University of Zurich[UZH]

Department of Physics

Scientific Analysis

Scientific Programming with Python

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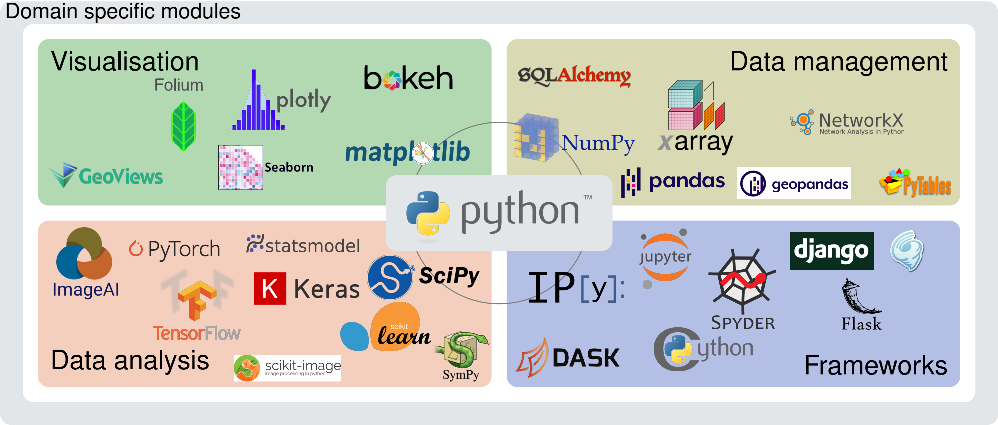
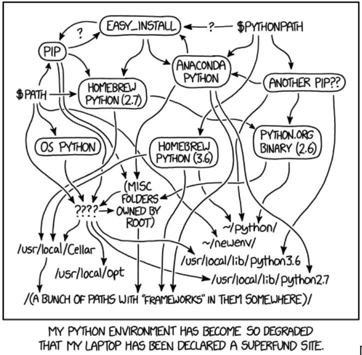
Python offers a large ecosystem for scientific analytics and beyond



We often treat modules like black boxes installed somehow on our machine



[xkcd]

The goal of this session is to deep-dive into some of the fundamental functionalities

Your Favourite Tools

You are . . .

- **analysing geographical data**
  - geopandas
  - shaply
  - rasterio
- **doing Machine Learning**
  - scikit-learn
  - Keras, TensorFlow, PyTorch
  - . . .
- **doing financial & economical modelling**
  - quantecon
  - statsmodels
- **dealing with images**
  - scikit-image
  - image AI

It is pretty difficult to satisfy all wishes!!!

$\Rightarrow$ Focus on **fundamental tools** (SciPy & NumPy) that are common to many areas!

Table of Contents

We focus on common challenges among the scientific disciplines:

- Root-finding
- Optimisation
- Numerical integration & differentiation
- Linear Algebra
- Distributions

You can find more details in the SciPy Lectures here!

SciPy – or Where the Fun Really Starts

- Offering a large number of functionality for numerical computation
  - `scipy.linalg` → Linear Algebra
  - `scipy.optimize` → Numerical optimisation (incl. least square)
  - `scipy.integrate` → Numerical integration
  - `scipy.stats` → Statistics including a large set of distributions
  - `scipy.spatial` → Spatial analysis like creation of Voroni sets, etc.
  - ...
  - more at http://docs.scipy.org/doc/scipy/reference/
- Eco-system of more advanced packages for data analysis

Remark: `import scipy` only imports the most basic tools ⇒ `from scipy import stats`

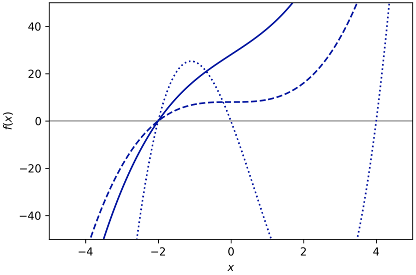
Use case 1 – Root-finding in non-linear functions

Problem:

- Finding roots of non-linear functions
- ...under sometimes non-trivial situations
- Basis to solve equations *i.e.* find x for $y = f(x) \Leftrightarrow f(x) - y = 0$

Goal:

- Understand what algorithms are available
- Understand their advantages and disadvantages as well as performance considerations



Libraries discussed: Optimisation (Root-finding part)

Root-finding Algorithms

Questions to ask:

- Smooth objective function?
- (Analytical) derivatives of first and second order available?
- Search constraint on a certain interval?
- Does a (or multiple) root exist?
- Fix-point formulation of the problem possible?

Available algorithms:

- Bracketing (Bisection)
- Quasi-Newton (Secant)
- Newton (Newton)
- Higher-order Householder (Halley)
- Hybrid (Brent)

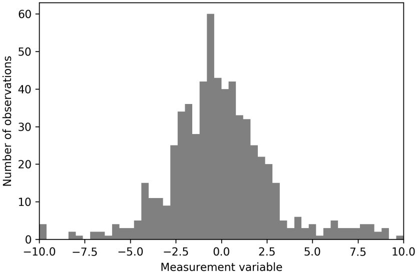
Use case 2 – Maximum-likelihood estimation

Problem:

- Parameter estimation of a distribution
- Evaluation of different models and if there are significant differences

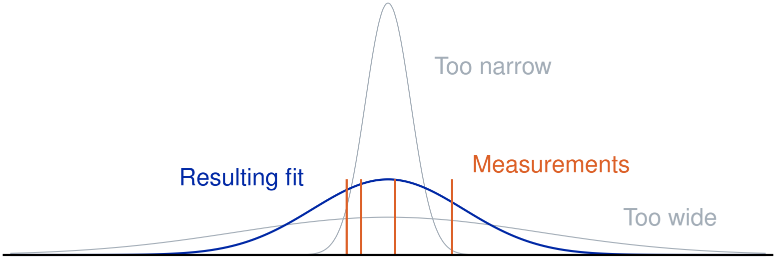
Goal:

- Understand available minimisation algorithms and their advantages and disadvantages
- Functionalities of distributions



Libraries discussed: Optimisation (Minimisation), Distributions

Maximum-Likelihood Estimation



For a given sample of (observed) values x_i find the parameters θ_j that are maximising the likelihood of the observation based on the distribution $f(x|\theta)$

Maximum-Likelihood Estimation

Fundamentals:

- For a given sample of (observed) values x_i find the parameters θ_j that are maximising the likelihood of the observation based on the distribution $f(x|\theta)$.
- $$\mathcal{L} = \prod_i f(x_i|\theta)$$
- Problem equivalent to minimise:

$$-_{\log}\mathcal{L} = -\sum_i \log(f(x_i|\theta))$$

Concrete case:

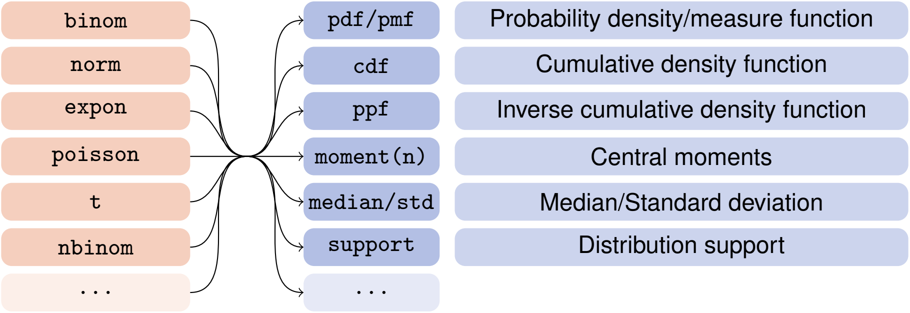
- Estimation of the daily returns by using a Gaussian distribution

$$f(x|\mu,\sigma) = \frac{1}{\sqrt{2\pi\sigma}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

- Single Gaussian case is trivial as the problem can be solved analytically with $\hat{\mu} = \overline{x}$ and $\hat{\sigma} = \sqrt{\overline{x^2} - \overline{x}^2}$
- But for most distributions a highly complex problem

Distributions and their functionality

The Scipy implementation of distributions offers a large range of distribution and statistical functionality



Minimisation Algorithms

Questions to ask:

- Smooth objective function?
- Convex objective function?
- Exact Jacobian vector or Hessian matrix available?
- Bound parameters?
- Constraints optimisation?

Available algorithms:

- Simplex (Nelder-Mead)
- Bi-directional (Powell)
- (Quasi-)Newton (BFGS)
- Trust-method (Dogleg,Newton)

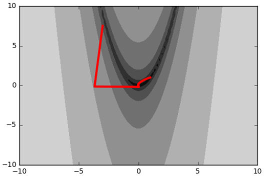
Check documentation of `scipy.optimize.minimize`

- **Choose the algorithm carefully based on your problem!**
- **A good conditioning (*i.e.* comparable scaling) is always beneficial**

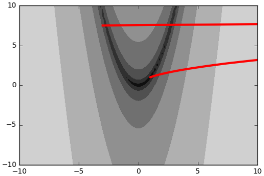
Minimisation Algorithms – Differences

Comparison of different algorithms with the Rosenbrock function
$f(x, y) = (x - 1)^2 + 100(y - x^2)^2$ and starting point $(-3, 7.5)$

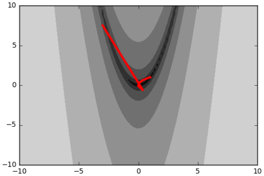
Nelder-Mead



BFGS



Conjugate Gradient



Convergence heavily dependent on the choice of the algorithm and the initial starting point.

More in the tutorial session!

Use case 3 – Linear Equation Solving

Python's matrix handling:

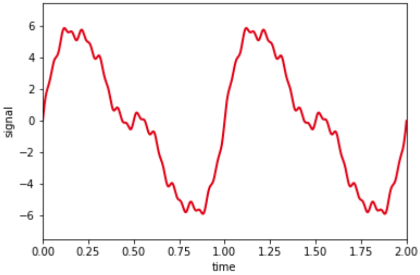
- Users should rely on the standard `ndarray` – `np.matrix` is depreciated
- Idea is to have only one type like MATLAB
- ...but with opposite default (array and not matrix)
- Inverse and Hermitian now only functions and not any more properties, multiplication via `@` operator

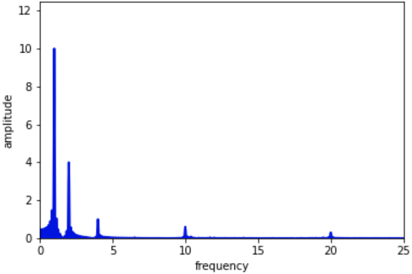
Linear Algebra Calculus:

- Numpy offers a light version of SciPy's linear algebra implementation at `np.linalg`
- Full functionality in `scipy.linalg` like matrix exponential `scipy.linalg.expm`
- The functions are wrappers of the LAPACK linear algebra package

Sparse matrices: SciPy offers under `scipy.sparse` various types and flavours of sparse matrices including corresponding linear algebra calculus `scipy.sparse.linalg`

Use case 4 – Signal Processing





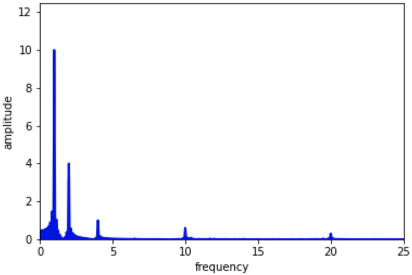
Use case 4 – Signal Processing

Problem:

- Spectrum determination of data or function
- Fast numerical integration

Goal:

- Understand numerical integration and differentiation in SciPy
- . . . as we use it to do spectral/Fourier analysis

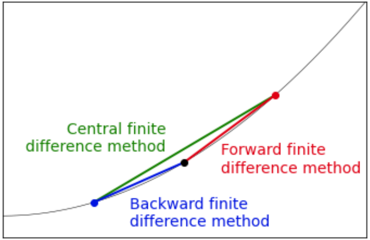


Libraries discussed: Differentiation, Integration

Numerical Differentiation

Differentiation

- Implemented as **Central finite difference method**
- Using weighting tables based on "Generation of Finite Difference Formulas on Arbitrarily Spaced Grids" (Bengt 1988)



Numerical Integration

Integration – Newton-Cotes methods

- Estimate the integral based on a sample of values $f(x_i)$ and x_i
  - Trapezoidal rule
  - Simpson's rule
  - Romberg's rule
- Integral based on polynomial between the different points x_i (spline)

Integration – Adaptive methods

- Quad methods based on Gauss–Kronrod quadrature
- Adaptive distance between evaluation points and able to dealing with "singularities"
- Based the Fortran library QUADPACK
- Sample of methods for particular situations *e.g.* to have a weight function $w(x)$ *i.e.*

$$I = \int_a^b \mathrm{d}x f(x) \times w(x)$$

Fourier Transformation

Problem to solve:

- Calculate for a given function $f(t)$ and frequency ω the amplitude

$$A(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t e^{-i\omega t} \times f(t)$$

or when focussing only on the real part

$$A'(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t \cos \omega t \times f(t)$$

- Idea: Evaluate the above integral numerically.

Strategy to solve it in Python:

1. Run the integration with the `quad` method
2. Use `np.vectorize` to evaluate the integral in parallel for different ω values

Advanced Python Modules

We omitted any modules with a large and specific purpose $\rightarrow$ otherwise you would sit here tomorrow

Left to the interested audience to explore them further

- NLTK (www.nltk.org) $\rightarrow$ Natural language processing
- scikit-learn (scikit-learn.org) $\rightarrow$ Machine learning
- scikit-image (scikit-image.org) $\rightarrow$ Image processing and analysis
- ...

Rapidly growing and improving landscape of python modules, but with still some “whitish” spots (*e.g.* time series) $\Rightarrow$ Reflection of available alternatives?

Conclusion

- SciPy together with NumPy offers a large number of fundamental tools for your everyday work in science and beyond . . .
- . . . and they let you built your own tools for research.
- Understanding these fundamental libraries is also helpful to understand the “under the hud” part of more specialised libraries.
- Take the time to understand the content of the package . . .
- . . . to avoid a reinvention of the wheel

Other relevant (fundamental) libraries will be discussed on Friday by Jonas together with the topic of visualisation.