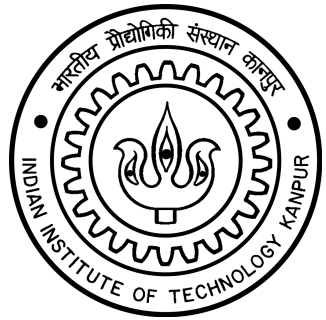
Scientific Computing using Python



Swaprava Nath

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IIT Kanpur

mini-course webpage: https://swaprava.wordpress.com/a-short-course-on-python/

Disclaimer: the contents of this lecture series are based on several texts and online resources

Outline of the Talk

1. Part 1: Preliminaries of Python
2. Part 2: Scientific Libraries
3. Part 3: Object Oriented Programming

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- Academic usage: companion of many courses – for 101 CS courses or for supportive computing

Relative popularity of Python

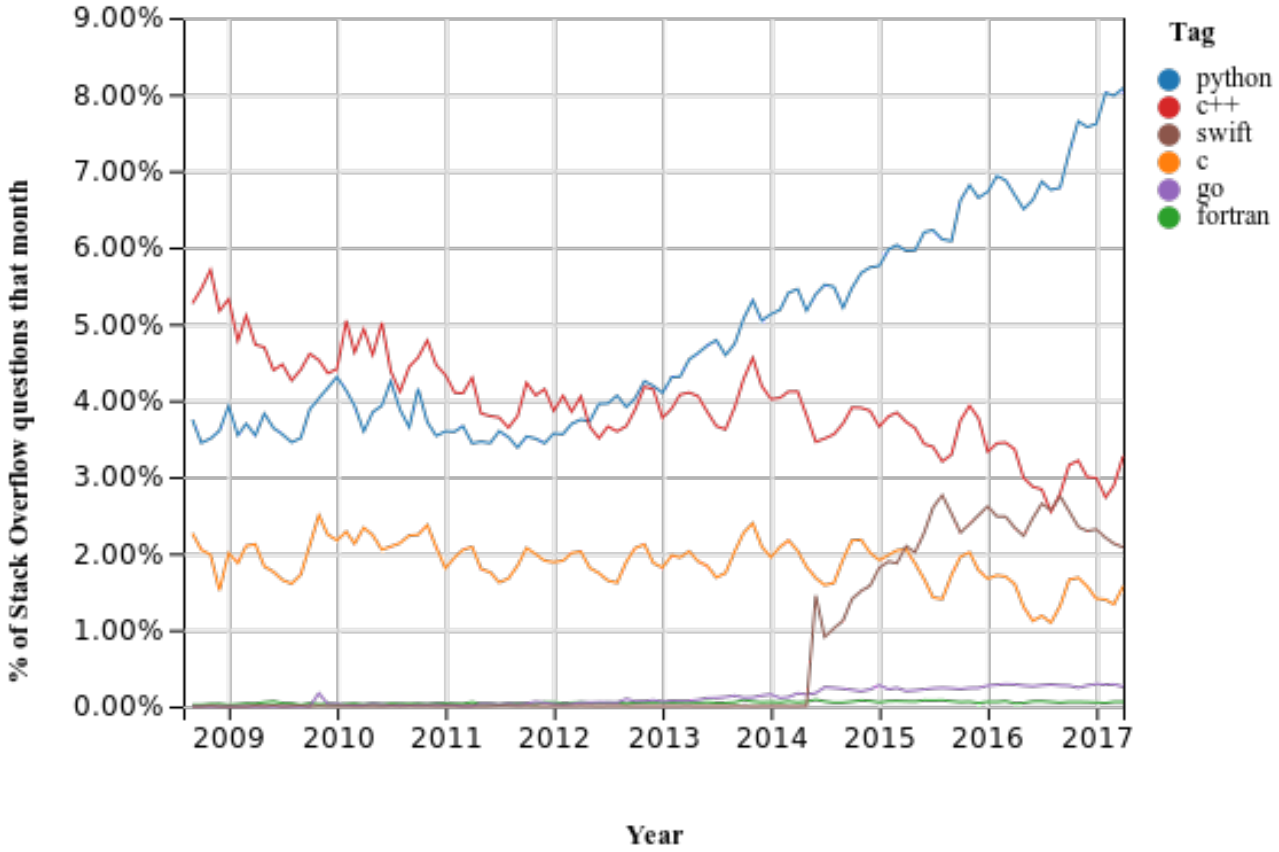

Image courtesy: www.quantecon.org

The plot, produced using Stack Overflow Trends, shows one measure of the relative popularity of Python

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- Usually implemented as interpreted as opposed to compiled (e.g. in C)
- Syntax and design of a python code makes it easier to read, debug, and develop

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  - Step-by-step execution also helps in identifying errors

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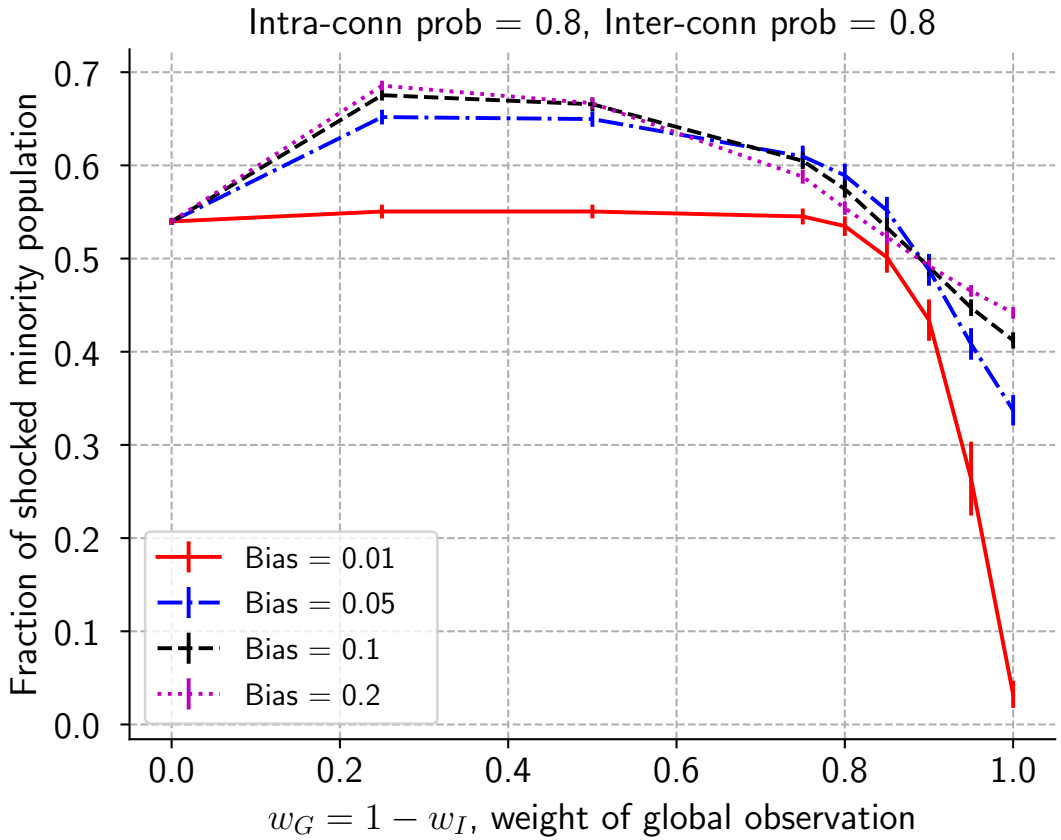
  - `pandas` – for data handling
- used in data science, machine learning, artificial intelligence, computational biology, computational physics, quantitative economics etc.

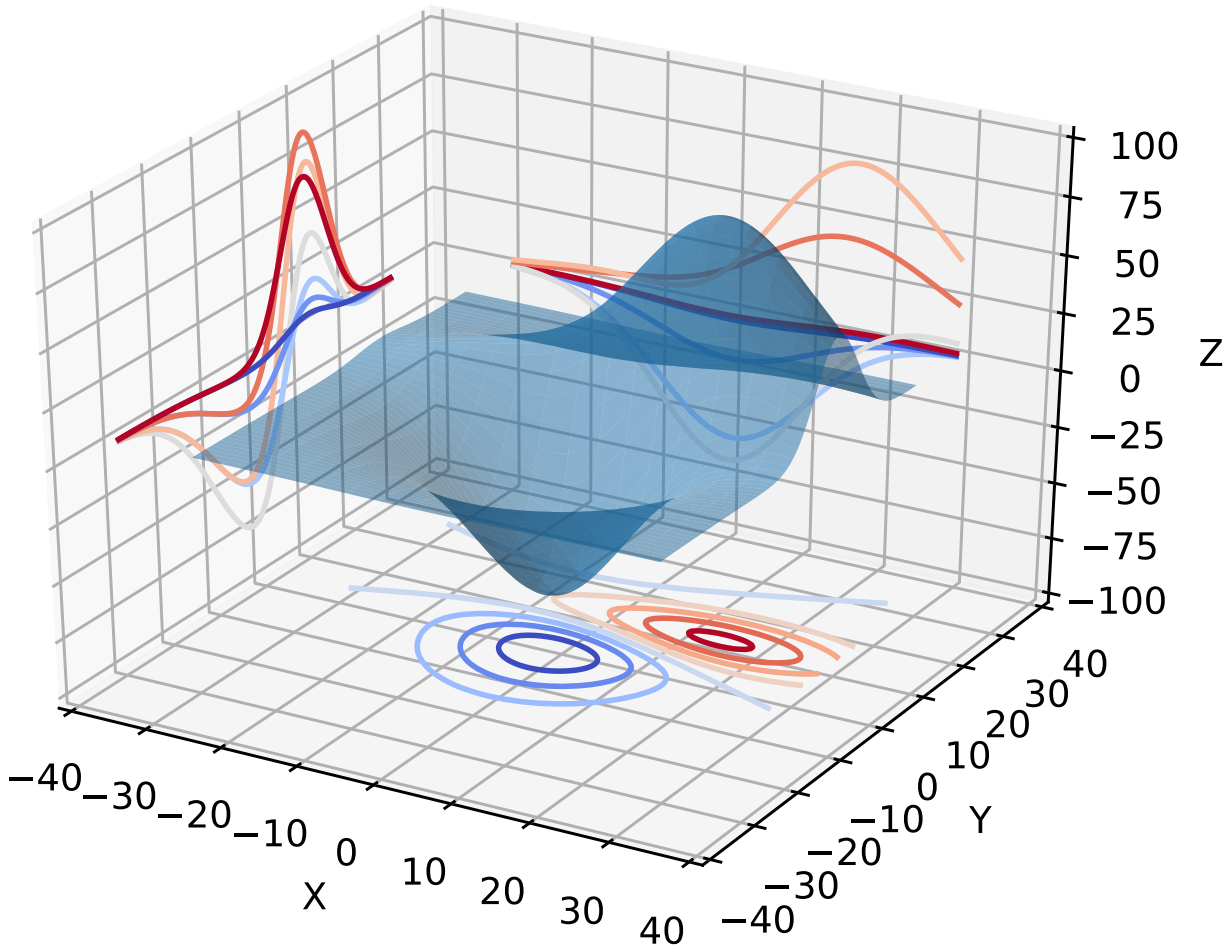
Example in action – 2D plot

- A plot of surprise in the Brexit election



- Used `pandas`, `numpy`, `matplotlib`

Example in action – 3D plot



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- `spyder` is useful for a long codebase development
- Examples

Some Introductory Python Programs

- Task 1: finding if a number is even/odd – `if-else` clause
- Task 2: finding the smallest of three numbers
- Task 3: finding if a natural number is prime or not – `while` loop and `for` loop

- Notice the indentation and absence of any braces or brackets
- Makes the code clutter-free and more readable

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$$x_{t+1} = x_t - \frac{f(x_t)}{f'(x_t)}$$

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Functions

- Example of a function – the root finding algorithm as a function
- Example of recursion of a function – checking a palindrome
- **Exercise**: solve the 'Tower of Hanoi' problem using recursion

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- A ton of useful functions on arrays
  - `linspace`, `amax`, `argmax`, `ones`, `zeros`, `sum`, `mean`, `var`, `std`, `cumsum`, `cumprod` and many more
  - `random` gives a bunch of random variables – `randn`, `beta`, `binomial`, `dirichlet`, `exponential`

Scientific Tools: `scipy`

- `numpy` $\subset$ `scipy`
- built on top of `numpy` for more focused scientific programming, e.g.,
  - linear algebra
  - numerical integration
  - interpolation
  - optimization
  - distributions and random number generation
  - signal processing
- similar ideas of using python over `C` and `Fortran` subroutines
- particularly useful for statistical methods – `scipy.stats`
- two specific functions – `bisect` and `newton`

Plotting: `matplotlib`

Features:

- high quality 2D and 3D plots
- output in all the usual formats (PDF, PNG, EPS, SVG etc.)
- LaTeX integration
- fine grained control over all aspects of presentation
- animation
- and many more

Some example usage of matplotlib

Data Handling: `pandas`

- Pandas is a package of fast, efficient data analysis tools for Python
- Similar to `numpy` that defines the basic array data type and fundamental operations on arrays
- `pandas` defines fundamental *structures* for working with data, and
- endows them with *methods* that facilitate operations such as
  - reading in data
  - adjusting indices
  - working with dates and time series
  - sorting, grouping, re-ordering, slicing, and general data manipulations
  - dealing with missing value
- Two fundamental *data types*: `series` and `dataframe`
  - `series`: an array of (possibly dissimilar) objects *with generalized index* – not as space consuming as dictionaries
  - `dataframe`: a matrix with generalized index – and various methods for data handling

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- Examples:
  1. simulating a 2D random walk
  2. simulation of a discrete random variable

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- **Example:** simulation of LUDO game

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how to draw a random variable of a given distribution

- inverse CDF method – true for discrete random variable too

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- Four important set of scientific libraries
- Object-oriented programming in python

References

- **[online course materials]** Python for scientific computing, by Swaprava Nath: `http://scientificcomputing.is-great.net/`
- **[book]** Introduction to Computation and Programming using Python, by John Guttag, Prentice Hall of India.
- **[online course materials]** Lectures in Quantitative Economics, Thomas J. Sargent and John Stachurski: `https://lectures.quantecon.org/py/index.html`