MAS212 Scientific Computing and Simulation

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Autumn 2018

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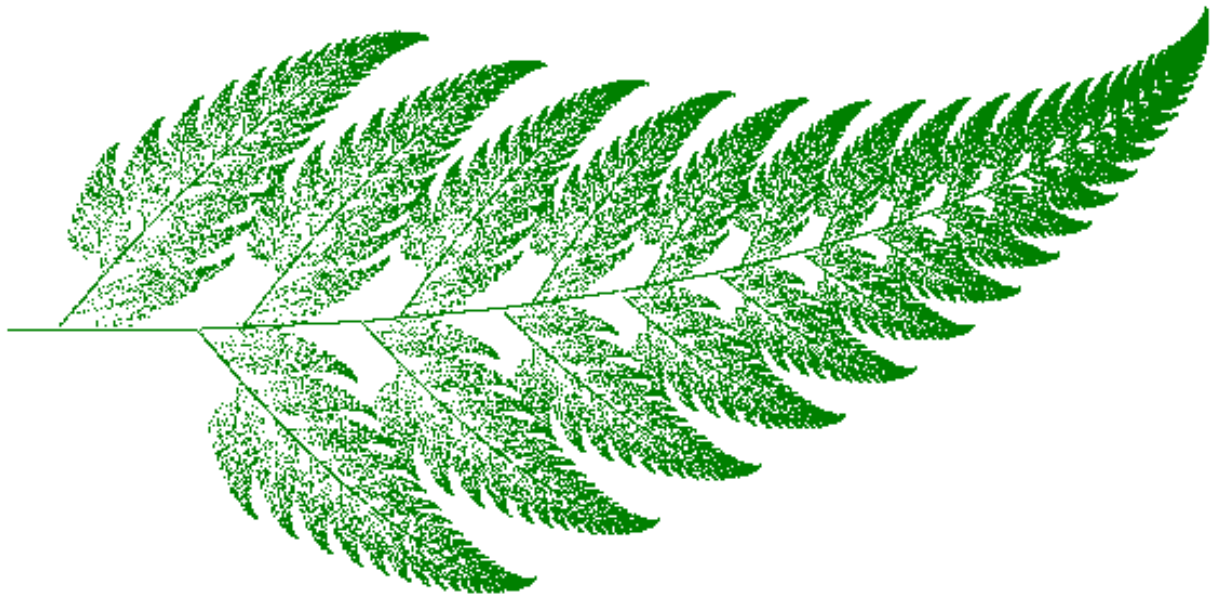


Example: The Barnsley Fern. Generated by repeated iteration of affine transformations of the form

$$\begin{pmatrix} x \\ y \end{pmatrix} \to \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} e \\ f \end{pmatrix}.$$

Course Summary (2018)

- 10 credit module in first semester.
- 10 lectures + 10 lab classes + 10 office hours
- **Assessment:** 3 assignments (90%) + 2 class tests (10%)
- Course website:
  `http://sam-dolan.staff.shef.ac.uk/mas212`
- Pre-requisite: MAS115.
- *Not a 'soft option'*.

Module description

Aims

- To further develop the students' programming skill in the context of scientific computing;
- To further develop the students' independent investigation skills;
- To introduce the knowledge of scientific computing;
- To further develop the skills of data analysis.

Outcomes

- To be able to use Python to investigate mathematical problems numerically.
- To learn basic numerical methods for solving ordinary differential equations and linear algebraic equations.
- To be able to implement basic numerical methods using Python.
- To be able to analyse the basic properties of the methods.

Syllabus

- **Week 1**: The Python language. Revision: variables; data types; arithmetic; list construction, comprehension, indexing, slicing & manipulation; `for` & `while` loops; control flow (`if-elif-else`; strings; string formatting.
  Introduction to Jupyter Notebook: Tab completion, getting help and `%magic` commands (e.g. `%timeit`).
- **Week 2**: Functions. Modules & scripts. Built-in modules (`math, cmath, random, decimal, datetime, io, os`). Simple file I/O and string processing. Debugging and testing. Workflow.
- **Week 3**: Introduction to `numpy`. Arrays (initialization, slicing). Basic linear algebra. Efficiency.
  Introduction to `matplotlib`. Simple plotting.
  Examples: (1) Estimating π by Monte Carlo integration; (2) the logistic map.
- **Week 4**: Introduction to `scipy`. Solving differential equations with `odeint`. Initial conditions. Time-domain plots. Phase plots. Critical points and limit cycles.
  Examples: (1) Logistic equation; (2) Damped harmonic oscillator; (3) van der Pol oscillator; (4) Predator-prey equations.

Syllabus

- **Week 5**: Animation with `matplotlib.animation.FuncAnimation`. Saving an animation. Examples: (1) The logistic map (again); (2) Driven damped oscillator and resonance.
- **Week 6**: Elementary numerical methods: Runge-Kutta and Adams-Bashforth methods. Implementation for initial value problems.
- **Week 7**: Error, order and stability of numerical methods.
- **Week 8**: Fitting models to data. `scipy.optimize.curve_fit`. Least-squares method and linear algebra.
- **Week 9**: Linear algebra. Gaussian elimination; iterative methods; convergence; condition number.
- **Week 10**: Plotting in 3D and visualisation. Data analysis with `pandas`. Other languages.

Books

- There are many books on Python, and on scientific computing.
- I recommend:
  "Learning Scientific Programming with Python", Christian Hill (Cambridge University Press, 2015). ISBN 978-1-107-42822-5.
- Copies available in Information Commons

Assessment guide: Assignments

- Three assignments (90%):

		Set	Due(*)
(1)	Assignment #1	Week 1	Week 4
(2)	Assignment #2	Week 4	Week 8
(3)	Assignment #3	Week 8	Week 12

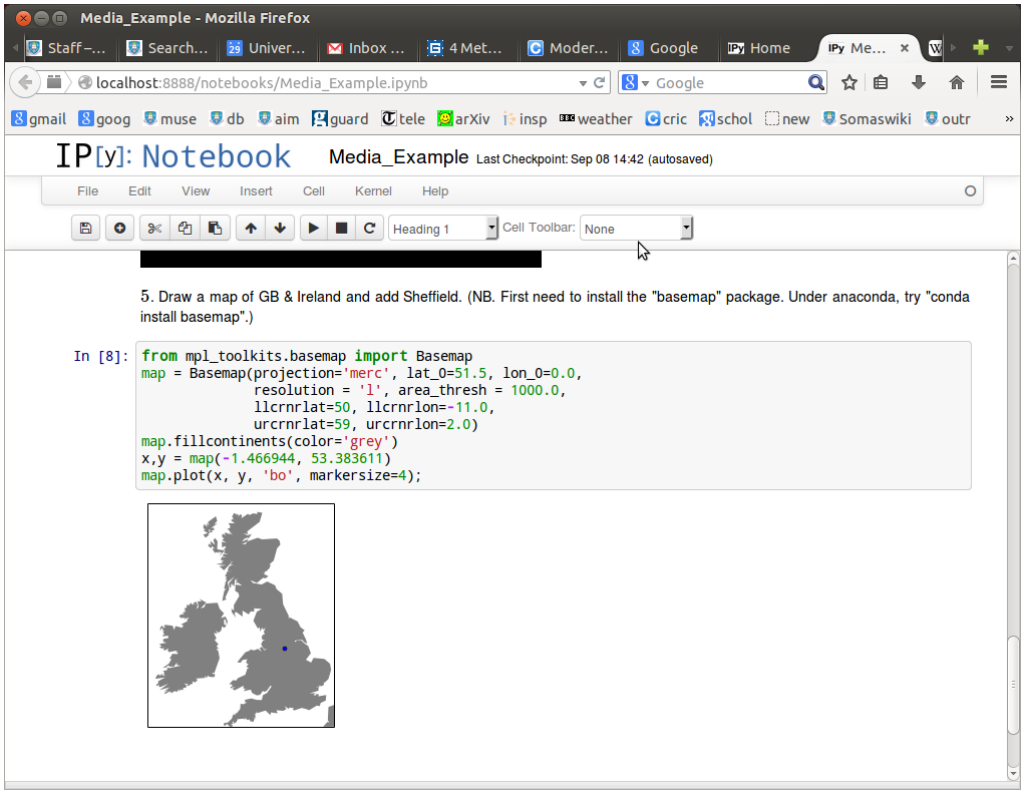
- (*) All dates provisional.
- In Assignment #1 you will submit one `.py` file
- In Assignment #2 you will submit code and write a report in LaTeX.
- In Assignment #3 you will submit code and a presentation.

Assessment guide: Class tests

- Two ‘open-book’ class tests: each 5% of module mark.
- Held in lab class in Weeks 2 and 11.
- Intended as ‘formative assessment’ (to improve skills).
- Test will use Jupyter Notebook.
- Tests for previous years are available on the course website.
- If you cannot attend your Week 2 lab class, please email me.
- Submit 1st class test by **midnight Sun 7th Oct 2018** via `http://somas-uploads.shef.ac.uk/mas212`

Jupyter Notebook

`http://jupyter.org/try`



Jupyter Notebook is . . .

. . . a web-based interactive computational environment where you can combine code execution, text, mathematics, plots and rich media into a single document.

Installing Jupyter Notebook

On your computer:

The simplest way is to get Jupyter Notebook is to install the Anaconda distribution of Python 3:
`https://www.anaconda.com/download/`
Choose Python 3.6 version.

This comes with the most popular libraries for scientific computing.

On the managed desktop:

The Anaconda distribution should be pre-installed. From the Start Menu, look for the folder `Anaconda3 (64-bit)`

Using Jupyter Notebook

- Enter Python code into a cell
- Press `Shift-Enter` to evaluate a cell
- Some example notebooks are shown on course website
  `http://sam-dolan.staff.shef.ac.uk/mas212`
- Notebooks can be converted to HTML or PDF.
- Notebooks may be shared on the web:
  `http://nbviewer.jupyter.org/`
- For an introduction to Jupyter Notebook see e.g.
  `http://opentechschool.github.io/python-data-intro/core/notebook.html`

Using Jupyter Notebook: Magic functions

Magic functions start with `%`. Examples:

- `%matplotlib inline` : include the plots in the workbook.
- `%timeit my_func()` : test the efficiency of your function.
- `%load my_module.py` : read the contents of `my_module.py` into a cell
- `%run my_module.py` : run the module as a script
- `?reversed` : get help on the `reversed` function (e.g.).
- `!` : execute a shell command.

Spyder

- Spyder is an Integrated Development Environment (IDE) for Python, . . .
- . . . the **S**cientific **PY**thon **D**evelopment **E**nvi**R**onment.
- It includes
  - A code editor with syntax colouring
  - An IPython console
  - Introspection: tab completion; go-to-definition, etc.
  - Online help
  - Object inspector
  - Debugging features, such as breakpoints
- You are encouraged to use Spyder and/or Jupyter Notebook :
  - The class test will use Jupyter Notebook;
  - Spyder is useful for developing code for the first assignment.

Checklist for Weeks 1–4

- ( ) Work through the 'Python basics' slides & **videos** on MOLE.
- ( ) Get started with Jupyter Notebook in Week 1 lab class
- ( ) Browse the course website & example notebooks. `http://sam-dolan.staff.shef.ac.uk/mas212`
- ( ) Try previous years class test(s).
- ( ) Week 2 lab class: **Class Test**. Submit by **Sunday 7th Oct**
- ( ) Assignment #1 (Rational approximations) is due **Sunday 21st Oct**

- NB. The **add/drop window** closes at the end of Week 3.