Python for scientific research

Number crunching with `NumPy` and `SciPy`

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Speedy express

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. Use string manipulation and regex to work with textual data
5. Interact with the file system
6. **Next**: Number crunching using `NumPy/SciPy`

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A taste of NumPy: vectors

- Example of a NumPy vector

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import numpy as np

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- Easy, however, to cast `np.ndarray` to a list

```python
x_list = list(x) # [1, 3, 4, 2 ]
x_list.reverse() # now x_list is [2, 4, 3, 1]
```

A taste of NumPy: matrices and linear algebra

- Specifying the matrix:

$$\mathbf{x} = \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

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np.dot(x, x) # matrix multiplication (dot product)
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# calculate eigenvalues and right eigenvectors
eival, eivec = np.linalg.eig(x)
# eigenvalues (eival):
# [-0.37228132  5.37228132]
# [-0.37228132  5.37228132]
#
# eigenvectors (eivec):
# [-0.82456484 -0.41597356]
# [ 0.56576746 -0.90937671]]
```

Numpy: number sequences

- Functions to create evenly spaced sequences of numbers:

```
# 0 to 1 (but not including 1) in steps of 0.1
np.arange(0, 1, 0.1)

# 100 evenly spaced values between 0 and 1 (including
    1)
np.linspace(0, 1, 100)

# 10 evenly spaced values between 10^0 and 10^1 (log
    scale)
np.logspace(0, 1, 10)
```

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- Random numbers using `numpy.random.default_rng`:

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# uniform distribution
rng_obj.uniform(size=5)

# normal distribution
rng_obj.normal(size=10)

# random integers from 0 to 9 (in this case: returns a
    5x5 matrix)
rng_obj.integers(low=0, high = 10, size=(5,5))
```

A taste of SciPy

- Basic statistics provided by `scipy.stats`
- For more advanced statistical tests (e.g., GLM, GLMM), check out the `statsmodels` package

```
import scipy.stats as sp

# Create two random arrays
x1 = rng_obj.normal(size=30)
x2 = rng_obj.normal(size=30)

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

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

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

Predator prey equations (Lotka Volterra)

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \alpha u - \beta uv$$

$$\frac{\mathrm{d}v}{\mathrm{d}t} = -\gamma v + \delta uv$$

Where:

- u: is the number of prey (e.g rabbits)
- v: 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

$$\frac{\mathrm{d}u}{\mathrm{d}t} = \alpha u - \beta uv$$

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

    # x = [u, v] describes prey and predator populations
    u, v = x

    # Define differential equation (u = x[0], v = x[1])
    du = alpha*u - beta*u*v
    dv = -gamma*v + delta*u*v

    return du, dv
```

Solve differential equations

```
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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plt.plot(time, x[:,0],"r", time, x[:,1], "b")
plt.xlabel("Time")
plt.ylabel("Population size of predator and prey")
fig.savefig("graph.pdf")
```
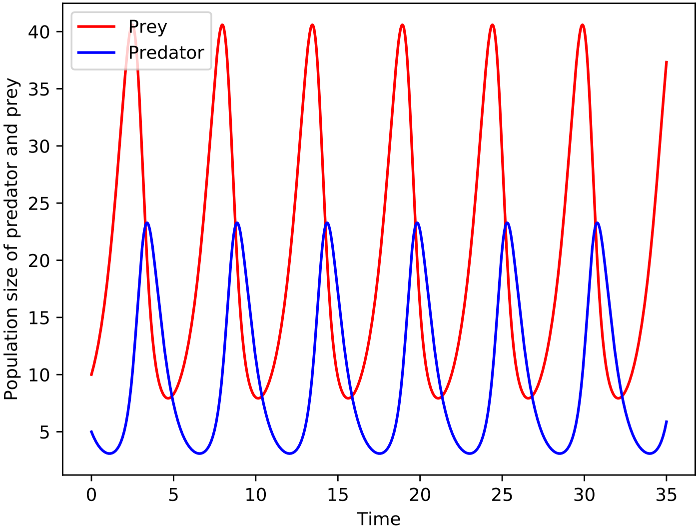

Solve differential equations: resulting graph



Fourier transform

```
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
```

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