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Introduction to linear algebra in \mathbb{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.

$$a = \begin{bmatrix} 2 \\ 1 \\ 3 \end{bmatrix}$$

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

$$a = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

where the a_i s are numbers, and this vector shall be written $a = (a_1, \dots, a_n)$.

A graphical representation of 2-vectors is shown Figure 1. Note that row and column vectors

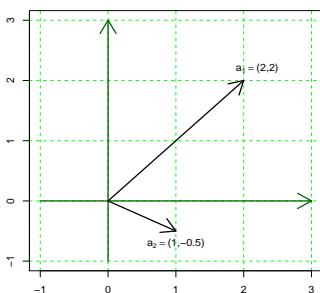


Figure 1: Two 2-vectors

are drawn the same way.

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

The vector \mathbf{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 “ \top ”.

Example 1

$$\begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix}^\top = [1, 3, 2] \quad \text{og} \quad [1, 3, 2]^\top = \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix}$$

□

Hence transposing twice takes us back to where we started:

$$a = (a^\top)^\top$$

```
> t(a)
      [,1] [,2] [,3]
[1,]    1    3    2
```

2.3 Multiplying a vector by a number

If a is a vector and α is a number then αa is the vector

$$\alpha a = \begin{bmatrix} \alpha a_1 \\ \alpha a_2 \\ \vdots \\ \alpha a_n \end{bmatrix}$$

See Figure 2.

Example 2

$$7 \begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} = \begin{bmatrix} 7 \\ 21 \\ 14 \end{bmatrix}$$

□

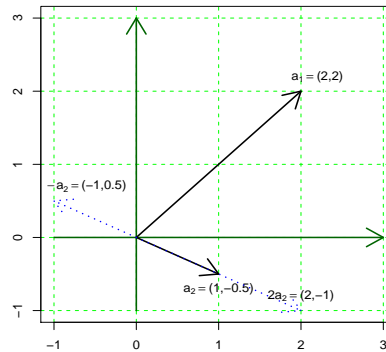


Figure 2: Multiplication of a vector by a number

> 7 * a

[1] 7 21 14

2.4 Sum of vectors

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

$$a + b = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} + \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} = \begin{bmatrix} a_1 + b_1 \\ a_2 + b_2 \\ \vdots \\ a_n + b_n \end{bmatrix} = b + a$$

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

Example 3

$$\begin{bmatrix} 1 \\ 3 \\ 2 \end{bmatrix} + \begin{bmatrix} 2 \\ 8 \\ 9 \end{bmatrix} = \begin{bmatrix} 1+2 \\ 3+8 \\ 2+9 \end{bmatrix} = \begin{bmatrix} 3 \\ 11 \\ 11 \end{bmatrix}$$

□

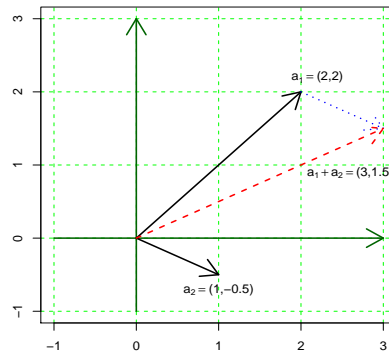


Figure 3: Addition of vectors

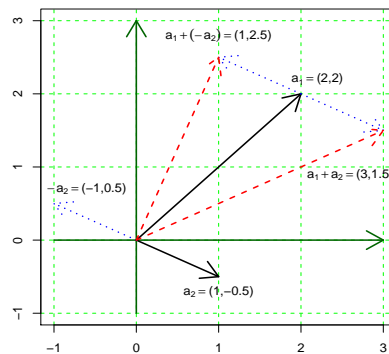


Figure 4: Addition of vectors and multiplication by a number

> a <- c(1, 3, 2)
> b <- c(2, 8, 9)
> a+b

```
[1] 3 11 11
```

2.5 Inner product of vectors

Let $a = (a_1, \dots, a_n)$ and $b = (b_1, \dots, b_n)$. The inner product of a and b is

$$a \cdot b = a_1 b_1 + \dots + a_n b_n$$

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

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

```
[1] 44
```

2.6 The length (norm) of a vector

The length (or norm) of a vector a is

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

```
> sqrt(sum(a * 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 (1_n) to emphasize that its length n .

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

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

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

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

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)
```

```
[1] 0
```

3 Matrices

3.1 Matrices

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

$$A = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1c} \\ a_{21} & a_{22} & \dots & a_{2c} \\ \vdots & \vdots & \ddots & \vdots \\ a_{r1} & a_{r2} & \dots & a_{rc} \end{bmatrix}$$

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

$$A = [a_1 : a_2 : \dots : a_c]$$

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

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

```
      [,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
```

```
      [,1] [,2] [,3]
[1,]    1    3    2
[2,]    2    8    9
```

3.2 Multiplying a matrix with a number

For a number α and a matrix A , the product αA is the matrix obtained by multiplying each element in A by α .

Example 4

$$7 \begin{bmatrix} 1 & 2 \\ 3 & 8 \\ 2 & 9 \end{bmatrix} = \begin{bmatrix} 7 & 14 \\ 21 & 56 \\ 14 & 63 \end{bmatrix}$$

□

```
> 7 * 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 “ \top ”.

Example 5

$$\begin{bmatrix} 1 & 2 \\ 3 & 8 \\ 2 & 9 \end{bmatrix}^\top = \begin{bmatrix} 1 & 3 & 2 \\ 2 & 8 & 9 \end{bmatrix}$$

□

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

$$\begin{bmatrix} 1 & 2 \\ 3 & 8 \\ 2 & 9 \end{bmatrix} + \begin{bmatrix} 5 & 4 \\ 8 & 2 \\ 3 & 7 \end{bmatrix} = \begin{bmatrix} 6 & 6 \\ 11 & 10 \\ 5 & 16 \end{bmatrix}$$

□

```
> B <- matrix(c(5, 8, 3, 4, 2, 7), ncol=3, byrow=T)
> A + B
```

```
      [,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 Ab is the $r \times 1$ matrix

$$Ab = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1c} \\ a_{21} & a_{22} & \dots & a_{2c} \\ \vdots & \vdots & \ddots & \vdots \\ a_{r1} & a_{r2} & \dots & a_{rc} \end{bmatrix} \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_c \end{bmatrix} = \begin{bmatrix} a_{11}b_1 + a_{12}b_2 + \dots + a_{1c}b_c \\ a_{21}b_1 + a_{22}b_2 + \dots + a_{2c}b_c \\ \vdots \\ a_{r1}b_1 + a_{r2}b_2 + \dots + a_{rc}b_c \end{bmatrix}$$

Example 7

$$\begin{bmatrix} 1 & 2 \\ 3 & 8 \\ 2 & 9 \end{bmatrix} \begin{bmatrix} 5 \\ 8 \end{bmatrix} = \begin{bmatrix} 1 \cdot 5 + 2 \cdot 8 \\ 3 \cdot 5 + 8 \cdot 8 \\ 2 \cdot 5 + 9 \cdot 8 \end{bmatrix} = \begin{bmatrix} 21 \\ 79 \\ 82 \end{bmatrix}$$

□

> A %% a

```

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

```

Note the difference to

> A * a

```

      [,1] [,2] [,3]
[1,]    1    4   24
[2,]    9    2   18

```

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. $B = [b_1 : b_2 : \dots : b_t]$. The product AB is the $r \times t$ matrix given by:

$$AB = A[b_1 : b_2 : \dots : b_t] = [Ab_1 : Ab_2 : \dots : Ab_t]$$

Example 8

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

□

Note that the product AB 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 AB and BA are not identical.

A [mnemonic for matrix multiplication](#) is :

$$\begin{bmatrix} 1 & 2 \\ 3 & 8 \\ 2 & 9 \end{bmatrix} \begin{bmatrix} 5 & 4 \\ 8 & 2 \end{bmatrix} = \begin{array}{cc|cc} & & 5 & 4 \\ & & 8 & 2 \\ \hline 1 & 2 & 1 \cdot 5 + 2 \cdot 8 & 1 \cdot 4 + 2 \cdot 2 \\ 3 & 8 & 3 \cdot 5 + 8 \cdot 8 & 3 \cdot 4 + 8 \cdot 2 \\ 2 & 9 & 2 \cdot 5 + 9 \cdot 8 & 2 \cdot 4 + 9 \cdot 2 \end{array} = \begin{bmatrix} 21 & 8 \\ 79 & 28 \\ 82 & 26 \end{bmatrix}$$

```

> A <- matrix(c(1, 3, 2, 2, 8, 9), ncol=2)
> B <- matrix(c(5, 8, 4, 2), ncol=2)
> A %*% B

```

```

      [,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 $A = A^T$.
- A matrix with 0 on all entries is the [0-matrix](#) and is often written simply as 0.
- A matrix consisting of 1s in all entries is often written J .
- A square matrix with 0 on all off-diagonal entries and elements d_1, d_2, \dots, d_n on the diagonal a [diagonal matrix](#) and is often written $diag\{d_1, d_2, \dots, d_n\}$
- A diagonal matrix with 1s on the diagonal is called the [identity matrix](#) and is denoted I . The identity matrix satisfies that $IA = AI = A$. Likewise, if x is a vector then $Ix = x$.

- 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(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] 1 2 3
```

```
> diag(A)
```

```
[1] 1 8
```

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,

$$AB = BA = I.$$

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

Example 9 Let

$$A = \begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} \quad B = \begin{bmatrix} -2 & 1.5 \\ 1 & -0.5 \end{bmatrix}$$

Now $AB = BA = I$ so $B = A^{-1}$. □

Example 10 If A is a 1×1 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
```

```

      [,1] [,2]
[1,]  -2  1.5
[2,]   1 -0.5

```

```
> A %% B
```

```

      [,1] [,2]
[1,]   1   0
[2,]   0   1

```

3.10 Solving systems of linear equations

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

$$\begin{aligned} x_1 + 3x_2 &= 7 \\ 2x_1 + 4x_2 &= 10 \end{aligned}$$

The system can be written in matrix form

$$\begin{bmatrix} 1 & 3 \\ 2 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 7 \\ 10 \end{bmatrix} \text{ i.e. } Ax = b$$

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

$$x = A^{-1}b = \begin{bmatrix} -2 & 1.5 \\ 1 & -0.5 \end{bmatrix} \begin{bmatrix} 7 \\ 10 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$

A geometrical approach to solving these equations is as follows: Isolate x_2 in the equations:

$$x_2 = \frac{7}{3} - \frac{1}{3}x_1 \quad x_2 = \frac{1}{4} \cdot 10 - \frac{2}{4}x_1$$

These two lines are shown in Figure 5 from which it can be seen that the solution is $x_1 = 1, x_2 = 2$.

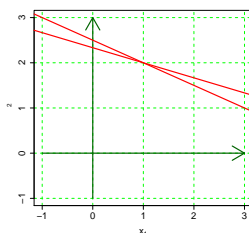


Figure 5: Solving two equations with two unknowns.

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.

□

```
> A <- matrix(c(1, 2, 3, 4), ncol=2)
> b <- c(7, 10)
> x <- solve(A) %*% b
> x
```

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

3.11 Some additional rules for matrix operations

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

$$\begin{aligned}(A + B)^\top &= A^\top + B^\top \\ (AB)^\top &= B^\top A^\top \\ A(B + C) &= AB + AC \\ AB = AC &\not\Rightarrow B = C\end{aligned}$$

In general $AB \neq BA$

$$AI = IA = A$$

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

3.12 Details on inverse matrices*

3.12.1 Inverse of a 2×2 matrix*

It is easy find the inverse for a 2×2 matrix. When

$$A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

then the inverse is

$$A^{-1} = \frac{1}{ad - bc} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

under the assumption that $ad - bc \neq 0$. The number $ad - bc$ is called the determinant of A , sometimes written $|A|$ or $\det(A)$. 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

$$A = \text{diag}(a_1, a_2, \dots, a_n)$$

where all $a_i \neq 0$. Then the inverse is

$$A^{-1} = \text{diag}\left(\frac{1}{a_1}, \frac{1}{a_2}, \dots, \frac{1}{a_n}\right)$$

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

$$AGA = A.$$

For many practical problems it suffice to find a generalized inverse.

```
> A <- matrix(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
```

```
> det(A)
```

```
[1] 0
```

```
> G <- MASS::ginv(A)
> A %*% G      # Not identity
```

```
      [,1]      [,2]      [,3]
[1,] 0.8333333 0.3333333 -0.1666667
[2,] 0.3333333 0.3333333 0.3333333
[3,] -0.1666667 0.3333333 0.8333333
```

```
> A %*% G %*% A # 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 method 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 AB :

```
> AB <- cbind(A, diag(c(1, 1, 1)))
> AB
```

```
      [,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 AB in a way such that one ends up with a 3×6 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. $AB[1,]$ extracts the entire first row of AB .

- First, we make sure that $AB[1,1]=1$. Then we subtract a constant times the first row from the second to obtain that $AB[2,1]=0$, 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 $AB[2,2]=1$. Afterwards we subtract a constant times the second row from the third to obtain that $AB[3,2]=0$:

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

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

```
> 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

> AB[1,] <- AB[1,] - 1.5 * AB[2,]
> AB

      [,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 AB 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,]  1.000000e+00  3.330669e-16  1.110223e-16
[2,] -4.440892e-16  1.000000e+00  2.220446e-16
[3,] -2.220446e-16  9.992007e-16  1.000000e+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 (x_i, y_i) 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.

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

$$y_i = \beta_0 + \beta_1 x_i \text{ for } i = 1, \dots, 5$$

Writing this in matrix form gives

$$y = \begin{bmatrix} y_1 \\ y_2 \\ \dots \\ y_5 \end{bmatrix} \approx \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_5 \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \mathbf{X}\boldsymbol{\beta}$$

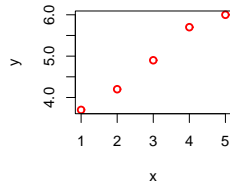


Figure 6: Regression

The first question is: Can we find a vector β 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

$$(X^T X)\beta = X^T y$$

If $(X^T X)$ is invertible, the (unique) solution is

$$\hat{\beta} = (X^T X)^{-1} X^T y$$

```
> y
[1] 3.7 4.2 4.9 5.7 6.0

> X

      x
[1,] 1 1
[2,] 1 2
[3,] 1 3
[4,] 1 4
[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] 3.68 4.29 4.90 5.51 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,] 1 4 5
[5,] 1 5 6
```

Then $(X_2^\top X_2)$ is not invertible. There are infinitely many solutions to the normal equations. One is:

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

```
      [,1]      [,2]      [,3]
[1,] 0.6333333 -0.4333333 0.2000000
[2,] -0.4333333 0.3000000 -0.1333333
[3,] 0.2000000 -0.1333333 0.0666667
```

```
> 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
```

```
> as.numeric(X2 %*% beta22.hat)
```

```
[1] 3.68 4.29 4.90 5.51 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: “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.