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MATRIX CALCULUS (brief revision)

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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 $(n \times n)$ 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 $(m \times 1)$ matrix

Row index changes

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

Row Matrix:

A $(1 \times n)$ 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 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 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

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

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

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.

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

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

EXERCISE 2.1.1

Problems

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

$$\begin{pmatrix} 1 & 3 & 4 \end{pmatrix}$$

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

$$\boldsymbol{A}=\begin{pmatrix} 3 & 0 \\ 0 & 2 \end{pmatrix} \quad \boldsymbol{B}=\begin{pmatrix} 3 & 4 \\ -4 & 1 \end{pmatrix} \quad \boldsymbol{C}=\begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix} \quad \boldsymbol{D}=\begin{pmatrix} 0 & 2 \\ -2 & 0 \end{pmatrix} \quad \boldsymbol{E}=\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\boldsymbol{F}=(3) \quad \boldsymbol{G}=\begin{pmatrix} 0 & 1 & -2 \\ -1 & 0 & 3 \\ 2 & -3 & 0 \end{pmatrix} \quad \boldsymbol{H}=\begin{pmatrix} 3 & 2 \\ 2 & 1 \\ 1 & 0 \end{pmatrix} \quad \boldsymbol{J}=\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix}$$

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

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

determine $3\boldsymbol{A}$.

Matrix addition and subtraction:

Let A_{ik} and B_{ik} be general elements of matrices ***A*** and ***B***.

A and ***B*** must be of the same size (i.e. same number of rows and columns). Then the sum and the difference ***A*** ± ***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 ***C*** is equal to the sum or difference of the elements A_{ik} and B_{ik} of ***A*** and ***B*** for any pair i,k:

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

EXERCISE 2.1.2

Problems

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

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

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

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

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

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

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

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

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

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

$\boldsymbol{C} \neq \boldsymbol{D}$, *i. e.* matrix multiplication is *not always commutative.*

However, it is *associative*, *e. g.*, $(\boldsymbol{A}\,\boldsymbol{B})\,\boldsymbol{D} = \boldsymbol{A}\,(\boldsymbol{B}\,\boldsymbol{D})$

and *distributive*, *i. e.* $(\boldsymbol{A} + \boldsymbol{B})\,\boldsymbol{C} = \boldsymbol{A}\,\boldsymbol{C} + \boldsymbol{B}\,\boldsymbol{C}$

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 $\boldsymbol{C} = \boldsymbol{AB}$.

Determine $\boldsymbol{C}$.

Determine $\boldsymbol{D}=\boldsymbol{BA}$, check if $\boldsymbol{C}=\boldsymbol{D}$ or not.

Multiplication
Product of matrix ***A*** with column ***a***:

Example: How to get element d_1:

$$\begin{pmatrix} d_1 \\ d_2 \\ \vdots \\ d_i \\ \vdots \\ d_m \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1k} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2k} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots & & \vdots \\ A_{i1} & A_{i2} & \dots & A_{ik} & \dots & A_{in} \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots \\ A_{m1} & A_{m2} & \dots & A_{mk} & \dots & A_{mn} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_k \\ \vdots \\ a_n \end{pmatrix}$$

$$d_1 = A_{11}\, a_1 + A_{12}\, a_2 + \ldots\ldots + A_{1k}\, a_k + \ldots\ldots + A_{1n}\, a_n$$

Example 3: Multiplication

Given that

$$A = \begin{pmatrix} 1 & 2 & 0 \\ \bar{1} & 0 & 3 \\ 2 & \bar{1} & 0 \end{pmatrix} \qquad B = \begin{pmatrix} 3 \\ \bar{5} \\ 6 \end{pmatrix}$$

and $\boldsymbol{C} = \boldsymbol{AB}$.

Determine $\boldsymbol{C}$.

Multiplication

Product of matrix *A* with row a^T:

Example: How to get elements d_1 and d_2:

$$(d_1\ d_2 \dots d_i \dots d_n) = (a_1\ a_2 \dots a_k \dots a_m) \begin{pmatrix} A_{11} & A_{12} & \dots & A_{1i} & \dots & A_{1n} \\ A_{21} & A_{22} & \dots & A_{2i} & \dots & A_{2n} \\ \vdots & \vdots & & \ddots\vdots & & \vdots \\ A_{k1} & A_{k2} & \dots & A_{ki} & \dots & A_{kn} \\ \vdots & \vdots & & \vdots & & \ddots\vdots \\ A_{m1} & A_{m2} & \dots & A_{mi} & \dots & A_{mn} \end{pmatrix}$$

$$d_1 = a_1A_{11} + a_2A_{21} + \dots\dots + a_kA_{k1} + \dots\dots + a_nA_{m1}$$

$$d_2 = a_1A_{12} + a_2A_{22} + \dots\dots + a_kA_{k2} + \dots\dots + a_nA_{m2}$$

Example 4: Multiplication

Given that

$$A = \begin{pmatrix} \bar{5} & 2 & 4 \end{pmatrix} \qquad B = \begin{pmatrix} 1 & 1 & 0 \\ 2 & 2 & 2 \\ 3 & 2 & 1 \end{pmatrix}$$

and $\boldsymbol{C} = \boldsymbol{AB}$.

Determine $\boldsymbol{C}$.

EXERCISE 2.1.3

Problems

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

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

2. Find the matrix products ***AB*** and ***BA*** of the row vector ***A***= $\begin{bmatrix} 1 & 2 & 3 \end{bmatrix}$, and the column vector ***B***= $\begin{bmatrix} -2 \\ 4 \\ 1 \end{bmatrix}$

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

A= $\begin{bmatrix} 1 & 2 \\ -1 & 3 \end{bmatrix}$ ***B***= $\begin{bmatrix} 1 & 0 & -1 \\ 2 & 1 & 0 \end{bmatrix}$ ***C***= $\begin{bmatrix} 1 & -1 \\ 3 & 2 \\ 2 & 1 \end{bmatrix}$

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

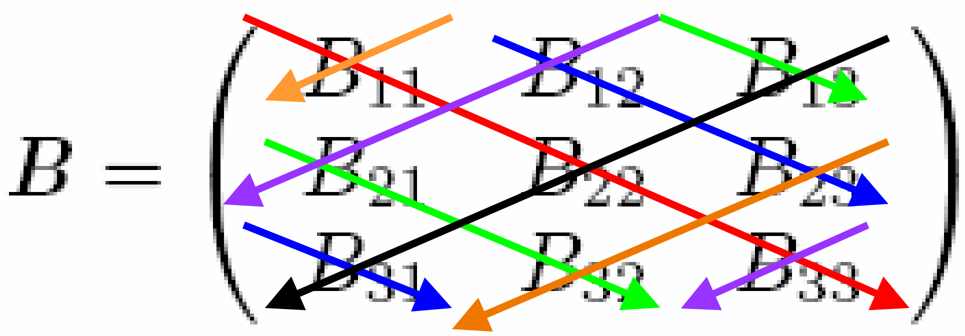
$$\text{Let } \boldsymbol{A} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

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

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

Determinants

(3×3) matrix



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

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

Example 6: Determinant

Given that

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

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

EXERCISE 2.1.4

Problems

1. Find the values of the traces and the determinants of $\boldsymbol{A}$ and $\boldsymbol{B}$ where

$\boldsymbol{A}=$

1	2
-1	3

$\boldsymbol{B}=$

0	4	2
4	-2	-1
5	1	3

2. Show that $\det(\boldsymbol{AB})=\det(\boldsymbol{A})\det(\boldsymbol{B})$ where

$\boldsymbol{A}=$

3	2
5	1

$\boldsymbol{B}=$

1	6
2	9

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

$\boldsymbol{A}=$

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 $\boldsymbol{A}$:

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

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

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

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

$$\boldsymbol{B}_{11} = \det \begin{bmatrix} 1 & 2 & 3 \\ 1 & 3 & 5 \\ 1 & 5 & 12 \end{bmatrix} = \det \begin{bmatrix} 3 & 5 \\ 5 & 12 \end{bmatrix} = 11$$

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

. . .

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

Is it correct?

EXERCISE 2.1.5

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

EXERCISE 2.1.5

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