Scientific Analysis

Scientific Programming with Python

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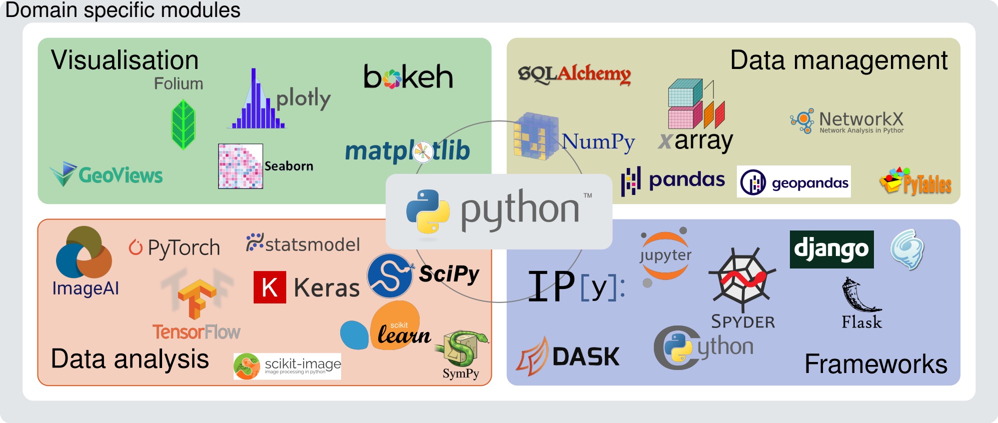
Python offers a large ecosystem for scientific analytics and beyond



Domain specific modules

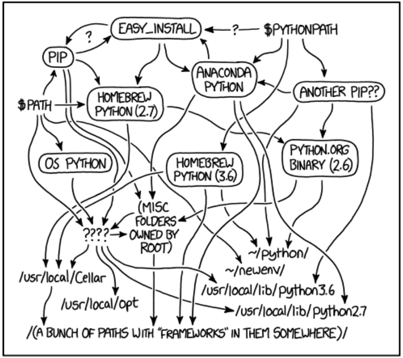
Visualisation

Data management

Data analysis

Frameworks

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



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

[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!!!

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

Outline

We focus on common challenges among the scientific disciplines:

Root Finding and Equation Solving

Optimization and Statistical Modeling

Linear Algebra and Matrix Operations

Integration and Differentiation

Conclusion and Advanced Topics

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`

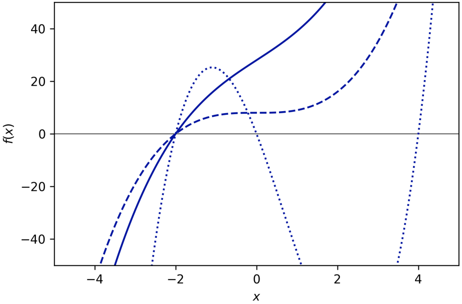
Use case 1 – Root-finding in non-linear functions

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)

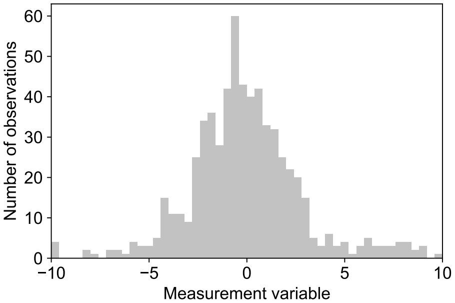
Use case 2 – Maximum-likelihood estimation

Problem:

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

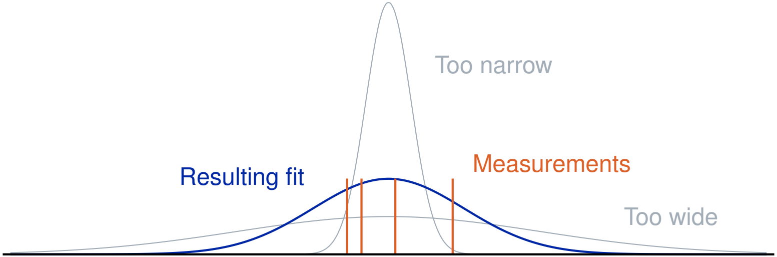
Goal:

- 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:

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

Concrete case:

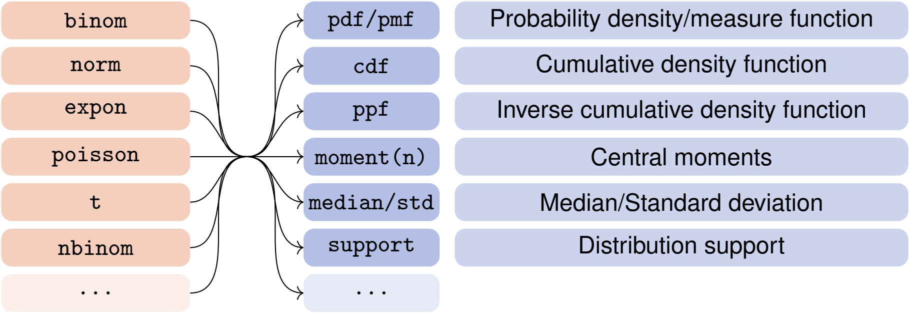
- Estimation of the parameters of a Gaussian distribution describing the data

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

- 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



- `binom`
- `norm`
- `expon`
- `poisson`
- `t`
- `nbinom`
- `...`

`pdf/pmf`	Probability density/measure function
`cdf`	Cumulative density function
`ppf`	Inverse cumulative density function
`moment(n)`	Central moments
`median/std`	Median/Standard deviation
`support`	Distribution support
`...`	

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)

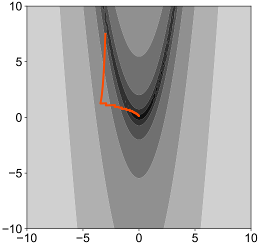
Check documentation of `scipy.optimize.minimize`

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

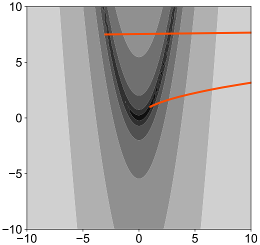
Minimisation Algorithms – Differences

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

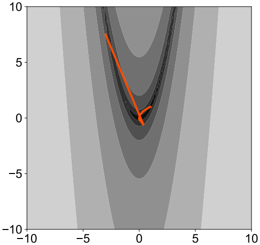
Nelder-Mead



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:

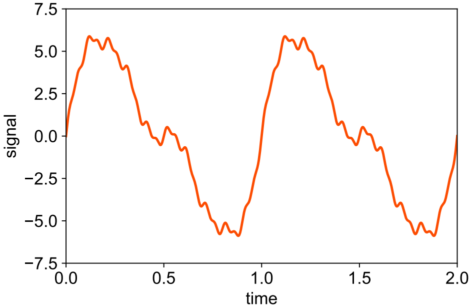
- Users should rely on the standard `ndarray` – `np.matrix` is depreciated
- Idea is to have only one type like MATLAB
- . . . but with opposite default (array and not matrix)
- Inverse and Hermitian now only functions and not any more properties, multiplication via `@` operator

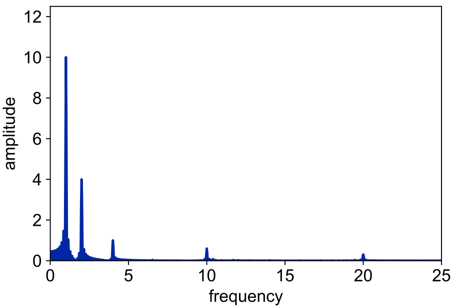
Linear Algebra Calculus:

- 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





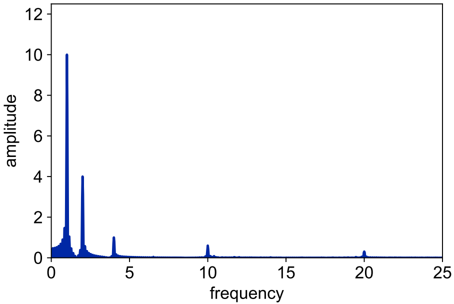
Use case 4 – Signal Processing

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

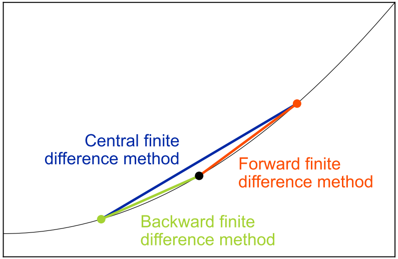


Libraries discussed: Differentiation, Integration

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)


Central finite difference method
Forward finite difference method
Backward finite difference method

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 → otherwise you would sit here tomorrow

Left to the interested audience to explore them further

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

Rapidly growing and improving landscape of python modules, but with still some “whitish” spots (*e.g.* time series) ⇒ 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