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MATRIX CALCULUS APPLIED TO CRYSTALLOGRAPHY

(short revision)

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MATRIX CALCULUS IN CRYSTALLOGRAPHY

(BRIEF REVISION)

Some of the slides are taken from the presentation "*Introduction to Matrix Algebra*" of **M. Rademeyer** given at the School on Fundamental Crystallography, Bloemfontein, South Africa, 2010

What is a matrix?

Definition:

- A rectangular array of numbers
- in m rows
- and n columns
- is called an $(m \times n)$ matrix $\boldsymbol{A}$

Use boldface italics upper case letters to indicate matrix, e.g. ***A*, *B*, *W***.

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{pmatrix}.$$

An item in a matrix is called an entry or element

Square Matrix:

An (n x n) matrix

rows = # columns

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix}$$

Column Matrix:

An (m x 1) matrix

Row index changes

$$\begin{pmatrix} A_{11} \\ A_{21} \\ \vdots \\ A_{m1} \end{pmatrix}$$

Row Matrix:

A (1 x n) matrix

Column index changes

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \end{pmatrix}$$

Index 1 is often omitted for column and row matrices.

Transposed Matrix $\boldsymbol{A}^T$

Let $\boldsymbol{A}$ be a (m x n) matrix
The (n x m) matrix obtained from
$\boldsymbol{A}$ = (A_{ik}) by exchanging rows and
columns is called the transposed
matrix $\boldsymbol{A}^T$.

$$\boldsymbol{A} = \begin{pmatrix} 1 & 0 & \bar{1} \\ 2 & 4 & \bar{3} \end{pmatrix} \qquad \boldsymbol{A}^{\mathrm{T}} = \begin{pmatrix} 1 & 2 \\ 0 & 4 \\ \bar{1} & \bar{3} \end{pmatrix}$$

Reminder: $\bar{z}$ means $-z$

Example 1: Transposed Matrix

Given that

$$\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix}$$

determine $\boldsymbol{A}^{\mathrm{T}}$.

Symmetric Matrix

A square matrix is symmetric if $\boldsymbol{A^T} = \boldsymbol{A}$

i.e. if $A_{ik} = A_{ki}$ for any pair i,k.

$$\begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & \bar{5} \\ 3 & \bar{5} & 6 \end{pmatrix}$$

Symmetric with respect to main diagonal

- Top left to bottom right

SKEW-SYMMETRIC MATRIX

$$\boldsymbol{A}^T = -\boldsymbol{A}$$

0	0	-5
0	0	6
5	-6	0

If $\boldsymbol{A}$ is a skew-symmetric matrix, then

$A_{ii}=0,\ i=1,2,3$

as $A_{ik}=-A_{ki}$

EXERCISES

Problems

1. Construct the transposed matrix of the (3x1) row matrix:

1	3	4

2. Determine which of the following matrices are symmetric and which are skew-symmetric:

A=

3	0
0	2

B=

3	4
-4	1

C=

2	-1
-1	1

D=

0	2
-2	0

E=

0	0
1	0

F= (3)

G=

0	1	-2
-1	0	3
2	-3	0

H=

3	2
2	1
1	0

J=

0	0
0	0

Matrix Calculations

Multiplication with a number (scalar product):

An (m x n) matrix $\boldsymbol{A}$ is multiplied with a number λ by multiplying each element with λ:

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{pmatrix} \longrightarrow \lambda\boldsymbol{A} = \begin{pmatrix} \lambda A_{11} & \lambda A_{12} & \dots & \lambda A_{1n} \\ \lambda A_{21} & \lambda A_{22} & \dots & \lambda A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda A_{m1} & \lambda A_{m2} & \dots & \lambda A_{mn} \end{pmatrix}$$

Example 2: Scalar product

Given that

$$\boldsymbol{A} = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix}$$

determine $3\boldsymbol{A}$.

Matrix addition and subtraction:

Let A_{ik} and B_{ik} be general elements of matrices $\boldsymbol{A}$ and $\boldsymbol{B}$.

$\boldsymbol{A}$ and $\boldsymbol{B}$ must be of the same size (i.e. same number of rows and columns). Then the sum and the difference $\boldsymbol{A} \pm \boldsymbol{B}$ is:

$$\boldsymbol{C} = \boldsymbol{A} \pm \boldsymbol{B} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mn} \end{pmatrix} \pm \begin{pmatrix} B_{11} & B_{12} & \dots & B_{1n} \\ B_{21} & B_{22} & \dots & B_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ B_{m1} & B_{m2} & \dots & B_{mn} \end{pmatrix} =$$

$$= \begin{pmatrix} A_{11} \pm B_{11} & A_{12} \pm B_{12} & \dots & A_{1n} \pm B_{1n} \\ A_{21} \pm B_{21} & A_{22} \pm B_{22} & \dots & A_{2n} \pm B_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1} \pm B_{m1} & A_{m2} \pm B_{m2} & \dots & A_{mn} \pm B_{mn} \end{pmatrix}$$

Element C_{ik} of $\boldsymbol{C}$ is equal to the sum or difference of the elements A_{ik} and B_{ik} of $\boldsymbol{A}$ and $\boldsymbol{B}$ for any pair i,k:

$C_{ik} = A_{ik} \pm B_{ik}$

EXERCISES

Problems

1. Find 3***A***-2***B***, where

$$\mathbf{A}=\begin{bmatrix}1 & 2\\ 3 & 0\end{bmatrix} \quad \mathbf{B}=\begin{bmatrix}1 & 3\\ 0 & -4\end{bmatrix}$$

2. Show that the sum of any matrix and its transpose is a symmetric matrix, *i.e.*

$$(\mathbf{A}+\mathbf{A}^{T})^{T}=\mathbf{A}+\mathbf{A}^{T}$$

3. Show that the difference of any matrix and its transpose is a skew-symmetric matrix, *i.e.*

$$(\mathbf{A}-\mathbf{A}^{T})^{T}=-(\mathbf{A}-\mathbf{A}^{T})$$

Matrix multiplication

The multiplication of two matrices is only defined when:

- the number $n_{(lema)}$ of columns of the *le*ft *ma*trix is the same as
- the number of $m_{(rima)}$ of rows on the *ri*ght *ma*trix
- no restriction on $m_{(lema)}$ or rows of the *le*ft *ma*trix
- no restriction on $n_{(rima)}$ or rows of the *ri*ght *ma*trix

columns of left matrix = # rows of right matrix

Multiplication
Product of two matrices *A* and *B*:

The matrix product ***C*** = ***AB*** or

$$\begin{pmatrix} C_{11} & C_{12} & \dots & C_{1k} & \dots & C_{1n} \\ C_{21} & C_{22} & \dots & C_{2k} & \dots & C_{2n} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ C_{i1} & C_{i2} & \dots & C_{ik} & \dots & C_{in} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ C_{m1} & C_{m2} & \dots & C_{mk} & \dots & C_{mn} \end{pmatrix} =$$

$$= \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1j} & \dots & A_{1r} \\ A_{21} & A_{22} & \dots & A_{2j} & \dots & A_{2r} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ A_{i1} & A_{i2} & \dots & A_{ij} & \dots & A_{ir} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mj} & \dots & A_{mr} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} & \dots & B_{1k} & \dots & B_{1n} \\ B_{21} & B_{22} & \dots & B_{2k} & \dots & B_{2n} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ B_{j1} & B_{j2} & \dots & B_{jk} & \dots & B_{jn} \\ \vdots & \vdots & & \vdots & \ddots & \vdots \\ B_{r1} & B_{r2} & \dots & B_{rk} & \dots & B_{rn} \end{pmatrix}$$

is defined by $C_{ik} = A_{i\,1} B_{1k} + A_{i\,2} B_{2k} + \ldots + A_{i\,j} B_{jk} + \ldots + A_{i\,r} B_{rk}$.

Examples: Matrix Multiplication

If $A = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$ and $B = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$,

then $C = A\,B = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

$$D = B\,A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$C \neq D$, *i. e.* matrix multiplication is *not always commutative.*
However, it is *associative*, *e. g.*, $(A\,B)\,D = A\,(B\,D)$
and *distributive*, *i. e.* $(A + B)\,C = A\,C + B\,C$.

Example 5: Multiplication

Given that

$$A = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 1 & 0 \\ 2 & 2 & 2 \\ 3 & 2 & 1 \end{pmatrix}$$

and ***C* = *AB***.
Determine ***C***.

Determine ***D*=*BA***, check if ***C*=*D*** or not.

EXERCISES

Problems

1. Find the products ***AB*** and ***BA***, if they exist, where

A =

1	2
3	-4

B =

3	-2	2
1	0	-1

2. Find the matrix products ***AB*** and ***BA*** of the row vector ***A*** =

1	2	3

, and the column vector ***B*** =

-2
4
1

3. Prove that ***A***(***BC***)=(***AB***)***C*** where

A =

1	2
-1	3

B =

1	0	-1
2	1	0

C =

1	-1
3	2
2	1

Trace of a Matrix

The trace of a (n x n) square matrix $\boldsymbol{A}$ is the sum of the elements on the main diagonal.

$$\boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix}$$

$$tr(\boldsymbol{A}) = A_{11} + A_{22} + \dots + A_{nn}$$

Determinants

The determinant det(***A***) or |***A***| of ***A*** can be calculated for any (n x n) square matrix.

(2×2) matrix

$$\text{Let } \boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

$$\det(\boldsymbol{A}) = \begin{vmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{vmatrix}$$

$$\det(\boldsymbol{A}) = \boxed{A_{11}A_{22}} - \boxed{A_{12}A_{21}}$$

Determinants

(3×3) matrix

$$\boldsymbol{B} = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix}$$

$$\det(\boldsymbol{B}) = \begin{vmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{vmatrix}$$

$$\begin{aligned} \det(\boldsymbol{B}) \quad = \quad & B_{11}\,B_{22}\,B_{33} + B_{12}\,B_{23}\,B_{31} + B_{13}\,B_{21}\,B_{32} - \\ & - B_{11}\,B_{23}\,B_{32} - B_{12}\,B_{21}\,B_{33} - B_{13}\,B_{22}\,B_{31} \end{aligned}$$

Example 6: Determinant

Given that

$$A = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix}$$

Determine det($\boldsymbol{A}$).

EXERCISES

Problems

1. Find the values of the traces and the determinants of ***A*** and ***B*** where

A=

1	2
-1	3

B=

0	4	2
4	-2	-1
5	1	3

2. Show that det(***AB***)=det(***A***)det(***B***) where

A=

3	2
5	1

B=

1	6
2	9

3. Show that det(***A***)= det($\boldsymbol{A}^T$) where

A=

1	1	3
2	2	2
3	2	3

Inverse of a Matrix

A matrix $\boldsymbol{C}$ which fulfills the condition $\boldsymbol{CA} = \boldsymbol{I}$ for a square matrix $\boldsymbol{A}$, is the inverse matrix $\boldsymbol{A}^{-1}$ of $\boldsymbol{A}$, i.e. $\boldsymbol{AA}^{-1} = \boldsymbol{I}$.

$\boldsymbol{A}^{-1}$ exists if and only if $\det(\boldsymbol{A}) \neq 0$.
Not all matrices have an inverse matrix.

Assume that $\boldsymbol{A}^{-1}$ exists. If $\boldsymbol{CA} = \boldsymbol{I}$ then $\boldsymbol{AC} = \boldsymbol{I}$ also holds.

A matrix is called orthogonal if $\boldsymbol{A}^{-1}=\boldsymbol{A}^{T}$, i.e. $\boldsymbol{AA}^{T}=\boldsymbol{A}^{T}\boldsymbol{A}=\boldsymbol{I}$

EXAMPLE

Inverse of a matrix $\boldsymbol{A}$:

$$(A^{-1})_{ik}=(\det A)^{-1}(-1)^{i+k}B_{ki}$$

Find the inverse, if it exists of $\boldsymbol{A}$, where $A=\begin{pmatrix}1&2&3\\1&3&5\\1&5&12\end{pmatrix}$

(i) $\det A=3$, $\det A\neq 0$

(ii) $(A^{-1})_{11}$: $(1/3)(-1)^{1+1}B_{11}= 11/3$

$$B_{11}=\det\begin{pmatrix}1&2&3\\1&3&5\\1&5&12\end{pmatrix}=\det\begin{pmatrix}3&5\\5&12\end{pmatrix}=11$$

(iii) $(A^{-1})_{12}$: $(1/3)(-1)^{1+2}B_{21}= -9/3$

• • •

$$A^{-1}=1/3\begin{pmatrix}11&-9&1\\-7&9&-2\\2&-3&1\end{pmatrix}$$

Is it correct?

EXERCISES

Problems

1. Determine the inverses of the following matrices:

A =

-1	0	0
0	-1	0
0	0	1

B =

0	-1	0
1	0	0
0	0	-1

C =

0	0	1
1	0	0
0	1	0

D =

1	-1	0
1	1	0
0	0	1

E =

-1	1	1
1	-1	1
1	1	-1

F =

0	1	1
1	0	1
1	1	0

2. Given that ***A*** =

1	2	0
-1	0	3
2	-1	0

, determine $\boldsymbol{A}^{-1}$.

EXERCISES

Problems

Given that $\boldsymbol{A}=$

1	2	0
-1	0	3
2	-1	0

, determine $\boldsymbol{A}^{-1}$.

SOLUTION

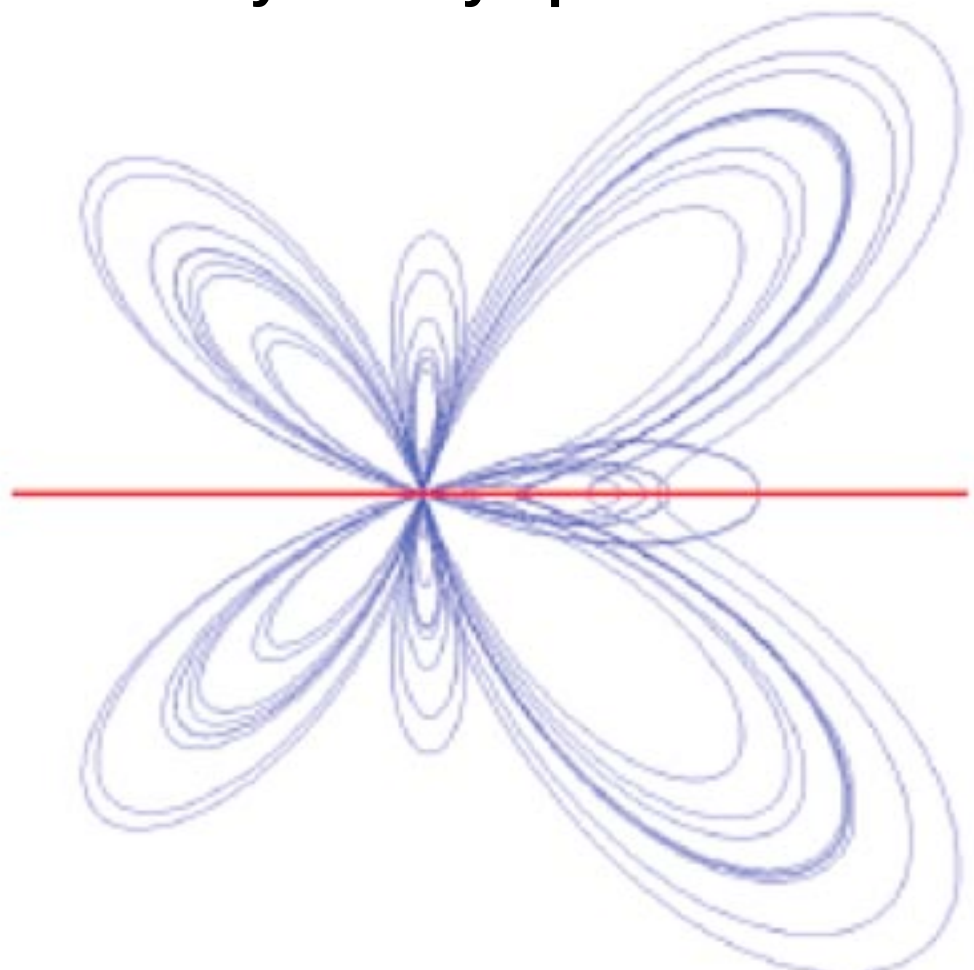
$\boldsymbol{A}^{-1}=$

1/5	0	2/5
2/5	0	-1/5
1/15	1/3	2/15

SYMMETRY OPERATIONS AND THEIR MATRIX-COLUMN PRESENTATION

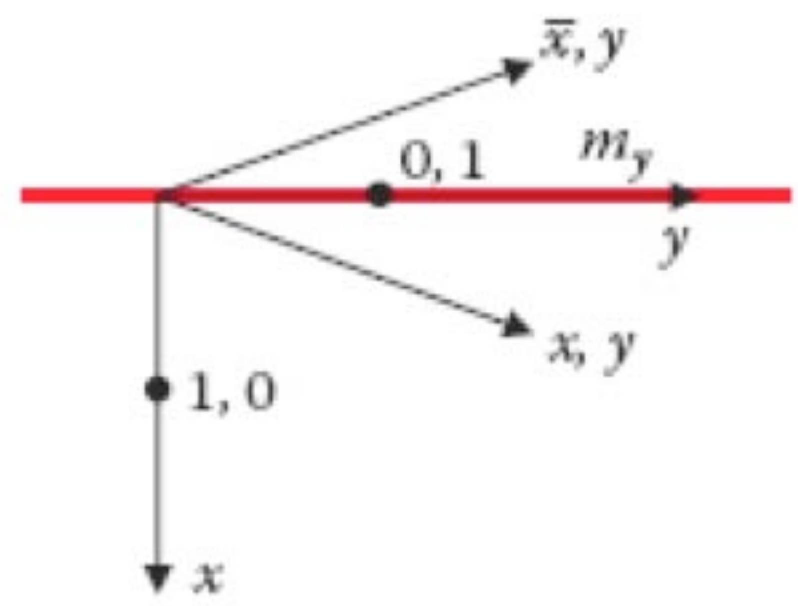
Example: Matrix presentation of symmetry operation

Mirror symmetry operation



drawing: M.M. Julian
Foundations of Crystallography

Mirror line m_y at 0,y



Fixed points

$$m_y \begin{pmatrix} x_f \\ y_f \end{pmatrix} = \begin{pmatrix} x_f \\ y_f \end{pmatrix}$$

Matrix representation

$$m_y \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -x \\ y \end{pmatrix} = \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\det \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} = ? \quad \mathrm{tr} \begin{pmatrix} -1 & \\ & 1 \end{pmatrix} = ?$$

Description of isometries

coordinate system: $\{O, \mathbf{a}, \mathbf{b}, \mathbf{c}\}$

isometry:

$\tilde{x} = F_1(x,y,z)$

$$\left|\begin{array}{lcl} \tilde{x} & = & W_{11}\,x + W_{12}\,y + W_{13}\,z + w_1 \\ \tilde{y} & = & W_{21}\,x + W_{22}\,y + W_{23}\,z + w_2 \\ \tilde{z} & = & W_{31}\,x + W_{32}\,y + W_{33}\,z + w_3 \end{array}\right.$$

Matrix notation for system of linear equations

$$
\begin{aligned}
\tilde{x} &= W_{11}\, x + W_{12}\, y + W_{13}\, z + w_1 \\
\tilde{y} &= W_{21}\, x + W_{22}\, y + W_{23}\, z + w_2 \\
\tilde{z} &= W_{31}\, x + W_{32}\, y + W_{33}\, z + w_3
\end{aligned}
$$

$$
\begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} W_{11} W_{12} W_{13} \\ W_{21} W_{22} W_{23} \\ W_{31} W_{32} W_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}
$$

Matrix-column presentation of isometries

$$\begin{pmatrix} \tilde{x} \\ \tilde{y} \\ \tilde{z} \end{pmatrix} = \begin{pmatrix} W_{11} W_{12} W_{13} \\ W_{21} W_{22} W_{23} \\ W_{31} W_{32} W_{33} \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$$

linear/matrix part

translation column part

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\,\boldsymbol{x} + \boldsymbol{w}$$

$$\tilde{\boldsymbol{x}} = (\,\boldsymbol{W},\,\boldsymbol{w})\,\boldsymbol{x} \quad \text{or} \quad \tilde{\boldsymbol{x}} = \{\,\boldsymbol{W}\,|\,\boldsymbol{w}\}\,\boldsymbol{x}$$

matrix-column pair

Seitz symbol

EXERCISES

Problem

Referred to an 'orthorhombic' coordinate system ($a \neq b \neq c$; $\alpha=\beta=\gamma=90$) two symmetry operations are represented by the following matrix-column pairs:

$$(W_1,w_1)=\left(\begin{array}{ccc|c} -1 & & & 0 \\ & 1 & & 0 \\ & & -1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine the images X_i of a point X under the symmetry operations (W_i,w_i) where

$$X=\begin{pmatrix} 0,70 \\ 0,31 \\ 0,95 \end{pmatrix}$$

Can you guess what is the geometric 'nature' of (W_1,w_1)?

And of (W_2,w_2)?

Hint:

A drawing could be rather helpful

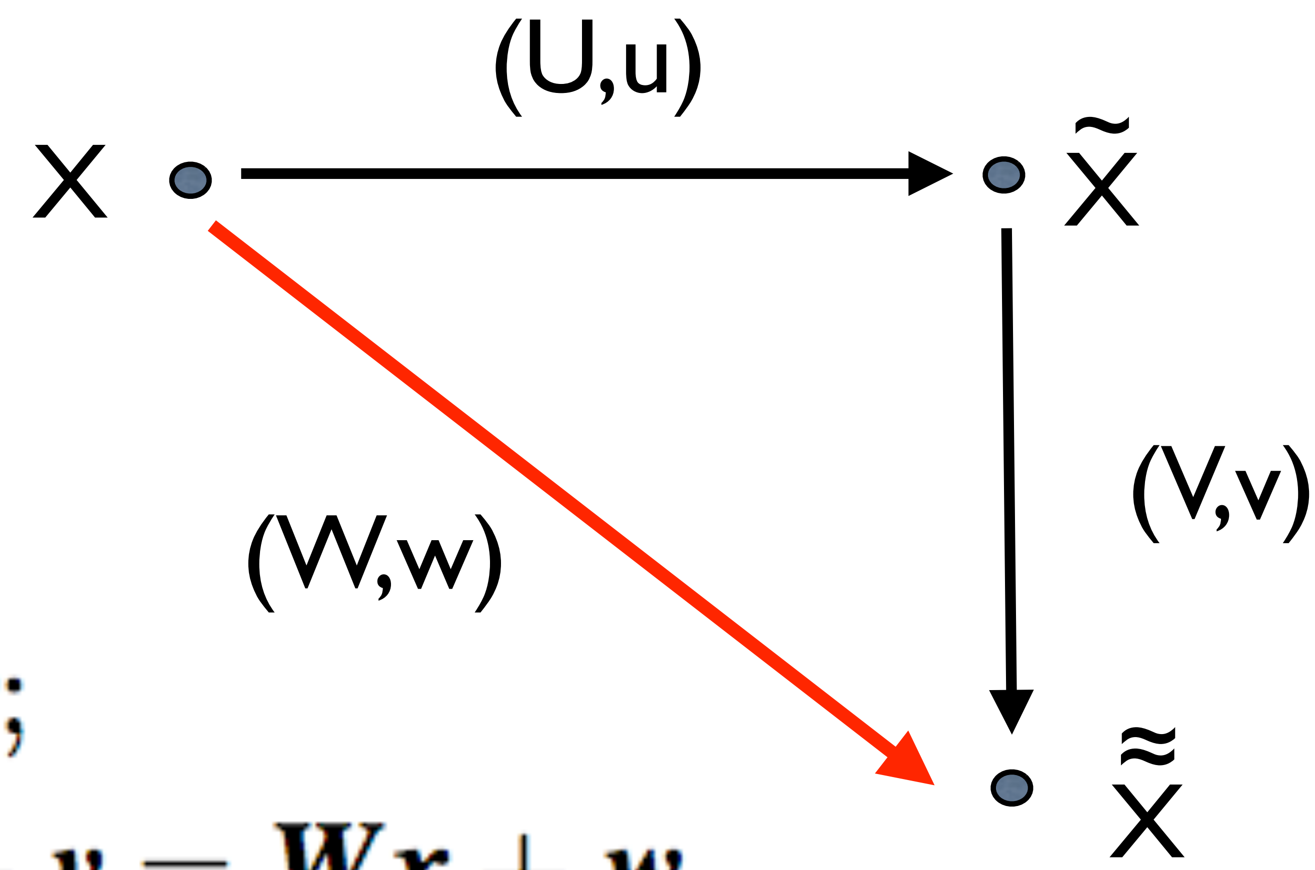
Characterization of the symmetry operations:

$$\det\begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix} = ? \qquad \mathrm{tr}\begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix} = ?$$

What are the fixed points of (W_1,w_1) and (W_2,w_2) ?

$$\left(\begin{matrix} -1 & & \\ & 1 & \\ & & -1 \end{matrix} \;\; \begin{matrix} 1/2 \\ 0 \\ 1/2 \end{matrix}\right) \begin{pmatrix} x_f \\ y_f \\ z_f \end{pmatrix} = \begin{pmatrix} x_f \\ y_f \\ z_f \end{pmatrix}$$

Combination of isometries



$$\tilde{\boldsymbol{x}} = \boldsymbol{U}\boldsymbol{x} + \boldsymbol{u};$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}\tilde{\boldsymbol{x}} + \boldsymbol{v};$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}(\boldsymbol{U}\boldsymbol{x} + \boldsymbol{u}) + \boldsymbol{v};$$
$$\tilde{\tilde{\boldsymbol{x}}} = \boldsymbol{V}\boldsymbol{U}\boldsymbol{x} + \boldsymbol{V}\boldsymbol{u} + \boldsymbol{v} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w}.$$

$$\tilde{\tilde{\boldsymbol{x}}} = (\boldsymbol{V},\, \boldsymbol{v})\,\tilde{\boldsymbol{x}} = (\boldsymbol{V},\, \boldsymbol{v})(\boldsymbol{U},\, \boldsymbol{u})\boldsymbol{x} = (\boldsymbol{W},\, \boldsymbol{w})\boldsymbol{x}.$$

$$(\boldsymbol{W},\, \boldsymbol{w}) = (\boldsymbol{V},\, \boldsymbol{v})(\boldsymbol{U},\, \boldsymbol{u}) = (\boldsymbol{V}\boldsymbol{U},\, \boldsymbol{V}\boldsymbol{u} + \boldsymbol{v}).$$

EXERCISES

Problem

Consider the matrix-column pairs of the two symmetry operations:

$$(W_1,w_1)=\left(\begin{array}{ccc|c} 0 & -1 & & 0 \\ 1 & 0 & & 0 \\ & & 1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine and compare the matrix-column pairs of the combined symmetry operations:

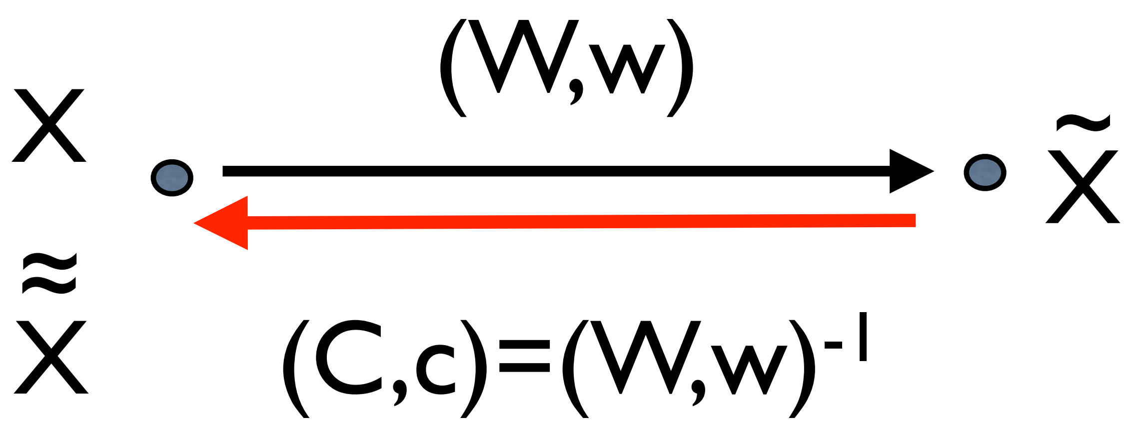
$$(W,w)=(W_1,w_1)(W_2,w_2)$$

$$(W,w)'=(W_2,w_2)(W_1,w_1)$$

combination of isometries:

$$(\boldsymbol{W}_2,\ \boldsymbol{w}_2)(\boldsymbol{W}_1,\ \boldsymbol{w}_1)=(\boldsymbol{W}_2\boldsymbol{W}_1,\ \boldsymbol{W}_2\boldsymbol{w}_1+\boldsymbol{w}_2)$$

Inverse isometries



$\boldsymbol{I}$ = 3x3 identity matrix

$\boldsymbol{o}$ = zero translation column

$$(C,c)(W,w) = (\boldsymbol{I},\boldsymbol{o})$$

$$(C,c)(W,w) = (CW, Cw+c)$$

$CW=\boldsymbol{I}$ → $C=W^{-1}$

$Cw+c=\boldsymbol{o}$ → $c=-Cw=-W^{-1}w$

EXERCISES

Problem

Determine the inverse symmetry operations $(W_1,w_1)^{-1}$ and $(W_2,w_2)^{-1}$ where

$$(W_1,w_1)=\left(\begin{array}{ccc|c} 0 & -1 & & 0 \\ 1 & 0 & & 0 \\ & & 1 & 0 \end{array}\right) \qquad (W_2,w_2)=\left(\begin{array}{ccc|c} -1 & & & 1/2 \\ & 1 & & 0 \\ & & -1 & 1/2 \end{array}\right)$$

Determine the inverse symmetry operation $(W,w)^{-1}$

$$(W,w)=(W_1,w_1)(W_2,w_2)$$

inverse of isometries:

$$(\boldsymbol{W},\boldsymbol{w})^{-1}=(\boldsymbol{W}^{-1},-\boldsymbol{W}^{-1}\boldsymbol{w})$$

EXERCISES

Problem

Consider the matrix-column pairs

$$(\boldsymbol{A}, \boldsymbol{a}) = \begin{pmatrix} 0\,1\,0 \\ 1\,0\,0 \\ 0\,0\,\bar{1} \end{pmatrix}, \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix} \text{ and } (\boldsymbol{B}, \boldsymbol{b}) = \begin{pmatrix} 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

(i) What is the matrix–column pair resulting from $(\boldsymbol{B},\ \boldsymbol{b})\,(\boldsymbol{A},\ \boldsymbol{a}) = (\boldsymbol{C}, \boldsymbol{c})$, and $(\boldsymbol{A},\ \boldsymbol{a})\,(\boldsymbol{B},\ \boldsymbol{b}) = (\boldsymbol{D}, \boldsymbol{d})$?

(ii) What is $(\boldsymbol{A}, \boldsymbol{a})^{-1}$, $(\boldsymbol{B}, \boldsymbol{b})^{-1}$, $(\boldsymbol{C}, \boldsymbol{c})^{-1}$ and $(\boldsymbol{D}, \boldsymbol{d})^{-1}$?

(iii) What is $(\boldsymbol{B}, \boldsymbol{b})^{-1}\,(\boldsymbol{A},\ \boldsymbol{a})^{-1}$?