

University of Ferrara



Stefano Bonnini

Multivariate problems and matrix algebra

Multivariate statistical analysis deals with data containing observations on two or more characteristics (variables) each measured on a set of objects (statistical units)

Example 1: examination marks, about 5 courses (Mechanics, Vectors, Algebra, Analysis, Statistics), achieved by 88 students

Example 2: weights of cork deposites (centigrams) for 28 trees in the four directions (N, E, S, W)

Example 3: flower measurements (sepal length, sepal width, petal length, petal width) on 50 flowers belonging to a certein species of iris



Available information \rightarrow Dataset $\rightarrow n \times k$ matrix

Example: data matrix with 5 students where X_1 =age in years at entry to university, X_2 =marks out of 100 in an examination at the end of the first year and X_3 =sex.



Some multivariate problems:

Example 1: study how the mark in the examination of «Statistics» (dependent variable) is affected by or can be predicted as function of the marks in other examinations or other variables such as age, sex, etc. (explanatory variables) \rightarrow regression problem

Example 2: study how to combine the information on the performance of the students on the 5 examinations to determine the global performance of each student with just one, or two or less than 5 values \rightarrow factor analysis, principal component analysis, composite indicator

Example 3: study how to group students with similar performances by considering the whole set of examinations \rightarrow cluster analysis

The general $n \times k$ matrix which represents a dataset with *n* statistical units and *k* variables can be written as follows:



This matrix can be denoted **X** or (x_{uv})

$$\mathbf{x}_{u} = \begin{pmatrix} x_{u1} \\ \cdots \\ x_{uv} \\ \cdots \\ x_{uk} \end{pmatrix} \qquad \qquad \mathbf{x}_{(v)} = \begin{pmatrix} x_{1v} \\ \cdots \\ x_{uv} \\ \cdots \\ x_{nv} \end{pmatrix}$$

5

A m \times n matrix *A* is a table with m rows and n columns:

$$\mathbf{A} = \begin{pmatrix} 3 & 8 & 3 & 5 \\ 9 & 1 & 1 & 8 \\ 4 & 6 & 4 & 2 \end{pmatrix} \longrightarrow a_{23} = 1$$

In this case the matrix has 3 rows and 4 columns. If *m*=*n* then it is called **square matrix**



A matrix with dimension $1 \times n$ is called **row vector**:

```
\mathbf{a}_{1\times 5} = \begin{pmatrix} 6 & 3 & 1 & 7 & 2 \end{pmatrix}
```

A matrix with dimension $m \times 1$ is called **column vector** or simply vector:

$$\mathbf{c}_{5\times 1} = \begin{pmatrix} 6\\3\\1\\7\\2 \end{pmatrix}$$

A **unit vector** is a vector of ones:

$$\mathbf{1}_{5\times 1} = \begin{pmatrix} 1\\1\\1\\1\\1\\1 \end{pmatrix}$$

Given the matrices **A** and **B**, their sum is defined as C=A+B, where $c_{ij} = a_{ij} + b_{ij}$

Example:

$$\mathbf{A} = \begin{pmatrix} 3 & 8 & 3 & 5 \\ 9 & 1 & 1 & 8 \\ 4 & 6 & 4 & 2 \end{pmatrix}, \mathbf{B} = \begin{pmatrix} 3 & 3 & 5 & 9 \\ 9 & 1 & 4 & 3 \\ 6 & 6 & 9 & 6 \end{pmatrix} \Rightarrow \mathbf{A} + \mathbf{B} = \mathbf{C} = \begin{pmatrix} 6 & 11 & 8 & 14 \\ 18 & 2 & 5 & 11 \\ 10 & 12 & 13 & 8 \end{pmatrix}$$
$$a_{23} = 1 \quad b_{23} = 4 \qquad \qquad c_{23} = 5$$

The product of a $m \times n$ matrix **A** and a scalar (single value) λ is called **scalar multiplication** and it consists in a matrix with the same dimension of **A**, obtained by multiplying each element of **A** by λ

$$\mathbf{C} = \lambda \mathbf{A} \iff c_{ij} = \lambda a_{ij}$$



The **inner product** of two vectors **a** and **b** is possible if the vectors have the same number of elements and it is equal to $\mathbf{a}'\mathbf{b} = \sum_i a_i b_i$

The **product between two matrices** A and B is possible if the number of columns of A is equal to the number of rows of B.

Given the $m \times n$ matrix A and the $n \times h$ matrix B, the product C=AB is a $m \times h$ matrix. The element in row i and column j is equal to the inner product between row i of A and column j of B.

C=AB
$$\Leftrightarrow c_{ij} = \mathbf{a}_i \mathbf{b}_{(j)}$$

Example:

...where the elements of **C** are equal to:

$$\mathbf{C} = \begin{pmatrix} c_{11} = 1 \cdot 1 + 2 \cdot 3 = 7 & c_{12} = 1 \cdot 2 + 2 \cdot 6 = 14 \\ c_{21} = -1 \cdot 1 + 0 \cdot 3 = -1 & c_{22} = -1 \cdot 2 + 0 \cdot 6 = -2 \\ c_{31} = 3 \cdot 1 + 1 \cdot 3 = 6 & c_{32} = 3 \cdot 2 + 1 \cdot 6 = 12 \end{pmatrix}$$

-

Note that:

$$\mathbf{A} \cdot \mathbf{B}_{(m \times h)} = \mathbf{C}_{(m \times h)}$$

Thus the product between a row vector and a column vector is a scalar; the product between a column vector and a row vector is a matrix:

$$\mathbf{a} \cdot \mathbf{b} = c \\ \underset{n \times 1}{\mathbb{b}} \sum_{n \times 1} \sum_{n \times 1} \mathbf{b} \cdot \mathbf{a} = \mathbf{C} \\ \underset{n \times 1}{\mathbb{b}} \sum_{n \times n} \sum_{n \times n} \sum_{n \times n} \mathbf{b} \cdot \mathbf{a} = \mathbf{C}$$

Examples:

$$\mathbf{a}_{1\times 2} = \begin{pmatrix} 2 & 4 \end{pmatrix} \quad \mathbf{b}_{2\times 1} = \begin{pmatrix} 5 \\ 2 \end{pmatrix} \qquad \qquad \mathbf{a} \times \mathbf{b} = 2 \cdot 5 + 4 \cdot 2 = 18$$

$$\mathbf{b}_{2\times 1} = \begin{pmatrix} 5 \\ 2 \end{pmatrix} \quad \mathbf{a}_{1\times 2} = \begin{pmatrix} 2 & 4 \end{pmatrix} \qquad \qquad \qquad \mathbf{b} \times \mathbf{a} = \begin{pmatrix} 10 & 20 \\ 4 & 8 \end{pmatrix}$$

The **transpose** of the matrix $\mathbf{A} = (a_{ij})$ is the matrix $\mathbf{A}' = (a_{ji})$ whose rows correspond to the columns of \mathbf{A} :

Example:

$$\mathbf{A} = \begin{pmatrix} 3 & 6 & 4 \\ 2 & 8 & 9 \\ 2 & 5 & 1 \end{pmatrix} \qquad \mathbf{A'} = \begin{pmatrix} 3 & 2 & 2 \\ 6 & 8 & 5 \\ 4 & 9 & 1 \end{pmatrix}$$

The square matrix $\mathbf{A} = (a_{ij})$ is symmetric if $a_{ij} = a_{ji}$ or equivalently if $\mathbf{A}' = \mathbf{A}$.

Example:

$$\mathbf{A} = \begin{pmatrix} 3 & 6 & 4 \\ 6 & 8 & 9 \\ 4 & 9 & 1 \end{pmatrix}$$

A null matrix is a matrix with all elements equal to 0.

$$\mathbf{0} = \begin{pmatrix} 0 & 0 & . & 0 \\ 0 & . & . & . \\ . & . & . & . \\ 0 & 0 & . & 0 \end{pmatrix}$$

A **diagonal matrix** is a square matrix whose elements not in the main diagonal are all equal to 0.

$$diag(a_1, \dots, a_n) = \begin{pmatrix} a_1 & 0 & \dots & 0 \\ 0 & a_2 & \dots & \dots \\ \vdots & \vdots & \ddots & \ddots \\ 0 & 0 & \dots & a_n \end{pmatrix}$$

The transpose satisfies the following properties:

- 1. (**A**')'=**A**
- 2. (**A**+**B**)'=**A**'+**B**'
- 3. (**AB**)'=**B**'**A**'

A **diagonal matrix** is a square matrix whose elements not in the main diagonal are all equal to 0.

The **trace** of $A = (a_{ij})$ is the sum of the elements in the main diagonal of **A**:

 $tr(\mathbf{A})=\Sigma_i a_{ii}$

Example:



The trace satisfies the following properties for

A ($m \times m$), **B** ($m \times m$), **C** ($m \times n$), **D** ($n \times m$) and a scalar λ :

- 1. $tr(\lambda) = \lambda$
- 2. tr(**A**)=tr(**A**')
- 3. tr(A+B)=tr(A)+tr(B)
- 4. $\operatorname{tr}(\mathbf{CD}) = \operatorname{tr}(\mathbf{DC}) = \Sigma_{i,j} C_{ij} d_{ji}$
- 5. $\operatorname{tr}(\mathbf{CC'})=\operatorname{tr}(\mathbf{C'C})=\Sigma_{i,j} C_{ij}^{2}$

Given the 2×2 matrix
$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

The determinant of A is

$$\det(\mathbf{A}) = |\mathbf{A}| = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = a_{11} \cdot a_{22} - a_{21} \cdot a_{12}$$

Given the *m×m* matrix

Case *m*=3:

A

The determinant of A is

$$\det(\mathbf{A}) = |\mathbf{A}| = \sum_{j=1}^{m} a_{ij} A_{ij} = \sum_{i=1}^{m} a_{ij} A_{ij} \text{ for any } i,j$$

where the **cofactor** A_{ij} is the product of $(-1)^{i+j}$ and the determinant of the matrix obtained after deleting *i*th row and *j*th column of **A** (minor)

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} \Rightarrow \det(\mathbf{A}) = |\mathbf{A}| = a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{32} \end{vmatrix} + a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$
$$= a_{11} (a_{22}a_{33} - a_{32}a_{23}) - a_{12} (a_{21}a_{33} - a_{31}a_{23}) + a_{13} (a_{21}a_{32} - a_{31}a_{22})$$

Computation of the determinant of a 3rd order matrix (Sarrus rule):

$$\det(\mathbf{A}) = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{11} & a_{12} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{22} \\ a_{31} & a_{32} & a_{33} & a_{31} & a_{32} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{12} \\ a_{21} & a_{22} & a_{23} & a_{24} & a_{22} \\ a_{31} & a_{32} & a_{33} & a_{31} & a_{32} \end{pmatrix} =$$

 $a_{11}a_{22}a_{33} + a_{12}a_{23}a_{31} + a_{13}a_{21}a_{32} - (a_{31}a_{22}a_{13} + a_{32}a_{23}a_{11} + a_{33}a_{21}a_{12})$

Example:

$$\mathbf{A} = \begin{pmatrix} 3 & 4 & 1 \\ 4 & 6 & 2 \\ 5 & 7 & 4 \end{pmatrix}$$
$$\det(A) = 3 \begin{vmatrix} 6 & 2 \\ 7 & 4 \end{vmatrix} - 4 \begin{vmatrix} 4 & 2 \\ 5 & 4 \end{vmatrix} + 1 \begin{vmatrix} 4 & 6 \\ 5 & 7 \end{vmatrix} = 3(24 - 14) - 4(16 - 10) + 1(28 - 30) = 4$$

or alternatively:

$$det(\mathbf{A}) = \begin{pmatrix} 3 & 4 & 1 & 3 & 4 \\ 4 & 6 & 2 & 4 & 6 \\ 5 & 7 & 4 & 5 & 7 \end{pmatrix} = \\ = 3 \cdot 6 \cdot 4 + 4 \cdot 2 \cdot 5 + 1 \cdot 4 \cdot 7 - (5 \cdot 6 \cdot 1 + 7 \cdot 2 \cdot 3 + 4 \cdot 4 \cdot 4) = \\ = 140 - 136 = 4$$

22

Properties of the determinant

- 1. If $\mathbf{A} = diag(a_1, \dots, a_n)$ then $det(\mathbf{A}) = a_1 \cdot a_2 \cdot \dots \cdot a_n = \Pi_i a_i$
- 2. $det(\lambda \mathbf{A}) = |\lambda \mathbf{A}| = \lambda^n |\mathbf{A}|$
- 3. $det(AB) = |AB| = |A| \cdot |B|$
- 4. If **A** has two equal rows or two equal columns then $det(\mathbf{A})=0$
- 5. If **A** has a row of zeros or a column of zeros then det(A)=0
- 6. If **B** is the matrix obtained exchanging the position of two rows or two columns of **A** then det(B) = -det(A)
- 7. *det*(**A**)=*det*(**A**')
- If *B* is the matrix obtained by summing to a row or a column of *A* a linear combination of the other rows or columns of *A* respectively then det(*B*)=det(*A*)
- A square matrix *A* is non-singular if det(*A*)≠0; otherwise *A* is singular

Example:

$$\mathbf{A} = \begin{pmatrix} 2 & 3 \\ 1 & 6 \end{pmatrix} \qquad \qquad \mathbf{B} = \begin{pmatrix} 2 & 5 \\ 7 & 3 \end{pmatrix}$$

 $det(\mathbf{A}) = 2 \cdot 6 - 3 \cdot 1 = 9 \qquad det(\mathbf{B}) = 2 \cdot 3 - 5 \cdot 7 = -29$ $det(\mathbf{A}) \cdot det(\mathbf{B}) = 9 \cdot (-29) = -261$

$$\mathbf{AB} = \begin{pmatrix} 2 & 3 \\ 1 & 6 \end{pmatrix} \cdot \begin{pmatrix} 2 & 5 \\ 7 & 3 \end{pmatrix} = \begin{pmatrix} 2 \cdot 2 + 3 \cdot 7 & 2 \cdot 5 + 3 \cdot 3 \\ 1 \cdot 2 + 6 \cdot 7 & 1 \cdot 5 + 6 \cdot 3 \end{pmatrix} = \begin{pmatrix} 25 & 19 \\ 44 & 23 \end{pmatrix}$$

 $det(AB) = 25 \cdot 23 - 19 \cdot 44 = -261$

The **inverse** of the square matrix **A** is the unique matrix **A**⁻¹ satisfying:



The inverse A^{-1} exists if and only if A is non singular, that is, if and only if det(A) \neq 0.

The **identity matrix** is a diagonal matrix where all the elements in the main diagonal are equal to 1.

$$\mathbf{I} = \begin{pmatrix} 1 & 0 & . & 0 & 0 \\ 0 & 1 & . & 0 & 0 \\ . & . & . & . \\ 0 & 0 & . & 1 & 0 \\ 0 & 0 & . & 0 & 1 \end{pmatrix}$$

Properties of **I**

 $A \times I = I \times A = A$ $A \times A^{-1} = I$ $A^{-1} \times A = I$

Properties of the inverse:

1. $(\lambda A)^{-1} = \lambda^{-1} A^{-1}$ 2. $(AB)^{-1} = B^{-1} A^{-1}$ 3. The unique solution of Ax = b is $x = A^{-1}b$

4.
$$A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \Rightarrow A^{-1} = \frac{1}{a_{11}a_{22}-a_{12}a_{21}} \begin{pmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{pmatrix}$$

Example 1:

$$\mathbf{AB} = \begin{pmatrix} 2 & 3 \\ 1 & 6 \end{pmatrix} \cdot \begin{pmatrix} 2 & 5 \\ 7 & 3 \end{pmatrix} \Rightarrow (\mathbf{AB})^{-1} = \begin{pmatrix} 25 & 19 \\ 44 & 23 \end{pmatrix}^{-1} = \frac{1}{(-261)} \begin{pmatrix} 23 & -19 \\ -44 & 25 \end{pmatrix} = \begin{pmatrix} -0.088 & 0.073 \\ 0.169 & -0.096 \end{pmatrix}$$

$$\mathbf{B}^{-1}\mathbf{A}^{-1} = \begin{pmatrix} 2 & 5 \\ 7 & 3 \end{pmatrix}^{-1} \cdot \begin{pmatrix} 2 & 3 \\ 1 & 6 \end{pmatrix}^{-1} \Rightarrow \begin{pmatrix} -0.103 & 0.172 \\ 0.241 & -0.069 \end{pmatrix} \cdot \begin{pmatrix} 0.667 & -0.333 \\ -0.111 & 0.222 \end{pmatrix} = \begin{pmatrix} -0.088 & 0.073 \\ 0.169 & -0.096 \end{pmatrix}$$

Example 2:

Let us consider the following system of equations

$$\begin{cases} 2x_1 + 3x_2 = 13 \\ x_1 + 2x_2 = 8 \end{cases} \implies \begin{pmatrix} 2 & 3 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 13 \\ 8 \end{pmatrix} \implies Ax = b$$

The solution is

$$\binom{x_1}{x_2} = \binom{2}{1} \binom{3}{2}^{-1} \binom{13}{8} = \frac{1}{2 \cdot 2 - 3 \cdot 1} \binom{2}{-1} \binom{13}{2} = \frac{1}{2 \cdot 2 - 3 \cdot 1} \binom{2}{-1} \binom{13}{2} \binom{13}{8} = \binom{2}{-1} \binom{2}{-1}$$

A square matrix **A** is **orthogonal** if **AA'=I** The following properties hold:

- **1.** $A' = A^{-1}$
- 2. A'A = I
- *3.* |**A**|=± 1
- 4. $a_i a_j = 0, i \neq j; a_i a_j = 0, \forall i; a_{(i)} a_{(j)} = 0, i \neq j; a_{(i)} a_{(i)} = 0, \forall i;$

Example:

$$A = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
$$A' = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} = A^{-1} \text{ because } AA' = I$$

Vectors $\boldsymbol{x}_1, \dots, \boldsymbol{x}_k$ are called **linearly dependent** if there exist numbers $\lambda_1, \dots, \lambda_K$ not all zero such that $\lambda_1 \boldsymbol{x}_1 + \dots + \lambda_K \boldsymbol{x}_k = \mathbf{0}$. Otherwise the *k* vectors are linearly independent.

Let W be a subspace of \mathbb{R}^n . Then a basis of W is a maximal linearly independent set of vectors.

Every basis of W contains the same (finite) number of elements. This number is the dimension of W.

If $x_1, ..., x_k$ is a basis for W then every element x in W can be expressed as a linear combination of $x_1, ..., x_k$.

Example:

The dimension of $W=R^3$ is 3. A basis for R^3 is $x_1=(1,0,0)'$, $x_2=(0,1,0)'$ and $x_3=(0,0,1)'$. As a matter of fact x_1 , x_2 and x_3 are linearly independent and every vector $a=(a_1,a_2,a_3)'$ can be expressed as linear combination of x_1 , x_2 and x_3 : $a=a_1x_1+a_2x_2+a_3x_3$

30

The **rank** of a $n \times k$ matrix **A** is defined as the maximum number of linearly independent columns (rows) in **A**.

The following properties hold for the rank of A, denoted with r(A):

- 1. r(A) is the largest order of those (square) submatrices of A with non null determinants.
- 2. $0 \le r(\mathbf{A}) \le min(n,k)$
- 3. r(**A**)=r(**A**')
- 4. $r(\mathbf{A}'\mathbf{A}) = r(\mathbf{A}\mathbf{A}') = r(\mathbf{A})$
- 5. If n=k then r(A)=k if and only if A is non-singular

Example:

$$\mathbf{A} = \begin{pmatrix} 1 & -1 & 3 \\ -2 & 2 & 5 \\ 1 & -1 & 9 \end{pmatrix} \quad \det(\mathbf{A}) = 0 \quad \begin{vmatrix} 1 & -1 \\ -2 & 2 \end{vmatrix} = 0 \quad \begin{vmatrix} -1 & 3 \\ 2 & 5 \end{vmatrix} = -11 \neq 0$$

Thus the r(A)=2

If **A** is a square matrix of order *n*, in some problems we are interested in finding a vector x and a scalar λ which satisfy the following property:



A trivial solution is x=0, any $\lambda \in R$

The *n* **eigenvalues** of **A** $\lambda_1, ..., \lambda_n$ are the *n* solutions of the characteristic equation

$$|\mathbf{A} - \lambda \mathbf{I}| = \mathbf{0}$$

Properties of the eigenvalues of A:

- 1. $|\mathbf{A}| = \Pi_i \lambda_i$
- 2. $tr(\mathbf{A}) = \Sigma_i \lambda_i$
- 3. $r(\mathbf{A})$ equals the number of non-zero eigenvalues
- 4. The set of all eigenvectors for an eigenvalue λ_i is called the eigenspace of **A** for λ_i
- 5. Any symmetric $n \times n$ matrix **A** can be written as $\mathbf{A} = \Gamma \Lambda \Gamma' = \Sigma_i \lambda_i \gamma_{(i)} \gamma_{(i)}'$ where Λ is a diagonal matrix of eigenvalues of **A** and Γ is an orthogonal matrix whose columns are eigenvectors with $\gamma_{((i)}' \gamma_{(i)} = 1_{33}$

Example:



By computing the determinant we have:

$$(2-\lambda) \cdot \begin{vmatrix} 1-\lambda & 1 \\ 3 & -1-\lambda \end{vmatrix} - 1 \cdot \begin{vmatrix} -2 & 3 \\ 3 & -1-\lambda \end{vmatrix} + 1 \cdot \begin{vmatrix} -2 & 3 \\ 1-\lambda & 1 \end{vmatrix} = (2-\lambda)[-1+\lambda^2-3] - 2 - 2\lambda + 9 - 2 - 3 + 3\lambda = (\lambda+2)(\lambda-1)(3-\lambda) = 0$$

The solutions represent the 3 eigenvalues of **A**:

$$\lambda_1 = 1$$
 $\lambda_2 = -2$ $\lambda_3 = 3$

34

The eigenvalue with maximum absolute value λ_3 =3 is called dominant

There is an infinite number of eigenvectors x which satisfy (A-3I)x = 0

$$\begin{pmatrix} -1 & -2 & 3 \\ 1 & -2 & 1 \\ 1 & 3 & -4 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

A possible solution is $\mathbf{x} = (1,1,1)'$, thus a standardized eigenvector is $\left(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right)'$