Chapter 2

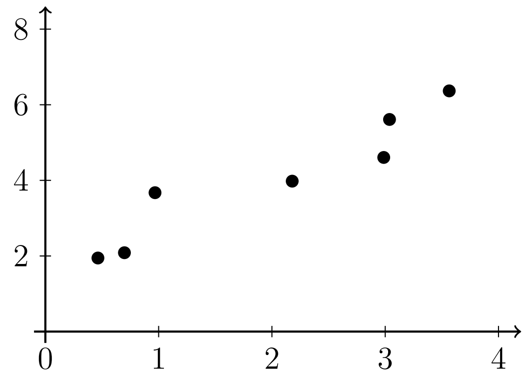
The method of least squares

2.1 Linear regression

We will start with a simple case: imagine you had a set of n data points, and wish to find a linear function that best approximates the data. For example, the data below has $n = 7$ data points.

i	1	2	3	4	5	6	7
x_i	0.464	0.698	0.968	2.179	2.987	3.038	3.565
y_i	1.946	2.086	3.674	3.979	4.606	5.611	6.367

These data points are plotted in the figure below.



To find a linear approximation to these points means to find coefficients b and c of the linear function

$$f(x) = bx + c.$$

To find the best linear approximation requires a proper definition of *best approximation*. There are many different ways this can be done, but by far the most common is the method of least squares.

For the given function $f(x) = bx + c$, the **residual** r_i of the point (x_i, y_i) is the difference between the actual value y_i and the predicted value $f(x_i)$, so:

$$r_i = y_i - bx_i - c.$$

The residuals can be viewed as a description of the error of the approximation. This is the first step towards a description of an objective function: intuitively, we would like to minimise the total error; i.e., minimise the sum of residuals. However, it turns out to be more effective to take the sum of *squared* residuals as the objective function instead. There are rigorous justifications for this that we will not go into, but an informal justification is that squaring the residuals penalises large errors more than small errors. Thus, the **least squares method** is to minimise the objective function

$$F(b, c) = \sum_{i=1}^{n} r_i^2,$$

where $r_i = y_i - f(x_i)$. For the linear function $f(x) = bx + c$, this becomes

$$\text{minimise } F(b, c) = \sum_{i=1}^{n} (y_i - bx_i - c)^2.$$

Before we describe the general approach, let's investigate this problem in more detail for our sample data set. The proposed function is $f(x) = bx + c$, so the i-th residual is

$$r_i = y_i - f(x_i) = y_i - bx - c.$$

There is one for each data point, tabulated below.

x_i	y_i	r_i
0.464	1.946	$1.946 - 0.464b - c$
0.698	2.086	$2.086 - 0.698b - c$
0.968	3.674	$3.674 - 0.968b - c$
2.179	3.979	$3.979 - 2.179b - c$
2.987	4.606	$4.606 - 2.987b - c$
3.038	5.611	$5.611 - 3.038b - c$
3.565	6.367	$6.367 - 3.565b - c$

Squaring and summing these residuals yields what looks like a rather unweildy objective function F:

$$\begin{aligned} F(b,c) = {} & (1.946 - 0.464b - c)^2 + (2.086 - 0.698b - c)^2 \\ & + (3.674 - 0.968b - c)^2 + (3.979 - 2.179b - c)^2 \\ & + (4.606 - 2.987b - c)^2 + (5.611 - 3.038b - c)^2 \\ & + (6.367 - 3.565b - c)^2. \end{aligned}$$

Finding a minimiser of this function will give us the coefficients. The objective function simplifies to

$$F(b,c) = 7c^2 + 27.798bc - 56.538c + 37.248403b^2 - 136.17668b + 130.706275,$$

and using the FONC, we want to set the partial derivatives to zero. The partial derivatives are:

$$\begin{aligned} \frac{\partial F}{\partial b} &= 74.496806b + 27.798c - 136.16778, \\ \frac{\partial F}{\partial c} &= 14c + 27.798b - 56.538, \end{aligned}$$

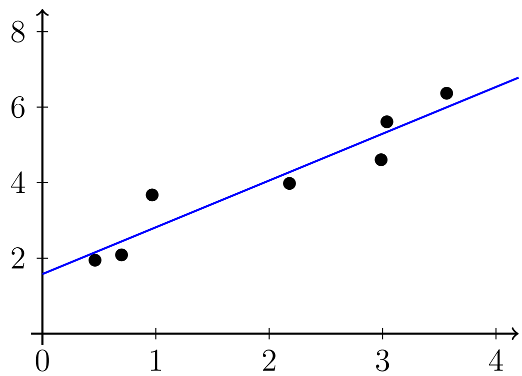
and setting these equal to zero results in the pair of linear equations,

$$\begin{aligned} 74.496806b + 27.798c &= 136.16778, \\ 14c + 27.798b &= 56.538. \end{aligned}$$

Finally, solving these simultaneous equations for b and c gives $b \approx 1.239$ and $c \approx 1.579$. Hence, the best approximation we find is (approximately)

$$f(x) = 1.239x + 1.579,$$

which is plotted below.



In this case, the specific example hides the elegance of the underlying solution. So let's now treat this in more generality. Suppose we have a data set with n entries of the form

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n),$$

and we aim to use the method of least squares to find a linear approximation to the data,

$$f(x) = bx + c.$$

The i-th residual is given by

$$r_i = y_i - f(x_i) = y_i - bx_i - c,$$

and then squaring it gives

$$r_i^2 = (y_i - bx_i - c)^2.$$

The partial derivatives of r_i^2 (with respect to b and c) are

$$\frac{\partial}{\partial b}\left(r_i^2\right) = -2x_i(y_i - bx_i - c),$$
$$\frac{\partial}{\partial c}\left(r_i^2\right) = -2(y_i - bx_i - c),$$

and so we have

$$F(b,c) = \sum_{i=1}^{n} r_i^2 = \sum_{i=1}^{n}(y_i - bx_i - c)^2,$$
$$\frac{\partial F}{\partial b} = \sum_{i=1}^{n}\left(-2x_i(y_i - bx_i - c)\right),$$
$$\frac{\partial F}{\partial c} = \sum_{i=1}^{n}\left(-2(y_i - bx_i - c)\right).$$

By making $\frac{\partial F}{\partial c}$ equal zero, we get:

$$\begin{aligned}\sum_{i=1}^{n} -2\left(y_i - bx_i - c\right) = 0 &\iff \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} c - \sum_{i=1}^{n} bx_i = 0\\ &\iff \sum_{i=1}^{n} y_i - nc - b\sum_{i=1}^{n} x_i = 0\\ &\iff nc + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i.\end{aligned}$$

Similarly, by making $\frac{\partial F}{\partial b}$ equal zero, we get:

$$\begin{aligned}\sum_{i=1}^{n}(-2x_i(y_i - bx_i - c) = 0 &\iff -2\sum_{i=1}^{n}(x_iy_i - x_ic - bx_i^2) = 0\\ &\iff \sum_{i=1}^{n} x_iy_i - c\sum_{i=1}^{n} x_i - b\sum_{i=1}^{n} x_i^2 = 0\\ &\iff c\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_iy_i.\end{aligned}$$

This results in two equations, linear in b and c, which can be solved to find the coefficients:

$$nc + b\sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i,$$
$$c\sum_{i=1}^{n} x_i + b\sum_{i=1}^{n} x_i^2 = \sum_{i=1}^{n} x_iy_i.$$

These equations are called the **normal equations** for the model, and solving them gives the coefficients.

Example: finding the normal equations

We will re-use the data from the earlier, but this time apply the normal equations directly. The data is:

i	1	2	3	4	5	6	7
x_i	0.464	0.698	0.968	2.179	2.987	3.038	3.565
y_i	1.946	2.086	3.674	3.979	4.606	5.611	6.367

Since we have 7 data points, we have $n = 7$. The sum of x_i values is

$$\sum_{i=1}^{n} x_i = 0.464 + 0.698 + 0.968 + 2.179 + 2.987 + 3.038 + 3.565 = 13.899,$$

and the sum of y_i values is

$$\sum_{i=1}^{n} y_i = 1.946 + 2.086 + 3.674 + 3.979 + 4.606 + 5.611 + 6.367 = 28.269.$$

So the first normal equation becomes

$$7c + 13.899b = 28.269.$$

For the second normal equation, we need the sum of squared x_i values:

$$\sum_{i=1}^{n} x_i^2 = 0.464^2 + 0.698^2 + 0.968^2 + 2.179^2 + 2.987^2 + 3.038^2 + 3.565^2 = 37.248403.$$

and the sum of the product of each x_i and y_i value:

$$\begin{aligned}\sum_{i=1}^{n} x_i y_i &= 0.464 \times 1.946 + 0.698 \times 2.086 + 0.968 \times 3.674 + 2.179 \times 3.979 \\ &\quad + 2.987 \times 4.606 + 3.038 \times 5.611 + 3.565 \times 6.367 \\ &= 68.08834.\end{aligned}$$

So the second normal equation becomes

$$13.899c + 37.24803b = 68.08834.$$

So to find the coefficients b and c, we need to solve the system of equations

$$\begin{aligned} 13.899b + 7c &= 28.269, \\ 37.24803b + 13.899c &= 68.08834. \end{aligned}$$

Observe that multiplying both sides of these equations by 2 results in the same equations found earlier.

Here, we have only considered data of the form (x_i, y_i). It is also possible to consider higher dimensional data; i.e., find coefficients $a_0, a_1, \ldots, a_m$ to fit a function of the form

$$f(x_1, x_2, \ldots, x_m) = a_0 + a_1x_1 + a_2x_2 + \ldots a_mx_m.$$

Normal equations can be found in a similar manner as above, but there will be more equations and more variables in the resulting system of linear equations. In the next section, we will see how systems of linear equations are best expressed and solved using matrix methods.

2.2 Systems of linear equations

In the last example of the previous section, we arrived at the following pair of linear equations:

$$13.899b + 7c = 28.269,$$
$$37.24803b + 13.899c = 68.08834.$$

Let's consider an alternative representation. Define the following matrices:

$$\mathbf{A} = \begin{pmatrix} 13.899 & 7 \\ 37.24803 & 13.899 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} b \\ c \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 28.269 \\ 68.08834 \end{pmatrix}. \tag{2.1}$$

Performing the matrix product $\mathbf{Ax}$ gives:

$$\mathbf{Ax} = \begin{pmatrix} 13.899 & 7 \\ 37.24803 & 13.899 \end{pmatrix} \begin{pmatrix} b \\ c \end{pmatrix} = \begin{pmatrix} 13.899b + 7c \\ 37.24803 + 13.899 \end{pmatrix}.$$

By demanding that $\mathbf{Ax} = \mathbf{B}$, we have the matrix equation

$$\begin{pmatrix} 13.899b + 7c \\ 37.24803b + 13.899c \end{pmatrix} = \begin{pmatrix} 28.269 \\ 68.08834 \end{pmatrix},$$

which is exactly the same pair of equations that we began with.

This matrix representation allows us to employ matrix methods to solve linear equations.

Background: matrix determinants and inverses

The $n \times n$ **identity matrix** is denoted by I_n, so

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad I_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad I_4 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \text{etc.}$$

Let $\mathbf{A}$ be an $n \times n$ matrix. The **determinant** of $\mathbf{A}$ is defined recursively. The determinant of a 1×1 matrix is the value of the one entry in that matrix. Otherwise, let $\mathbf{A}_{ij}$ denote the determinant of the $(n-1) \times (n-1)$ matrix obtained by deleting row i and column j from $\mathbf{A}$. Then, the determinant can be determined by an expansion on any row i,

$$\det(\mathbf{A}) = \sum_{j=1}^{n} (-1)^{i+j} a_{ij} \mathbf{A}_{ij},$$

or by an expansion on any column j,

$$\det(\mathbf{A}) = \sum_{i=1}^{n} (-1)^{i+j} a_{ij} \mathbf{A}_{ij}.$$

In particular, if $\mathbf{A}$ is 2×2, so that

$$\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix},$$

then $\det(\mathbf{A}) = ad - bc$. Some properties of determinants:

- $\det(I_n) = 1$.

- $\det(\mathbf{A}^T) = \det(\mathbf{A})$.
- For compatible matrices $\mathbf{A}$ and $\mathbf{B}$, $\det(\mathbf{AB}) = \det(\mathbf{A})\det(\mathbf{B})$.

The determinant of $\mathbf{A}$ is sometimes also denoted by $|\mathbf{A}|$. We say that $\mathbf{A}$ is **singular** if $\det(\mathbf{A}) = 0$ and **nonsingular** otherwise.

The matrix $\mathbf{A}$ is **invertible** if there is another matrix, denoted by $\mathbf{A}^{-1}$ and called the **inverse** of $\mathbf{A}$, such that $\mathbf{A}\mathbf{A}^{-1} = \mathbf{A}^{-1}\mathbf{A} = I_n$. The invertibility of a matrix can be deduced from its determinant: a matrix is invertible if and only if it is nonsingular.

In particular, if $\mathbf{A}$ is a 2 by 2 invertible matrix,

$$\mathbf{A} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad ad - bc \neq 0,$$

then its inverse is given by

$$\mathbf{A}^{-1} = \frac{1}{\det(\mathbf{A})}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}.$$

Some properties of inverses:

- $I_n^{-1} = I_n$.
- If $\mathbf{A}$ is invertible, then $\det(\mathbf{A}^{-1}) = \frac{1}{\det(\mathbf{A})}$.
- If $\mathbf{A}$ and $\mathbf{B}$ are invertible, then $\mathbf{AB}$ is invertible, with inverse $\mathbf{B}^{-1}\mathbf{A}^{-1}$.

As long as the matrix $\mathbf{A}$ is invertible, we can solve $\mathbf{Ax} = \mathbf{B}$ as follows:

$$\mathbf{Ax} = \mathbf{B} \implies \mathbf{x} = \mathbf{A}^{-1}\mathbf{B}.$$

For instance, using the matrices (2.1), we have:

$$\det(\mathbf{A}) = 13.899 \cdot 13.899 - 7 \cdot 37.24803 = -67.554009 \neq 0,$$

so

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{B} = \frac{1}{-67.554009}\begin{pmatrix} 13.899 & -7 \\ -37.24803 & 13.899 \end{pmatrix}\begin{pmatrix} 28.269 \\ 68.08834 \end{pmatrix} \approx \begin{pmatrix} 1.239 \\ 1.578 \end{pmatrix},$$

which is the desired solution.

In general, the normal equations of Section 2.1 can be reformulated using matrices. Suppose we have a data set with n entries of the form

$$(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n),$$

and we wish to fit the data to a linear function $f(x) = bx + c$. Define the following matrices:

$$\mathbf{A} = \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}, \quad \mathbf{a} = \begin{pmatrix} b \\ c \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}.$$

We can then write the normal equations as

$$\mathbf{A}^T\mathbf{A}\mathbf{a} = \mathbf{A}^T\mathbf{y}.$$

Thus, assuming $\mathbf{A}^T\mathbf{A}$ is invertible, the coefficient vector $\mathbf{a}$ can be found using a single matrix product:

$$\mathbf{a} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}.$$

Example: linear regression using matrices

We wish to fit the linear function $f(x) = bx + c$ to the data below:

i	1	2	3	4	5	6	7
x_i	0.464	0.698	0.968	2.179	2.987	3.038	3.565
y_i	1.946	2.086	3.674	3.979	4.606	5.611	6.367

The required matrices are

$$\mathbf{A} = \begin{pmatrix} 1 & 0.464 \\ 1 & 0.698 \\ 1 & 0.968 \\ 1 & 2.179 \\ 1 & 2.987 \\ 1 & 3.038 \\ 1 & 3.565 \end{pmatrix}, \quad \mathbf{a} = \begin{pmatrix} b \\ c \end{pmatrix}, \quad \mathbf{y} = \begin{pmatrix} 1.946 \\ 2.086 \\ 3.674 \\ 3.979 \\ 4.606 \\ 5.611 \\ 6.367 \end{pmatrix}.$$

We use the following MATLAB code to construct the required matrices:

```
% Store x and y as column matrices
x = [0.464 0.698 0.968 2.179 2.987 3.038 3.565]';
y = [1.946 2.086 3.674 3.979 4.606 5.611 6.367]';
% Initialise the matrix A (as a list of columns)
A = [ones([7,1]) x];
```

The term $\mathbf{A}^T\mathbf{A}$ in left-hand side of the matrix equation $\mathbf{A}^T\mathbf{A}\mathbf{a} = \mathbf{A}^T\mathbf{y}$ can be computed using the following MATLAB code, which results in the matrix $\mathbf{A}$ as written in (2.1):

```
A'*A
```

Likewise, the matrix $\mathbf{B}$ as written in (2.1) is obtained using:

```
A'*y
```

The following MATLAB code will find the coefficient vector $\mathbf{a} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\mathbf{y}$:

```
a = inv(A'*A)*A'*y
```

To four decimal places, this gives

$$\mathbf{a} = \begin{pmatrix} 1.5782 \\ 1.2391 \end{pmatrix}.$$

More generally, a **system of linear equations** with n variables and m equations is a system of equations of the form

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n &= b_2 \\ \vdots \qquad\quad \vdots \qquad\qquad &\quad \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \ldots + a_{mn}x_n &= b_m, \end{aligned}$$

where $x_1, x_2, \ldots, x_n$ are the variables, each a_{ij} is a coefficient, and $b_1, b_2, \ldots, b_m$ are the constant terms.

This can then be represented using the matrix equation

$$\mathbf{A}\mathbf{x} = \mathbf{B},$$

where

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_m \end{pmatrix}.$$

The matrix $\mathbf{A}$ is called the **coefficient matrix**, the matrix $\mathbf{x}$ is the column vector of variables, and the matrix $\mathbf{B}$ is the column matrix of constant terms.

Example: a system of linear equations

Consider the following system of linear equations:

$$\begin{aligned} -3x + 7y - 8z + 4w &= 0, \\ x - 2y - 2z + w &= -5, \\ 5x + 5z + 2w &= 3. \end{aligned}$$

We can represent this in matrix form $\mathbf{Ax} = \mathbf{B}$, where

$$\mathbf{A} = \begin{pmatrix} -3 & 7 & -8 & 4 \\ 1 & -2 & -2 & 1 \\ 5 & 0 & 5 & 2 \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x \\ y \\ z \\ w \end{pmatrix}, \quad \mathbf{B} = \begin{pmatrix} 0 \\ -5 \\ 3 \end{pmatrix}.$$

Henceforth, we will describe systems of linear equations using the matrix form,

$$\mathbf{Ax} = \mathbf{B}.$$

If the matrix $\mathbf{A}$ is invertible, then the solution can be obtained immediately using

$$\mathbf{x} = \mathbf{A}^{-1}\mathbf{B}.$$

This is not always possible (e.g., if the matrix $\mathbf{A}$ is not square).

Given a system of linear equations $\mathbf{Ax} = \mathbf{B}$, the **augmented matrix** for the system is the matrix obtained by appending the columns of $\mathbf{B}$ to the columns of $\mathbf{A}$, separated by a vertical line and denoted by $\big(\mathbf{A} \mid \mathbf{B}\big)$.

Example: augmented matrices

The augmented matrix for the previous example is

$$\left(\begin{array}{cccc|c} -3 & 7 & -8 & 4 & -3 \\ 1 & -2 & -2 & 1 & -5 \\ 5 & 0 & 5 & 2 & 3 \end{array}\right).$$

The goal of the rest of this section is to see how to transform an augmented matrix into a simplified form that allows us to read any solutions directly from the matrix. A *non-augmented* matrix is in **reduced row-echelon** form if all of the following are satisfied:

- any row consisting of only zeros is at the bottom of the matrix,
- the leftmost non-zero entry (called a **row leader**) in each non-zero row is 1,
- each row leader appears to the right of any row leader in a row above it,

- every column containing a row leader otherwise contains only zeros.

An augmented matrix $(\mathbf{A} \mid \mathbf{B})$ is in reduced row-echelon form if the coefficient part $\mathbf{A}$ is in reduced row-echelon form.

Example: reduced row-echelon form

The following three augmented matrices are in reduced row-echelon form:

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 5 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 \end{array}\right), \quad \left(\begin{array}{cccc|c} 0 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right), \quad \left(\begin{array}{ccc|c} 1 & 0 & 0 & 100 \\ 0 & 1 & 0 & -100 \\ 0 & 0 & 1 & 0.95 \end{array}\right).$$

The following three augmented matrices are not in reduced row-echelon form:

$$\left(\begin{array}{cc|c} 3 & 0 & 5 \\ 0 & 1 & 0 \end{array}\right), \quad \left(\begin{array}{cccc|c} 1 & 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 1 & 3 \end{array}\right), \quad \left(\begin{array}{ccc|c} 0 & 1 & 0 & -100 \\ 1 & 0 & 0 & 100 \\ 0 & 0 & 1 & 0.95 \end{array}\right).$$

In the first case, the row leader of the first row is 3 instead of 1. In the second case, the row leader of the second row is correctly 1, but it has a non-zero entry above it. In the third case, the row leader of the second row is *not* to the right of the row leader in the first row.

For an augmented matrix $(\mathbf{A} \mid \mathbf{B})$ in reduced row-echelon form, the solutions can be read from the matrix by reinterpreting the augmented matrix as a matrix equation $\mathbf{A}\mathbf{x} = \mathbf{B}$. In more detail:

- Each variable in the system is associated to a column of the coefficient part of the augmented matrix.
- If a column has a row leader, then the variable associated to that column is called a **leading variable**.
- The non-leading variables will be parameters of the solution set.
- Express each of the leading variables in terms of the non-leading variables.

There are three possible outcomes:

- There may be no solutions, which occurs only if one of the rows takes the form

$$\begin{array}{cccc|c} 0 & 0 & \cdots & 0 & c \end{array},$$

  for some non-zero number c.
- There may be a unique solution, which occurs only if all variables are leading variables.
- There may be infinitely many solutions, which occurs only if some variables are non-leading variables.

Example: reading the solutions

The following system has no solutions:

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 5 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 3 \end{array}\right).$$

This is because the last row asserts that $0 = 3$.

Now consider the following matrix:

$$\left(\begin{array}{cccc|c} 0 & 1 & 2 & 0 & 0 \\ 0 & 0 & 0 & 1 & 3 \end{array}\right).$$

The leading variables are x_2 and x_4, so x_1 and x_3 are parameters. Thus there are infinitely many solutions, which we express parametrically. The first row gives

$$x_2 + 2x_3 = 0 \iff x_2 = -2x_3,$$

and the second row gives $x_4 = 3$. Thus the solution set (a subset of $\mathbb{R}^4$) is

$$\{(x_1, -2x_3, x_3, 3) \mid x_1, x_3 \in \mathbb{R}\}$$

Finally, consider the following matrix:

$$\left(\begin{array}{ccc|c} 1 & 0 & 0 & 100 \\ 0 & 1 & 0 & -100 \\ 0 & 0 & 1 & 0.95 \end{array}\right).$$

The first row asserts $x_1 = 100$, the second row asserts $x_2 = -100$, and the third row asserts $x_3 = 0.95$. So there is exactly one solution, and the solution set is $\{(100, -100, 0.95)\}$.

To any matrix (augmented or not), we can apply the following **row operations**:

- interchange two rows,
- multiply a row by a non-zero constant,
- leave one row unchanged while adding multiples of it to one or more other rows.

The important property of these row operations is that, when applied to an augmented matrix, the solutions to the corresponding system of linear equations stay the same.

Applying row operations to an augmented matrix until it is in reduced row-echelon form is called **Gaussian elimination**. From that point, any solutions to the corresponding system of linear equations can be read immediately from the matrix. The typical strategy for performing Gaussian elimination is to identify an element to *pivot* on, which means to turn a row leader into a 1, and then use that 1 to clear out the column it is in.

Example: applying Gaussian elimination

To solve the following system of linear equations,

$$\begin{aligned} -2x + 3y - z &= 8, \\ 4x + 2y + 4z &= 12, \\ 6x - 2y + 4z &= -1, \end{aligned}$$

we start with the augmented matrix

$$\left(\begin{array}{ccc|c} -2 & 3 & -1 & 8 \\ 4 & 2 & 4 & 12 \\ 6 & -2 & 4 & -1 \end{array}\right).$$

Note that we depict the row operations that we apply at each step to the right of each matrix.

We start by pivoting on row 1, column 1. This entails dividing the first row by -2 (to turn the (1,1)-entry into a row leader), and then add multiples of row 1 to the other rows to clear column 1.

$$\begin{aligned}
&\left(\begin{array}{ccc|c} -2 & 3 & -1 & 8 \\ 4 & 2 & 4 & 12 \\ 6 & -2 & 4 & -1 \end{array}\right) \\
\equiv &\left(\begin{array}{ccc|c} 1 & -3/2 & 1/2 & -4 \\ 4 & 2 & 4 & 12 \\ 6 & -2 & 4 & -1 \end{array}\right) \quad R_1' = -\tfrac{1}{2}R_1 \\
\equiv &\left(\begin{array}{ccc|c} 1 & -3/2 & 1/2 & -4 \\ 0 & 8 & 2 & 28 \\ 0 & 7 & 1 & 23 \end{array}\right) \quad \begin{array}{l} R_2' = R_2 - 4R_1 \\ R_3' = R_3 - 6R_1 \end{array}
\end{aligned}$$

Next, we pivot on row 2, column 2. First, we divide by 8 to turn the entry into a row leader, and then use the row leader to clear out its column.

$$\begin{aligned}
&\left(\begin{array}{ccc|c} 1 & -3/2 & 1/2 & -4 \\ 0 & 1 & 1/4 & 7/2 \\ 0 & 7 & 1 & 23 \end{array}\right) \quad R_2' = \tfrac{1}{8}R_2 \\
\equiv &\left(\begin{array}{ccc|c} 1 & 0 & 7/8 & 5/4 \\ 0 & 1 & 1/4 & 7/2 \\ 0 & 0 & -3/4 & -3/2 \end{array}\right) \quad \begin{array}{l} R_1' = R_1 + \tfrac{3}{2}R_2 \\ \\ R_3' = R_3 - 7R_2 \end{array}
\end{aligned}$$

Finally, we pivot on row 3, column 3. First, we divide by $-\frac{3}{4}$ to turn the entry into a row leader, and then use the row leader to clear out its column.

$$\begin{aligned}
&\left(\begin{array}{ccc|c} 1 & 0 & 7/8 & 5/4 \\ 0 & 1 & 1/4 & 7/2 \\ 0 & 0 & 1 & 2 \end{array}\right) \quad R_3' = -\tfrac{4}{3}R_3 \\
\equiv &\left(\begin{array}{ccc|c} 1 & 0 & 0 & -1/2 \\ 0 & 1 & 0 & 3 \\ 0 & 0 & 1 & 2 \end{array}\right) \quad \begin{array}{l} R_1' = R_1 - \tfrac{7}{8}R_3 \\ R_2' = R_2 - \tfrac{1}{4}R_3 \end{array}
\end{aligned}$$

The matrix is now in reduced row-echelon form, so we can read the solution from the matrix:

$$(x, y, z) = (-\tfrac{1}{2}, 3, 2).$$

In Chapter 4, we will employ an algorithm that is very similar to Gaussian elimination when we study linear programming.