

CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

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Lecture 22: Combining Translation with Point Symmetries-II

In this lecture, we will see how to represent translation in matrix form. We have already seen rotation and reflection operations. One key property of rotation and reflection transformations is that they are linear transformations.

What does this mean? Suppose we have a transformation T represented by a matrix, and we apply it to vectors \bar{a} and \bar{b} . If T is linear, then:

- $T(\bar{a} + \bar{b}) = T(\bar{a}) + T(\bar{b})$
- $T(c\bar{a}) = cT(\bar{a})$, where c is a scalar.

Now, let us look at translation. Suppose we have a vector $\bar{v} = (v_x, v_y)$ and a translation vector $\bar{t} = (T_x, T_y)$. The translation is simply

$$\bar{v} + \bar{t} = (v_x + T_x, v_y + T_y)$$

However, this is not a linear transformation, because it does not satisfy the linearity properties above. Therefore, we cannot use regular matrix multiplication directly as we did for rotations or reflections.

For example, in the previous lecture with two perpendicular mirrors M_1 and M_2 , the reflection matrices for σ_1 and σ_2 could be multiplied:

$$\sigma_2 * \sigma_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

which corresponds to a 180° rotation at the intersection of the mirrors, giving a two-fold rotational symmetry (A_π).

To handle translation in a similar matrix form, we use homogeneous coordinates. In 2D, we attach a third coordinate with value 1 to a point (x, y) :

$$p = \begin{pmatrix} x \\ y \\ 1 \end{pmatrix}$$

The translation matrix for $\bar{t} = (T_x, T_y)$ becomes:

$$T = \begin{pmatrix} 1 & 0 & T_x \\ 0 & 1 & T_y \\ 0 & 0 & 1 \end{pmatrix}$$

Multiplying T with p gives:

$$Tp = \begin{pmatrix} x + T_x \\ y + T_y \\ 1 \end{pmatrix}$$

This correctly performs the translation. Homogeneous coordinates are widely used in computer graphics to combine translations with rotations and reflections. Sometimes the third coordinate is written as w , a scaling factor, but for our purposes, we keep it as 1.

In 3D, the translation matrix becomes 4×4 , and the point coordinates become $(x, y, z, 1)$:

$$T = \begin{pmatrix} 1 & 0 & 0 & T_x \\ 0 & 1 & 0 & T_y \\ 0 & 0 & 1 & T_z \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad p = \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

Then $Tp = (x + T_x, y + T_y, z + T_z, 1)^T$. To combine with rotation or reflection in 3D, these matrices are also extended to 4×4 .

$$\begin{pmatrix} 1 & 0 & 0 & T_x \\ 0 & 1 & 0 & T_y \\ 0 & 0 & 1 & T_z \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} = \begin{pmatrix} x + T_x \\ y + T_y \\ z + T_z \\ 1 \end{pmatrix}$$

Now, let us see an application. Suppose we want a rotation not about the origin, but about a point (a, b) . We know the rotation matrix at the origin for an angle α is:

$$A_\alpha(0, 0) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

To rotate about (a, b) , we first translate the point (a, b) to the origin using a translation by $(-a, -b)$:

$$T(-a, -b) = \begin{pmatrix} 1 & 0 & -a \\ 0 & 1 & -b \\ 0 & 0 & 1 \end{pmatrix}$$

Once at the origin, we apply the rotation A_α . After rotation, we translate back by (a, b) .

This combination of translation and rotation using homogeneous coordinates allows us to perform transformations at arbitrary points using simple matrix multiplication.

To perform a rotation at a point (a, b) rather than the origin, we first translate the point (a, b) to the origin using $(-a, -b)$. After performing the rotation at the origin, we then translate back by (a, b) .

Mathematically, the rotation matrix $A_\alpha(a, b)$ at the point (a, b) is given by:

$$A_\alpha(a, b) = T(a, b) A_\alpha(0, 0) T(-a, -b)$$

where

$$T(a, b) = \begin{pmatrix} 1 & 0 & a \\ 0 & 1 & b \\ 0 & 0 & 1 \end{pmatrix}, \quad A_\alpha(0,0) = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$T(-a, -b) = \begin{pmatrix} 1 & 0 & -a \\ 0 & 1 & -b \\ 0 & 0 & 1 \end{pmatrix}$$

Multiplying these matrices gives:

$$A_\alpha(a, b) = \begin{pmatrix} \cos\alpha & -\sin\alpha & a(1 - \cos\alpha) + B\sin\alpha \\ \sin\alpha & \cos\alpha & -a\sin\alpha + b(1 - \cos\alpha) \\ 0 & 0 & 1 \end{pmatrix}$$

This is the rotation matrix about (a, b) .

Similarly, for a reflection across a mirror not passing through the origin, for example a mirror at $x = a$ parallel to the yz -plane, we first translate by $(-a, 0)$ to bring the mirror to the origin, perform the reflection σ_{yz} , and then translate back by $(a, 0)$.

The resulting reflection matrix is:

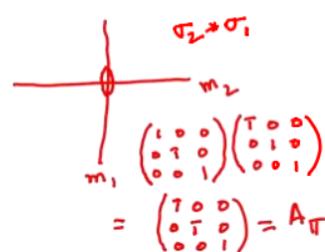
$$\sigma_{yz}(a) = \begin{pmatrix} -1 & 0 & 2a \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

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Translation Matrix

* Rotation & Reflection Transformations:
 - Linear Transformation (T)
 $T(\vec{a}) + T(\vec{b}) = T(\vec{a} + \vec{b})$
 $T(c\vec{a}) = cT(\vec{a})$

* Translation
 $\vec{v} = \begin{pmatrix} v_x \\ v_y \end{pmatrix}$ $\vec{t} = \begin{pmatrix} t_x \\ t_y \end{pmatrix}$
 $\vec{v} + \vec{t} = \begin{pmatrix} v_x \\ v_y \end{pmatrix} + \begin{pmatrix} t_x \\ t_y \end{pmatrix} = \begin{pmatrix} v_x + t_x \\ v_y + t_y \end{pmatrix}$
 → NOT A LINEAR TRANSFORM



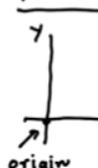
$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} T & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} T & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = A_T$

Use homogeneous coordinates

2D $\begin{pmatrix} 1 & 0 & t_x \\ 0 & 1 & t_y \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ 1 \end{pmatrix} = \begin{pmatrix} x + t_x \\ y + t_y \\ 1 \end{pmatrix}$
 scaling

3D $\vec{t} = (t_x, t_y, t_z)$
 $\begin{pmatrix} 1 & 0 & 0 & t_x \\ 0 & 1 & 0 & t_y \\ 0 & 0 & 1 & t_z \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix} = \begin{pmatrix} x + t_x \\ y + t_y \\ z + t_z \\ 1 \end{pmatrix}$

Rotation Matrix at (a, b)



$A_d(a, b) = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$
 $x T(a, b) = A_d(a, b) T(-a, -b) = A_d(a, b)$

$A_d(a, b) = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
 $= \begin{pmatrix} \cos^2 \theta - \sin^2 \theta & a[-\cos \theta] + b \sin \theta & 0 \\ \sin \theta \cos \theta & -a \sin \theta + b[1 - \cos \theta] & 0 \\ 0 & 0 & 1 \end{pmatrix}$

$T(a, b) = \sigma_{y_2}(a) = T(-a, 0) = \sigma_{y_2}(a) = \begin{pmatrix} T & 2a \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$



Applying this matrix to a point $(x, y, 1)^T$ gives:

$$(x, y, 1)^T \rightarrow (-x + 2a, y, 1)^T$$

Graphically, this works as follows: a point at distance $a - x$ from the mirror is reflected to the other side by the same distance, giving the new x-coordinate $-x + 2a$, and the y-coordinate remains the same. This matches the result from the matrix approach.

Finally, consider the problem of two mirrors M_1 and M_2 , where M_2 is at $x = a$. Using matrices, the reflection matrices are:

$$\sigma_2 = \begin{pmatrix} -1 & 0 & 2a \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Multiplying them:

$$\sigma_2 * \sigma_1 = \begin{pmatrix} 1 & 0 & 2a \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Comparing with the translation matrix, we see that this corresponds to a translation by $(2a, 0)$.

This shows how two reflection operations can be combined using matrices. In the next lecture, we will explore combining rotation and translation, which will lead us to the development of plane groups.

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$$\sigma_2 * \sigma_1 = \begin{pmatrix} 1 & 0 & 2a \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\sigma_2 * \sigma_1 = \begin{pmatrix} 1 & 0 & 2a \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 2a \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \underline{\underline{T(2a, 0)}}$$

$$T(t_x, t_y) = \begin{pmatrix} 1 & 0 & t_x \\ 0 & 1 & t_y \\ 0 & 0 & 1 \end{pmatrix}$$

$t_x = 2a$
 $t_y = 0$