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## Introduction to linear algebra in R

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# Introduction to linear algebra in R 

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## 1 Introduction

The first version of these notes were written in 2005. These notes/slides have two aims: 1) Introducing linear algebra (vectors and matrices) and 2) showing how to work with these concepts in $R$. They were written in an attempt to give a specific group of students a "feeling" for what matrices, vectors etc. are all about. Hence the notes/slides are not suitable for a course in linear algebra.

## 2 Vectors

### 2.1 Vectors

A column vector is a list of numbers stacked on top of each other, e.g.

$$
a=\left[\begin{array}{l}
2 \\
1 \\
3
\end{array}\right]
$$

A row vector is a list of numbers written one after the other, e.g.

$$
b=(2,1,3)
$$

In both cases, the list is ordered, i.e.

$$
(2,1,3) \neq(1,2,3) .
$$

We make the following convention:

- In what follows all vectors are column vectors unless otherwise stated.
- However, writing column vectors takes up more space than row vectors. Therefore we shall frequently write vectors as row vectors, but with the understanding that it really is a column vector.

A general $n$-vector has the form

$$
a=\left[\begin{array}{c}
a_{1} \\
a_{2} \\
\vdots \\
a_{n}
\end{array}\right]
$$

where the $a_{i} \mathrm{~s}$ are numbers, and this vector shall be written $a=\left(a_{1}, \ldots, a_{n}\right)$.
A graphical representation of $2-$ vectors is shown Figure 1 .


Figure 1: Two 2-vectors
Note that row and column vectors are drawn the same way.

```
>a<-c(1, 3, 2)
> a
```

[1] 132
The vector a is in R printed "in row format" but can really be regarded as a column vector, cfr. the convention above.

### 2.2 Transpose of vectors

Transposing a vector means turning a column (row) vector into a row (column) vector. The transpose is denoted by "T".

## Example 1

$$
\left[\begin{array}{l}
1 \\
3 \\
2
\end{array}\right]^{\top}=[1,3,2] \text { og }[1,3,2]^{\top}=\left[\begin{array}{l}
1 \\
3 \\
2
\end{array}\right]
$$

Hence transposing twice takes us back to where we started:

$$
a=\left(a^{\top}\right)^{\top}
$$

```
> t(a)
```

```
[ [,1] [,2] [,3]
```


### 2.3 Multiplying a vector by a number

If $a$ is a vector and $\alpha$ is a number then $\alpha a$ is the vector

$$
\alpha a=\left[\begin{array}{c}
\alpha a_{1} \\
\alpha a_{2} \\
\vdots \\
\alpha a_{n}
\end{array}\right]
$$

See Figure 2.
Example 2

$$
7\left[\begin{array}{l}
1 \\
3 \\
2
\end{array}\right]=\left[\begin{array}{c}
7 \\
21 \\
14
\end{array}\right]
$$



Figure 2: Multiplication of a vector by a number

$$
>7 * \mathrm{a}
$$

### 2.4 Sum of vectors

Let $a$ and $b$ be $n$-vectors. The sum $a+b$ is the $n$-vector

$$
a+b=\left[\begin{array}{c}
a_{1} \\
a_{2} \\
\vdots \\
a_{n}
\end{array}\right]+\left[\begin{array}{c}
b_{1} \\
b_{2} \\
\vdots \\
b_{n}
\end{array}\right]=\left[\begin{array}{c}
a_{1}+b_{1} \\
a_{2}+b_{2} \\
\vdots \\
a_{n}+b_{n}
\end{array}\right]=b+a
$$

See Figure 3 and 4. Only vectors of the same dimension can be added.

Example 3

$$
\left[\begin{array}{l}
1 \\
3 \\
2
\end{array}\right]+\left[\begin{array}{l}
2 \\
8 \\
9
\end{array}\right]=\left[\begin{array}{l}
1+2 \\
3+8 \\
2+9
\end{array}\right]=\left[\begin{array}{c}
3 \\
11 \\
11
\end{array}\right]
$$



Figure 3: Addition of vectors


Figure 4: Addition of vectors and multiplication by a number

$$
\begin{aligned}
& >a<-c(1,3,2) \\
& >b<-c(2,8,9) \\
& >a+b
\end{aligned}
$$

[1] 311111

### 2.5 Inner product of vectors

Let $a=\left(a_{1}, \ldots, a_{n}\right)$ and $b=\left(b_{1}, \ldots, b_{n}\right)$. The inner product of $a$ and $b$ is

$$
a \cdot b=a_{1} b_{1}+\cdots+a_{n} b_{n}
$$

Note, that the inner product is a number - not a vector.

```
> sum(a * b)
```


### 2.6 The length (norm) of a vector

The length (or norm) of a vector $a$ is

$$
\|a\|=\sqrt{a \cdot a}=\sqrt{\sum_{i=1}^{n} a_{i}^{2}}
$$

$>\operatorname{sqrt}(\operatorname{sum}(\mathrm{a} * \mathrm{a}))$
[1] 3.741657

### 2.7 The 0-vector and 1-vector

The 0 -vector (1-vector) is a vector with 0 (1) on all entries. The 0 -vector ( 1 -vector) is frequently written simply as 0 (1) or as $0_{n}\left(1_{n}\right)$ to emphasize that its length $n$.

```
> rep(0, 5)
```

```
[1] 0 0 0 0 0
```

```
> rep(1, 5)
```

[1] $\begin{array}{llllll}1 & 1 & 1 & 1 & 1\end{array}$

### 2.8 Orthogonal (perpendicular) vectors

Two vectors $v_{1}$ and $v_{2}$ are orthogonal if and only if their inner product is zero, written

$$
v_{1} \perp v_{2} \Leftrightarrow v_{1} \cdot v_{2}=0
$$

Note that any vector is orthogonal to the 0 -vector.

```
> v1 <- c(1, 1)
> v2 <- c(-1, 1)
> sum(v1 * v2)
```


## 3 Matrices

### 3.1 Matrices

An $r \times c$ matrix $A$ (reads "an $r$ times $c$ matrix") is a table with $r$ rows og columns

$$
A=\left[\begin{array}{cccc}
a_{11} & a_{12} & \ldots & a_{1 c} \\
a_{21} & a_{22} & \ldots & a_{2 c} \\
\vdots & \vdots & \ddots & \vdots \\
a_{r 1} & a_{r 2} & \ldots & a_{r c}
\end{array}\right]
$$

Note that one can regard $A$ as consisting of $c$ columns vectors put after each other:

$$
A=\left[a_{1}: a_{2}: \cdots: a_{c}\right]
$$

Likewise one can regard $A$ as consisting of $r$ row vectors stacked on to of each other.

$$
\begin{aligned}
& >\mathrm{A}<-\operatorname{matrix}(\mathrm{c}(1,3,2,2,8,9), \mathrm{ncol}=3) \\
& >\mathrm{A}
\end{aligned}
$$

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 1 | 2 | 8 |
| $[2]$, | 3 | 2 | 9 |

Note that the numbers $1,3,2,2,8,9$ are read into the matrix column-by-column. To get the numbers read in row-by-row do

```
> A2 <- matrix(c(1, 3, 2, 2, 8, 9), ncol=3, byrow=T)
```

> A2

```
lrrrer
```


### 3.2 Multiplying a matrix with a number

For a number $\alpha$ and a matrix $A$, the product $\alpha A$ is the matrix obtained by multiplying each element in $A$ by $\alpha$.

## Example 4

$$
7\left[\begin{array}{ll}
1 & 2 \\
3 & 8 \\
2 & 9
\end{array}\right]=\left[\begin{array}{rr}
7 & 14 \\
21 & 56 \\
14 & 63
\end{array}\right]
$$

$$
>7 * \mathrm{~A}
$$

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 7 | 14 | 56 |
| $[2]$, | 21 | 14 | 63 |

### 3.3 Transpose of matrices

A matrix is transposed by interchanging rows and columns and is denoted by "T".

Example 5

$$
\left[\begin{array}{ll}
1 & 2 \\
3 & 8 \\
2 & 9
\end{array}\right]^{\top}=\left[\begin{array}{lll}
1 & 3 & 2 \\
2 & 8 & 9
\end{array}\right]
$$

Note that if $A$ is an $r \times c$ matrix then $A^{\top}$ is a $c \times r$ matrix.

```
t (A)
```

|  | $[, 1]$ | $[, 2]$ |
| ---: | ---: | ---: |
| $[1]$, | 1 | 3 |
| $[2]$, | 2 | 2 |
| $[3]$, | 8 | 9 |

### 3.4 Sum of matrices

Let $A$ and $B$ be $r \times c$ matrices. The sum $A+B$ is the $r \times c$ matrix obtained by adding $A$ and $B$ elementwise.
Only matrices with the same dimensions can be added.

## Example 6

$$
\left[\begin{array}{ll}
1 & 2 \\
3 & 8 \\
2 & 9
\end{array}\right]+\left[\begin{array}{ll}
5 & 4 \\
8 & 2 \\
3 & 7
\end{array}\right]=\left[\begin{array}{rr}
6 & 6 \\
11 & 10 \\
5 & 16
\end{array}\right]
$$

$$
\begin{aligned}
& >B \quad<-\operatorname{matrix}(c(5,8,3,4,2,7), \text { ncol=3, byrow=T) } \\
& >A+B
\end{aligned}
$$

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 6 | 10 | 11 |
| $[2]$, | 7 | 4 | 16 |

### 3.5 Multiplication of a matrix and a vector

Let $A$ be an $r \times c$ matrix and let $b$ be a $c$-dimensional column vector. The product $A b$ is the $r \times 1$ matrix
$A b=\left[\begin{array}{cccc}a_{11} & a_{12} & \ldots & a_{1 c} \\ a_{21} & a_{22} & \ldots & a_{2 c} \\ \vdots & \vdots & \ddots & \vdots \\ a_{r 1} & a_{r 2} & \ldots & a_{r c}\end{array}\right]\left[\begin{array}{c}b_{1} \\ b_{2} \\ \vdots \\ b_{c}\end{array}\right]=\left[\begin{array}{c}a_{11} b_{1}+a_{12} b_{2}+\cdots+a_{1 c} b_{c} \\ a_{21} b_{1}+a_{22} b_{2}+\cdots+a_{2 c} b_{c} \\ \vdots \\ a_{r 1} b_{1}+a_{r 2} b_{2}+\cdots+a_{r c} b_{c}\end{array}\right]$
Example 7

$$
\left[\begin{array}{ll}
1 & 2 \\
3 & 8 \\
2 & 9
\end{array}\right]\left[\begin{array}{l}
5 \\
8
\end{array}\right]=\left[\begin{array}{l}
1 \cdot 5+2 \cdot 8 \\
3 \cdot 5+8 \cdot 8 \\
2 \cdot 5+9 \cdot 8
\end{array}\right]=\left[\begin{array}{l}
21 \\
79 \\
82
\end{array}\right]
$$

$$
>\mathrm{A} \% * \% \mathrm{a}
$$

```
    [,1]
[1,] 23
[2,] 27
```

Note the difference to

```
>A*a
    [,1] [,2] [,3]
[1,] 1 4 24
[2,] 
```

Please figure out yourself what goes on!

### 3.6 Multiplication of matrices

Let $A$ be an $r \times c$ matrix and $B$ a $c \times t$ matrix, i.e. $B=\left[b_{1}: b_{2}: \cdots: b_{t}\right]$. The product $A B$ is the $r \times t$ matrix given by:

$$
A B=A\left[b_{1}: b_{2}: \cdots: b_{t}\right]=\left[A b_{1}: A b_{2}: \cdots: A b_{t}\right]
$$

Example 8

$$
\begin{aligned}
{\left[\begin{array}{ll}
1 & 2 \\
3 & 8 \\
2 & 9
\end{array}\right]\left[\begin{array}{ll}
5 & 4 \\
8 & 2
\end{array}\right] } & =\left[\left[\begin{array}{ll}
1 & 2 \\
3 & 8 \\
2 & 9
\end{array}\right]\left[\begin{array}{l}
5 \\
8
\end{array}\right]:\left[\begin{array}{ll}
1 & 2 \\
3 & 8 \\
2 & 9
\end{array}\right]\left[\begin{array}{l}
4 \\
2
\end{array}\right]\right] \\
& =\left[\begin{array}{ll}
1 \cdot 5+2 \cdot 8 & 1 \cdot 4+2 \cdot 2 \\
3 \cdot 5+8 \cdot 8 & 3 \cdot 4+8 \cdot 2 \\
2 \cdot 5+9 \cdot 8 & 2 \cdot 4+9 \cdot 2
\end{array}\right]=\left[\begin{array}{cc}
21 & 8 \\
79 & 28 \\
82 & 26
\end{array}\right]
\end{aligned}
$$

Note that the product $A B$ can only be formed if the number of rows in $B$ and the number of columns in $A$ are the same. In that case, $A$ and $B$ are said to be conforme.

In general $A B$ and $B A$ are not identical.
A mnemonic for matrix multiplication is:

$$
\left[\begin{array}{ll}
1 & 2 \\
3 & 8 \\
2 & 9
\end{array}\right]\left[\begin{array}{ll}
5 & 4 \\
8 & 2
\end{array}\right]=\begin{array}{cccc} 
& & 5 & 4 \\
\hline 1 & 2 & 1 \cdot 5+2 \cdot 8 & 1 \cdot 4+2 \cdot 2 \\
3 & 8 & 3 \cdot 5+8 \cdot 8 & 3 \cdot 4+8 \cdot 2 \\
2 & 9 & 2 \cdot 5+9 \cdot 8 & 2 \cdot 4+9 \cdot 2
\end{array}=\left[\begin{array}{cc}
21 & 8 \\
79 & 28 \\
82 & 26
\end{array}\right]
$$

$$
\begin{aligned}
& >\mathrm{A}<-\operatorname{matrix}(\mathrm{c}(1,3,2,2,8,9), \mathrm{ncol}=2) \\
& >\mathrm{B}<-\operatorname{matrix}(\mathrm{c}(5,8,4,2), \mathrm{ncol}=2) \\
& >\mathrm{A} \% * \% \mathrm{~B}
\end{aligned}
$$

|  | $[, 1]$ | $[, 2]$ |
| :--- | ---: | ---: |
| $[1]$, | 21 | 8 |
| $[2]$, | 79 | 28 |
| $[3]$, | 82 | 26 |

### 3.7 Vectors as matrices

One can regard a column vector of length $r$ as an $r \times 1$ matrix and a row vector of length $c$ as a $1 \times c$ matrix.

### 3.8 Some special matrices

- An $n \times n$ matrix is a square matrix
- A matrix $A$ is symmetric if $A=A^{\top}$.
- A matrix with 0 on all entries is the $\underline{0-m a t r i x}$ and is often written simply as 0 .
- A matrix consisting of 1 s in all entries is often written $J$.
- A square matrix with 0 on all off-diagonal entries and element $d_{1}, d_{2}, \ldots, d_{n}$ on the diagonal a diagonal matrix and is often written $\operatorname{diag}\left\{d_{1}, d_{2}, \ldots, d_{n}\right\}$
- A diagonal matrix with 1 s on the diagonal is called the identity matrix and is denoted $I$. The identity matrix satisfies that $I A=A I=A$. Likewise, if $x$ is a vector then $I x=x$.
- 0-matrix and 1-matrix
$>$ matrix(0, nrow=2, ncol=3)

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 0 | 0 | 0 |
| $[2]$, | 0 | 0 | 0 |

matrix(1, nrow=2, ncol=3)

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 1 | 1 | 1 |
| $[2]$, | 1 | 1 | 1 |

- Diagonal matrix and identity matrix

| > diag $(\mathrm{c}(1,2,3)$ |  |  |  |
| :---: | :---: | :---: | :---: |
|  | [,1] | [,2] | [,3] |
| [1,] | 1 | 0 | 0 |
| [2,] | 0 | 2 | 0 |
| [3,] | 0 | 0 | 3 |

> diag(1, 3)

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 1 | 0 | 0 |
| $[2]$, | 0 | 1 | 0 |
| $[3]$, | 0 | 0 | 1 |

Note what happens when diag is applied to a matrix:

```
> diag(diag(c(1, 2, 3)))
```

[1] 123
> diag(A)
[1] 18

### 3.9 Inverse of matrices

In general, the inverse of an $n \times n$ matrix $A$ is the matrix $B$ (which is also $n \times n$ ) which when multiplied with $A$ gives the identity matrix $I$. That is,

$$
A B=B A=I
$$

One says that $B$ is $A^{\prime}$ s inverse and writes $B=A^{-1}$. Likewise, $A$ is $B$ s inverse.

Example 9 Let

$$
A=\left[\begin{array}{ll}
1 & 3 \\
2 & 4
\end{array}\right] \quad B=\left[\begin{array}{rr}
-2 & 1.5 \\
1 & -0.5
\end{array}\right]
$$

Now $A B=B A=I$ so $B=A^{-1}$.
Example 10 If $A$ is a $1 \times 1$ matrix, i.e. a number, for example $A=4$, then $A^{-1}=1 / 4$.

Some facts about inverse matrices are:

- Only square matrices can have an inverse, but not all square matrices have an inverse.
- When the inverse exists, it is unique.
- Finding the inverse of a large matrix $A$ is numerically complicated (but computers do it for us).
Finding the inverse of a matrix in R is done using the solve() function:

```
> A <- matrix(c(1, 3, 2, 4), ncol=2,byrow=T)
> A
```

|  | $[, 1]$ | $[, 2]$ |
| :--- | ---: | ---: |
| $[1]$, | 1 | 3 |
| $[2]$, | 2 | 4 |

```
> #M2 <- matrix(c(-2,1.5,1,-0.5),ncol=2,byrow=T)
> B <- solve(A)
> B
```

$$
\begin{array}{rrr} 
& {[, 1]} & {[, 2]} \\
{[1,]} & -2 & 1.5 \\
{[2,]} & 1 & -0.5
\end{array}
$$

$$
>\mathrm{A} \% * \% \quad \mathrm{~B}
$$

$$
\begin{array}{|lrr}
\hline & {[, 1]} & {[, 2]} \\
{[1,]} & 1 & 0 \\
{[2,]} & 0 & 1
\end{array}
$$

### 3.10 Solving systems of Linear equations

Example 11 Matrices are closely related to systems of Linear equations. Consider the two equations

$$
\begin{aligned}
x_{1}+3 x_{2} & =7 \\
2 x_{1}+4 x_{2} & =10
\end{aligned}
$$

The system can be written in matrix form

$$
\left[\begin{array}{ll}
1 & 3 \\
2 & 4
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]=\left[\begin{array}{r}
7 \\
10
\end{array}\right] \text { i.e. } A x=b
$$

Since $A^{-1} A=I$ and since $I x=x$ we have

$$
x=A^{-1} b=\left[\begin{array}{rr}
-2 & 1.5 \\
1 & -0.5
\end{array}\right]\left[\begin{array}{r}
7 \\
10
\end{array}\right]=\left[\begin{array}{l}
1 \\
2
\end{array}\right]
$$

A geometrical approach to solving these equations is as
follows: Isolate $x_{2}$ in the equations:

$$
x_{2}=\frac{7}{3}-\frac{1}{3} x_{1} \quad x_{2}=\frac{1}{0} 4-\frac{2}{4} x_{1}
$$

These two lines are shown in Figure 5 from which it can be seen that the solution is $x_{1}=1, x_{2}=2$.


Figure 5: Solving two equations with two unknowns.
From the Figure it follows that there are 3 possible cases of solutions to the system

1. Exactly one solution - when the lines intersect in one point
2. No solutions - when the lines are parallel but not identical
3. Infinitely many solutions - when the lines coincide.
```
\(>\mathrm{A}<-\operatorname{matrix}(\mathrm{c}(1,2,3,4)\), \(\mathrm{ncol}=2)\)
\(>\mathrm{b}<-\mathrm{c}(7,10)\)
\(>\mathrm{x}<-\operatorname{solve}(\mathrm{A}) \% * \% \mathrm{~b}\)
\(>\mathrm{x}\)
```

```
    [,1]
[1,] 1
[2,] 2
```


### 3.11 Some additional rutes for matrix operations

For matrices $A, B$ and $C$ whose dimension match appropriately: the following rules apply

$$
\begin{gathered}
(A+B)^{\top}=A^{\top}+B^{\top} \\
(A B)^{\top}=B^{\top} A^{\top} \\
A(B+C)=A B+A C \\
A B=A C \nRightarrow B=C
\end{gathered}
$$

In genereal $A B \neq B A$

$$
A I=I A=A
$$

If $\alpha$ is a number then $\alpha A B=A(\alpha B)$

### 3.12 Details on inverse matrices*

3.12.1 Inverse of a $2 \times 2$ matrix*

It is easy find the inverse for a $2 \times 2$ matrix. When

$$
A=\left[\begin{array}{ll}
a & b \\
c & d
\end{array}\right]
$$

then the inverse is

$$
A^{-1}=\frac{1}{a d-b c}\left[\begin{array}{rr}
d & -b \\
-c & a
\end{array}\right]
$$

under the assumption that $a b-b c \neq 0$. The number $a b-b c$ is called the determinant of $A$, sometimes written $|A|$ or $\operatorname{det}(A)$. A matrix $A$ has an inverse if and only if $|A| \neq 0$.

### 3.12.2 Inverse of diagonal matrices*

Finding the inverse of a diagonal matrix is easy: Let

$$
A=\operatorname{diag}\left(a_{1}, a_{2}, \ldots, a_{n}\right)
$$

where all $a_{i} \neq 0$. Then the inverse is

$$
A^{-1}=\operatorname{diag}\left(\frac{1}{a_{1}}, \frac{1}{a_{2}}, \ldots, \frac{1}{a_{n}}\right)
$$

If one $a_{i}=0$ then $A^{-1}$ does not exist.

### 3.12.3 Generalized inverse*

Not all square matrices have an inverse. However all square matrices have an infinite number of generalized inverses. A generalized inverse of a square matrix $A$ is a matrix $G$ satisfying that

$$
A G A=A .
$$

For many practical problems it suffice to find a generalized inverse.
$>\mathrm{A}<-\operatorname{matrix}(\mathrm{c}(1,2,3,2,3,4,3,5,7)$, ncol=3)
> A \# 3rd column is sum of the two first; the inverse does not exist

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 1 | 2 | 3 |
| $[2]$, | 2 | 3 | 5 |
| $[3]$, | 3 | 4 | 7 |

$>\operatorname{det}(\mathrm{A})$
[1] 0
$>\mathrm{G}<-\mathrm{MASS}:: \operatorname{ginv}(\mathrm{A})$
$>\mathrm{A} \% * \% \mathrm{G} \quad$ \# Not identity

| $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | :--- | :--- | :--- |

$[1] \quad 0.83333330 .3333333-$,
$[2] \quad 0.33333330 .3333333 \quad$,
$[3]-,0.1666667 \quad 0.3333333 \quad 0.8333333$
$\square$
$>\mathrm{A} \% * \% \mathrm{G} \% * \% \mathrm{~A} \quad \#$ This is A

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| ---: | ---: | ---: | ---: |
| $[1]$, | 1 | 2 | 3 |
| $[2]$, | 2 | 3 | 5 |
| $[3]$, | 3 | 4 | 7 |

### 3.12.4 Inverting an $n \times n$ matrix*

In the following we will illustrate one frequently applied methopd for matrix inversion. The method is called Gauss-Seidels method and many computer programs use variants of the method for finding the inverse of an $n \times n$ matrix.

Consider the matrix $A$ :

```
> A <- matrix (c(2, 2, 3, 3, 5, 9, 5, 6, 7), ncol=3)
>A
```

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 2 | 3 | 5 |
| $[2]$, | 2 | 5 | 6 |
| $[3]$, | 3 | 9 | 7 |

We want to find the matrix $B=A^{-1}$. To start, we append to $A$ the identity matrix and call the result $A B$ :
$\mid>A B<-\operatorname{cbind}(A, \operatorname{diag}(c(1,1,1)))$

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ | $[, 4]$ | $[, 5]$ | $[, 6]$ |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $[1]$, | 2 | 3 | 5 | 1 | 0 | 0 |
| $[2]$, | 2 | 5 | 6 | 0 | 1 | 0 |
| $[3]$, | 3 | 9 | 7 | 0 | 0 | 1 |

On a matrix we allow ourselves to do the following three operations (sometimes called elementary operations) as often as we want:

1. Multiply a row by a (non-zero) constant.
2. Multiply a row by a (non-zero) constant and add the result to another row.
3. Interchange two rows.

The aim is to perform such operations on $A B$ in a way such that one ends up with a $3 \times 6$ matrix which has the identity matrix in the three leftmost columns. The three rightmost columns will then contain $B=A^{-1}$.

Recall that writing e.g. $A B[1$,$] extracts the enire first row of A B$.

- First, we make sure that $\mathrm{AB}[1,1]=1$. Then we subtract a constant times the first row from the second to obtain that $A B[2,1]=0$, and similarly for the third row:

```
> AB[1,] <- AB[1,] / AB[1,1]
> AB[2,] <- AB[2,] - 2 * AB[1,]
> AB[3,] <- AB[3,] - 3*AB[1,]
>AB
```

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ | $[, 4]$ | $[, 5]$ | $[, 6]$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| $[1]$, | 1 | 1.5 | 2.5 | 0.5 | 0 | 0 |
| $[2]$, | 0 | 2.0 | 1.0 | -1.0 | 1 | 0 |
| $[3]$, | 0 | 4.5 | -0.5 | -1.5 | 0 | 1 |

- Next we ensure that $\mathrm{AB}[2,2]=1$. Afterwards we subtract a constant times the second row from the third to obtain that $\mathrm{AB}[3,2]=0$ :

```
> AB[2,] <- AB[2,] / AB[2,2]
> AB[3,] <- AB[3,] - 4.5 * AB[2,]
```

- Now we rescale the third row such that $\mathrm{AB}[3,3]=1$ :

```
> AB[3,] <- AB[3,] / AB[3,3]
> AB
```

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ | $[, 4]$ | $[, 5]$ | $[, 6]$ |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| $[1]$, | 1 | 1.5 | 2.5 | 0.5000000 | 0.0000000 | 0.0000000 |
| $[2]$, | 0 | 1.0 | 0.5 | -0.5000000 | 0.5000000 | 0.0000000 |
| $[3]$, | 0 | 0.0 | 1.0 | -0.2727273 | 0.8181818 | -0.3636364 |

Then AB has zeros below the main diagonal.

- We then work our way up to obtain that AB has zeros above the main diagonal:

```
> AB[2,] <- AB[2,] - 0.5 * AB[3,]
> AB[1,] <- AB[1,] - 2.5 * AB[3,]
> AB
```

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ | $[, 4]$ | $[, 5]$ | $[, 6]$ |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $[1]$, | 1 | 1.5 | 0 | 1.1818182 | -2.04545455 | 0.9090909 |
| $[2]$, | 0 | 1.0 | 0 | -0.3636364 | 0.09090909 | 0.1818182 |
| $[3]$, | 0 | 0.0 | 1 | -0.2727273 | 0.81818182 | -0.3636364 |

$$
\begin{aligned}
& >\mathrm{AB}[1,]<-\mathrm{AB}[1,]-1.5 * \mathrm{AB}[2,] \\
& >\mathrm{AB}
\end{aligned}
$$

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ | $[, 4]$ | $[, 5]$ | $[, 6]$ |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $[1]$, | 1 | 0 | 0 | 1.7272727 | -2.18181818 | 0.6363636 |
| $[2]$, | 0 | 1 | 0 | -0.3636364 | 0.09090909 | 0.1818182 |
| $[3]$, | 0 | 0 | 1 | -0.2727273 | 0.81818182 | -0.3636364 |

Now we extract the three rightmost columns of $A B$ into the matrix $B$. We claim that $B$ is the inverse of $A$, and this can be verified by $a$ simple matrix multiplication

```
> B <- AB[,4:6]
> A%*% B
```

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| ---: | ---: | ---: | ---: |
| $[1]$, | $1.000000 \mathrm{e}+00$ | $3.330669 \mathrm{e}-16$ | $1.110223 \mathrm{e}-16$ |
| $[2]$, | $-4.440892 \mathrm{e}-16$ | $1.000000 \mathrm{e}+00$ | $2.220446 \mathrm{e}-16$ |
| $[3]$, | $-2.220446 \mathrm{e}-16$ | $9.992007 \mathrm{e}-16$ | $1.000000 \mathrm{e}+00$ |

So, apart from rounding errors, the product is the identity matrix,
and hence $B=A^{-1}$. This example illustrates that numerical precision and rounding errors is an important issue when making computer programs.

## 4 Least squares

Consider the table of pairs $\left(x_{i}, y_{i}\right)$ below.

| x | 1.00 | 2.00 | 3.00 | 4.00 | 5.00 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| y | 3.70 | 4.20 | 4.90 | 5.70 | 6.00 |

A plot of $y_{i}$ against $x_{i}$ is shown in Figure 6.


Figure 6: Regression

The plot in Figure 6 suggests an approximately linear relationship between $y$ and $x$, i.e.

$$
y_{i}=\beta_{0}+\beta_{1} x_{i} \text { for } i=1, \ldots, 5
$$

Writing this in matrix form gives

$$
y=\left[\begin{array}{c}
y_{1} \\
y_{2} \\
\cdots \\
y_{5}
\end{array}\right] \approx\left[\begin{array}{rr}
1 & x_{1} \\
1 & x_{2} \\
\vdots & \vdots \\
1 & x_{5}
\end{array}\right]\left[\begin{array}{c}
\beta_{0} \\
\beta_{1}
\end{array}\right]=\boldsymbol{X} \boldsymbol{\beta}
$$

The first question is: Can we find a vector $\beta$ such that $y=X \beta$ ? The answer is clearly no, because that would require the points to lie exactly on a straight line.

A more modest question is: Can we find a vector $\hat{\beta}$ such that $X \hat{\beta}$ is in a sense "as close to $y$ as possible". The answer is yes. The task
is to find $\hat{\beta}$ such that the length of the vector

$$
e=y-X \beta
$$

is as small as possible. This leads to the so-called system of normal equations

$$
\left(X^{\top} X\right) \beta=X^{\top} y
$$

If $\left(X^{\top} X\right)$ is invertible, the (unique) solution is

$$
\hat{\beta}=\left(X^{\top} X\right)^{-1} X^{\top} y
$$

$>y$
[1] $3.74 .24 .95 .7 \quad 6.0$
$>\mathrm{X}$
$[1]$,
$[2]$,

```
[3,] 1 3
[4,] 14
[5,] 1 5
```

beta.hat <- solve(t(X) $\% * \%$ X) $\% * \%$ t (X) $\% * \%$ y
beta.hat

```
    [,1]
3.07
x 0.61
```

The fitted values are

```
> as.numeric(X %*% beta.hat)
```

[1] $3.684 .294 .90 \quad 5.51 \quad 6.12$

### 4.1 Least squares with generalized inverse

Expand the setting above: Let $X_{2}$ be $X$ with an extra column added: The sum of the columns of $X$.

```
> X2 <- cbind(X, rowSums(X))
> X2
```

```
    x
[1,] 1 1 2
[2,] 1 2 3
[3,] 1 3 4
[4,] 145
[5,] 1 5 6
```

Then $\left(X_{2}^{\top} X_{2}\right)$ is not invertible. There are infinitely many solutions to the normal equations. One is:

```
\(>G<-\) MASS : : ginv (t (X2) \(\% * \%\) X2)
\(>G\)
```

$[, 1] \quad[, 2] \quad[, 3]$

```
[1,] 0.6333333-0.4333333 0.20000000
[2,] -0.4333333 0.3000000-0.13333333
[3,] 0.2000000 -0.1333333 0.06666667
```

$>$ beta2.hat <-G $\% * \%$ t(X2) $\% * \%$ y
> beta2.hat

```
    [,1]
[1,] 1.8433333
[2,] -0.6166667
[3,] 1.2266667
```

Another solution is (why?)
beta22.hat <- c(beta.hat, 0)

## The fitted values are the same:

as.numeric(X2 \%*\% beta2.hat)

```
[1] 3.68 4.29 4.90 5.51 6.12
```

$\square$
as.numeric (X2 \%*\% beta22.hat)
[1] $3.684 .294 .90 \quad 5.51 \quad 6.12$

## 5 A neat little exercise - from a bird's perspective

On a sunny day, two tables are standing in an English country garden. On each table birds of unknown species are sitting having the time of their lives.

A bird from the first table says to those on the second table: " $\mathrm{Hi}-$ if one of you come to our table then there will be the same number of us on each table". "Yeah, right", says a bird from the second table, "but if one of you comes to our table, then we will be twice as many on our table as on yours".

Question: How many birds are on each table? More specifically,

- Write up two equations with two unknowns.
- Solve these equations using the methods you have learned from linear algebra.
- Simply finding the solution by trial-and-error is considered cheating.

