Python for scientific research
Number crunching using `NumPy/SciPy`

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What we've done so far

1. Declare variables using built-in data types and execute operations on them

2. Use flow control commands to dictate the order in which commands are run and when

3. Encapsulate programs into reusable functions, modules and packages

4. **Next**: Introducing the popular `NumPy` and `SciPy` packages

Motivation

- We are typically faced by numerical tasks, such as, computing Pearson's correlation coefficient or generating random numbers

- The NumPy (numeric python) package provides a comprehensive set of mathematical data structures (e.g vector, matrix) and functions (e.g trigonometry, random number generator)

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  - Statistics (e.g correlation coefficient)
  - Signal processing (e.g Fourier transform, filtering)
  - Solving differential equations
  - Optimisation
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A taste of NumPy

```python
import numpy as np

# 1D array/vector
x = np.array([1, 2, 3, 4])
x.min() # return min of array
x.max() # return max of array
x.sum() # sum all elements in array

# 2D array/matrix
x = np.array([[1, 2, 3, 4], [5, 6, 7, 8]])
x*x # element-element-multiplication
x.shape # return dimensions of matrix
np.dot(x, x.transpose()) # matrix multiplication
```

A taste of NumPy

```python
# Generate random numbers
np.random.rand() # from a uniform distribution
np.random.randn() # from a normal distribution
np.random.randn(5, 5) # 5 x 5 matrix of random numbers

# Create number sequences
np.arange(0, 1, 0.1) # 0 to 1 in steps of 0.1
np.linspace(0, 1, 100) # 100 values between 0 and 1
np.logspace(0, 1, 10) # 10 values between 10^0 and 10^1
```

A taste of SciPy

```python
import scipy.stats

# Create two random arrays
x1 = np.random.randn(30)
x2 = np.random.randn(30)

# Correlation coefficientss
scipy.stats.pearsonr(x1, x2) # pearson correlation
scipy.stats.spearmanr(x1, x2) # spearman correlation
scipy.stats.kendalltau(x1, x2) # kendall correlation

# Statistical tests
scipy.stats.ttest_ind(x1, x2) # independent t-test
scipy.stats.mannwhitneyu(x1, x2) #  Mann-Whitney rank test
scipy.stats.wilcoxon(x1, x2) # Wilcoxon signed-rank test

# Least-squares regression
scipy.stats.linregress(x1, x2)
```

Predator prey equations (Lotka Volterra)

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \alpha x - \beta xy$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = -\gamma y + \delta xy$$

Where:

x: is the number of prey (e.g rabbits)

y: is the number of predators (e.g foxes)

α: prey growth rate in the absence of predators

β: dying rate of prey due to predation

γ: dying rate of predators in the absence of prey

δ: predator growth rate when consuming prey

Predator prey equations in Python

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \alpha x - \beta xy$$

$$\frac{\mathrm{d}y}{\mathrm{d}t} = -\gamma y + \delta xy$$

```python
def predator_prey(x, t):
    """
    Predator prey model (Lotka Volterra)
    """
    # Constants
    alpha = 1
    beta = 0.1
    gamma = 1.5
    delta = 0.075

    # Define differential equation (x = x[0], y = x[1])
    dx_dt = alpha*x[0] - beta*x[0]*x[1]
    dy_dt = -gamma*x[1] + delta*x[0]*x[1]

    return dx_dt, dy_dt
```

Solve differential equations

```python
from scipy.integrate import odeint

time = np.linspace(0, 35, 1000) # time vector
init = [10, 5] # initial condition: 10 prey, 5 predators
x = odeint(predator_prey, init, time) # solve
```

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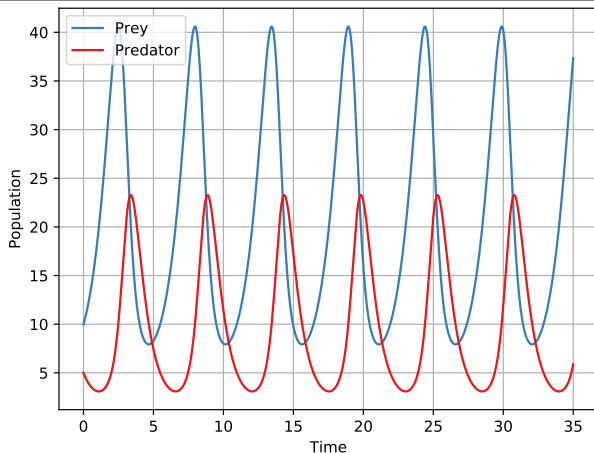
Fourier transform

```python
from scipy.fftpack import fftfreq, fft

# Create frequency vector
N = len(time)
freq = fftfreq(N, np.mean(np.diff(time)))
freq = freq[range(int(N/2))]

# Compute Fast Fourier Transform
y = fft(x[:, 0])/N # compute and normalise fft
y = y[range(int(N/2))] # keep only positive frequencies
```

Fourier transform