SciPy & other packages

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Reusing this material

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SciPy

- NumPy provides arrays, basic linear algebra, random number generation, and Fourier transforms

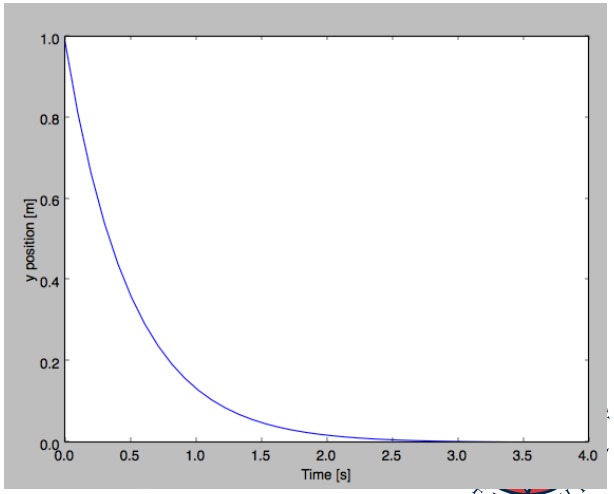
- SciPy builds on NumPy (e.g. by using arrays) and expands this with (additional) routines for:
  - Numerical integration
  - Interpolation
  - Linear algebra and wrappers to LAPACK & BLAS
  - Sparse linear algebra
  - Image processing
  - Optimisation
  - Signal processing
  - Statistical functions
  - Spatial data structures and algorithms
  - Airy functions

- Note: no PDE solvers (though other packages exist)

Integration

- Routines for numerical integration – single, double and triple integrals
- Function to integrate can be given by function object or by fixed samples
- e.g. solve the ODE
  - dy/dt = -2y between t = 0..4, with the initial condition y(t=0) = 1

```
import numpy as np
from scipy.integrate import odeint
def calc_derivative(ypos, time):
        return -2*ypos
time_vec = np.linspace(0, 4, 40)
yvec = odeint(calc_derivative, 1, time_vec)
pl.plot(time_vec, yvec)
```



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Optimisation

- Several classical optimisation algorithms
  - Quasi-Newton type optimisations
  - Least squares fitting
  - Simulated annealing
  - General purpose root finding
- Rosenbrock function

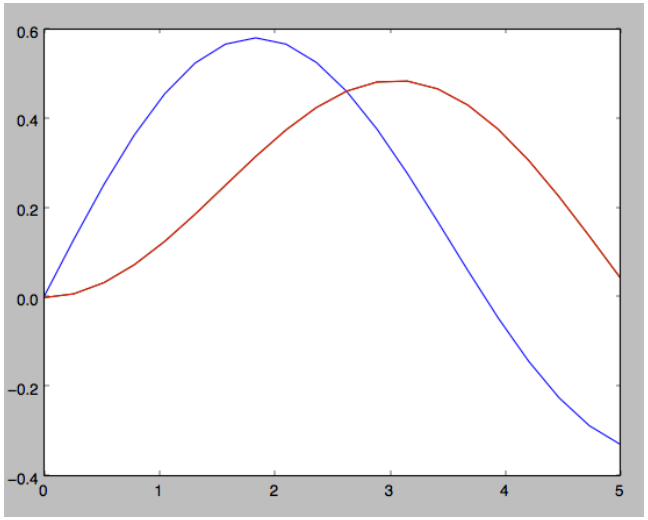
$$f(\mathbf{x}) = \sum_{i=1}^{N-1} (x_i - x_{i-1}^2)^2 + (1 - x_{i-1})^2$$

```
>>> from scipy.optimize import fmin
>>> def rosen(x):
... return sum(100.0*(x[1:]-x[:-1]**2.0)**2.0 + (1-x[:-1])**2.0)
>>> x0 = [1.3, 0.7, 0.8, 1.9, 1.2]
>>> xopt = fmin(rosen, x0, xtol=1e-8)
 Optimization terminated successfully.
         Current function value: 0.000000
         Iterations: 339
         Function evaluations: 571
```

Special functions

- SciPy contains huge set of special functions – Bessel functions
  - Legendre functions
  - Gamma functions
  - Bessel function →

```
>>> from scipy.special import *
>>> x = np.linspace(0, 5, 20)
>>> plot(x, jv(1, x))
>>> plot(x, jv(2, x))
```



Linear Algebra

- Wider set of linear algebra operations than in Numpy
  - decompositions,
  - matrix exponentials
- Routines also for sparse matrices
  - storage formats
  - iterative algorithms

```
>>> import numpy as np
>>> from scipy.sparse.linalg import LinearOperator, cg
>>> # Define “Sparse” matrix-vector product
>>> def mv(v):
>>>       return np.array([ 2*v[0], 3*v[1]])
>>> A = LinearOperator( (2,2), matvec=mv, dtype=float )
>>> b = np.array((4.0, 1.0))
>>> x = cg(A, b) # Solve linear equation Ax = b with conjugate gradient
>>> x
(array([ 2.        ,  0.33333333]), 0)
```

Other packages

- Pandas
  - Offers R-like statistical analysis of numerical tables and time series
- SymPy
  - Python library for symbolic computing
- scikit-image
  - Advanced image processing
- scikit-learn
  - Package for machine learning
- Sage
  - Open source replacement for Mathematica / Maple / Matlab (built using Python)