

MAS212 Scientific Computing and Simulation

#1: Getting Started with Jupyter Notebook

<https://jupyter.org/about.html>

<http://sam-dolan.staff.shef.ac.uk/mas212>

1. Getting started. Start Jupyter (Start → Anaconda3 (64-bit) → Jupyter Notebook). A terminal window will appear; ignore this. A new tab should appear in a web browser, showing the directory structure. Create a new folder MAS212 under ManWin/Documents, in which to save your work. On the right-hand side, press the New button, and choose Python 3. When the notebook opens, click on Untitled (next to the jupyter logo), and change the notebook title to Lab_Class_1 or similar. Save via the menu: File → Save and Checkpoint.

- **Code cells.** Enter Python code in the first cell, e.g. `print("Hello")`. Press Shift-Enter to execute the code snippet. The output appears below. Add new cells from the menu: Insert → Insert Cell Below.
- **Cell types.** There are different types of cells: code, markdown, heading, etc. To toggle the cell type, use the drop-down box situated below the menu. Try the following:
 - Add some HTML to a markdown cell and press Shift-Enter e.g. `<h1>Heading!</h1>`.
 - Add some LaTeX to a markdown cell and press Shift-Enter e.g. `$ x = \frac{3}{4} $`
 - Add another code cell and calculate the first 10 square numbers using list comprehension, e.g. `[x**2 for x in range(1,11)]`
- **Keyboard shortcuts.** For a list see Help → Keyboard Shortcuts. Example: to insert a new cell, press Esc to go into command mode, and then press a or b (to insert cell above or below). To change the cell type press y (code) or m (markdown). You may wish to take the User Interface Tour.

2. Sample notebooks. Go to 'Notebooks' section of course homepage. Right-click on a .ipynb link in the right column, and download (Save Link As ...). Under Save as type, change from Text Document to All Files. Save the file in the directory Documents/MAS212. **N.B.** You cannot open the file by double-clicking. Instead open the notebook through the Jupyter

tab in the browser. Now, starting at the top, try executing the cells with **Shift-Enter**. Try editing the cells. Try improving any plots by (e.g.) adding titles and axis labels.

3. Mock class test. Go to ‘Class Tests’ section of course homepage. Right-click the `.ipynb` link next to (Mock) Class Test 1. Save in `My Documents/MAS212`. Open the notebook. Read the rubric. Try taking the class test, by adding a new cell below each question.

4. Revision of Python. There are lots of code snippets in these slides: https://sam-dolan.staff.shef.ac.uk/mas212/docs/python_basics.pdf Work through these slides, by entering the snippets in code cells, and executing with **Shift-Enter**. Add markdown cells (or Python comments) to explain what the code does.

Videos of the lecturer working through these slides can be found on MOLE (Week 0 folder).

5. Coding exercises.

(a) **Iteration.** Compute $\sqrt{2}$ using the recurrence relation

$$x \rightarrow \frac{1}{2}(x + 2/x)$$

starting from $x = 1$. Now use the `decimal` module to compute $\sqrt{2}$ to 100 decimal places (<https://docs.python.org/3.5/library/decimal.html>). How many iterations are needed?

(b) **Pisano periods.** Write a function to compute the Fibonacci sequence. Now modify the function to compute the Fibonacci sequence modulo N . For example, modulo $N = 4$ the sequence 0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, ... becomes 0, 1, 1, 2, 3, 1, 0, 1, 1, 2, 3, 1, ... Can you see a repeating sequence here? Write a function to compute the Pisano period $\pi(N)$: the length of the repeating sequence for a given N . What is $\pi(N = 144)$? Read more at http://en.wikipedia.org/wiki/Pisano_period

(c) Using the `cmath` module for complex numbers, and the Newton–Raphson method

$$z_{n+1} = z_n - \frac{f(z_n)}{f'(z_n)},$$

find the three complex roots of the cubic $f(z) = z^3 - 1$. Try choosing the initial guess close to $z = 0$ in the complex plane. Which root does the method converge upon? Read more at http://en.wikipedia.org/wiki/Newton%27s_method#Complex_functions