A taste of SciPy

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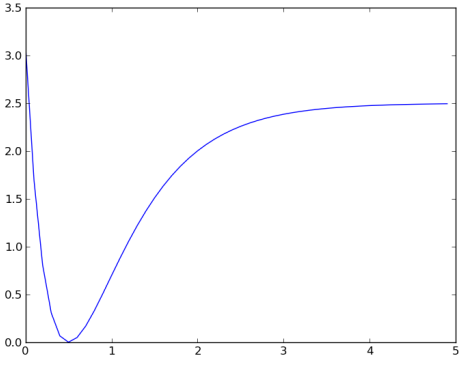
Learning objectives

- Overview of the SciPy library
- Minimizing
- Curve fitting
- Least-square optimization

Example

In the examples below we use the Morse potential




```
def morse(r, r0=0.5, a=1.5, d=2.5):
    import math
    e = math.exp(-a*(r-r0))
    return d*(1-e)**2
```

Interpretation

- `r0`: minimum
- `a`: inversly related to width
- `d`: asympototic

Methods for function minimization

- A very common problem in science
- Associated to the variational principle
- A model parameterized function that minimized some criterion

The Brent method

- Bracketing approach
- No derivatives

```
scipy.optimize.brent(f)
```

Conjugant gradient method

- Gradient function can be given
- Approximate gradient used if not

```
scipy.optimize.fmin_cg(f)
```

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scipy.optimize.fmin_cg(f)
```

With gradient

```
scipy.optimize.fmin_cg(f, [1], fprime=g)
```

The Newton method

- Based on a local second-order expansion
- Iterative method

```
x = x_0 - f'(x_0)/f''(x_0)
```

- Hessian is optional - numerical requires more gradient evaluations

```
minx = optimize.fmin_ncg(f, [1], fprime=g)
```

- with Hessian

```
optimize.fmin_ncg(f, [1], fprime=g, fhess=h)
```

The quasi-Newton method

- some approximation of the Hessian is maintained
- when the Hessian is too expensive

```
optimize.fmin_bfgs(f, [1], fprime=g)
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```
optimize.fmin_bfgs(f, [1], fprime=g)
```

The lBFGS

- inprinciple as BFGS - does not store explicit Hessians

```
optimize.fmin_l_bfgs_b(f, [1], fprime=g)
```

Curve-Fitting Illustration

- Consider the Morse example `d=2.5, a=1.5 r0=0.5`
- Add some numerical noise
- Given input numerical data the optional parameters (r0, a, d) are optimized to fit data

```
x = numpy.arange(0, 5, .1)
y = f(x) + 0.01*numpy.random.normal(size=len(x))
optimize.curve_fit(f, x, y)
```

Least-Square fitting

- Simple least square fitting to a straight line
- Initialize arrays

```
import numpy
from scipy.optimize import leastsq
x = numpy.arange(0, 10, .01)
k0 = 3.0
l0 = 1.0
y = k0 * x + l0 + numpy.random.randn(len(x))
```

- Define a residual function
- The parameters to be optimize are the first argument (tuple)

```
def resid(p, y, x):
k,l = p
return y - k*x - l
```

- The arguments to `leastsq` are the residual function, the initial parameters `p0` and the data set `(y, x)` in `args`

```
p0 = numpy.array([k0, l0])
scipy.optimize.leastsq(resid, p0, args=(y, x))
```

Integration

- uses package `scipy.integrate`
- definite integrals in 1-3 dimensions

Example

The integral of a Gaussian distribution

```
from scipy.integrate import quad
sqrtpi = math.sqrt(math.pi)
def e2(x):
   return math.exp(-x*x)
scipy.integrate.quad(e2, -10, 10)
```

Other SciPy submodules

- Special functions
- Interpolation
- Linear algebra
- Statistics

Links:

- http://docs.scipy.org/doc/
- http://scipy-lectures.github.com