Introductory Scientific Computing with Python

Basic SciPy

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Outline

Solution of equations

Consider,

$$3x + 2y - z = 1$$
$$2x - 2y + 4z = -2$$
$$-x + \frac{1}{2}y - z = 0$$

Solution:

$$x = 1$$
$$y = -2$$
$$z = -2$$

Solving using Matrices

Let us now look at how to solve this using **matrices**

```
In []: A = array([[3,2,-1],
                  [2,-2,4],
                  [-1, 0.5, -1]])
In []: b = array([1, -2, 0])
In []: x = solve(A, b)
```

Solution:

```
In []: x
Out[]: array([ 1., -2., -2.])
```

Let's check!

```
In []: Ax = dot(A, x)
In []: Ax
Out[]: array([  1.00000000e+00,  -2.00000000e+00,
-1.11022302e-16])
```

The last term in the matrix is actually 0!
We can use `allclose()` to check.

```
In []: allclose(Ax, b)
Out[]: True
```

10 m

Problem

Solve the set of equations:

$$
\begin{aligned}
x + y + 2z - w &= 3 \\
2x + 5y - z - 9w &= -3 \\
2x + y - z + 3w &= -11 \\
x - 3y + 2z + 7w &= -5
\end{aligned}
$$

Solution

Use `solve()`

$$
\begin{aligned}
x &= -5 \\
y &= 2 \\
z &= 3 \\
w &= 0
\end{aligned}
$$

15 m

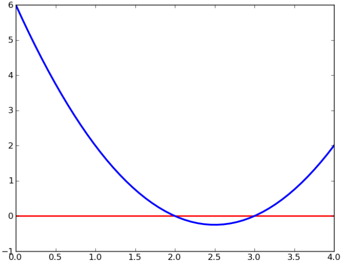
Outline

1. Solving linear systems
2. Finding Roots
3. ODEs
4. FFTs

SciPy: `roots`

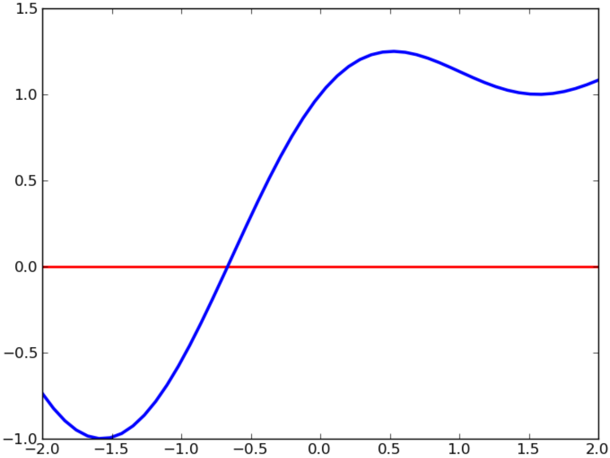
- Calculates the roots of polynomials
- To calculate the roots of $x^2 - 5x + 6$

```
In []: coeffs = [1, -5, 6]
In []: roots(coeffs)
Out[]: array([3., 2.])
```



SciPy: `fsolve`

Find the root of $sin(z) + cos^2(z)$ nearest to 0



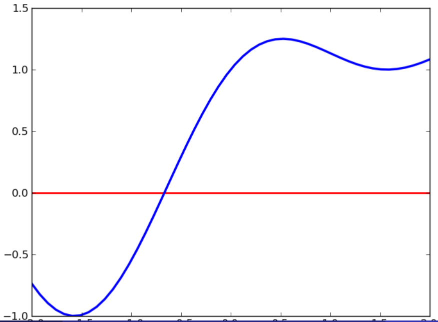
fsolve

```
In []: from scipy.optimize import fsolve
```

- Finds the roots of a system of non-linear equations
- Input arguments - Function and initial estimate
- Returns the solution

fsolve ...

```
In []: def g(z):
 ....:     return sin(z)+cos(z)*cos(z)
In []: fsolve(g, 0)
Out[]: -0.66623943249251527
```

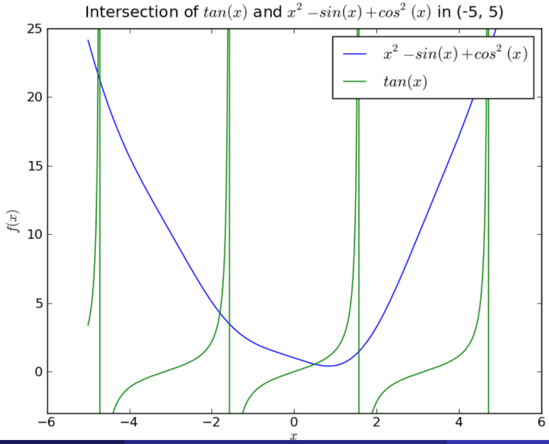


Exercise Problem

Find the root of the equation
$x^2 - sin(x) + cos^2(x) = tan(x)$ nearest to 0

Solution

```
def g(x):
    return x**2 - sin(x) + cos(x)*cos(x) - tan(x)
fsolve(g, 0)
```



30 m

Outline

Solving ODEs using SciPy

- Consider the spread of an epidemic in a population
- $\frac{dy}{dt} = ky(L - y)$ gives the spread of the disease
- L is the total population.
- Use $L = 2.5E5, k = 3E-5, y(0) = 250$

Solving ODEs using SciPy

Define a function as below

```
In []: from scipy.integrate import odeint
In []: def epid(y, t):
  ...:     k = 3.0e-5
  ...:     L = 2.5e5
  ...:     return k*y*(L-y)
  ...:
```

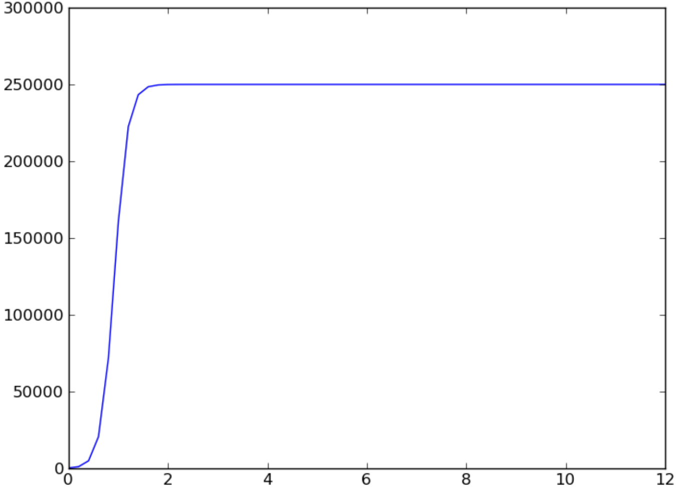
Solving ODEs using SciPy . . .

```
In []: t = linspace(0, 12, 61)

In []: y = odeint(epid, 250, t)

In []: plot(t, y)
```

Result



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ODEs - Simple Pendulum

We shall use the simple ODE of a simple pendulum.

$$\ddot{\theta} = -\frac{g}{L} sin(\theta)$$

- This equation can be written as a system of two first order ODEs

$$\dot{\theta} = \omega \quad (1)$$

$$\dot{\omega} = -\frac{g}{L} sin(\theta) \quad (2)$$

$$\text{At } t = 0 :$$

$$\theta = \theta_0(10^o) \quad \& \quad \omega = 0 \ (\textit{Initial values})$$

ODEs - Simple Pendulum . . .

- Use **odeint** to do the integration

```
In []: def pend_rhs(state, t):
....       theta = state[0]
....       omega = state[1]
....       g = 9.81
....       L = 0.2
....       F=[omega, -(g/L)*sin(theta)]
....       return F
....
```

ODEs - Simple Pendulum . . .

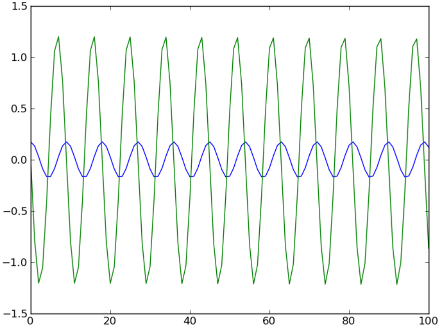
- `t` is the time variable
- `initial` has the initial values

```
In []: t = linspace(0, 20, 101)
In []: initial = [10*2*pi/360, 0]
```

ODEs - Simple Pendulum . . .

```
In []: from scipy.integrate import odeint
In []: pend_sol = odeint(pend_rhs,
                         initial,t)
```

Result



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Outline

The FFT

- We have a simple signal $y(t)$
- Find the FFT and plot it

```
In []: t = linspace(0, 2*pi, 500)
In []: y = sin(4*pi*t)

In []: f = fft.fft(y)
In []: freq = fft.fftfreq(500,
   ...:                      t[1] - t[0])

In []: plot(freq[:250], abs(f)[:250])
In []: grid()
```

FFTs cont. . .

```
In []: y1 = fft.ifft(f) # inverse FFT
In []: allclose(y, y1)
Out[]: True
```

FFTs cont. . .

Let us add some noise to the signal

```
In []: yr = y +
   ...:     random.random(size=500)*0.2
In []: yn = y +
   ...:     random.normal(size=500)*0.2

In []: plot(t, yr)
In []: figure()
In []: plot(freq[:250],
   ...:         abs(fft.fft(yr))[:250])
```

- **random**: produces uniform deviates in $[0, 1)$
- **normal**: draws random samples from a Gaussian

FFTs cont. . .

Filter the noisy signal:

```
In []: from scipy import signal
In []: yc = signal.wiener(yn, 5)
In []: clf()
In []: plot(t, yc)
In []: figure()
In []: plot(freq[:250],
   ...:        abs(fft.fft(yc))[:250])
```

Only scratched the surface here . . .

55 m

Things we have learned

- Solving Linear Equations
- Defining Functions
- Finding Roots
- Solving ODEs
- FFTs and basic signal processing

Further reading

- ipython.github.com/ipython-doc
- matplotlib.sf.net/contents.html
- scipy.org/Tentative_NumPy_Tutorial
- docs.scipy.org/doc/scipy/reference/tutorial