UQ IN PYTHON - INTRO

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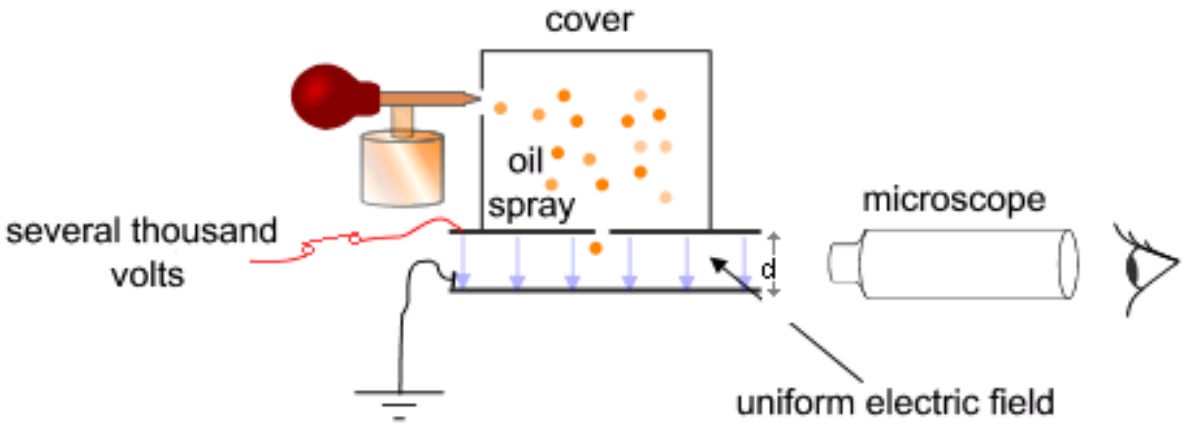
Measuring the charge of an electron

- Robert Millikan held a famous experiment published in 1910.
  - Part of the reason for his 1923 Nobel prize in physics



- By varying the charge of the electric field, the (charged) oil particles would rise or fall.
  - Millikan discovered that that charge was discrete, and had a value of $1.5924(17)\times10^{-19}$ coulomb with a very small margin of error
  - The value is today believed to be $1.602176487(40)\times10^{-19}$ coulomb

Oil-drop experiment image, CC-BY-SA 3.0, Theresa Knott

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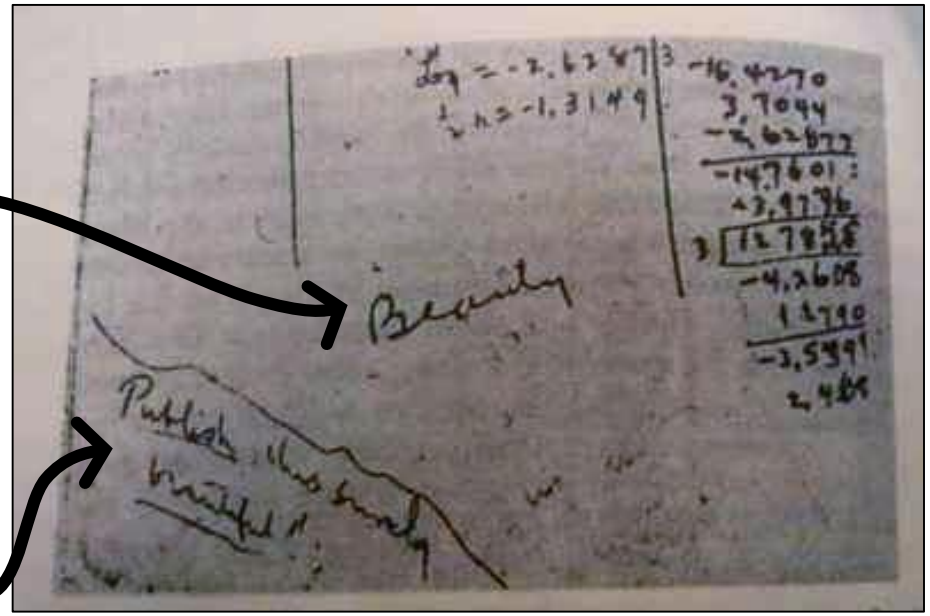
Measuring the charge of an electron

Beauty

Publish this surely
Beautiful!!



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Measuring the charge of an electron

- Millikan had almost exactly the correct value, but extremely small error margins in published result.

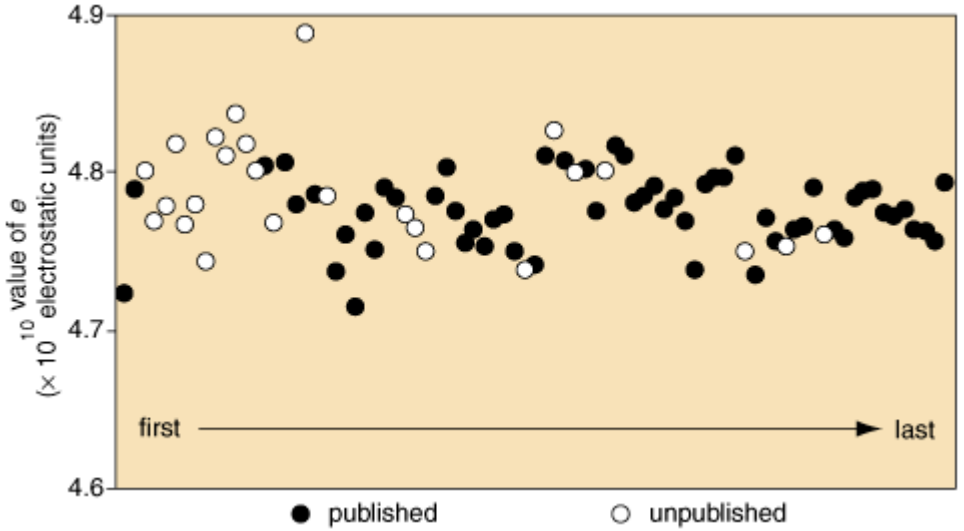

Figure by David Schneider

- A lot of data excluded from publication

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Tenfold increase in scientific research papers retracted for fraud since 1975: Two thirds retracted for scientific misconduct, not error

Findings in six of 53 landmark studies in cancer research can be confirmed

Source:

- Tenfold increase in scientific research papers retracted for fraud, Alok Jha, The Guardian, Monday 1 October 2012
- Drug development: Raise standards for preclinical cancer research, C. Glenn Begley and Lee M. Ellis, Nature 483, 2012

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A chemist treats the laboratory with thorough respect, having strict security procedures, careful note taking during experiments, etc. So should we also treat our computers, as it is the laboratory of computational science.

"In academia, software quality, user interfaces, documentation, testing and reproducibility, will all be sacrificed at the altar of publications"

Working reproducibly should become a central part of your everyday work cycle: it is not enough to think of it as a post publication step (which never happens, anyway…)

Python and Jupyter Notebooks

Python

- Almost 30 years old!
- Two "versions"
  - "Jurassic" version 2.7
  - Modern version 3.x
  - Mostly compatible with each other
- Runs on everything from cellphones to supercomputers

python™

Paradigm	Multi-paradigm: functional, imperative, object-oriented, reflective
Designed by	Guido van Rossum
Developer	Python Software Foundation
First appeared	1990; 29 years ago[1]
Stable release	3.7.2 / 24 December 2018; 30 days ago[2] 2.7.15 / 1 May 2018; 8 months ago[3]
Typing discipline	Duck, dynamic, gradual (since 3.5),[4] strong
License	Python Software Foundation License
Filename extensions	.py, .pyc, .pyd, .pyo (prior to 3.5),[5] .pyw, .pyz (since 3.5)[6]
Website	www.python.org

Python ecosystem

- Mature and fast libraries
- Numpy – matrices and arrays in Python
- Pandas – statistics and data analysis
- Scikit-learn – Machine learning (see 2018 winter school!)
- Matplotlib – interactive plotting similar to Matlab
- Mayavi – 3D interactive visualization
- …

Jupyter Notebook

- Major part of 2013 Geilo Winter School on Reproducible Research
- Makes Python interactive (what Julien is using)
- REPL environment
  Read-Eval-Print-loop
- Interactive prototyping workbench

Exercise 1: Plot unit circle

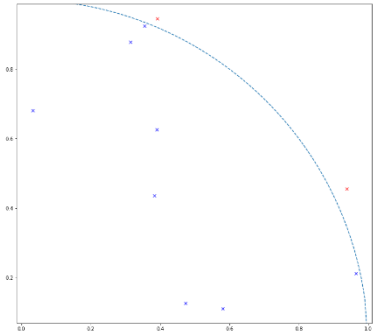
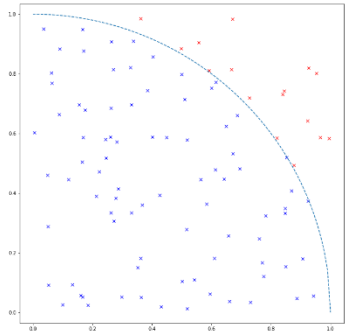
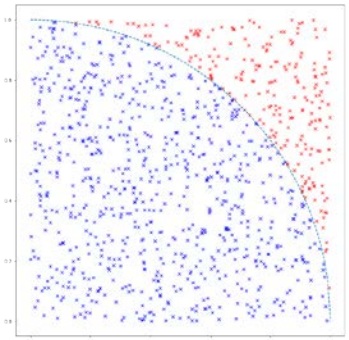
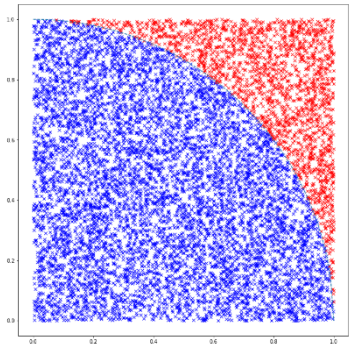
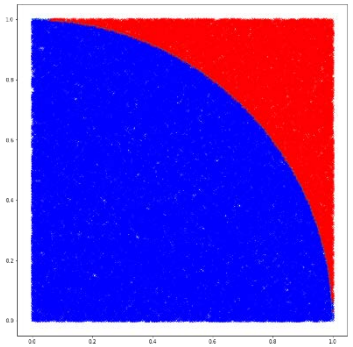
- Unit circle: y = +/- sqrt(1 – x^2)

- import numpy as np
  from matplotlib import pyplot as plt
- Generate x as a linear space (linspace) in numpy
- Use sqrt from numpy to generate y
- Use plt.plot(x, y, 'r.-') to plot

- Use question mark (?) to get help on commands!
- Add legend, change plot color, line type, add marker

Exercise 2: Monte Carlo integration of Pi

- Sample n random points in 2d (np.random.random)
- Estimate area of circle, and use pi = A / r^2

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