Python and Programming 1

Programming basics and algorithms

Dr.ir. Ivo Roghair, Prof.dr.ir. Martin van Sint Annaland

Chemical Process Intensification group Eindhoven University of Technology

Numerical Methods (6E5X0), 2023-2024

Today's outline

- Introduction
 - General programming
 - First steps
 - Further reading
- Data structure:
 - Data types
 - Lists
 - Strings
 - Tuples
 - Dictionaries
- Control flow
 - Loops
 - Branching

- Functions
 - Defining functions
 - Recursion
 - Scope
 - Lambda functions
- Modules
 - Using modules
 - Math module
 - The random module
- Conclusions
- Exercises



Why should you learn something about programming?

- Scientific analyses depend more than ever on computer programs and simulation methods
- Knowledge of programming allows you to automate routine tasks
- Ability to understand algorithms by inspection of the code
- Learn to think by dissecting a problem into smaller, easier to solve, parts









Introduction to programming

What is a program?

Introduction

A program is a sequence of instructions that is written to perform a certain task on a computer.

 The computation might be something mathematical, a symbolic operation, image analysis, etc.

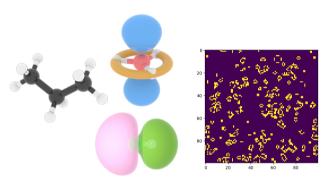
Program layout

- 1 Input (Get the radius of a circle)
- Operations (Compute and store the area of the circle)
- 3 Output (Print the area to the screen)



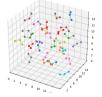
 Introduction
 Data structures
 Control flow occood
 Functions occood
 Modules occood
 Conclusions occood
 Exercises occood

Versatility of Python



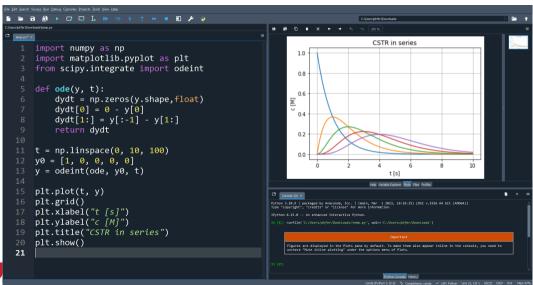
```
A melyany ("Obsergine Orden champement on a particular party ("Obsergine Orden champement on a party of the champement o
```







Versatility of Python: ODE solver





Versatility of Python: Image analysis

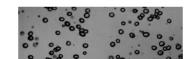
```
# Importing necessary libraries
import numpy as np
from scipy import ndimage
from PIL.Image import fromarray
from skimage import io, color, feature, measure

# Loading and processing image
I = io.imread('bub0.png')
BW = color.rgb2gray(I)
E = feature.canny(BW)
F = ndimage.binary_fill_holes(E)

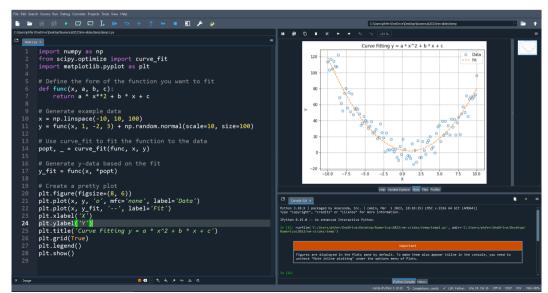
# Show final image
fromarray(F).show()
```







Versatility of Python: Curve fitting



Getting started

Introduction

- Start the Python REPL (read-eval-print loop) by running python or ipython
- Enter the following commands on the command line. Evaluate the output.

```
>>> 2 + 3  # Some simple calculations

>>> 2 * 3

>>> 2 * 3**2  # Powers are done using **

>>> a = 2  # Storing values into the workspace

>>> b = 3

>>> c = (2 * 3)**2  # Parentheses set priority

>>> 10_000_000 / b

>>> print(a)

>>> print(a,b)

>>> print(a,b,c,sep='--')

>>> print("Numerical methods")
```

```
5
6
18
3333333.33333333335
2
2, 3
2--3--36
Numerical methods
```



Printing and formatting results

You can control the formatting of variables in string literals using various methods - we recommend f-strings. Note that formatting only changes how numbers are *displayed*, not the underlying representation.

```
>>> a = 19/4
>>> print("Few digits {:.2f}".format(a)) # 2 decimal places
>>> print("Many digits {:.10f}".format(a)) # 10 decimal places
>>>
>>> b = 22/7
>>> i = 13
>>> print("Almost pi: %1.4f" % b)
>>> print("i = %d, a = %1.4f and b = %1.8f" % (i.a.b))
>>>
>>> # Using f-strings (Pvthon 3.6+)
>>> c = (21)**0.5 # sqrt of 21
>>> print(f"{c:.10f}") # Float with 10 decimal places
>>> mystr = f"{c:.2e}" # Scientific notation with 2 decimal places in a string object
>>> print(mystr) # Print the string object
>>> print(f"{b=}") # Use = to print variable name and value
>>> print(f"{b=:_^15.2}") # Adjust spacing and spacer character
```



A few helpful things

- Using the $\ \ \$ and $\ \ \$ keys, you can cycle through recent commands
- Typing part of a command and pressing Tab completes the command and lists the possibilities
- If a computation takes too long, you can press ctrl + c to stop the program and return to the command line. Stored variables may contain incomplete results.
- Sequences of commands (programs, scripts) are contained as py-files, plain text files with the .py extension.
- Python scripts (and notes/markdown) can also be contained in jupyter notebooks, which have extension .ipynb.
- Such py-files must be in the *current working directory* or in the Python *path*, the locations where Python searches for a command. If you try to run a script that is not in the path, Python will throw an Exception/Error.
- Anything following a # symbol is regarded as a comment
- There are several keyboard shortcuts (vary with text editor) that will make coding much more efficient.

Scripts, notebooks and REPL

- The REPL, indicated by the >>> prompt, has the advantage of immediate result after typing a command.
- Larger programs are better written in separate files; either Jupyter notebooks (.ipynb files) or plain script files (.py files).
- Defining functions in such files will put them in the scope, but will not run them until they are actually called.
- The snippets in these slides will continue to use the REPL for single-line commands, and move towards scripts when larger functions are being constructed.



Python help, documentation, resources

- Refer to the Python documentation at Official documentation.
 - Try for instance: help(print) or help(help).
- Other packages that we will use:
 - NumPy documentation
 - Matplotlib documentation
 - SciPy documentation
- We supply a number of basic practice/reference modules: Python Crash Course.
- Python Crash Course, 3rd Edition by Eric Matthes
- A Whirlwind Tour of Python by Jake Vanderplas
- Introduction to Scientific Programming with Python by Joakim Sundnes
- Python Programming And Numerical Methods: A Guide For Engineers And Scientists by Kong, Siauw and Bayen
- Search the web, Reddit, YouTube, etc.



Today's outline

- Introduction
 - General programming
 - First steps
 - Further reading
- Data structures
 - Data types
 - Lists
 - Strings
 - Tuples
 - Dictionaries
- Control flow
 - Loops
 - Branching

- Functions
 - Defining functions
 - Recursion
 - Scope
 - Lambda functions
- Modules
 - Using modules
 - Math module
 - The random module
- Conclusions
- Exercises



Terminology

- Variable Piece of data stored in the computer memory, to be referenced and/or manipulated
- Function Piece of code that performs a certain operation/sequence of operations on given input
- Operators Mathematical operators (e.g. + * or /), relational (e.g. < >or ==, and logical operators (and, or)
 - Script Piece of code that performs a certain sequence of operations without specified input/output
- Expression A command that combines variables, functions, operators and/or values to produce a result.



Variables in Python

- Python stores variables in the namespace
- You should recognize the difference between the identifier of a variable (its name, e.g. x, setpoint_p), and the data that it actually stores (e.g. 0.5)
- Python also defines a number of functions by default, e.g. min, max or sum.
 - A list of built-in methods is given by dir(__builtins__)
- You can assign a variable by the = sign:

```
>>> x = 4*3
>>> x
12
```

- If you don't assign a variable, it will be stored in _
- In most text editors, all variables are cleared automatically before the next execution.



Datatypes and variables

Python uses different types of variables:

Datatype	Example
str	'Wednesday'
int	15
float	0.15
list	[0.0, 0.1, 0.2, 'Hello', ['Another','List']]
dict	{'name': 'word', "n": 2}
bool	False
tuple	(True, False)

Everything in Python is an object. You can use the dir() function to query the possible methods on an object of a datatype (e.g. (dir(List)), dir(28) or dir("Yes!")).



Lists in Python (1)

- Lists are containers of collections of objects
- A list is initialized using square brackets with comma-separated elements

```
>>> brands = ['Audi', 'Toyota', 'Honda', 'Ford', 'Tesla']
```

• Lists can contain and mix any object type, even other lists:

```
>>> another_list = [0.0, 0.1, 0.2, 'Hello', brands]
>>> print(another_list)
```

```
[0.0, 0.1, 0.2, 'Hello', ['Audi', 'Toyota', 'Honda', 'Ford', 'Tesla']]
```

• Access (i.e., read) an entry in a list. Note that indexing starts at 0:

```
>>> print(another_list[0],another_list[3])
```

0.0 Hello



Lists in Python (2)

• Manipulate the value of an entry goes likewise:

```
>>> another_list[3] = 'Bye' # Becomes: [0.0, 0.1, 0.2, 'Bye', ['Audi', ...]]
```

• Slicing is used to retrieve multiple elements:

```
>>> another_list[1:4] # This will give the elements from index 1 to index 3
[0.1, 0.2, 'Bye']
```

Lists can be unpacked into individual variables:

```
>>> a,b,c,d,e = brands
>>> print(f"The first list element was {a}, then {b}, {c}, {d} and finally {e}.")
```

The first list element was Audi, then Toyota, Honda, Ford and finally Tesla.

• From here onwards, we will omit the print statements from the slides



Lists in Python (3)

[0, 0, 0, 0, 0, 0, 0, 0, 0, 0]

 Lists can be concatenated or repeated by the addition and multiplication operators respectively:

```
>>> more_brands = ['Nissan','Kia'] + brands

['Nissan', 'Kia', 'Audi', 'Toyota', 'Honda', 'Ford', 'Tesla']

>>> zeros = 10*[0]
```

```
• Find out which methods can be performed on a list by using dir(more_brands):
```

Find out which methods can be performed on a list by using air(more_brands).

```
more_brands.append('Volvo') # Append object (here: string literal) at the end of the list
more_brands.insert(1,'BMW') # Insert object at index 1
more_brands.sort() # Sorts the list in-place
item = more_brands.pop(3) # Removes element at index 3 from the list, stores it as item
```



Lists in Python (4)

Ranges of numbers are set using the range(start=0, stop, step=1) command:

Create a list with a range of numbers:

```
>>> a = list(range(1, 11))  # Creates a list from 1 to 10
```

• List comprehensions can be used to create lists with more complex patterns:

```
>>> x = [i/10 \text{ for i in range}(-10, 11)] # Creates a list from -1 to 1 with a step of 0.1
```

Manipulating multiple components using slicing and a loop:

```
>>> y = list(range(11)) # Creates a list from 0 to 10
>>> for i in [0, 3, 4, 5, 6]:
>>> y[i] = 1
```

• Or (by supplying a list instead of a scalar):

```
>>> y[0:2] = [16, 19] # Sets y[0] to 16 and y[1] to 19
```



Assignment of variables; value or reference

Consider the following code snippets:

```
1 >>> i = 3
2 >>> j = i
3 >>> j = i + 3
4 >>> print(i,j)
5 >>> print(id(i), id(j)) # Print
    memory address of data
```

```
3, 6
8885416 8885544
```

```
1 >>> list_a = ['aa', 1, 'bb', 12, True, 1.618]
2 >>> list_b = list_a
3 >>> list_b[2] = 'cc'
4 >>> print(list_a, list_b, sep='\n')
5 >>> print(id(list_a), id(list_b))
```

```
['aa', 1, 'cc', 12, True, 1.618]
['aa', 1, 'cc', 12, True, 1.618]
140285003056512 140285003056512
```

- Primitive or immutable data types (e.g. int, float, str, tuple) are assigned by value; the value is copied and changes do not affect the original variables.
- Mutable data types (e.g. list, set, dict) are assigned by reference; they are two
 names pointing to the same data, changing one affects the values of the other.



Practice

Given a vector

- Define the vector using range's, without typing all individual elements
- Investigate the meaning of the following commands:

```
>>> x[2]

>>> x[0:5]

>>> x[:-1]

>>> y = x[4:]

>>> y[3]

>>> y.pop(3)

>>> sum(x)

>>> max(x)

>>> min(x)

>>> x[::-1]
```



Strings in Python (1)

Creating a string:

```
>>> s = "Hello, world!"
>>> len(s)
13
```

Accessing a character in a string:

```
>>> s[7]
'w'
```

Getting a substring:

```
>>> s[7:12]
'world'
```

Or separate by whitespace using a string method (see dir(s)):

```
>>> s.split()
['Hello,', 'world!']
```



Strings in Python (2)

Replacing a substring with another string:

```
>>> s.replace('world', 'Python')
'Hello, Python!'
```

Converting to upper and lower case:

```
>>> s.upper()
'HELLO, WORLD!'
>>> s.lower()
'hello, world!'
```

You can combine methods with string literals too:

```
>>> s.replace('WoRlD'.lower(), 'Python')
'Hello, Python!'
>>> s.startswith('hello'.title())
True
```

Finding the starting index of a substring:

```
>>> s.index("world")
7
TUP UNIVERSITY OF TECHNOLOGY
```

Practice

Given a string

```
>>> s = "Python programming is fun!"
```

- Find and print the index of the word "is".
- Create a new string where "fun" is replaced with "awesome".
- Print the string in uppercase.



Tuples in Python

A tuple is a built-in data type that contains an immutable sequence of values. Creating a tuple:

```
>>> t = (1, 2, 3)
```

Accessing an element of a tuple:

```
>>> t[1]
2
```

Tuples are immutable, so we can't change their elements. However, we can create a new tuple based on the old one:

```
>>> t = t + (4, )
```

Finding the length of a tuple:

```
>>> len(t)
4
```



Practice

Given a tuple

- Access and print the third element of the tuple.
- Try to change the value of the second element of the tuple.
- Create a new tuple by concatenating a second tuple (7,8,9) to the original tuple.



Dictionaries in Python (1)

Creating a dictionary:

```
>>> d = {'a': 1, 'b': 2, 'c': 3}
```

Accessing a value by its key:

```
>>> d['b']
2
```

Modifying a value associated with a key:

```
>>> d['b'] = 47
```

Adding a new key-value pair:

```
>>> d['d'] = 4
```

Removing a key-value pair using pop:

```
>>> d.pop('d')
4
```



Dictionaries in Python (2)

Get all keys as a list:

```
>>> list(d.keys())
['a', 'b', 'c']
```

Get all values as a list:

```
>>> list(d.values())
[1, 47, 3]
```

Get all key-value pairs as a list of tuples:

```
>>> list(d.items())
[('a', 1), ('b', 47), ('c', 3)]
```



Practice

Given a dictionary

```
>>> d = { 'Alice': 24, 'Bob': 27, 'Charlie': 22, 'Dave': 30}
```

- Access and print the age of 'Charlie'.
- Update 'Alice' age to 25.
- Add a new entry for 'Eve' with age 29.
- Print all the keys in the dictionary.



Today's outline

- Introduction
 - General programming
 - First steps
 - Further reading
- Data structures
 - Data types
 - Lists
 - Strings
 - Tuples
 - Dictionaries
- Control flow
 - Loops
 - Branching

- Functions
 - Defining functions
 - Recursion
 - Scope
 - Lambda functions
- Modules
 - Using modules
 - Math module
 - The random module
- Conclusions
- Exercises



Loops in Python (1)

The for loop is used to iterate over a sequence (e.g. lists, sets, tuples, dictionaries, strings). Any *iterable* object can be listed over:

```
>>> for i in range(5):
... print(i)
0
1
2
3
4
```

You can iterate over a list directly:

```
>>> my_list = [1, 2, 3, 4, 5]
>>> for num in my_list:
... print(num)
1
2
3
4
5
```



Loops in Python (2)

The enumerate keyword returns both the *index* as well as the *list element*:

```
>>> my_list = ['aa', 1, 'bb', 12, True, 1.618034, []]
>>> for idx,elm in enumerate(my_list):
... print(f'Element {elm} of type {type(elm)} at index {idx}')
```

```
Element aa of type <class 'str'> at index 0
Element 1 of type <class 'int'> at index 1
Element bb of type <class 'str'> at index 2
Element 12 of type <class 'int'> at index 3
Element True of type <class 'bool'> at index 4
Element 1.618034 of type <class 'float'> at index 5
Element [] of type <class 'list'> at index 6
```



roduction Data structures Control flow Functions Modules Conclusions Exercises

Loops in Python (3)

The 'while' loop keeps going as long as a condition is **True**:

```
>>> i = 0

>>> while i < 3:

... print(i)

... i += 1

0

1
```

Use break to exit a loop prematurely, and continue to skip to the next iteration:



Practice

Given a list

- Use a for loop to print each element of the list.
- Use a while loop to print the values at indices 0 to 4.
- Use a loop to find and print the index of the number 7 in the list.



Conditional Statements in Python

The Boolean type bool has only 2 possible values: True or False
The if statement is used to execute a block of code only if a condition is evaluated to
True:

```
>>> x = 5
>>> if x > 0:
... print("x is positive")
x is positive
```

Use **elif** to specify additional conditions, and **else** to define what to do if no conditions are met:

```
>>> if x > 10:
...     print("x is greater than 10")
... elif x == 10:
...     print("x is exactly 10")
... else:
...     print("x is less than 10")
x is less than 10
```



Nested conditionals

Nesting conditions allows for more complex conditionals:

```
>>> if x > 0:
...     if x % 2 == 0: # The modulo operator % yields the remainder of a division
...         print("x is positive and even")
...         else:
...         print("x is positive but odd")
...         else:
...         print("x is non-positive")
x is positive but odd
```

The in keyword can be used to check membership in a sequence:

```
>>> my_list = [1, 2, 3, 4, 5]
>>> if 3 in my_list:
... print("3 is a member of the list")
3 is a member of the list
```



Combined conditionals

Leap year determination

To be a leap year, the year number must be divisible by four, except for end-of-century years, which must be divisible by 400.

We can create combined conditions using not, and and or to determine whether we have a leap year:

```
>>> year = 2024
>>> if year % 4 == 0 and (not year % 100 == 0 or year % 400 == 0):
... print(f"{year} is a leap year.")
... else:
... print(f"{year} is not a leap year.")
```



Conditionals in list comprehensions

List comprehensions can be extended with conditionals too:

```
>>> x = [i for i in range(0,31) if i%3 == 0]
>>> print(x)
[0, 3, 6, 9, 12, 15, 18, 21, 24, 27, 30]
```

Conditions are not restricted to modulo's. Here we select artists who have an 'r' or 'R' in their name:



Practice

Consider the list:

```
>>> my_list = [x**3 for x in range(1,25,2)] # Cubes of odd numbers
```

- Use an **if** statement to check if 125 is in my_list, and print a message indicating the result.
- Write a statement that checks and prints whether my_list[3] is divisible by 3, and if not, print the remainder.
- Use a list comprehension to create a list of all numbers in my_list that are not divisible by 5.



Today's outline

- Introduction
 - General programming
 - First steps
 - Further reading
- Data structures
 - Data types
 - Lists
 - Strings
 - Tuples
 - Dictionaries
- Control flow
 - Loops
 - Branching

- Functions
 - Defining functions
 - Recursion
 - Scope
 - Lambda functions
- Modules
 - Using modules
 - Math module
 - The random module
- Conclusions
- Exercises



Functions in Python (1)

Functions are defined using the def keyword followed by the function name and a list of parameters in parentheses. The function body starts after the colon:

```
>>> def greet(name):
... print(f"Hello, {name}!")
```

Call the function with the necessary arguments:

```
>>> greet("Alice")
Hello, Alice!
```

Functions can return values using the return keyword:

```
>>> def add(a, b):
... return a + b
```

Capture the return value in a variable, e.g. result:

```
>>> result = add(2, 3)
>>> print(result)
5
```



Functions in Python (2)

Default argument values can be specified, making the argument optional:

```
>>> def greet(name, greeting="Hello"):
... print(f"{greeting}, {name}!")
```

Call the function with or without the optional argument:

```
>>> greet("Bob")
Hello, Bob!
>>> greet("Bob", "Buzz off")
Buzz off, Bob!
```

Python supports functions with a variable number of arguments:

```
>>> def my_function(*args):
... print(args)
```

Call the function with a varying number of arguments:

```
>>> my_function(1, 2, 3, "Hello")
(1, 2, 3, "Hello")
```



Functions in Python (3)

Functions can also return multiple values (also >2)

```
>>> def statistics(numbers):
... return max(numbers), min(numbers)
```

Let's call the function with some list:

```
>>> numlist = [94,12,6,19,33,14,81,56,43,22]
>>> print(statistics(numlist))
(94, 6)
```

Store the elements in separate variables:

```
>>> a,b = statistics(numlist)
>>> print(f'{a=}, {b=}')
a=94, b=6
```



Functions in Python (4)

- Functions are very useful for *abstraction*:
 - You can compartmentalize and 'hide' complex pieces of code
 - Retain flexibility through arguments
 - You can reuse often used pieces of code, limiting copy-paste of code
- Extending functionality or fixing bugs is done in 1 place
- Documentation is crucial!

```
>>> def statistics(numbers):
... """Return the maximum and minimum of a list of numbers
... Function arguments:
... numbers: list of numbers"""
... return max(numbers), min(numbers)
```

```
>>> help(statistics)
```

```
Help on function statistics in module __main__:

statistics(numbers)

Return the maximum and minimum of a list of numbers

Function arguments:
numbers: list of numbers
```

Passing arguments by value or reference?

Recall that certain Python variables are assigned by value, and others reference; the same goes for passing arguments ¹:

- Primitive or immutable data types are *passed by value*; the value is copied and changes made inside the function will not affect the values stored in the variables passed to the function.
- Mutable data types (e.g. list, set, dict) are passed to a function by reference; changes that are made inside the function do affect the values outside of the function.

Consider the function:

```
def func(x, y):
    x = x - 1 # Subtract 1
    y.pop() # Remove last item

i = 1
l = ['a', 'b']
func(i, l)
print(i, l)
```

```
1, ['a']
```

¹ https://k0nze.dev/posts/python-copy-reference-none/

Practice

Define a function that computes the factorial of a number, *n*!:

$$n! = 1 \times 2 \times 3 \times ... \times (n-1) \times n$$

Compute $\exp(x)$ using the Taylor series, iterate until the change is smaller than $1 \cdot 10^{-6}$:

$$\exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots + \frac{x^n}{n!}$$



Advanced topic: Recursion

- In order to understand recursion, one must first understand recursion
- A recursive function includes a call to itself (a function within a function)
 - This could lead to infinite calls:
 - A base case is required so that recursion is stopped;
 - Base case does not call itself, simply returns.





Advanced topic: Recursion

- In order to understand recursion, one must first understand recursion
- A recursive function includes a call to itself (a function within a function)
 - This could lead to infinite calls:
 - A base case is required so that recursion is stopped;
 - Base case does not call itself, simply returns.





Recursion: example

```
def mystery(a, b):
   if b == 1:
        # Base case
        return a
else:
        # Recursive function call
        return a + mystery(a, b-1)
```

- What does this function do?
- Can you spot the error?
- How deep can you go? Which values of b don't work anymore?



Practice

Define a function that computes the factorial of a number, n!, using recursion:

$$n! = 1 \times 2 \times 3 \times ... \times (n-1) \times n$$



Scope of functions and variables in Python

In Python, the scope of a variable refers to the regions of a program where that variable is accessible. Understanding the scope of variables helps to avoid bugs and maintain a clean codebase. The scopes in Python are categorized as follows:

- Local Scope Variables defined inside a function are in the local scope of that function. They can only be accessed within that function.
- Enclosing Scope In the case of nested functions, a function will have access to the variables of the functions it is nested within.
- Global Scope Variables defined at the top-level of a script are global and can be accessed by all functions in the script, unless overridden within a function.
- Built-in Scope Python has a number of built-in identifiers that should not be used as variable names as they have special significance. Examples include *print, list, dict,* etc.



Examples Variable Scope

1. Local Scope:

```
def my_func():
local_var = 100 # Local scope
print(local_var)
```

2. Enclosing Scope:

```
def outer_func():
    outer_var = 200  # Enclosing scope

def inner_func():
    print(outer_var)

inner_func()
```

3. Global Scope:

```
global_var = 300 # Global scope

def another_func():
    print(global_var)
```

4. Built-in Scope:

```
print(max, min, len, str, int, list)
```

Exercise Variable Scope

Investigate the behavior of the following nested functions and variables with the same name:

```
def outer_func():
    outer_var = 200

def inner_func():
    outer_var = 500
    print(outer_var)

inner_func()
```



Lambda functions (1)

Consider the mathematical function $f(x) = x^2 + e^x$ defined as a Python function block:

```
def f(x):
    from math import exp
return x**2 + np.exp(x)
```

Note:

- The function is defined using the def keyword.
- The variables and exp function used are defined locally. They will not be available globally unless defined as such.
- The function is defined in a Python script, not in a separate file.



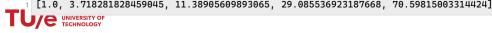
Lambda functions (2)

If you do not want to create a new function block, you can create an *lambda function*: Lambda functions are small, anonymous functions that can be instantiated in a single line, or even as an argument to a function.

```
from math import exp
f = lambda x: x**2 + exp(x)
```

- f: the name of the function
- Lambda: used to define the inline function
- x: the input argument (can be multiple, comma separated)
- :: colon indicating the function definition will start
- x**2 + exp(x): the actual function

```
1 xsqr_exp = [f(x) for x in range(5)]
2 print(xsqr_exp)
```



Today's outline

- Introduction
 - General programming
 - First steps
 - Further reading
- Data structures
 - Data types
 - Lists
 - Strings
 - Tuples
 - Dictionaries
- Control flow
 - Loops
 - Branching

- Functions
 - Defining functions
 - Recursion
 - Scope
 - Lambda functions
- Modules
 - Using modules
 - Math module
 - The random module
- Conclusions
- Exercises



Using Modules in Python (1)

Modules are files containing Python code, used to organize functionalities and reuse code across projects. To use a module, it must first be imported using the import keyword. Here, we import the entire math module:

```
>>> import math
```

Once imported, use the dot notation to access functions and variables defined in the module:

```
>>> math.sqrt(16)
4.0
```

You can import specific attributes from a module using the from ... import ... syntax:

```
>>> from math import sqrt
>>> sqrt(16)
4.0
```



Using Modules in Python (2)

Alias module names using the as keyword to shorten module names and avoid naming conflicts:

```
>>> import numpy as np
```

To view the list of all functions and variables in a module, use the dir() function:

```
>>> import math
>>> dir(math)
```

Get help on how to use a module or a function using the help() function:

```
>>> help(math.sqrt)
```



The math module

Many mathematical operations and concepts are available in the math module:

```
from math import pi,sin,sqrt,log10\
, exp,floor,ceil,factorial,inf,log
print(pi)

print(sin(0.2*pi))
print(sqrt(2))
print(log10(10_000))
print(exp(1))
print(floor(2.57))
print(floor(2.57))
print(floor(-2.57))
print(floor(-2.57))
print(floor(4.5))
print(factorial(5))
print(f"1 divided by infinity equals {1/inf}")
```

```
3.141592653589793
0.5877852522924731
1.4142135623730951
4.0
2.718281828459045
2.0
-3
120
1 divided by infinity equals 0.0
```



Practice

Use the math module to compute $y = \sin(x)$ for 8 equidistant points $x \in [0, 2\pi]$

• Use *list comprehensions* to generate the lists x and y



The random module (1)

Random number generators and sampling tools are available through the random module. A few examples for integers and sequences:

```
import random as rnd
# Random integers
random_integers = [rnd.randint(0,10) for i in range(10)]
print(f'{random_integers = }')
# Sample from given population
my_range = range(12) # [0, 1, 2, ..., 11]
select_from_range = rnd.sample(my_range,8)
print(f'{select_from_range = }') # Selected 8 elements
# Choose 1 element from list
days_of_week = ['Monday'.'Tuesday'.'Wednesday'.'Thursday'.'Friday'.'Saturday'.'Sunday']
day = rnd.choice(days_of_week)
print(f"I've chosen {dav} as mv luckv dav!")
```

```
random_integers = [6, 6, 2, 5, 5, 8, 3, 7, 3, 4]
select_from_range = [2, 3, 10, 1, 6, 4, 8, 5]
I've chosen Wednesday as my lucky day!
```

The random module (2)

Examples for real valued distributions:

```
import random as rnd

# Random number (uniform distribution) 0 < x < 1
x = [rnd.random() for i in range(5)]
print(x)

# Random number (uniform distribution) between given bounds
x = [rnd.uniform(1,3) for i in range(5)]
print(x)

# Random number from a Gauss distribution (mu=0, sigma=2)
x = [rnd.gauss(0,2) for i in range(5)]
print(x)</pre>
```

```
[0.6697878114597362, 0.4136014290205997, 0.5108247513505662, 0.44260043089156076, 0.9902269207988261]
[2.4749381508841077, 2.943448233960596, 2.516639180020423, 1.0481550073898795, 1.961356325508141]
[1.8199856149229392, 2.000097897306016, -2.4604868187736026, -0.46836605162997846, -2.5069012642608803]
```



Practice

- Create a function that returns a list of N dice throws (cubic dice, values 1-6)
- Throw the dice many times
- Print for each value how often it has been thrown

```
[5, 1, 1, 4, 6, 3, 3, 1, 5, 6, 1, 1, 1, 1, 5, 5, 2, 1, 1, 2, 2, 5, 5, 4, 6, 1, 3, 5, 6, 3, 1, 5, 6, 2, 3, 1, 6, 3, 2, 1]
Value 1 was thrown 13 times
Value 2 was thrown 6 times
Value 3 was thrown 6 times
Value 4 was thrown 2 times
Value 5 was thrown 8 times
Value 6 was thrown 8 times
```



Today's outline

- Introduction
 - General programming
 - First steps
 - Further reading
- Data structures
 - Data types
 - Lists
 - Strings
 - Tuples
 - Dictionaries
- Control flow
 - Loops
 - Branching

- Functions
 - Defining functions
 - Recursion
 - Scope
 - Lambda functions
- Modules
 - Using modules
 - Math module
 - The random module
- Conclusions
- Exercises



In conclusion...

- Python: A versatile development language. Easy to use libraries makes this language multi-purpose and easy to use.
- Programming basics: variables, operators and functions, locality of variables, modules and recursive operations
- For now: exercises on slide deck and Python modules



Practice vectors and arrays

- 1 Create a list x with the elements:
 - [2, 4, 6, 8, ..., 16]
 - [0, 0.5, 2/3, 3/4, ..., 99/100]
- 2 Create a list x with the elements: $x_n = \frac{(-1)^n}{2n-1}$ for n = 1, 2, 3, ..., 200. Find the sum of the first 50 elements $x_1, ..., x_{50}$.
- 3 Let x = List(range(20, 201, 10)). Create a list y of the same length as x such that:
 - y[i] = x[i] 3
 - y[i] = x[i] for every even index i and y[i] = x[i] + 11 for every odd index i.
- 4 Let τ = np.array([[3, 4, 6], [1, 8, 6], [-4, 3, 6], [5, 6, 6]]). Perform the following operations on T:
 - Retrieve a list consisting of the 2nd and 4th elements of the 3rd row.
 - Find the minimum of the 3rd column.
 - Find the maximum of the 2nd row.
 - Compute the sum of the 2nd column
 - Compute the mean of the row 1 and the mean of row 4



Practice plotting

- 1 Plot the functions f(x) = x, $g(x) = x^3$, $h(x) = e^x$ and $z(x) = e^{x^2}$ over the interval [0.4] on the normal scale and on the log-log scale. Use an appropriate sampling to get smooth curves. Describe your plots by using the functions: plt.xlabel, plt.ylabel, plt.title and plt.legend.
- 2 Make a plot of the functions: f(x) = sin(1/x) and g(x) = cos(1/x) over the interval [0.01, 0.1]. How do you create x so that the plots look sufficiently smooth?



Practice control flow and loops (1)

• Write a function that uses two logical input arguments with the following behaviour:

```
f(\text{true}, \text{true}) \mapsto \text{false}

f(\text{false}, \text{true}) \mapsto \text{true}

f(\text{true}, \text{false}) \mapsto \text{true}

f(\text{false}, \text{false}) \mapsto \text{false}
```

2 Write a function that computes the factorial of x:

$$f(x) = x! = 1 \times 2 \times 3 \times 4 \times \ldots \times x$$

Using a loop-construction



EIND OVEN SING recursion

Practice control flow and loops (2)

• Write a function that computes the exponential function using the Taylor series

$$e^{x} = 1 + x + \frac{x^{2}}{2!} + \frac{x^{3}}{3!} + \dots$$

until the last term is smaller than 10^{-6} .

Use a script to compute the result of the following series:

$$f_n = \sum_{n=1}^{\infty} \frac{1}{\pi^2 n^2}$$

This should give you an indication of the fraction this series converges to.

• Now plot in two vertically aligned subplots i) The result as a function of *n*, and ii) the difference with the earlier mentioned fraction as a function of n. For the latter, consider carefully the axis scale!



Practice logical indexing

- 1 Let x = np.linspace(-4, 4, 1000), $y_1 = 3x^2 4x 6$ and $y_2 = 1.5x 1$. Use logical indexing to determine function $y_3 = max(max(y_1, y_2), 0)$. Plot the function.
- Consider these data concerning the age (in years), length (in cm) and weight (in kg) of twelve adult men: A = [41 25 33 29 64 34 47 38 49 32 26 26]; H = [165 186 177 190 156 174 164 205 184 190 165 171]; W = [75 90 97 60 74 65 101 85 91 75 87 70];.
 - Calculate the average of all vectors (age, weight and length).
 - Combine the command Length with logical indexing to determine how many men in the group are taller than 182 cm.
 - What is the average age of men with a body-mass index ($B \equiv \frac{W}{L^2}$ with W in kg and L in m) larger than 25? And for men with a B < 25?
 - How many men are older than the average and at the same time have a BMI below 25?



Exercises

Practice algorithm: Fourier series for heat equation

The unsteady 1D heat equation in 1D in a slab of material is given as:

$$\frac{\partial T}{\partial t} = k \frac{\partial^2 T}{\partial x^2}$$

We can express the temperature profile T(x,t) in the slab using a Fourier sine series. For an initial profile T(x,0) = 20 and fixed boundary values T(0,t) = T(L,t) = 0, the solution is given as:

$$T(x,t) = \sum_{n=1}^{n=\infty} \frac{40(1-(-1)^n)}{n\pi} \sin\left(\frac{n\pi x}{L}\right) \exp\left(-kt\frac{n\pi^2}{L}\right)$$

• Create a script to solve this equation using loops and/or conditional statements

