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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1 import numpy as np
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3 # 1D array/vector
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```
1 x_list = list(x) # [1, 3, 4, 2 ]
2 x_list.reverse() # now x_list is [2, 4, 3, 1]
```

A taste of NumPy: matrices and linear algebra

- Specifying the matrix:

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6 np.dot(x, x) # matrix multiplication (dot product)
```

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8
9  # calculate eigenvalues and right eigenvectors
10 eival, eivec = np.linalg.eig(x)
11 # eigenvalues (eival):
12 # [-0.37228132  5.37228132]
13 # [-0.37228132  5.37228132]
14 #
15 # eigenvectors (eivec):
16 # [-0.82456484 -0.41597356]
17 # [ 0.56576746 -0.90937671]]
```

Numpy: number sequences

- Functions to create evenly spaced sequences of numbers:

```
1 # 0 to 1 (but not including 1) in steps of 0.1
2 np.arange(0, 1, 0.1)
3
4 # 100 evenly spaced values between 0 and 1 (including
      1)
5 np.linspace(0, 1, 100)
6
7 # 10 evenly spaced values between 10^0 and 10^1 (log
      scale)
8 np.logspace(0, 1, 10)
```

Numpy: random numbers

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

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7  rng_obj = default_rng(seed=3434)
8
9  # uniform distribution
10 rng_obj.uniform(size=5)
11
12 # normal distribution
13 rng_obj.normal(size=10)
14
15 # random integers from 0 to 9 (in this case: returns a
       5x5 matrix)
16 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

```
1  import scipy.stats as sp
2
3  # Create two random arrays
4  x1 = rng_obj.normal(size=30)
5  x2 = rng_obj.normal(size=30)
6
7  # Correlation coefficientss
8  sp.pearsonr(x1, x2) # pearson correlation
9  sp.spearmanr(x1, x2) # spearman correlation
10 sp.kendalltau(x1, x2) # kendall correlation
11
12 # Statistical tests
13 sp.ttest_ind(x1, x2) # independent t-test
14 sp.mannwhitneyu(x1, x2) #  Mann-Whitney rank test
15 sp.wilcoxon(x1, x2) # Wilcoxon signed-rank test
16
17 # Least-squares regression
18 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

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

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

```python
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

```
1 from scipy.integrate import odeint
2
3 time = np.linspace(0, 35, 1000) # time vector
4 init = [10, 5] # initial condition: 10 prey, 5 predators
5 x = odeint(predator_prey, init, time) # solve
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20 plt.xlabel("Time")
21 plt.ylabel("Population size of predator and prey")
22 fig.savefig("graph.pdf")
```
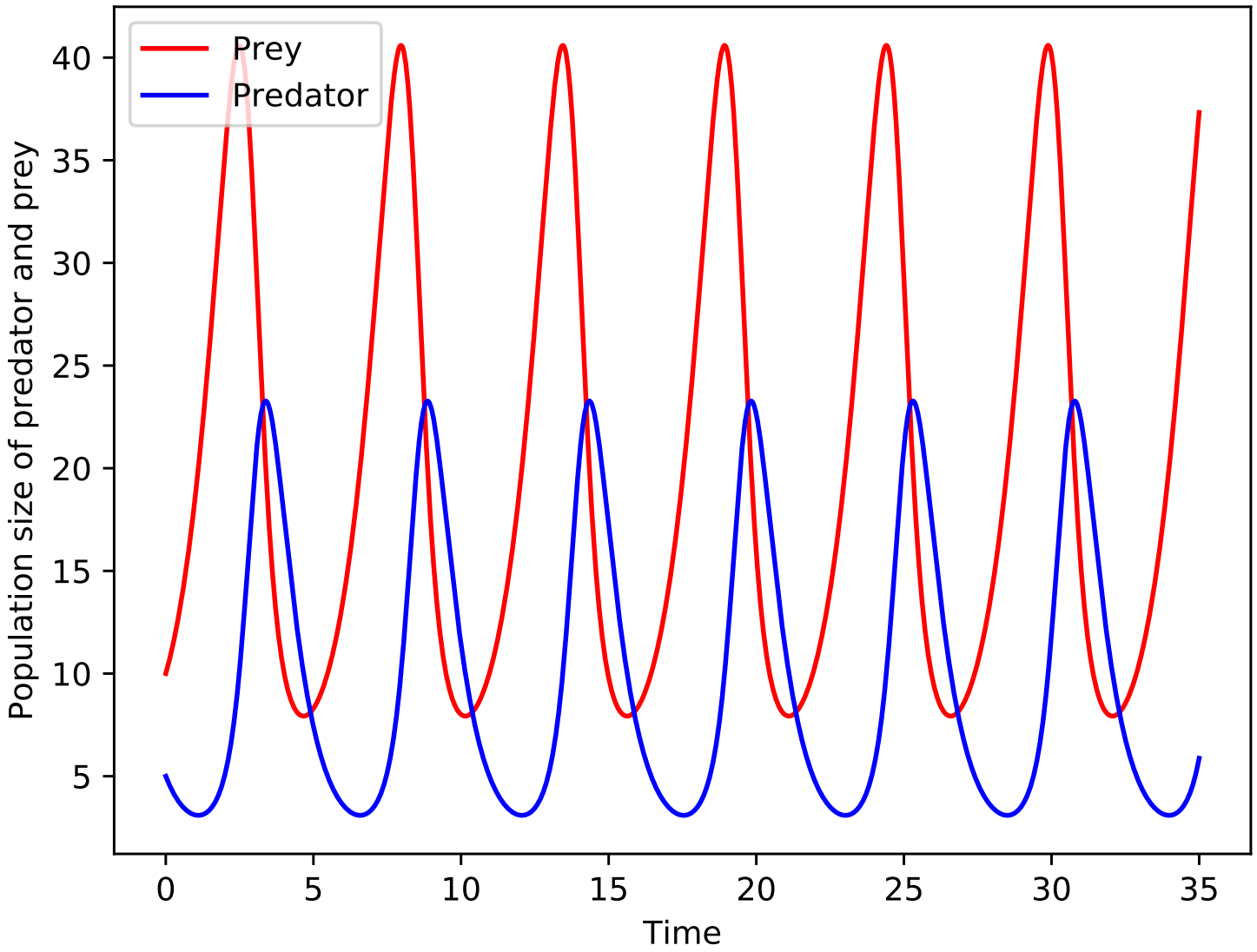

Solve differential equations: resulting graph



Fourier transform

```
1  from scipy.fftpack import fftfreq, fft
2
3  # Create frequency vector
4  N = len(time)
5  freq = fftfreq(N, np.mean(np.diff(time)))
6  freq = freq[range(int(N/2))]
7
8  # Compute Fast Fourier Transform
9  y = fft(x[:, 0])/N # compute and normalise fft
10 y = y[range(int(N/2))] # keep only positive frequencies
```

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