## STAT0023 Workshop 3: simple programming in R

In this workshop you'll start writing your own scripts to produce some simple functions. You will need the slides / handouts from the lecture which explain the key concepts: these can be downloaded from the STAT0023 Moodle page, under the 'Course overview and useful materials' tab.

## 1 Setting up

For this workshop, in addition to the lecture slides / handouts you will need the following, all of which can be downloaded from the 'Week 3' tab of the Moodle page:

- These instructions.
- The R scripts ConvertTemp.r, MandelbrotFunctions.r and MandelbrotDemo.r. You should save these to the appropriate place on your N: drive, as you created it during Workshop S1 Relarible Edition of the Court for Workshop Tree Stary and remember to make sure that your web browser doesn't change the filenames when downloading them (Section 1.3 of the Workshop 1 notes).

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Having downloaded the files, start up RStudio and use the Session menu to set the working directory appropriately, as usual (refer to your notes from Workshop 1 if necessary).

# WeChat: cstutorcs 1.1 Defining and saving functions

In this workshop, you'll get some practice at writing R scripts and functions from scratch. To define a function in R, the following method is recommended:

- Use the <u>F</u>ile menu in RStudio to open a new R script (<u>F</u>ile  $\rightarrow$  New <u>F</u>ile  $\rightarrow$  <u>R</u> Script). You will get a blank pane in which to type your function.
- Save the file with a sensible name in your current working directory. For example, in the first exercise below you're asked to write a function called taylor.sin. You might choose to save the R script for this function in a file called TaylorSin.r.
- Click the button in RStudio, to run the script. If your script is correct, you won't see anything on screen but you will now be able to use your function. If it contains syntax errors, R will let you know! Sometimes however, the error messages are not directly related to the cause of the problem. At this stage, the cause is usually something like:
  - Mismatched brackets e.g. a missing opening or closing '(' or ')', or an opening '(' that gets closed with a ']', or something like that. If you have used curly brackets '{' and '}' to define blocks of code, make sure these are all balanced. Use the

<u>Code</u> menu in RStudio to help with this: in particular, if you highlight a sequence of lines and then choose the <u>Reindent Lines</u> or <u>Reformat Code</u> options, RStudio will try and arrange the code logically according to how you've *actually* defined it (rather than how you *think* you've defined it!). This can help you to spot where the problem lies, because the indentation will look wrong.

– Mismatched quotes "". The syntax highlighting in RStudio is helpful here: make sure that things that are supposed to be inside quotes (like file names) are in an appropriate colour and that this colour has not "escaped" to the rest of your code!

Be aware that the cause of the problem may be on an earlier line than the one where R starts complaining. Also, be aware that if can source your function definition without error, this does *not* mean that your function is correct: it merely means that there is nothing obviously wrong with the basic syntax of your function.

### 2 Power Series for the Sine Function

Let's start was signment h Projects Examble 1p

https://tutorcs.
$$\frac{x^3}{5}$$
. $\frac{x^5}{5}$ . $\frac{x^7}{5}$ . $\frac{x^7}{5}$ ...

In order to investigate the accuracy of this power series, create the following function (called taylor.sin) using the approach described in Section 1.1 above, and click the button to load it into R CSTULTORS

```
taylor.sin <- function(x) {
#
# Taylor approximation to sin(x)
#
    x - (x^3)/6 + (x^5)/120
}</pre>
```

This function computes the Taylor expansion up to the third term. Now you can use your function. Type the following commands at the Console prompt:

```
> taylor.sin(0)
> taylor.sin(pi/4)
> sin(pi/4)
> taylor.sin(pi/4)-sin(pi/4)
```

The last command is the error between the Taylor approximation and the accurate value for  $\sin(\pi/4)$ . So far the approximations are reasonable, but as the value of x gets larger, so the approximation gets worse . . .

```
> taylor.sin(pi/2)
> taylor.sin(pi)
> taylor.sin(2*pi)
```

Create a plot to compare the two functions:

```
> theta <- pi*(-200:200) / 150 # Fine grid of values from -4*pi/3 to 4*pi/3
> plot(theta, sin(theta), type="l", col="red") # Exact value
> lines(theta,taylor.sin(theta), col="blue", lty=2) # Approximation
```

Now change your function taylor.sin so that the expansion is calculated up to the fourth term. Repeat the above commands to see how much more accurate the method is.

#### 3 The '...' Argument

In the lectual she following function Project Exam Help

```
convert.temp <- function(degrees.F, plot.wanted=TRUE, ...) {</pre>
 degrees.C <- (degrees.F - 32) * 5/9
 if (plot.wanted nub ) Segree UI Octos COM
  degrees.C
}
```

Open the file ConvertTemp.r that you downloaded earlier, by clicking on it in the 'Files' tab of the lower right-hand pane in RStudio. This file contains the convert.temp function definition, together with some comments about its use and purpose: these comments follow the general layout of an R help page (you might not like this, but you're just going to have to get used to it!). Specifically, the comments tell you:

- What is the purpose of the function;
- What its arguments are, including what kinds of objects they are e.g. that degrees. F is a vector. This is not just fluffy waffle: it tells the user that if they want to use the function successfully, the input degrees. F must be a vector. Almost all of the help pages in the core R package will provide similar information: be aware, and use it! Unfortunately, the help pages for the add-on libraries (the ones that you access using the library() command) are of variable quality. You can't complain, though: you get more than you pay for.
- What is the 'value' of the function i.e. what kind of object dog would be if you typed dog <- convert.temp() with some appropriate arguments.

<sup>&</sup>lt;sup>1</sup>In R, to find out whether an object is a vector you can use the is.vector() function which returns either TRUE or FALSE.

• Any other side effects (in this case, the optional creation of a plot on the current graphics device).

Click the Source button to load this function into R. Then, at the Console prompt, create a vector of Fahrenheit temperatures

```
> fahrtemps <- c(0,20,32,61,70,80,90,100,110,212)
```

Now do the following:

- 1. Call the function convert.temp using these temperatures (i.e. convert.temp(fahrtemps))
- 2. Call the function again, this time with the additional argument type="b".
- 3. Add a title by calling the function with yet another additional argument main="Celsius against Fahrenheit".
- 4. One more time; call the function gain, but now so that the points and lines appear in real your hight want colors at like people for part here examples from previous workshops to find out how colours are specified).

Can you see how the arting://twtsacshyctopaful?

### 3.1 Adding more detail

You should have the convert.temp() function definition open in RStudio. This means that you can edit the function to 'improve' it. So: change the line

```
if (plot.wanted) plot(degrees.F, degrees.C, ...)

if (plot.wanted) {
  plot(degrees.F, degrees.C, ...)
  if (min(degrees.C) <= 0) {
    abline(h=0, col="blue")
    abline(v=32, col="blue")
  }
  if(max(degrees.C) >= 100){
    abline(h=100, col="red")
    abline(v=212, col="red")
  }
}
```

Reload the function into R (click the button ...) and call it again. Can you see what the function abline does and how the if statements work?

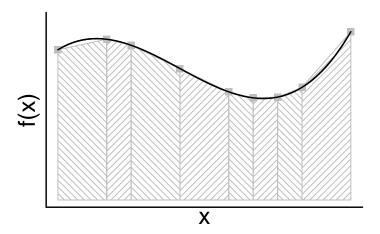


Figure 1: Illustration of the trapezium rule

## 4 Nu Assignment Project Exam Help

A common mathematical problem is to integrate a function f between two points i.e. to evaluate  $\int_a^b f(x)dx$  [TB] we using He Ope Surction its mathematical sense now, rather than the computational sense of the previous section). For many simple functions (e.g.  $f(x) = x^2 + 4$ ), humans can do this using rules learned in school or university, but these rules can't be implemented easily in most computing environments. Moreover, it is common to encounter functions that can't be integrated using standard rules (for example, if you want to find probabilities under the standard normal curve).

An alternative exploits the fact that an integral is just the area under a curve. This area can be calculated approximately by evaluating the function at values  $x_0, \ldots, x_n$  to to get  $f(x_0), f(x_2), \ldots f(x_n)$ , joining up the points with straight lines and calculating the areas of the resulting trapezia as illustrated in Figure 1. This leads to the *trapezium rule* to approximate the integral of f. For equally-spaced x-values, the trapezium rule is

$$\int_{x_0}^{x_n} f(x)dx \approx \frac{h}{2} \left[ f(x_0) + 2f(x_1) + \dots + 2f(x_{n-1}) + f(x_n) \right],$$

where

$$h = \frac{x_n - x_0}{n}.$$

**Exercise:** we will write an R function called trapezium, to approximate an integral using the trapezium rule with equally spaced x values. The R function will have three arguments, as follows:

 $v : a \text{ vector containing the values } v[1] = f(x_0), v[2] = f(x_1), \dots v[n+1] = f(x_n);$ 

a: the lower limit of integration  $a = x_0$ ;

b: the upper limit of integration  $b = x_n$ .

Use the following code as a template for your function, filling in the gaps where indicated:

We can check the method using a couple of examples for which the answer is known. For example, the value of  $\int_{1}^{10} 1 dx$  can be proximated using trapezium (rep(1,11),0,10) (there are 11 x values 0,1,2,...,10). How accurate is the answer? Can you explain this?

As another example, we can use the function to evaluate the integral  $\int_0^{\pi/2} \sin(x) dx$ . In the first instance, this can be done using trapezium( $\sin((0.6)*pi/12)$ , 0, pi/2) (the vector v contains function values from  $\sin(0)$  to  $\sin(\pi/2)$  and the integration limits are defined as a=0 and b=pi/2). Answer the following questions:

- 1. What value do why got for transezium (stu (10:6) rpic(12),0,pi/2)?
- 2. What is the exact answer for this integral? How big is the approximation error from the trapezium rule?
- 3. It should be clear from Figure 1 that the accuracy of the trapezium rule will improve as the number of evaluation points increases i.e. as n increases (although this comes with an increase in computational cost, obviously). The most human-friendly way of doing this is to change the argument sin((0:6)\*pi/12) in the call above to something like sin(seq(0,pi/2,length.out=10)) or sin(seq(0,pi/2,length.out=20)) or sin(seq(0,pi/2,length.out=50)). How fast does your approximation improve as you increase the number of evaluation points? By what fraction does the error decrease as you double the number of evaluation points? Will this increase in accuracy continue forever?

## WARNING!!!

You may be tempted to see what happens if you try a *very* large number of evaluation points, such as 1e9. DO NOT ATTEMPT THIS!!! The reason is that if you do, R will try to store the evaluation points in a vector containing 10<sup>9</sup> elements. Each element uses 8 bytes of the computer's memory, and the entire vector uses 8 gigabytes. Your computer probably doesn't have this much memory, and it will grind to a halt — possibly for more than an hour.

## 5 To loop or not to loop?

In the lecture, we discussed the fact that you should avoid loops in R where possible. This section demonstrates the problem.

#### 5.1 How not to calculate a sum

We'll start with a very simple example. Following the procedure described in Section 1.1, define a function called sillysum() as follows:

```
sillysum <- function(x) {
  z <- 0
  for (i in 1:x) z <- z+i
  z
}</pre>
```

Before you Anting: what do contain this function does an Help Check that silly sum (10) gives the same result as sum (1:10). Then check that silly sum (1e6) gives the same results as sum (as.numeric(1:1e6)) (the 'as.numeric()' is needed to stop R from trying to stope the numbers as integers; the largest integer it can store is  $2^{31} - 1$ ). Do you notice the difference in speed! You can quantify this:

```
> system.time(sillysum(1e6))
[output ...] WeChat: cstutorcs
> system.time(sum(as.numeric(1:1e6)))
[output ...]
```

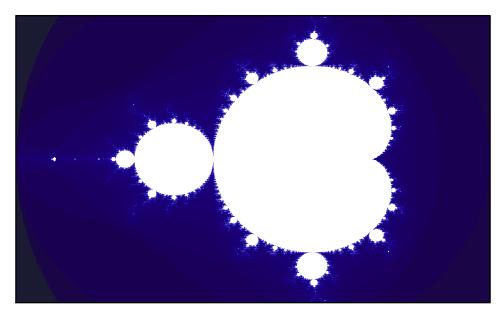
How much slower are the loops?

It doesn't hurt to repeat the warning from the previous section: do *not* be tempted to try even bigger numbers here, because of the memory required to store very large vectors.

### 5.2 A more challenging example: plotting a Mandelbrot set

The example in this section is considerably more advanced, but it demonstrates clearly the benefits of avoiding loops in R. It's mathematical rather than statistical: it involves the computation of the Mandelbrot set (Figure 2). This set is constructed using the function  $f(z) = z^2 + c$  where z and c are complex numbers. The function is iterated starting from  $z_0 = 0$  to give a sequence  $z_1 = f(z_0) = z_0^2 + c$ ,  $z_2 = f(z_1) = z_1^2 + c = (z_0^2 + c)^2 + c$ , and so on. The Mandelbrot set is defined as the set of values  $\{c\}$  for which this sequence remains bounded. Remarkably for such a simple concept, the set has an extremely complex structure — indeed, many of you have probably encountered it before as a well-known example of a fractal set (i.e. a set that has structure at all scales).

To draw the Mandelbrot set, the 'obvious' approach is to set up a fine grid of values  $\{c = c_x + ic_y\}$  in the complex plane and, for each pair  $(c_x, c_y)$ , to determine whether the sequence



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 $z_0, z_1, z_2, z_3, \ldots$  remains bounded./Then draw the grid, with each point  $(c_x, c_y)$  shaded black (say) if the sequence remains bounded and white otherwise.

This is easier said than done, however! One useful thing to know is that if there is some k with  $|z_k| \geq 2$  then the sequence definitely does not remain bounded. This means that if you start at  $z_0 = 0$  and an expected adjusted  $S_0$ , the sequence  $S_0$  particular value of c, and at some stage you produce a value with modulus greater than 2, then this value of c is not in the Mandelbrot set. In practice of course, the sequence is infinite so you can't calculate every element. An operational procedure, therefore, is to calculate a finite version of the sequence  $z_0, z_1, z_2, \ldots, z_K$  where K is some large number: if  $|z_K|$  is still less than 2 then your value of c may be in the Mandelbrot set, although you can't be sure. This is called the escape time algorithm.

When using the escape time algorithm, it is common to indicate not just whether or not a grid node is in the set, but instead to draw a 'map' of the first integer k for which  $|z_k| > 2$ . Thus, Figure 2 shows a part of the complex plane (the axes are omitted because they spoil the view!), with  $-2 \le c_x \le 1$  and  $-1 \le c_y \le 1$ . This part of the plane has been divided into a regular grid of dimensions  $1000 \times 1000$ , and for each grid node the escape time algorithm has been used with a maximum iteration number of K = 1000: at each grid node, the colour indicates the first value of k with  $|z_k| > 2$ . Dark blue and purple values indicate low values of k, with white indicating K = 1000 so that the corresponding points may be in the Mandelbrot set.

In the script MandelbrotFunctions.r that you downloaded earlier, there are two functions that implement the escape time algorithm. Open the script and look through the definition of the function Mandelbrot1(). This is a direct translation into R of the 'pseudo-code' given on the Wikipedia page at https://en.wikipedia.org/wiki/Mandelbrot\_set. You should

not attempt to understand all the details here! Notice the following, however:

• The function has several arguments: nx and ny to control the numbers of grid nodes in the x and y directions, xlim and ylim to set the overall ranges of values for the grid, max.iter to control the maximum number of iterations (i.e. the value of K in the algorithm description above), ColourScale so that the user can specify their own colours for the image. xlim and ylim have default values corresponding to the image shown in Figure 2; max.iter has a default value of 1000; and ColourScale has a default value of NULL: this is a special value, discussed further below. The '...' argument is also used, because this enables the user to define additional graphics parameters to the image() command later on.

By setting default values for most of the arguments, the function can be called very easily. Try it:

> Mandelbrot1(50,50)

NB do Sory Environment bers that be cre! Explain the interpret. If you do this, after a few seconds you should see a plot which is just about recognisable as a very coarse-resolution approximation to Figure 2: it's so coarse (50 grid nodes in each direction) that prices still see the pair exactor of the image.

- The NULL default value for ColourScale is used because the code to set up the default colour scale takes up a couple of lines, and it would be hard to read if if this code were included as part of the argument specification of stead, the function starts by testing whether ColourScale is NULL (i.e. the default value): if so, the built-in colour scale is explicitly computed, and otherwise the user-supplied value is used. This is a common way to set non-trivial default values (note that you shouldn't worry about the precise code used to set up the colour scale here it was produced by trial and error!).
- The main calculations are in a pair of *nested* for loops:

```
for (i in 1:nx) {
  for (j in 1:ny) {
    ...
}
```

The 'i' loop here deals with one row of the grid at a time; and, for each row, the 'j' loop moves along the columns. By doing this, we deal with each grid node in turn, which makes the calculations easy to think about.

• For each grid node, some relevant quantities are initialised (x < 0 and y < 0, corresponding to the real and imaginary parts of  $z_0$  in the algorithm as described above; and iter < 0 to initialise the iteration counter i.e. k in the algorithm description). Then a while loop is used:

```
while (x^2 + y^2 < 4 & iter < max.iter) { # NB escape clause!
   ...
   iter <- iter + 1
}</pre>
```

There are two conditions in the while() statement here: the first is  $x^2 + y^2 < 4$ , which corresponds to the condition  $|z_k| < 2$  in the escape time algorithm (x and y get continuously updated so that, at each iteration, they represent the real and imaginary parts of  $z_k$ ). The second condition is iter < max.iter: this will be TRUE unless the iteration count exceeds the maximum number of iterations allowed. The two conditions are linked by the '&' sign which means "and": the entire expression is TRUE only if both of the individual conditions are TRUE, and FALSE otherwise. The while loop will therefore continue until either  $|z_k| \geq 2$ , or the maximum number of iterations is reached (because the iteration count iter is incremented on each pass through the loop). The condition iter < max.iter is an 'escape clause' ensuring that the loop will always terminate and you don't get stuck on the infinite staircase (if you don't know about this staircase, see the lecture slides / handouts).

ASSIGNMENT Project Exam Help You shouldn't worry about anything else in the function: there are some tricks to get the colour scale to display sensibly, and to return the matrix result invisibly (you didn't really want to see a  $50 \times 10$  matrix on your screen when you typed Mandelbrot1(50,50), did you?); but these are not particularly happrent for this worldshop.

That seems all very well: but you may have noticed that it took a few seconds to run the Mandelbrot1(50,50) command and the results are nowhere near as impressive as Figure 2. To produce such a Mgr esolution for Figure 2 is  $1000 \times 1000$  rather than  $50 \times 50$ . Whatever you do, resist the temptation to deal with this by typing Mandelbrot1(1000,1000)! Think about it: a  $1000 \times 1000$  grid contains 400 times as many nodes as a  $50 \times 50$  grid, so you can expect the computations to take 400 times as long.<sup>2</sup> On my laptop, the  $50 \times 50$  computations take around 2.75 seconds: the  $1000 \times 1000$  computations might take about 18 minutes, therefore.

This is where function Mandelbrot2() comes in. It implements exactly the same algorithm as before, but this time there are no for loops: the entire grid is updated at each operation, simply by using R's facilities for componentwise multiplication of matrix elements (here representing grid nodes). The key to this is to create additional matrices for the quantities x and y, as well as for the co-ordinates of the grid nodes themselves; and, additionally, to keep track of which grid nodes have already 'escaped' from the region |z| < 2 on an earlier iteration. This 'tracking' is done by creating a matrix called NotDone, with elements that are TRUE for those grid nodes that have not yet escaped and FALSE otherwise. Then, at each iteration, the calculations are only performed on the subset of grid nodes for which NotDone is TRUE (as always, using the [] construction to select the required subset): this ensures that we don't waste computer time doing calculations for nodes that have already escaped and therefore don't need to be considered further. This technique (the use of a logical matrix to restrict the set of elements considered in a calculation) is sometimes called masking.

<sup>&</sup>lt;sup>2</sup>This isn't *quite* correct, because the computations for some grid nodes are quicker than others — but it's roughly right.

Don't worry if you don't understand all of this: it is quite advanced programming, and you aren't expected to get to that level in STAT0023! What you *are* expected to do, however, is to appreciate the benefits of avoiding loops. Try it:

#### > Mandelbrot2(50,50)

Do you notice the difference in speed compared with Mandelbrot1? On my laptop, it runs more than 10 times faster; and it allows Figure 2 to be produced in under 90 seconds. If you want to relax a bit and entertain yourself, open the file MandelbrotDemo.r and run the last few lines:

These lines illustrate the following points:

- The inclusion of arguments such as xlab="" and ylab="" in the Mandelbrot2() command: these are interpreted as part of the ... argument, and hence passed through to the underlying image() call.
- The use of a for loop to generate a sequence of plots. In this kind of situation a for loop is permissible: recall from the lecture that the reason to avoid these loops is that it takes time for R to interpret each line of code before executing it. In this case however, the time taken to *interpret* the code is tiny by comparison with the time taken to *execute* it (because the execution involves a call to Mandelbrot2(), which takes a few seconds). Compare with the for loops in Mandelbrot1(), where each loop only involved a small amount of computation and the interpretation time was therefore substantial by comparison.
- The locator() function can be used to select co-ordinates of points on an R graphics device. As each plot is produced therefore, you will be prompted to click two points: these will be taken as the opposite corners of a rectangle, and the next plot will 'zoom in' on that rectangle. This illustrates the usefulness of the locator() function as a

way to help you interact with R graphics. There are, apparently, an infinite number of seahorses, nautiluses and other strange creatures hiding in the Mandelbrot set: see if you can find one!

• Functions provide an extremely powerful way to carry out complex tasks with a single command. Thus, to produce a plot for a different region of the complex plane, we don't have to type out all of the Mandelbrot2 code again: we simply call the command with different values of the xlim and ylim arguments.

## 6 Logical operations and comparison of objects

In the previous section we saw the use of the '&' symbol to test whether two logical conditions are both TRUE. This is an example of a *logical operator*, in the same way that +, -, \*, / and ^ are arithmetic operators. Like arithmetic operators, '&' can be used with vectors. For example:

```
> x <- 1: Assignment Project Exam Help

> y <- c(2,-1,1,4,3)

> (x > y) & (y > 0)

[1] FALSE FALSE TRUE FALSE / TRUE TOURS.com
```

The conditions are combined elementwise, as you might expect.

## 6.1 The main Wge Chat: Cstutorcs

You need to be familiar with the following logical operators:

- '&': x & y is TRUE if the corresponding elements of x and y are both TRUE, and FALSE otherwise.
- '|': x | y is TRUE if at least one of the corresponding elements of x and y is TRUE. Think of it as 'or': 'x or y is true'.
- '%in%': x %in% y returns, for each element of x, the value TRUE if that value appears in the object y and FALSE otherwise. For example (the LETTERS object was introduced in the lecture):

```
> x <- c("L","o","n","d","o","n")
> x %in% LETTERS
[1] TRUE FALSE FALSE FALSE FALSE FALSE
```

## 6.2 Further work with logical operations

You also need to be familiar with the following:

• The '!' ('not') symbol swaps round the TRUE and FALSE elements of an object:

```
> !(x %in% LETTERS)
[1] FALSE TRUE TRUE TRUE TRUE TRUE
```

• The any() and all() commands can be used to determine whether any, or all, of the elements of a logical object are TRUE.

```
> any(x %in% LETTERS)
[1] TRUE
> all(x %in% LETTERS)
[1] FALSE
```

These commands can be useful in if() and while() conditions (for example, the any(NotDone) condition in the Mandelbrot2 function).

Notice that the conditions in an if() or while() statement must evaluate to a *single* TRUE or FALSE value S It 2 in 10 to 10

```
Warning message: https://tutorcs.com

In if (your condition has length > 1 and only the first element will be used
```

## 6.3 Comparison & Chat: cstutorcs

When you're using if() or while() statements, or selecting subsets of an object using [] based on some condition, the condition itself often involves the comparison of vectors or matrices. The main comparison operators are:

'==': x==y is TRUE if the corresponding elements of x and y are equal, and FALSE otherwise. Note, however, that computers can't do calculations with 100% accuracy, and small rounding errors can lead to unexpected results. For example:

```
> sin(2*pi) == 0
[1] FALSE
> sin(2*pi)
[1] -2.449213e-16
```

To get round this problem, if you need to test for equality of objects that have been produced by some calculation process, it is usually safer to test whether the absolute difference between them is less than some small number.

'!=': x!=y is TRUE if the corresponding elements of x and y are different, and FALSE if they're the same. So, for example, if x and y are vectors of the same length then x!=y is an alternative way of writing !(x==y).

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'<', '>': x<y (resp. x>y) return TRUE for those elements of x that are less (resp. greater) than the corresponding elements of y, and FALSE otherwise. To test whether the absolute difference between x and y is less than some small number — say  $10^{-12}$  — therefore, you can use abs(x-y) < 1e-12.

'<=', '>=': as '<' and '>', but now representing 'less / greater than or equal to'. You saw some examples of their use in Section 3.1 above.

## 7 Moodle quiz

There is just one new Moodle quiz this week. If you have time left in the workshop, try it a few times.

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