

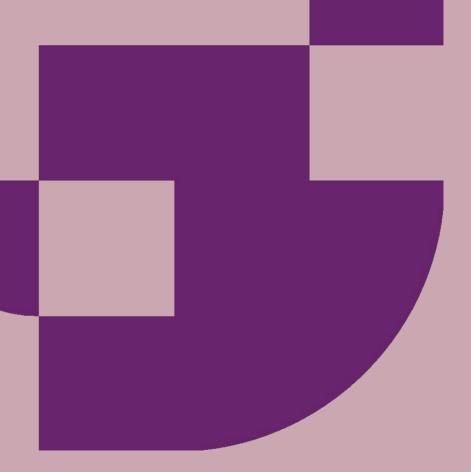
Intermediate Python

Teachers: Dmitry Nikolaenko, Samantha Finnigan

Assistant: Jordan Byers

Advanced Research Computing, Durham University

June 12, 2023



Welcome and icebreaker

- Thank you for joining!
- 2-hours course (10am-12pm); a coffee-break for 10 minutes
- Icebreaker introduction
- Link to the exercises for today: <u>Exercises link</u>





Course structure

- 'Beginners Python' recap
 - variables, lists, control flow statements, and functions
- 'Pythonic' concepts
 - List comprehension, ternary expressions, *args and **kwargs
 - Lambda functions
- More advanced string manipulation
- Introduction to libraries and modules
- Data structures and containers
 - Mutability
- Brief introduction to classes





Python Setup

- In this lesson, we will be using Python 3
- As an interactive computing environment to run Python exercises, there are several options:
 - a web-based interactive environment: jupyter notebook
 - the standard interactive shell: *python*
 - an enhanced interactive shell: *ipython*





Recap(a): Python fundamentals

- **Variables**: a name for a value ([A-Za-z0-9_], case-sensitive)
 - # this is a comment
- Basic data types: integers, floating-point numbers, strings, bool
 - pi = 3.14, n = 5, name = "John"
 - n = n + 1, n += 1
 - str(37), float('3.14'), int(pi)
 - Expressions and operators: +, -, *, /, //, %, **
 - Assignment statements:

•
$$w = x = y = z = 0 \# chain assignment$$

- Built-in functions: type, print, input, eval, int, float, str, len, range, ...
 - print(type(str(1.234)))
 - value1 = eval(input('Please enter a number: '))





 $^{\circ}C = \frac{5}{9} \times (^{\circ}F - 32)$

Recap(b): Lists

- List: a mutable sequence type
- Holds a collection of objects in a defined order (indexed by integers)
- A user-friendly <u>data container</u> to store objects of any type, even a mix of types
- Dynamic type system:
 - no need to declare the type of a variable explicitly

```
random_stuff = [1, 'apples', 3.14, ['Mars', 'Venus', 'Pluto']]
print(random_stuff[3][2])
Pluto
```

Appending to lists:

```
chem_elements = ["oxygen"]
for i in range(2):
    chem_elements.append("hydrogen")
print(chem_elements)
```

Easy to process lists in for loops (in the next slides)



```
L = [1, 2, 3, 4, 5]
print(type(L))
<class 'list'>
```



Recap(b): Lists (cont.), similarities to strings

- len function: the number of items in a list/string
- in operator: tells if a list/string contains something
- + and * operators: concatenating and repeating

```
[7,8]+[3,4,5] [0]*5
[7, 8, 3, 4, 5] [0, 0, 0, 0, 0]
```

Indexing: simple to "grab" an item/character in a list/string if you know where it sits:

```
L = ['a','b','c','d','e','f','g','h','i','j']
print(L[4])
```

е

- Slicing: use: to "grab" a range defined subsection of a list/string:
- Looping:



```
for i in range(len(L)):
    print(L[i])

for item in L:
    print(item)
```

```
L = "abcdefghii"
                                 The :stop value
print(L[4])
                              represents the first
                                 value not in the
                                       slice
   start=3
   stop=7
    print(L[start:stop]) # items start to stop-1
    ['d', 'e', 'f', 'q']
    print(L[start:]) # items start to the end of list
    ['d', 'e', 'f', 'q', 'h', 'i', 'j']
    print(L[:stop]) # items from beginning of list to stop-1
    ['a', 'b', 'c', 'd', 'e', 'f', 'g']
    print(L[:]) # whole list
    ['a', 'b', 'c', 'd', 'e', 'f', 'g', 'h', 'i', 'j']
```

Recap(c): Control Flow

Conditional statements:
 if, elif, else

```
grade = eval(input( ' Enter your score: ' ))
if grade>=90:
    print('A')
elif grade>=80:
    print('B')
else:
    print('C')
```

 Loop control statements: break, continue

```
a = ['Mary', 'had', 'a', 'little', 'lamb', '.']
for i in range(len(a)+2):
    if(i < len(a)):
        print(i, a[i])
    elif (i == len(a)):
        print("The sentence has ended,")
        continue #break
    else:
        print("The end.")</pre>
```

Loop statements: for, while

```
for i in range(10):
    print(i)
    i=0
    while i<10:
        print(i)
        i=i+1</pre>
```

Nested loops

```
for x_axis in range(2):
    for y_axis in range(2):
        print('(' + str(x_axis) + ',' + str(y_axis) + ')')
```

Range objects:

range(stop), range(start, stop[, step])

```
range(5)
range(0, 5)

list(range(5))

[0, 1, 2, 3, 4]

list(range(1,10,2))

[1, 3, 5, 7, 9]
len(random_stuff)

4
```





Recap(c): Control Flow (cont.), iterators

But what is the *for* loop doing under the hood?

 iter() is called on the container object returning an <u>iterator object</u>

'h'

- The <u>iterator object</u> defines a <u>__next__()</u> function which facilitates access to elements one at a time
- 3. __next__() tells for loop when there are no more elements raising *StopIteration* exception

```
uni = 'Durham'
                                                 next(it)
             it = iter(uni)
                                                 'a'
             <str iterator at 0x7f1208f38f70>
                                                 next(it)
             next(it)
             ים י
                                                 next(it)
             next(it)
             'u'
                                                                                               Traceback (most recent call last)
                                                 StopIteration
                                                 <ipython-input-31-bclab118995a> in <module>
             next(it)
Durham
                                                 ----> 1 next(it)
  University
                                                 StopIteration:
             next(it)
```

Recap(d): Functions

- Principle of encapsulation
 - Enables maintainability and readability alongside complexity
 - Reusable code

def name (parameter list):

- Why to write functions:
- It is difficult to write correctly
- It is difficult to debug
- It is difficult to extend

- Important parts of function definition:
 - Name
 - Parameters
 - Body
 - Indentation

```
# function definition
def increment(number):
    number += 1
    new_number = number
    return new_number

# function invocation
print("4+1 =", increment(4))

4+1 = 5
```

```
# only function invocation
from math import sqrt
print(sqrt(16.0))
4.0

sqrt

4
```



- Every Python function has two aspects:
 - 1) Function definition
 - 2) Function invocation





Building on the above(a): *args and **kwargs

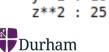
Collecting an arbitrary number of arguments into a tuple, when number of arguments is unknown, *args:
 def product(*nums):

def product(*nums):
 prod = 1
 for i in nums:
 prod*=i
 return prod
print(product(3,4), product(2,3,4), sep=' ')
12 24

Collecting an arbitrary number of keyword arguments into a dictionary,
 **kwarqs:

```
def f(**kwargs):
    for k in kwargs:
        print(k, '**2 : ', kwargs[k]**2, sep='')
f(x=3, y=4, z=5)
```

```
x**2 : 9
y**2 : 16
z**2 : 25
```



University

```
def f(**kwargs):
    for key, value in kwargs.items():
        print(key, "=", value, sep='', end=", ")
f(x=3, y=4, z=5)
x=3, y=4, z=5,
```

Building on the above(b): more on expressions and lists

Ternary expressions

```
hungry = True
state = "grumpy" if hungry else "content"
print(state)
grumpy
```

List comprehension

```
multiples_of_three = [i for i in range(20) if i%3==0]
print(multiples_of_three)

[0, 3, 6, 9, 12, 15, 18]
```

List methods (more after exercise)

```
L = [33, 84, 57, 11, 29, 0, 57]

L.remove(57)

print(L)

[33, 84, 11, 29, 0, 57]

L.remove(57)

print(L)

[33, 84, 11, 29, 0]
```





Exercises

Ask us questions!





Building on the above(c): list methods

- Inserting an element
- Reversing
 - Note: reversed() returns a 'reverse iterator' that then needs to be turned back into a list with list()
- Sorting
- Searching
- Emptying

University

- Removing duplicates
 - by converting list→set→list
- Note: As we can see from examples, some functions actively modified whereas some returned a copy of the modified list

 Durham

```
L = [33, 84, 11, 29, 0]
L.insert(2, 57)
print(L)
[33, 84, 57, 11, 29, 0]
```

```
print(list(reversed(L)))
[0, 29, 11, 57, 84, 33]
```

```
print(sorted(L))
[0, 11, 29, 33, 57, 84]
```

```
if 57 in L:
    position = L.index(57)
    print("57 is in the list. "
        "It is at position", position)
```

57 is in the list. It is at position 2

```
print(L.clear())
```

None

```
L2 = [1, 2, 2, 2, 3, 3]
print(list(set(L2)))
```





Building on the above (d): lambda functions

- Lambda functions for compact inline function definitions
- Useful when you don't want to use a function twice

lambda arguments : expression

Or more generally:

Functionally equivalent

```
somefunc = lambda a1, a2, ...: some_expression
```

def somefunc(a1, a2, ...):
 return some_expression

Example

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

```
def diff2(f, x, h=1E-6):
    r = (f(x-h) - 2*f(x) + f(x+h))/float(h*h)
    return r
```

```
def f(x):
    return x**2 - 1

df2 = diff2(f,1.5)
print(df2)
```



```
df2 = diff2(lambda x: x**2-1,1.5)
print(df2)
```

1.999733711954832



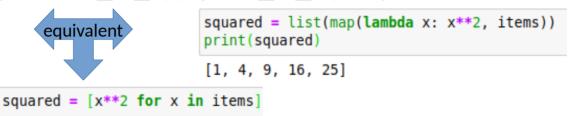


Building on the above (d): lambda functions (cont.)

Map applies a function to all the items in an iterable:

map(function_to_apply, list_of_inputs)

```
items = [1, 2, 3, 4, 5]
squared = []
for i in items:
     squared.append(i**2)
print(squared)
```



• **Filter** creates a list of elements for which a function returns true:

Note: **list comprehensions** can accomplish everything what **map** and **filter** do

```
number_list = range(-5, 5)
less_than_zero = list(filter(lambda x: x<0, number_list))
print(less_than_zero)

def is_less_than_zero(x):
    return True if x<0 else False

negative_nums = []
for num in number_list:
    if is_less_than_zero(num):
        negative_nums.append(num)
print(negative_nums)

negative_nums = [num for num in number_list if num < 0]
print(negative_nums)

[-5, -4, -3, -2, -1]</pre>
```



Mastering strings (a)

- Adjusting case
- Formatting strings
 - Note: Modification requires assignment, because these functions return a copy, not modifying the original string

```
line = "the quick brown fox jumped over a lazy dog"
print(line.find('fox'))
print(line.startswith('the'))
print(line.endswith('fox'))
print(line.replace('brown', 'red'))
print(line.split())
try:
    index = line.index('bear')
    print(index)
except ValueError:
    print("A bear isn't mentioned in the text")
```

```
16
True
False
the quick red fox jumped over a lazy dog
['the', 'quick', 'brown', 'fox', 'jumped', 'over', 'a', 'lazy', 'dog']
A bear isn't mentioned in the text
```



```
arc_update = "ThE HAmILton suPercompUTER is beiNg UPGraded"
print(arc_update.upper())
print(arc_update.title())
print(arc_update.capitalize())
print(arc_update)
arc_update = " RSE "
print(arc_update.strip())
print(arc_update.rstrip())
print(arc_update.lstrip())
```

arc

```
THE HAMILTON SUPERCOMPUTER IS BEING UPGRADED
RSE
RSE
```

- Find() and index(): return index of a substring, but the latter raises a ValueError exception when not found (exception handling)
- Querying the existence, replacing, splitting

Mastering strings (b)

The canonical way to search a string (if not interested in the index) is very simple:

```
line = "the quick brown fox jumped over a lazy dog"
if "fox" in line:
    print("A fox has been seen")
```

A fox has been seen

F-strings provide a way to embed expressions inside string literals, using a minimal

syntax

 expressions are evaluated at runtime and replaced with their values

```
interests = ["football", "zoom"]
print(f"Bob enjoys {interests[0]} and {interests[1]}")

weekdays = ['Mon', 'Tue', 'Wed', 'Thu', 'Fri']
for weekday in weekdays:
    print(f"Today is {weekday}")

age = 70
print(f"Soon I'll be {age+1}!")

Bob enjoys football and zoom
Today is Mon
Today is Tue
Today is Tue
Today is Thu
Today is Fri
Soon I'll be 71!
```





Exercises

Ask us questions!





Modules

Several ways of importing modules:

```
import os, sys, time # several modules at once
import numpy as np # changing module name
import math # the whole module

import module list

print(math.sqrt(16.0))

• Another example

from module import function list
```

```
from math import sqrt # only specific functions from a module
print(sqrt(16.0))

from math import * # all functions from a module
from math import log as ln # changing function name
```





Some standard and 3rd-party modules

- math: contains familiar math functions including:
 - sin, cos, tan, exp, log, log10, factorial, sqrt, floor, ceil
- numpy: fundamental package for scientific computing
 - a multidimensional array object, various derived objects (such as masked arrays and matrices), and an assortment of routines for fast operations on arrays, including mathematical, logical, shape manipulation, sorting, selecting, I/O, discrete Fourier transforms, basic linear algebra, basic statistical operations, random simulation and much more
- scipy: a collection of mathematical algorithms and convenience functions built on the NumPy extension
 - high-level commands and classes for the manipulation and visualization of data
- matplotlib: library for plotting
- sympy: symbolic computations
- Other useful modules: os, random, itertools, time, datetime and many more
- Durham
- Python comes with a program called *pip* which will automatically fetch packages released and listed on PyPI: *pip install <some-module>*

Other useful modules in the standard library

Tools for interfacing with the operating system: **os**

Facilitates portability

```
import os
root = "/Users"
print(os.path.join(root, os.environ["USER"], "holiday_planning"))
# out /Users/kgkc25/holiday_planning
os.listdir("Desktop")
if not os.path.exists("blahblah.txt"):
    print("File not found")
    exit(1)
```

Very useful when processing multiple data files





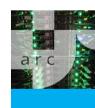
Using the csv module (part 1)

- Very convenient module for parsing and writing csv files
- Writing a csv

```
import csv

with open("example.csv", "w") as out_f:
    writer = csv.writer(out_f, delimiter=",")
    writer.writerow(["x_axis", "y_axis"])
    x_axis = [x * 0.1 for x in range(0, 100)]
    for x in x_axis:
        writer.writerow([x, math.cos(x)])
```





For the sake of visualization, here is the first part of the csv we just made:

x_axis	y_axis
0	1
0.1	0.99500417
0.2	0.98006658
0.3	0.95533649
0.4	0.92106099
0.5	0.87758256
0.6	0.82533561
0.7	0.76484219
0.8	0.69670671
0.9	0.62160997
1	0.54030231
1.1	0.45359612
1.2	0.36235775
1.3	0.26749883
1.4	0.16996714
1.5	0.0707372





Using the csv module (part 2)

 Now let's extract the value for y_axis when x_axis is 1.0 for the csv we just wrote:

```
import csv
with open("example.csv", "r") as in_file:
    reader = csv.reader(in_file, delimiter=",")
    next(reader) # skip header
    for row in reader:
        if row[0] == "1.0":
            print(row[1])
            break
# out: 0.5403023058681398
```





- Dictionaries: flexible mappings of keys to values
 - an unordered collection of key-value pairs
 - dictionary items are colon-connected (:) key-value pairs
 - an associative container permitting access based on a key (not an index)

```
capitals = {'Norway':'Oslo','Sweden':'Stockholm','France':'Paris'}
# capitals = dict(Norway='Oslo', Sweden='Stockholm', France='Paris') # the same
capitals['Germany'] = 'Berlin' # instead of append() for list
for country in capitals:
    print(f'The capital of {country} is {capitals[country]}')
```

```
The capital of Norway is Oslo
The capital of Sweden is Stockholm
The capital of France is Paris
The capital of Germany is Berlin
```





- Sets: unordered collections of unique elements
 - represents a mathematical set
 - curly braces (♂) enclose the elements of a literal set

```
S = {10, 3, 7, 2, 11}
S {2, 3, 7, 10, 11}
```

```
L = [10, 13, 10, 5, 6, 13, 2, 10, 5]
S = set(L)
L
```

[10, 13, 10, 5, 6, 13, 2, 10, 5]

```
S
```

{2, 5, 6, 10, 13}





- Tuples: immutable sequences
 - essentially a constant list which can't be changed

```
t = (2, 4, 6, 'temp.pdf')
t = 2, 4, 6, 'temp.pdf' # can skip parentheses
t

(2, 4, 6, 'temp.pdf')
```

much of the same functionality as lists, including indexing and slicing

```
t = t + (-1.0, -2.0)
t
(2, 4, 6, 'temp.pdf', -1.0, -2.0)
t[1] t[3:]
4 ('temp.pdf', -1.0, -2.0) True
```

<u>Lists</u> are typically for homogeneous data sequences (ingredients, names)
 whereas <u>tuples</u> are ideal for heterogeneous data (entries with different meanings)

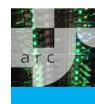


- Namedtuple is handy, but also <u>immutable</u>
- Namedtuple is a factory function for making a tuple class
 - In the example, NINumber becomes a factory function that can encapsulate data from any employee

```
from collections import namedtuple
NINumber = namedtuple('national_insurance_number', 'name NI')
employee_data = NINumber('Simon', '12345678')
print(f'Employee {employee_data.name} has NI: {employee_data.NI}')
```



```
# assignment creates error!
# employee_data.NI = '4444'
```



Very brief introduction to classes

Class = code template (like previously seen factory function)

```
class FootballTeam:
    players = ['Kane', 'Sterling', 'Pickford']
    def get_players(self):
        return self.players
england_team = FootballTeam()
print(england_team.get_players())
# out: ['Kane', 'Sterling', 'Pickford']
```



Very brief introduction to classes

We can generalise the template



```
class Football Team:
    def __init__(self, players):
        self.players = players
    def get_players(self):
        return self.players
england_team = FootballTeam(["Kane", "Sterling", "Pickford"])
print(england_team.get_players())
# out: ['Kane', 'Sterling', 'Pickford']
spanish_team = FootballTeam(["Moreno", "Llorente"])
print(spanish_team.get_players())
# out: ['Moreno', 'Llorente']
```





Very brief introduction to classes

We can encapsulate complexity

```
class FootballTeam:
    def __init__(self, players):
        self.players = players
    def make_substitution(self, player_off, player_on):
        self.players = [player if player != player_off else player_on
                        for player in self.players]
    def get_players(self):
        return self.players
england_team = FootballTeam(["Kane", "Sterling", "Pickford"])
print(england_team.get_players())
# out: ['Kane', 'Sterling', 'Pickford']
england_team.make_substitution("Kane", "Grealish")
print(england_team.get_players())
# out: ['Grealish', 'Sterling', 'Pickford']
```





Exercises

Ask us questions!







Thank you!

- Feedback would really be appreciated: https://bit.ly/arc_trainingfeedback
- Other training courses at ARC
- RSE support

Solutions to the exercises can be found here:

Solutions link

