Python for scientific research

Introduction

John Joseph Valletta

University of Exeter, Penryn Campus, UK

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Acknowledgements

- The workshop is funded by Exeter's researcher-led initiative award
- Thanks to Jeremy Metz for sharing his notes used in the Biomedical Informatics Hub, from which I borrowed some examples
- Last but not least, big thanks to Mario Recker, Thomas Holding, Warren Tennant and James Clewett for helping out putting this workshop together

Housekeeping

Day 1

09:00 - 10:30	Introduction to Python
10:30 - 11:00	Coffee/Tea break
11:00 - 12:30	Flow control
12:30 - 13:30	Lunch
13:30 - 15:00	Functions, modules and packages
15:00 - 15:30	Coffee/Tea break
15:30 - 17:00	Number crunching using Numpy/Scipy

Housekeeping

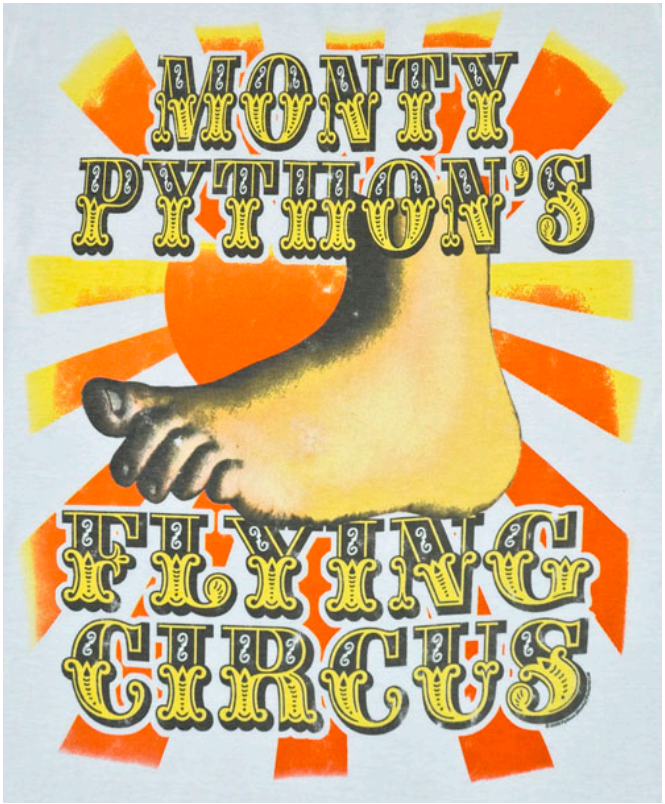
Day 2

09:00 - 10:30	Plotting with Matplotlib
10:30 - 11:00	Coffee/Tea break
11:00 - 12:30	Data analysis with Pandas
12:30 - 13:30	Lunch
13:30 - 15:00	Data visualisation with Seaborn
15:00 - 15:30	Coffee/Tea break
15:30 - 17:00	Advanced topics

References

- A Byte of Python
- Think Python
- Python for Computational Science and Engineering
- A Primer on Scientific Programming with Python
- Introduction to Python for Econometrics, Statistics and Numerical Analysis

What is Python?



- A scripted high-level programming language created by Guido Van Rossum and named after Monty Python's Flying Circus
- Easy-to-use, versatile and with an emphasise on readability
- It has a minimalistic English-like syntax, relying on indentation instead of curly brackets, semicolons etc.

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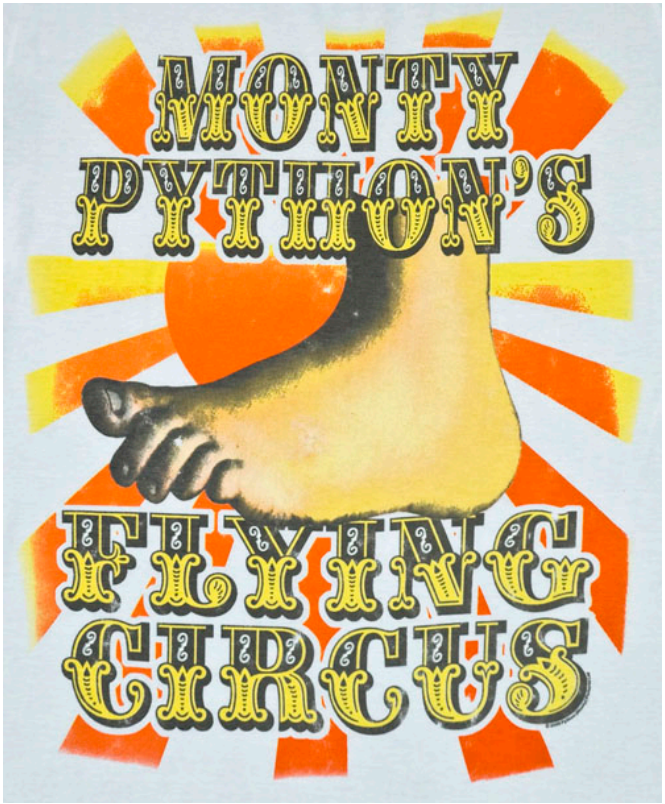

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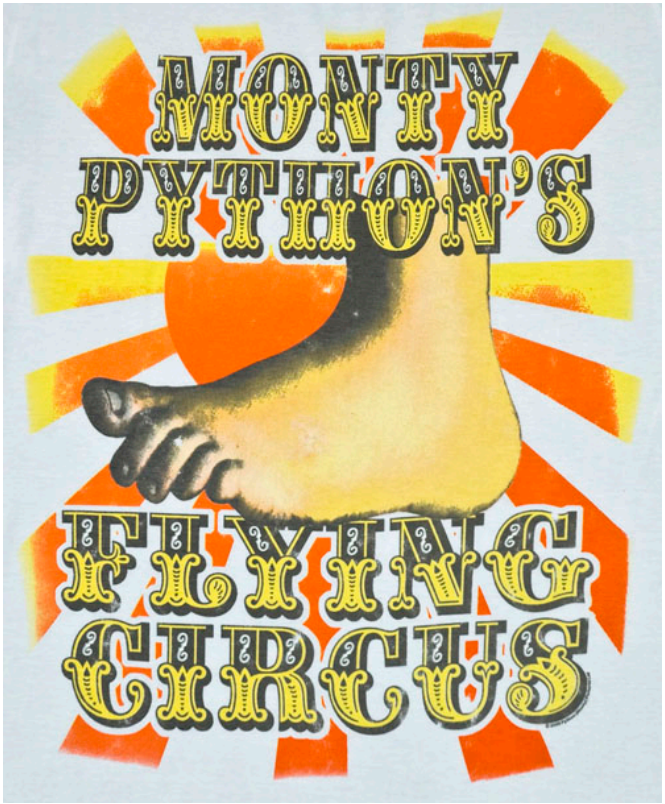

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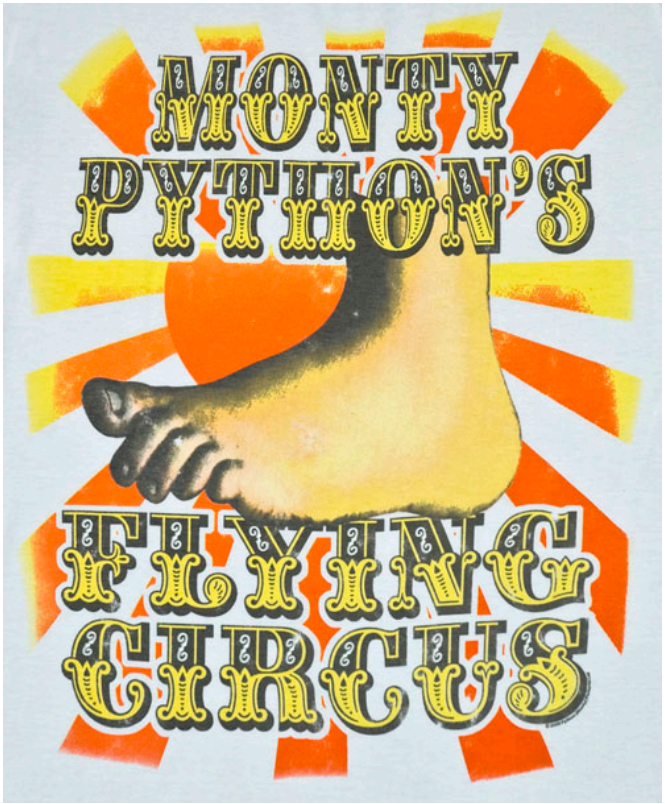

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Why Python?

The TIOBE index is a measure of the popularity of programming languages

May 2017	May 2016	Change	Programming Language	Ratings	Change
1	1		Java	14.639%	-6.32%
2	2		C	7.002%	-6.22%
3	3		C++	4.751%	-1.95%
4	5	↑	Python	3.548%	-0.24%
5	4	↓	C#	3.457%	-1.02%
6	10	⇈	Visual Basic .NET	3.391%	+1.07%
7	7		JavaScript	3.071%	+0.73%
8	12	⇈	Assembly language	2.859%	+0.98%
9	6	↓	PHP	2.693%	-0.30%
10	9	↓	Perl	2.602%	+0.28%
11	8	↓	Ruby	2.429%	+0.09%
12	13	↑	Visual Basic	2.347%	+0.52%
13	15	↑	Swift	2.274%	+0.68%
14	16	↑	R	2.192%	+0.86%
15	14	↓	Objective-C	2.101%	+0.50%
16	42	⇈	Go	2.080%	+1.83%
17	18	↑	MATLAB	2.063%	+0.78%

Why Python?

- It is free! No licence costs
- Runs on all platforms (Mac, Windows, Linux)
- Because of it's ease of programming (e.g no neeed to worry about memory allocation), Python minimises development effort
- A huge number of libraries, written by an active community
- Python can "glue" together functions written in C/C++ and Fortran to speed things up (we can also call R and MATLAB functions)
- Compared to other high-level scientific languages such as MATLAB and R, Python offers a much wider range of additional functionality (e.g web and GUI development)

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Horses for courses

- Python is becoming the de facto standard for exploratory and interactive scientific research

BUT

- Python is no programming silver bullet
- Your application will ultimately dictate the tool (and a mixture of more than one language *is* ok). For example:
  - MATLAB excels at interfacing with hardware, e.g. connecting to configure an integrated circuit board or connecting to a
  - R is great for data wrangling and visualization and statistical modelling
  - (a probabilistic programming language) is an excellent choice for performing full Bayesian statistical inference

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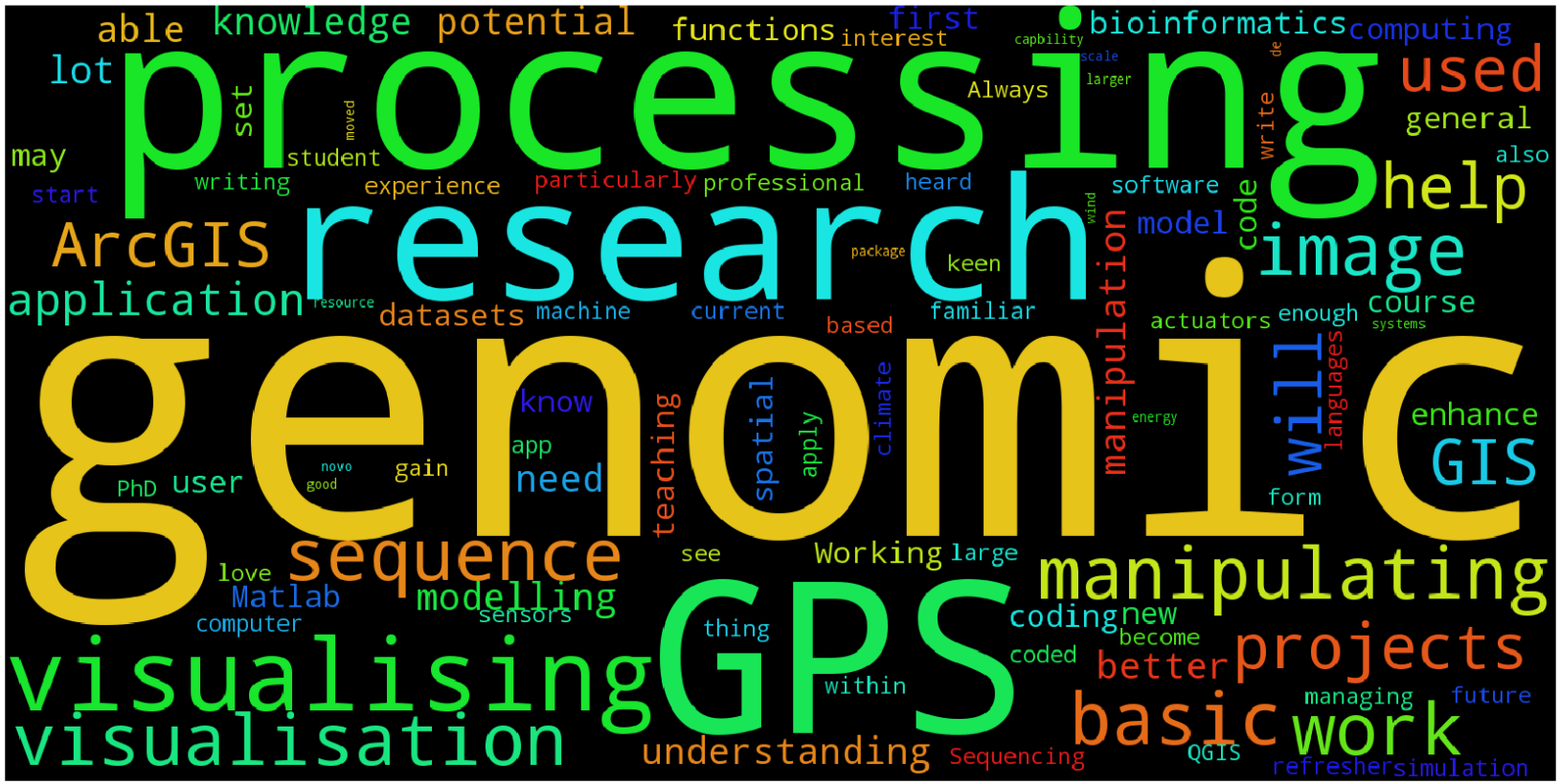
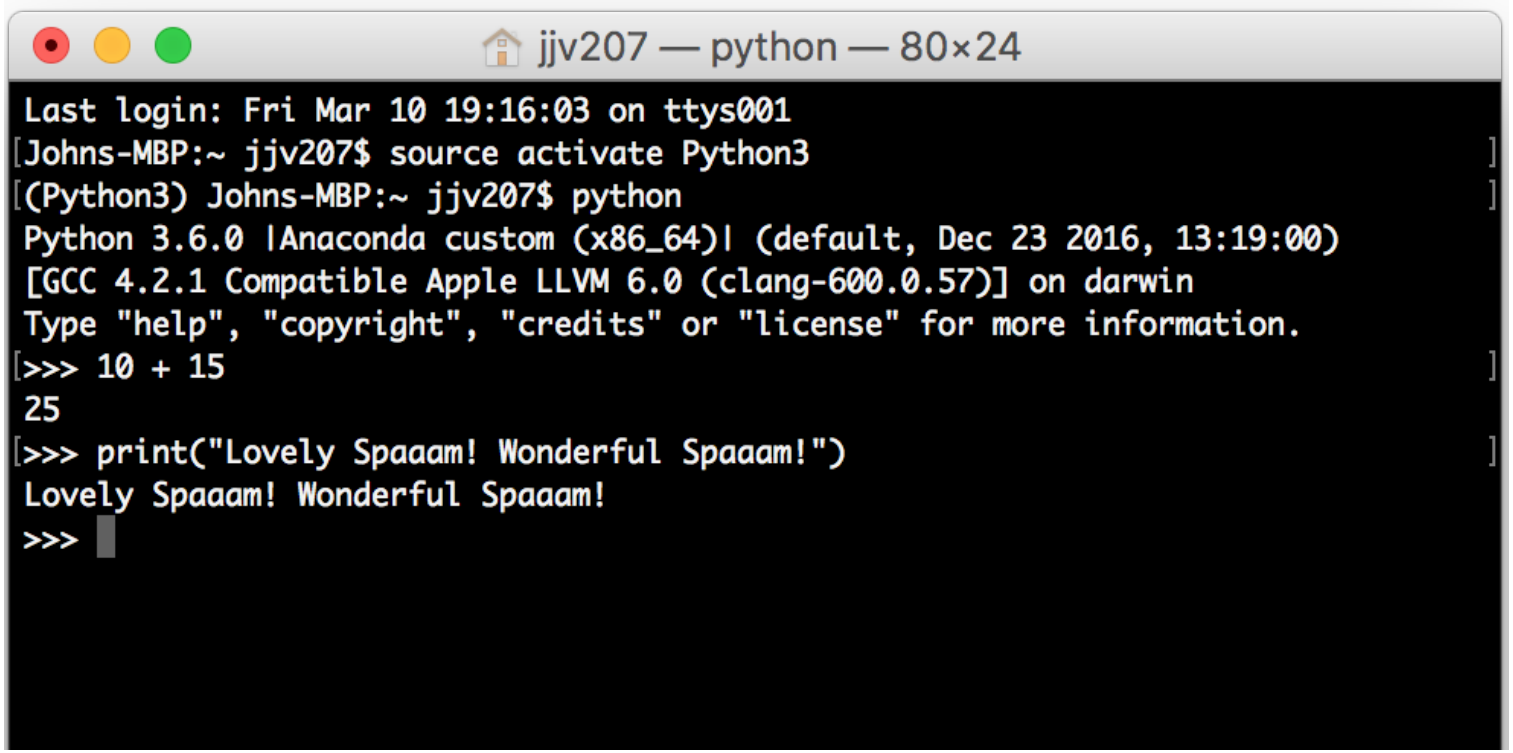
Why do *you* want to learn Python?



Executing Python code: No frills Python interpreter

- Type `python` in your terminal window to invoke the interpreter
- Any Python code you type in is executed once you press enter

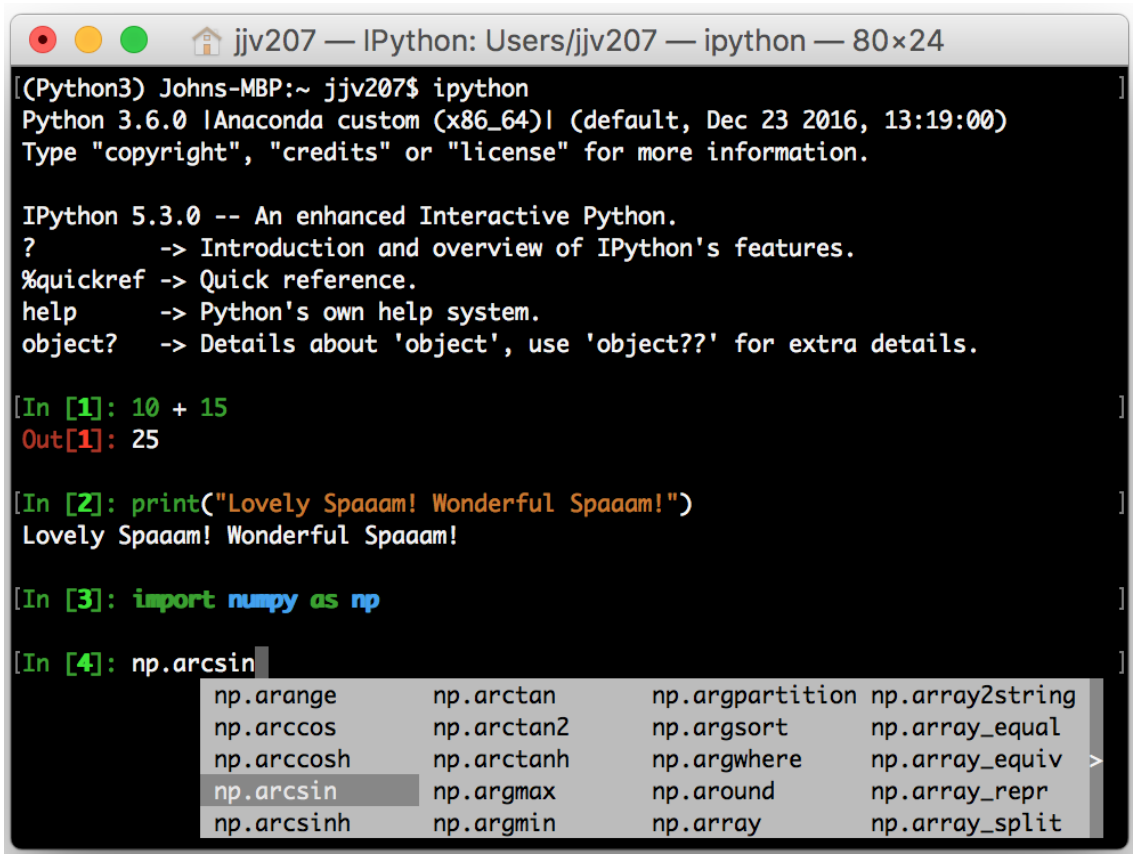


- Alternatively if your code is written in a text file, e.g `my_script.py`:

```
python my_script.py
```

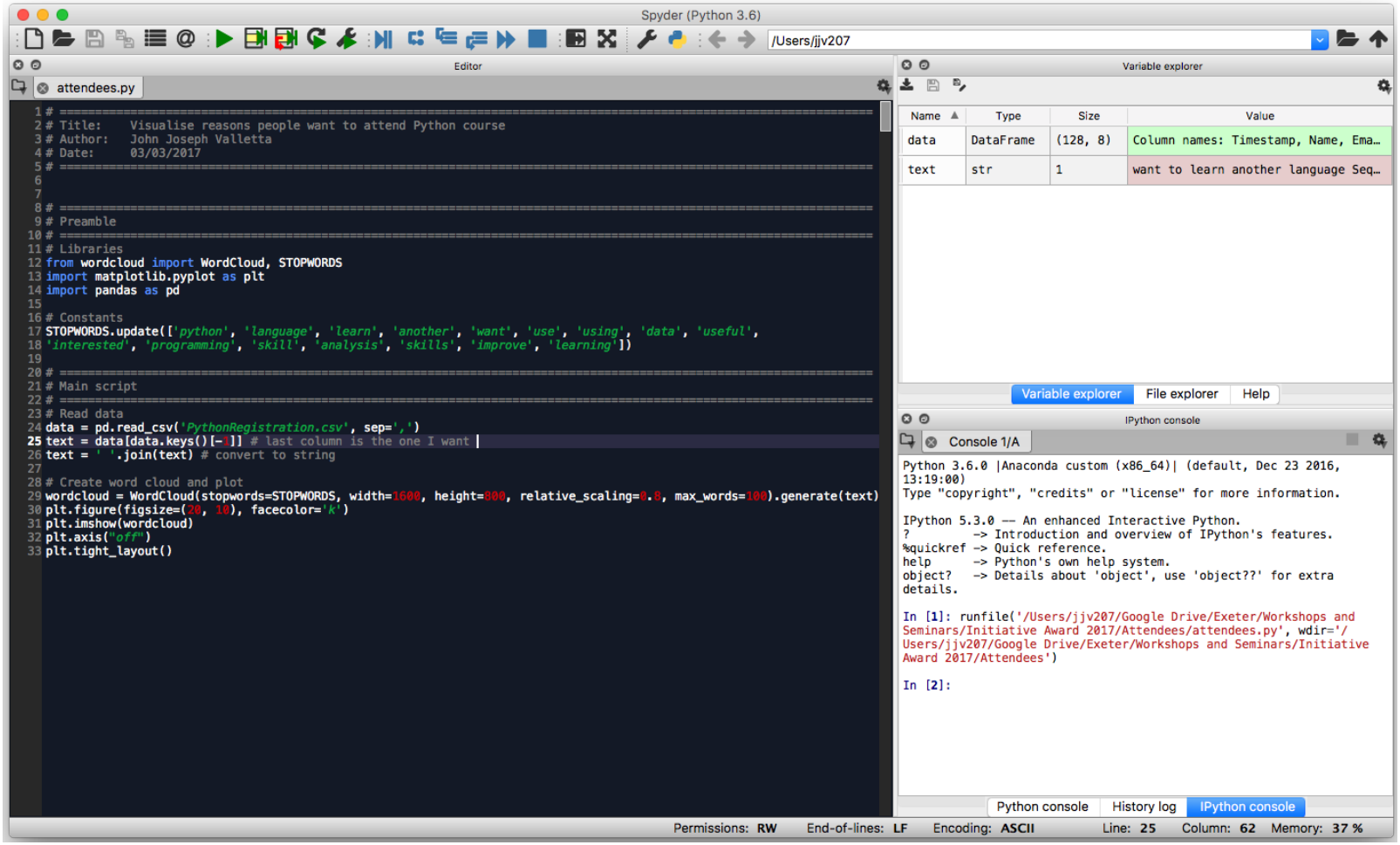
Executing Python code: IPython interpreter

- IPython is an interactive shell (similar to R Console), adding "frills" to the vanilla interpreter, such as:
  - syntax highlighting (making it easier to read code)
  - tab auto-completion (minimises typeos and lists available functions)



Executing Python code: Spyder IDE

- Spyder is an integrated development environment (IDE) for scientific computing, akin to RStudio and MATLAB
- One place to write, execute and debug code, and explore variables



The Zen of Python

- Coding standards are important in *every* programming language
- PEP 8 is a style guide for python code

```
Beautiful is better than ugly.
Explicit is better than implicit.
Simple is better than complex.
Complex is better than complicated.
Flat is better than nested.
Sparse is better than dense.
Readability counts.
Special cases aren't special enough to break the rules.
Although practicality beats purity.
Errors should never pass silently.
Unless explicitly silenced.
In the face of ambiguity, refuse the temptation to guess.
There should be one-- and preferably only one --obvious way to do it.
Although that way may not be obvious at first unless you're Dutch.
Now is better than never.
Although never is often better than *right* now.
If the implementation is hard to explain, it's a bad idea.
If the implementation is easy to explain, it may be a good idea.
Namespaces are one honking great idea -- let's do more of those!
```

Python 2.x vs 3.x

- Python 2.x and Python 3.x are the two main versions of Python
- Python 2.x is legacy, Python 3.x is the present and future of the language
- However, not all Python 3.x code is backwards-compatible
- Be aware of key differences between the two
- Here we will use Python 3.x, the language actively being developed

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Installing Python

- The easiest way to get started is to download and install a cross-platform Python distribution such as:
  - Anaconda
  - Enthought Canopy
- These distributions contain most libraries you need to get started
- Here we will use Anaconda which should be installed on your machines