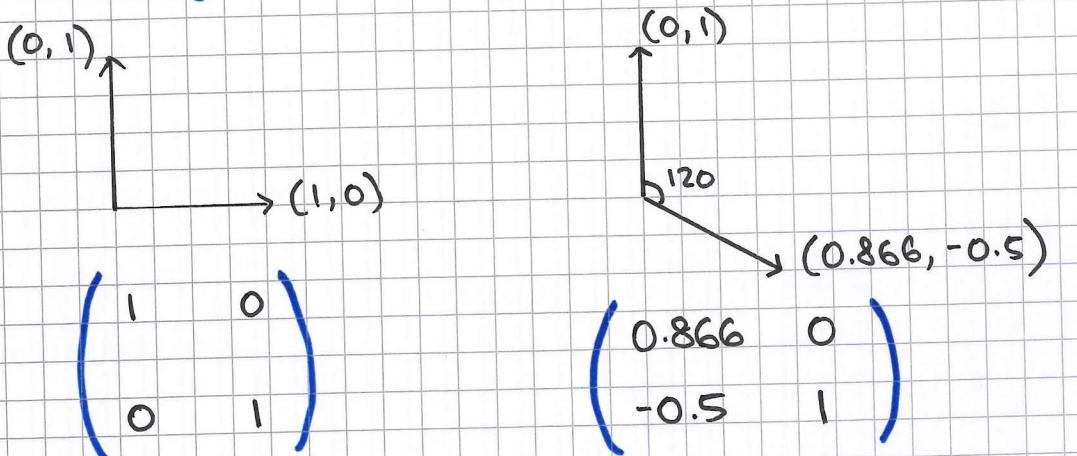
Orthogonal coordinate systems are those where angles between each pair of basis vectors are  $90^\circ$ .

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This matrix will map fractional coordinates (i.e. the coordinate system of the identity matrix) onto positions in the real space unit cell. For example, to find the centre of the unit cell (e.g. for an alternative origin):

$$\begin{pmatrix} 60 & 0 & 0 \\ 0 & 30 & 0 \\ 0 & 0 & 30 \end{pmatrix} \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \end{pmatrix} = \begin{pmatrix} 30 \\ 15 \\ 15 \end{pmatrix} \rightarrow \text{centre of unit cell is at } (30, 15, 15) \text{ \AA}.$$

### Describing a non-orthogonal 2D system



For example, a two-dimensional crystal with three-fold crystallographic symmetry needs a unit cell with a  $120^\circ$  angle. Calculating the centre of the unit cell is no longer intuitive.

$$\begin{pmatrix} 0.866 & 0 \\ -0.5 & 1 \end{pmatrix} \begin{pmatrix} 0.5 \\ 0.5 \end{pmatrix} = \begin{pmatrix} 0.433 \\ 0.25 \end{pmatrix} \rightarrow \text{centre of unit cell converted into "identity coordinates"}$$

### Unit cell parameters of a triclinic system

PDB code 5i40 is used in this example. The PDB coordinate system can be described using this matrix:

$$\begin{pmatrix} 24.58 & 9.01 & 11.34 \\ 0 & 32.52 & 10.56 \\ 0 & 0 & 36.34 \end{pmatrix} \begin{matrix} \uparrow \\ \mathbf{a} \\ \uparrow \\ \mathbf{b} \\ \uparrow \\ \mathbf{c} \end{matrix} \times \text{What are the unit cell dimensions of 5i40?}$$

Working out lengths of basis vectors:

$$\mathbf{a} \text{ axis} = (24.58, 0, 0); |\mathbf{a}| = 24.58 \text{ \AA}.$$

$$\mathbf{b} \text{ axis} = (9.01, 32.52, 0); |\mathbf{b}| = \sqrt{(9.01^2 + 32.52^2)} = 33.75 \text{ \AA}.$$

$$\mathbf{c} \text{ axis} = (11.34, 10.56, 36.34);$$

$$|\mathbf{c}| = \sqrt{(11.34^2 + 10.56^2 + 36.34^2)} = 39.50 \text{ \AA}.$$

The  $\alpha$  angle is the angle between the  $\mathbf{b}$  and  $\mathbf{c}$  basis vectors and can be determined using the dot product rule:

$$\cos \alpha = \frac{\mathbf{b} \cdot \mathbf{c}}{|\mathbf{b}| |\mathbf{c}|}$$

Evaluating this in the above example:

$$\cos \alpha = \frac{(9.01 \times 11.34 + 32.52 \times 10.56 + 0 \times 36.34)}{33.75 \times 39.50}$$

$$\cos \alpha = 0.3342; \alpha = \cos^{-1}(0.3342) = 70.47^\circ.$$

Note that this can be used on basis vectors which have been rotated by a rotation matrix as the lengths and angles will remain internally consistent!

### Coordinate system from unit cell dimensions

From some unit cell ( $a, b, c, \alpha, \beta, \gamma$ ), find some matrix to describe the corresponding coordinate system. There is no fixed method but by convention this formulation is widely used:

$$\begin{pmatrix} a & b \cdot \cos\gamma & c \cdot \cos\beta \\ 0 & b \cdot \sin\gamma & \frac{c(\cos\alpha - \cos\beta \cdot \cos\gamma)}{\sin\gamma} \\ 0 & 0 & \frac{\text{volume}}{a \cdot b \cdot \sin\gamma} \end{pmatrix}$$

$$\text{volume} = a \cdot b \cdot c \cdot \sqrt{1 - \cos^2\alpha - \cos^2\beta - \cos^2\gamma + 2\cos\alpha\cos\beta\cos\gamma}$$

### Real to reciprocal unit cell coordinates

- \* The inverse matrix of the real space coordinate system is the reciprocal space coordinate system.
- \* Applying the reciprocal space coordinate system to a real space vector brings it into fractional space (the identity matrix).

e.g. from earlier, we had real space unit cell presented as:

$$\begin{pmatrix} 60 & 0 & 0 \\ 0 & 30 & 0 \\ 0 & 0 & 30 \end{pmatrix}$$

the inverse  
of which is:

$$\begin{pmatrix} \frac{1}{60} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{30} \end{pmatrix}$$

So now to convert the centre of the unit cell back to fractional coordinates:

$$\begin{pmatrix} \frac{1}{60} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} 30 \\ 15 \\ 15 \end{pmatrix} = \begin{pmatrix} 0.5 \\ 0.5 \\ 0.5 \end{pmatrix}$$

The reciprocal matrix also describes separations of Miller indices in reciprocal space. Bragg peaks will be located at whole number multiples of the basis vectors in reciprocal space: for example, where and at what resolution is Miller index (2, 5, 1)?

$$\begin{pmatrix} \frac{1}{60} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{30} \end{pmatrix} \begin{pmatrix} 2 \\ 5 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.0333 \\ 0.1667 \\ 0.0333 \end{pmatrix}$$

in reciprocal space  
i.e.  $\text{\AA}^{-1}$ .

The reciprocal distance from the origin is  $d^*$  in  $\text{\AA}^{-1}$ , or the inverse of the resolution.

$$d^* = \sqrt{(0.0333^2 + 0.1667^2 + 0.0333^2)} = \sqrt{0.03} = 0.1732 \text{\AA}^{-1}$$

$$d = 0.1732^{-1} = 5.77 \text{\AA}$$

Therefore the (2, 5, 1) reflection in this space group contains information about the crystal at 5.77  $\text{\AA}$  resolution.

- \* Note that if you are placing atoms in a unit cell in real space, you will generally be working with fractional coordinates, each dimension of which will occupy values between 0 and 1.
- \* If instead you are working with locations of Bragg peaks, you will be working in integer coordinates where each dimension has whole number values.

### Rotations of crystals

- Particularly important for indexing as crystals are rotated during X-ray exposure and are already at arbitrary rotations. These can be handled with rotation matrices in various ways.

#### Do I have a rotation matrix?

If you receive a rotation matrix, how can you tell?

$$\begin{pmatrix} 0.977 & -0.158 & -0.144 \\ 0.094 & 0.922 & -0.374 \\ 0.192 & 0.352 & 0.916 \end{pmatrix} \quad \begin{matrix} \uparrow x \\ \uparrow y \\ \uparrow z \end{matrix} \quad \rightarrow \text{this encodes a small rotation so has minor deviations from the identity}$$

Rotation matrices must have unit vectors:

$$x_0^2 + x_1^2 + x_2^2 = 1; \quad y_0^2 + y_1^2 + y_2^2 = 1; \quad z_0^2 + z_1^2 + z_2^2 = 1$$

Dot products are all 0, indicating orthogonal vectors:

$$\underline{x} \cdot \underline{y} = 0; \quad \underline{y} \cdot \underline{z} = 0; \quad \underline{z} \cdot \underline{x} = 0$$

Therefore determinant of matrix will be  $\pm 1$ . Positive determinant maintains handedness, and is highly recommended.

Rotation matrices can be constructed or deconstructed in many ways. Two I find particularly useful are Tait-Bryan angles (closely related to Euler angles and good for small-angle applications). Axis/angle definitions are great for goniometer-like scenarios.

### Tait-Bryan angles

- These define some angle to rotate around the x, y and z axes. As the angles get larger, the order of operations matters more (matrix operations are non-commutative).
- Individual axis rotation definitions are available on Wikipedia (August 2018) on page "Rotation\_matrix".

Reproduced here:

$$R_x(\alpha) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix} \quad \leftarrow \text{n.b. as this rotates around the } x \text{ axis, the } x \text{ axis basis vector is unaffected by this operation.}$$

$$R_y(\beta) = \begin{pmatrix} \cos\beta & 0 & \sin\beta \\ 0 & 1 & 0 \\ -\sin\beta & 0 & \cos\beta \end{pmatrix}$$

$$R_z(\gamma) = \begin{pmatrix} \cos\gamma & -\sin\gamma & 0 \\ \sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- From these, we can apply these operations in some arbitrary order.

$$R_x(\alpha) R_y(\beta) R_z(\gamma) =$$

$$\begin{pmatrix} \cos\beta \cos\gamma & -\sin\gamma \cos\beta & \sin\beta \\ \cos\alpha \sin\gamma + \sin\alpha \sin\beta \cos\gamma & \cos\alpha \cos\gamma - \sin\alpha \sin\beta \sin\gamma & -\sin\alpha \cos\beta \\ \sin\alpha \sin\gamma - \cos\alpha \sin\beta \cos\gamma & \sin\alpha \cos\gamma + \cos\alpha \sin\beta \sin\gamma & \cos\alpha \cos\beta \end{pmatrix}$$

You can decompose an existing rotation matrix into  $\alpha$ ,  $\beta$  and  $\gamma$  angles by solving simple equations from the matrix components. For a matrix:

$$\begin{pmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{pmatrix}$$

$$\begin{aligned} z_0 &= \sin\beta && \text{(solve for } \beta) \\ z_1 &= -\cos\beta \sin\alpha && \text{(solve for } \alpha) \\ y_0 &= -\cos\beta \sin\gamma && \text{(solve for } \gamma) \end{aligned}$$

n.b. beware of multiple solutions.

### Rotation around axis and angle.

- \* Definition is also on Wikipedia on page "Rotation\_matrix" but also reproduced here: Clockwise rotation of  $\theta$  around unit vector  $(u_x, u_y, u_z)$ .

Rotation matrix:

$$\begin{matrix} \cos\theta + u_x^2(1-\cos\theta) & u_x u_y (1-\cos\theta) - u_z \sin\theta & u_x u_z (1-\cos\theta) + u_y \sin\theta \\ u_y u_x (1-\cos\theta) + u_z \sin\theta & \cos\theta + u_y^2(1-\cos\theta) & u_y u_z (1-\cos\theta) - u_x \sin\theta \\ u_z u_x (1-\cos\theta) - u_y \sin\theta & u_z u_y (1-\cos\theta) + u_x \sin\theta & \cos\theta + u_z^2(1-\cos\theta) \end{matrix}$$

- \* If you have a rotation matrix, extracting the angle and axis is not too difficult. Consider adding the elements of the body diagonal:

$$\begin{aligned} x_0 + y_1 + z_2 &= \cos\theta + u_x^2(1-\cos\theta) + \cos\theta + u_y^2(1-\cos\theta) \\ &\quad + \cos\theta + u_z^2(1-\cos\theta) \\ &= 3\cos\theta + (1-\cos\theta)(u_x^2 + u_y^2 + u_z^2) \end{aligned}$$

We know the axis is a unit vector, so this simplifies:

$$x_0 + y_1 + z_2 = 2\cos\theta + 1$$

This allows us to solve for  $\theta$ , which can then be used to extract the axis from the individual components of the body diagonal.

### Inverting a rotation matrix.

Due to the restrictions on rotation matrices, their inverses are also their transposes.

$$R^{-1} = R^T$$

$$\begin{pmatrix} x_0 & y_0 & z_0 \\ x_1 & y_1 & z_1 \\ x_2 & y_2 & z_2 \end{pmatrix} = \begin{pmatrix} x_0 & x_1 & x_2 \\ y_0 & y_1 & y_2 \\ z_0 & z_1 & z_2 \end{pmatrix}$$

The rotation needed to get from P to Q is therefore:

$$Q \cdot P^{-1} = Q \cdot P^T$$