This intro; descriptive
next: algebra; geometry
statistical
multivariate analysis: broad
definition: inference, prediction
and/or decision-making with data
involving 2 or more variables
measured on 2 or more individuals/
objects/
subjects/elements; this includes
many topics we won't cover here
(e.g., multiple linear regression).
2-dimensional table (variables, objects)
is a matrix: ex. random sample of 50 flowers (1 flower/plant) from each of 3 species of iris: (Fisher, 1936) (unit: $cm$)

Table 1.2.2 Measurements on three types of iris (after Fisher, 1936)

<table>
<thead>
<tr>
<th>Iris setosa</th>
<th>Iris versicolor</th>
<th>Iris virginica</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sepal width</td>
<td>Petal length</td>
<td>Sepal length</td>
</tr>
<tr>
<td>5.1</td>
<td>3.5</td>
<td>1.4</td>
</tr>
<tr>
<td>4.9</td>
<td>3.0</td>
<td>1.4</td>
</tr>
<tr>
<td>4.7</td>
<td>3.2</td>
<td>1.3</td>
</tr>
<tr>
<td>4.6</td>
<td>3.1</td>
<td>1.5</td>
</tr>
<tr>
<td>5.0</td>
<td>3.6</td>
<td>1.4</td>
</tr>
<tr>
<td>5.2</td>
<td>3.4</td>
<td>1.2</td>
</tr>
<tr>
<td>5.5</td>
<td>3.5</td>
<td>1.7</td>
</tr>
<tr>
<td>4.9</td>
<td>3.2</td>
<td>1.4</td>
</tr>
<tr>
<td>5.0</td>
<td>3.4</td>
<td>1.5</td>
</tr>
<tr>
<td>4.4</td>
<td>2.9</td>
<td>1.5</td>
</tr>
<tr>
<td>5.1</td>
<td>3.7</td>
<td>1.5</td>
</tr>
<tr>
<td>4.8</td>
<td>3.6</td>
<td>1.2</td>
</tr>
<tr>
<td>4.6</td>
<td>3.2</td>
<td>1.1</td>
</tr>
<tr>
<td>4.0</td>
<td>3.0</td>
<td>1.0</td>
</tr>
<tr>
<td>4.8</td>
<td>3.3</td>
<td>0.9</td>
</tr>
<tr>
<td>4.8</td>
<td>3.1</td>
<td>1.1</td>
</tr>
<tr>
<td>5.0</td>
<td>3.4</td>
<td>0.9</td>
</tr>
</tbody>
</table>
By convention people usually specify rows = objects, columns = variables and call the resulting data matrix $\mathbf{X}$ (with $n$ rows & $p$ columns):

$\begin{bmatrix}
  x_{11} & \cdots & x_{1j} & \cdots & x_{1p} \\
  \vdots & \ddots & \vdots & \ddots & \vdots \\
  x_{n1} & \cdots & x_{nj} & \cdots & x_{np}
\end{bmatrix}
$

Iris data has $n=150$ rows & $p=5$ columns ($s=\text{sepal}$, $r=\text{petal}$, $l=\text{length}$, $w=\text{width}$: $s_L, s_W, p_L, p_W$, (quantitative continuous)
and a qualitative (categorical) nominal variable at 3 levels indicating the species (setosa, versicolor, virginica), as in the R dataset iris. I'll use upper case ($\mathbf{X}$) for matrices and lower case ($x$) for (scalars) (here in MKB vectors); by convention, vectors are always column vectors; if you want to talk about a row vector you have to write it as the transpose $^\top x$ of a column vector. Notation (MKB):

$\mathbf{X} = \begin{pmatrix} x_{1j} & \cdots & x_{nj} \end{pmatrix}$; column $j$ is $x_{oj}$; the rows of $\mathbf{X}$ are $x_1, \ldots, x_n$.
\[ \overline{X} = \begin{bmatrix}
\vdots \\
x_i' \\
\vdots \\
x_n'
\end{bmatrix} = \begin{bmatrix}
x_{i1}, \ldots, x_{ip}
\end{bmatrix} \]

where

\[ x_i' = \begin{bmatrix}
x_{i1} \\
\vdots \\
x_{ip}
\end{bmatrix} \quad \text{and} \quad x_{ij} = \begin{bmatrix}
x_{ij}
\end{bmatrix} \]

\((i = 1, \ldots, n)\) \quad \((j = 1, \ldots, p)\).

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Review of matrix algebra:

(from MKB Appendix A)
Appendix A
Matrix Algebra

A.1 Introduction

This appendix gives (i) a summary of basic definitions and results in matrix algebra with comments and (ii) details of those results and proofs which are used in this book but normally not treated in undergraduate Mathematics courses. It is designed as a convenient source of reference to be used in the rest of the book. A geometrical interpretation of some of the results is also given. If the reader is unfamiliar with any of the results not proved here he should consult a text such as Graybill (1969, especially pp. 4–52, 163–196, and 222–235) or Rao (1973, pp. 1–78). For the computational aspects of matrix operations see for example Wilkinson (1965).

Definition A matrix \( A \) is a rectangular array of numbers. If \( A \) has \( n \) rows and \( p \) columns we say it is of order \( n \times p \). For example, \( n \) observations on \( p \) random variables are arranged in this way.

Notation 1 We write matrix \( A \) of order \( n \times p \) as

\[
A = \begin{bmatrix}
a_{11} & a_{12} & \cdots & a_{1p} \\
a_{21} & a_{22} & \cdots & a_{2p} \\
\vdots & \vdots & \ddots & \vdots \\
a_{n1} & a_{n2} & \cdots & a_{np}
\end{bmatrix} = (a_{ij}), \quad (A.1.1)
\]

where \( a_{ij} \) is the element in row \( i \) and column \( j \) of the matrix \( A \), \( i = 1, \ldots, n; j = 1, \ldots, p \). Sometimes, we write \( (A)_{ij} \) for \( a_{ij} \).
**Definition** A matrix written in terms of its sub-matrices is called a partitioned matrix.

**Notation 3** Let $A_{11}$, $A_{12}$, $A_{21}$, and $A_{22}$ be submatrices such that $A_{11}(r \times s)$ has elements $a_{ij}$, $i = 1, \ldots, r$; $j = 1, \ldots, s$ and so on. Then we write

$$A(n \times p) = \begin{bmatrix}
A_{11}(r \times s) & A_{12}(r \times (p-s)) \\
A_{21}((n-r) \times s) & A_{22}((n-r) \times (p-s))
\end{bmatrix}.$$ 

Obviously, this notation can be extended to contain further partitions of $A_{11}$, $A_{22}$, etc.

A list of some important types of particular matrices is given in Table A.1.1. Another list which depends on the next section appears in Table A.3.1.

**Table A.1.1** Particular matrices and types of matrix (List 1). For List 2 see Table A.3.1.

<table>
<thead>
<tr>
<th>Name</th>
<th>Definition</th>
<th>Notation</th>
<th>Trivial Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Scalar</td>
<td>$p = n = 1$</td>
<td>$a, b$</td>
<td>(1)</td>
</tr>
<tr>
<td>2a Column vector</td>
<td>$p = 1$</td>
<td>$a, b, \ldots$</td>
<td>(2)</td>
</tr>
<tr>
<td>2b Unit vector</td>
<td>$(1, \ldots, 1)'$</td>
<td>$1$ or $1_p$</td>
<td>(1)</td>
</tr>
<tr>
<td>3 Rectangular</td>
<td>$p \times n$</td>
<td>$A(n \times p)$</td>
<td></td>
</tr>
<tr>
<td>4 Square</td>
<td>$p = n$</td>
<td>$A(p \times p)$</td>
<td>(1 3)</td>
</tr>
<tr>
<td>4a Diagonal</td>
<td>$p = n, a_{ij} = 0, i \neq j$</td>
<td>diag $(a_{ii})$</td>
<td>(2 0)</td>
</tr>
<tr>
<td>4b Identity</td>
<td>diag $(1)$</td>
<td>$I$ or $I_p$</td>
<td>(1 0)</td>
</tr>
<tr>
<td>4c Symmetric</td>
<td>$a_{ii} = a_{ii}$</td>
<td></td>
<td>(2 5)</td>
</tr>
<tr>
<td>4d Unit matrix</td>
<td>$p = n, a_{ii} = 1$</td>
<td>$I_p = 1_p$</td>
<td>(1 1)</td>
</tr>
<tr>
<td>4e Triangular matrix (upper)</td>
<td>$a_{ii} = 0$ below the diagonal</td>
<td>$\Delta'$</td>
<td>(1 0 0)</td>
</tr>
<tr>
<td>Triangular matrix (lower)</td>
<td>$a_{ii} = 0$ above the diagonal</td>
<td>$\Delta$</td>
<td>(2 2 0)</td>
</tr>
<tr>
<td>5 Asymmetric</td>
<td>$a_{ii} \neq a_{ii}$</td>
<td></td>
<td>(3 2 5)</td>
</tr>
<tr>
<td>6 Null</td>
<td>$a_{ii} = 0$</td>
<td>0</td>
<td>(0 0 0)</td>
</tr>
</tbody>
</table>
We may write the matrix \( A \) as \( A(n \times p) \) to emphasize the row and column order. In general, matrices are represented by boldface upper case letters throughout this book, e.g. \( A, B, X, Y, Z \). Their elements are represented by small letters with subscripts.

**Definition** The transpose of a matrix \( A \) is formed by interchanging the rows and columns:

\[
A' = \begin{pmatrix}
    a_{11} & a_{21} & \cdots & a_{n1} \\
    a_{12} & a_{22} & \cdots & a_{n2} \\
    \vdots & \vdots & \ddots & \vdots \\
    a_{1p} & a_{2p} & \cdots & a_{np}
\end{pmatrix}
\]

**Definition** A matrix with column-order one is called a column vector. Thus

\[
a = \begin{pmatrix}
    a_1 \\
    a_2 \\
    \vdots \\
    a_n
\end{pmatrix}
\]

is a column vector with \( n \) components.

In general, boldface lower case letters represent column vectors. Row vectors are written as column vectors transposed, i.e.

\[
a' = (a_1, \ldots, a_n).
\]

**Notation 2** We write the columns of the matrix \( A \) as \( a_{(1)}, a_{(2)}, \ldots, a_{(p)} \) and the rows (if written as column vectors) as \( a_1, a_2, \ldots, a_n \) so that

\[
A = (a_{(1)}, a_{(2)}, \ldots, a_{(p)}) = \begin{bmatrix}
    a_1' \\
    a_2' \\
    \vdots \\
    a_n'
\end{bmatrix}, \quad (A.1,2)
\]

where

\[
a_{(j)} = \begin{pmatrix}
    a_{1j} \\
    \vdots \\
    a_{nj}
\end{pmatrix}, \quad a_i = \begin{pmatrix}
    a_{i1} \\
    \vdots \\
    a_{ip}
\end{pmatrix}
\]
As shown in Table A.1.1 a square matrix $A(p \times p)$ is diagonal if $a_{ij} = 0$ for all $i \neq j$. There are two convenient ways to construct diagonal matrices. If $\mathbf{a} = (a_1, \ldots, a_p)'$ is any vector and $\mathbf{B}(p \times p)$ is any square matrix then
\[
\text{diag} (\mathbf{a}) = \text{diag} (a_i) = \text{diag} (a_1, \ldots, a_p) = \begin{pmatrix} a_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & a_p \end{pmatrix}
\]
and
\[
\text{Diag} (\mathbf{B}) = \begin{pmatrix} b_{11} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & b_{pp} \end{pmatrix}
\]
each defines a diagonal matrix.

### A.2 Matrix Operations

Table A.2.1 gives a summary of various important matrix operations. We deal with some of these in detail, assuming the definitions in the table.

#### Table A.2.1 Basic matrix operations

<table>
<thead>
<tr>
<th>Operation</th>
<th>Restrictions</th>
<th>Definitions</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 Addition</td>
<td>$A, B$ of the same order</td>
<td>$A + B = (a_i + b_i)$</td>
<td></td>
</tr>
<tr>
<td>2 Subtraction</td>
<td>$A, B$ of the same order</td>
<td>$A - B = (a_i - b_i)$</td>
<td></td>
</tr>
<tr>
<td>3a Scalar</td>
<td>$A, B$ of the same order</td>
<td>$cA = (ca_i)$</td>
<td>$AB \neq BA$</td>
</tr>
<tr>
<td>3b Multiplication</td>
<td>inner product</td>
<td>$\mathbf{a} \cdot \mathbf{b} = \sum a_i b_i$</td>
<td></td>
</tr>
<tr>
<td>3c Multiplication</td>
<td>$A$ of the same order number of columns in $A$ equals number of rows in $B$</td>
<td>$AB = (a_i b_{ij})$</td>
<td></td>
</tr>
<tr>
<td>4 Transpose</td>
<td>$A$ square</td>
<td>$A' = (a_1, a_2, \ldots, a_n)$</td>
<td>Section A.2.1</td>
</tr>
<tr>
<td>5 Trace</td>
<td>$A$ square</td>
<td>$\text{tr} A = \sum a_i$</td>
<td>Section A.2.2</td>
</tr>
<tr>
<td>6 Determinant</td>
<td>$A$ square</td>
<td>$</td>
<td>A</td>
</tr>
<tr>
<td>7 Inverse</td>
<td>$A$ square and $</td>
<td>A</td>
<td>\neq 0$</td>
</tr>
<tr>
<td>8 g-inverse ($A^{-1}$)</td>
<td>$A(n \times p)$</td>
<td>$AA^{-1} = A$</td>
<td>Section A.8</td>
</tr>
</tbody>
</table>

#### A.2.1 Transpose

The transpose satisfies the simple properties
\[
(A')' = A, \quad (A + B)' = A' + B', \quad (AB)' = B'A'. \tag{A.2.1}
\]
\[ p(0|\gamma) \cdot \lambda(\theta) \]
\[ \frac{\text{outcomes}}{\text{species}} \]
\[ \text{SL}, \text{SW}, \text{PL}, \text{PW} \]

- **Species**: setosa, versicolor, virginica
- **Quantitative**: SL, SW, PL, PW

**Predictors**

- If 2 species, logistic regression