Python for Scientific Computing

Lecture 2: Data Structures

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Review π

$$\pi = 2 \prod_{i=1}^{\infty} \frac{4i^2}{4i^2 - 1}$$

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```
1  pi = 2.
2  for i in range(1,n):
3     pi *= 4.*i**2 / (4.*i**2 - 1)
4  print pi
```

Containers

- tuples, lists and strings
  - Elements are accessed with `container[ ]`
    - Indexed starting at 0
  - Arguments for `len(container)`
  - Each type has special features

Tuples

- Tuple = (1,3.,'red')
- Contain *references* to other objects
- The structure cannot be changed
- A convenient way to pass multiple objects
  - Packing and un-packing

Lists

- List = `['red','green','blue']`
- Resizable
- List-of-Lists is a multi-dimensional list
- Lists are not arrays
- `range()` is a list

Dictionaries

- Key - value pairs

  Protons = {'Oxygen': 8, 'Hydrogen': 1}

  Protons['Carbon'] = 6

  - Any type can be a key or value
  - Look-up tables
  - Sorting and searching operations

Indexing Lists and tuples

- Slicing just like Fortran 90

  L[start : stop : stride]

  $\text{start} \leq i < \text{stop}; i+ = \text{stride}$
- Negative indices start at the end of the list
  - -1 is the last element

Other operations

- Search for value with `in`
- Concatenate with `+` or `*`
- Count number of occurrences

Loops

- Iterate over any sequence
  - string, list, keys in dictionary, lines in file

```
1  vowels = 'aeiouy'
2  for i in 'orbital':
3      if i in vowels:
4          print(i)
```

Loops

- Keep a counter

```
1  shells = ('s', 'p', 'd', 'f')
2  for index, thisShell in enumerate(shells):
3      print index, thisShell
```

Loops

- List comprehension

```
1  even = [i for i in range(100) if i%2 == 0]
2
3  listX = [-1, 0, 1]
4  listY = [2, 4]
5  myTuple = [(x,y) for x in listX for y in listY]
```

Mutability of objects

- Immutable objects get created and destroyed upon assignment and collection
  - Strings
  - Numbers (no $++$ operator)
  - Tuples
- Mutable objects create references to contained objects upon assignment
  - Lists
  - Dictionaries

Hands-on: Mutability

Tuples or Lists?

- List: homogeneous data
  - Elements can be added or deleted
  - Elements can be in any order
  - Mutable

- Tuples: heterogeneous data (`structs`)
  - Constant size
  - Order matters
  - Immutable

Container examples

- List
  - Particles
  - Lines in an input file
- Tuple
  - Position data
- Dictionary
  - Associated lists
  - Look-up tables
  - Histograms
  - Networks
  - Graphs

Functions

- Doc strings
- Default values
- Optional arguments
- Returns

Functions

```
1  def divide(x,y):
2    """Divide takes two integers as input
3    returns a tupe of quotient and remainder"""
4    return x/y,x%y
```

Mathematical Exercises

- Write a function to differentiate another function

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

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- $f(x)$ and h are arguments
  - make $h = 0.01$ the default value
- Practice with the following functions
  - $f(x) = x^2$ at $x = 1$
  - $f(x) = cos(x)$ at $x = 2\pi$
  - $f(x) = e^{-2x^2}$ at $x = 0$

recursions

$$n! = \prod_{k=1}^{n} k$$

```
1  def factorial(n):
2    if(n==0):
3      return 1
4    return n*factorial(n-1)
```