

# Advanced Data Analytics — Lecture 3a

## A Crash Course on Programming in Python

Simon Scheidegger  
Department of Economics, University of Lausanne, Switzerland

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# Before we start — some resources

**!!! Lecture slides and codes available on Nuvolos !!!**

**Extended tutorial on python here: [python\\_refresher](#)**

If you are new to Python, this is a pre-requisite!!!

# Outline of this mini-course in Python

1. Motivation — why Python.
2. First steps in Python.
3. Nonlinear equations and optimization.
4. Pointers to tutorials and literature.

# Computational science in general

- ▶ **Computational science**: a rapidly growing multidisciplinary field that uses **advanced computing** capabilities to understand and solve complex problems.
- ▶ It is an area of science which spans many disciplines (comp. finance, comp. econ, comp. physics, comp. biology).
- ▶ At its core it involves the **development of models** and **simulations** to understand complex systems.

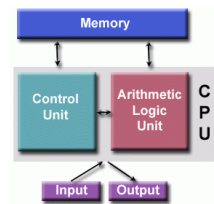
⇒ computational science aims to make the complexity of those systems tractable.



# Basics: von Neumann Architecture

[https://computing.llnl.gov/tutorials/parallel\\_comp](https://computing.llnl.gov/tutorials/parallel_comp)

- ▶ Virtually all computers have followed this basic design.  
Comprised of **four main components**: **Memory**, **Control Unit**, **Arithmetic Logic Unit**, **Input/Output**.
- ▶ **Read/write, random access memory** is used to store both program instructions and data:
  - ▶ Program instructions are coded data which tell the computer to do something.
  - ▶ Data is simply information to be used by the program.
- ▶ **Control unit**
  - ▶ fetches instructions/data from memory, decodes the instructions and then sequentially coordinates operations to accomplish the programmed task.
- ▶ **Arithmetic unit**
  - ▶ performs basic arithmetic operations.
- ▶ **Input/Output**
  - ▶ interface to the human operator.



# From a programming language to hardware

<http://cse-lab.ethz.ch/index.php/teaching/42-teaching/classes/577-hpcsei>

- ▶ A computer is a “stupid” device, only understands “on” and “off”
- ▶ The symbols for these states are 0 and 1 (binary).
- ▶ First, programmers communicated in 0 and 1.
- ▶ Later, programs were developed to translate from symbolic notation to binary. The first was called “**assembly**”.

```
> add A, B (programmer writes in assembly language)
>1000110010100000 (assembly translates to machine language)
```

Advanced programming languages are better than “assembly”:

- ▶ programmer thinks in a more natural language.
- ▶ productivity of software development.
- ▶ portability.

***There are only two kinds of (programming) languages: the ones people complain about and the ones nobody uses.***

— Bjarne Stroustrup (designer of C++)

Let's complain about...



# What is Python?

- ▶ Python is a **general purpose** programming language conceived in 1989 by Dutch programmer Guido van Rossum.
- ▶ Python is **free and open source**, with development coordinated through the **Python Software Foundation** (<https://www.python.org/psf/>).
- ▶ Python has experienced rapid adoption in the last decade, and is now one of the most popular programming languages.

# Common uses

Python is a general purpose language used in almost all application domains:

- ▶ communications
- ▶ web development
- ▶ graphical user interfaces
- ▶ games, multimedia, data processing, security, etc.
- ▶ Machine Learning, Artificial Intelligence

Used extensively by Internet service and high tech companies such as

- ▶ Google
- ▶ Dropbox
- ▶ Reddit
- ▶ YouTube
- ▶ Walt Disney Animation,...

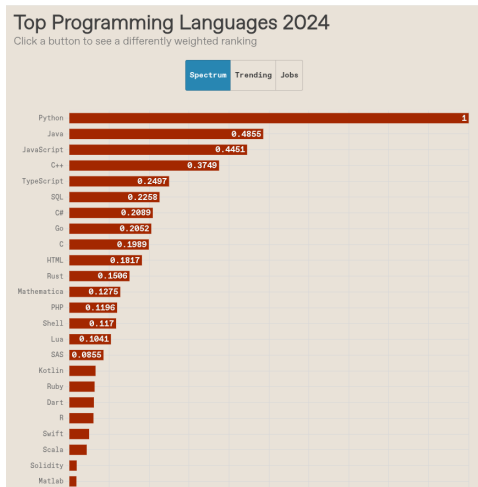
→ **Often used to teach computer science and programming**

→ **For reasons we will discuss, Python is particularly popular within the scientific community**

# Top Programming Languages 2024

<https://spectrum.ieee.org/the-top-programming-languages-2024>

- ▶ Python is one of the most popular programming languages worldwide.
- ▶ Python is a major tool for scientific computing, accounting for a rapidly rising share of scientific work around the globe.



# Some features

- ▶ Python is a **high level language** suitable for rapid development.
- ▶ It has a relatively small core language **supported by many libraries.**
- ▶ A **multi-paradigm language**, in that multiple programming styles are supported (procedural, object-oriented, functional,...)
- ▶ **Interpreted rather than compiled.**



# Syntax and Design

- ▶ One nice feature of Python is its **elegant syntax** — we'll see many examples later on.
- ▶ **Elegant code** might sound superfluous but in fact it's highly beneficial because it makes the syntax **easy to read and easy to remember**.
- ▶ **Remembering** how to read from files, sort dictionaries and other such routine tasks means that **you don't need to break your flow** in order to hunt down correct syntax.
- ▶ Closely related to **elegant syntax** is **elegant design**.
- ▶ Features like iterators, generators, list comprehensions, etc. make Python highly expressive, **allowing you to get more done with less code**.

# Get Python

- ▶ You can download and install Python directly from <https://www.python.org>
- ▶ Since we're going to use several libraries for numerical computation (numpy), data analysis (pandas), machine learning (scikit-learn), and visualization (matplotlib), it is easier to install Anaconda, which bundles all things required  
<https://www.continuum.io/downloads>



## Download

Download these documents

## Docs by version

Python 3.13 (in development)  
Python 3.12 (stable)  
Python 3.11 (stable)  
Python 3.10 (security-fixes)  
Python 3.9 (security-fixes)  
Python 3.8 (security-fixes)  
Python 3.7 (EOL)  
Python 3.6 (EOL)  
Python 3.5 (EOL)  
Python 3.4 (EOL)  
Python 3.3 (EOL)  
Python 3.2 (EOL)  
Python 3.1 (EOL)  
Python 3.0 (EOL)  
Python 2.7 (EOL)  
Python 2.6 (EOL)  
All versions

## Other resources

PEP Index  
Beginner's Guide  
Book List  
Audio/Visual Talks  
Python Developer's Guide

# Python 3.12.0 documentation

Welcome! This is the official documentation for Python 3.12.0.

## Parts of the documentation:

### What's new in Python 3.12?

*or all "What's new" documents since 2.0*

### Tutorial

*start here*

### Library Reference

*keep this under your pillow*

### Language Reference

*describes syntax and language elements*

### Python Setup and Usage

*how to use Python on different platforms*

### Python HOWTOs

*in-depth documents on specific topics*

## Indices and tables:

### Global Module Index

*quick access to all modules*

### General Index

*all functions, classes, terms*

### Glossary

*the most important terms explained*

### Installing Python Modules

*installing from the Python Package Index & other sources*

### Distributing Python Modules

*publishing modules for installation by others*

### Extending and Embedding

*tutorial for C/C++ programmers*

### Python/C API

*reference for C/C++ programmers*

### FAQs

*frequently asked questions (with answers!)*

### Search page

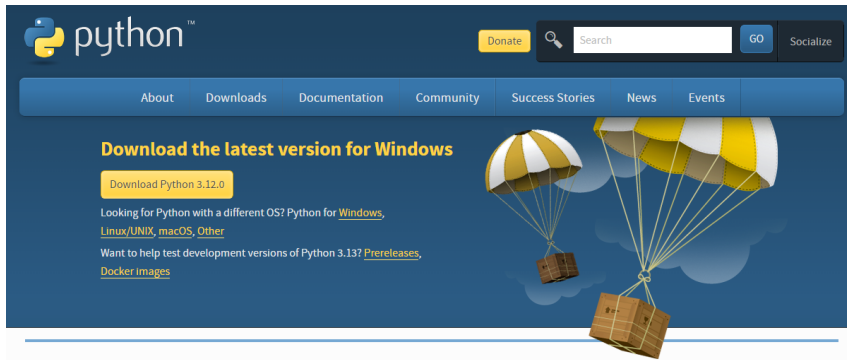
*search this documentation*

### Complete Table of Contents

*lists all sections and subsections*

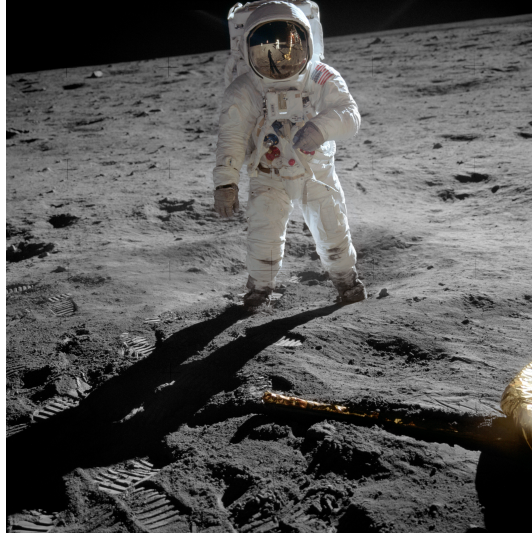
# Install Python

<https://www.python.org/downloads/>



Find the installation you need (Linux, MacOS, Windows)

## 2. First steps in Python → action required



# List of examples

- ▶ 2.0. Setting up your environment.
- ▶ 2.1. Python basics.
- ▶ 2.2. Loops and Lists.
- ▶ 2.3. Functions and Branching.
- ▶ 2.4. Reading/writing Data.

# Python Setup

A bare-bones development environment consists of:

- A text editor (e.g., `gedit`, `emacs`, `vim`)
- The Python interpreter (it is installed by default on Ubuntu and almost any other Linux distribution)
- A terminal application to run the interpreter in.

See <http://wiki.python.org/moin/IntegratedDevelopmentEnvironments> for a commented list of IDEs with Python support.

# Another helpful online tool

The **Online Python Tutor** is a free tool to visualize the execution of programs step-by-step.

Python Tutor: Visualize code in [Python](#), [JavaScript](#), [C](#), [C++](#), and [Java](#)

The screenshot displays the Python Tutor interface. On the left, a code editor shows Python 3.6 code with line numbers 1 to 21. The code defines a list `x`, appends elements to it, and defines a function `foo`. The execution is paused at line 18. On the right, the 'Frames' and 'Objects' panels show the current state of memory. The 'Global frame' contains variables `x` (pointing to a list object), `y` (pointing to the string 'hello'), `foo` (pointing to a function object), and `bar` (pointing to a function object). The 'list' object is shown as a table with indices 0 to 6, containing values [1, 2, 3, 4, 5, 6, 7]. The 'function' objects are shown as tables with indices 0 to 4, containing values [1, 2, 3, 4, 5]. The 'Print output' panel is empty. At the bottom, navigation buttons and a step indicator 'Step 18 of 31' are visible.

```
Python 3.6
known limitations

1 x = [1, 2, 3]
2 y = [4, 5, 6]
3 z = y
4 y = x
5 x = z
6
7 x = [1, 2, 3] # a different [1, 2, 3] list!
8 y = x
9 x.append(4)
10 y.append(5)
11 z = [1, 2, 3, 4, 5] # a different list!
12 x.append(6)
13 y.append(7)
14 y = "hello"
15
16
17 def foo(lst):
18     lst.append("hello")
19     bar(lst)
20
21 def bar(myList):
```

Print output (drag lower right corner to resize)

Frames

Objects

Global frame

list

list

function foo(lst)

function bar(myList)

Step 18 of 31

Feel free to use it for the course exercises and your own code:

<http://pythontutor.com/visualize.html>

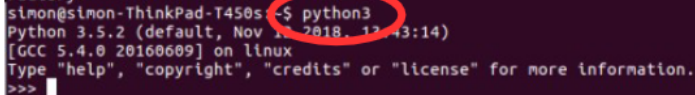


## 2.1 Python Basics

Python is an interpreted language.

It also features an interactive “**shell**” for evaluating expressions and statements immediately.

The Python shell is started by invoking the command python in a terminal window.



```
simon@simon-ThinkPad-T450s ~$ python3
Python 3.5.2 (default, Nov 12 2018, 13:43:14)
[GCC 5.4.0 20160609] on linux
Type "help", "copyright", "credits" or "license" for more information.
>>> 
```

## Python Basics (II)

Expressions can be entered at the Python shell prompt (the '>>>' at the start of a line); they are evaluated and the result is printed:

```
>>> 2+2  
4
```

A line can be continued onto the next by ending it with the character '\'; for example:

```
>>> "hello" + \  
... " world!"  
'hello world!'
```

The prompt changes to '...' on continuation lines.

Reference:

[http://docs.python.org/reference/lexical\\_analysis.html#line-structure](http://docs.python.org/reference/lexical_analysis.html#line-structure)

# Basic Types

Basic object types in Python:

`bool` The class of the two boolean constants  
True, False.

`int` Integer numbers: 1, -2, ...

`float` Double precision floating-point numbers,  
e.g.: 3.1415, -1e-3.

`str` Text (strings of byte-size characters).

`list` Mutable list of Python objects

`dict` Key/value mapping

**No type declaration needed — Python does that for you on the fly**

# Type Conversions

`str(x)` Converts the argument `x` to a string; for numbers, the base 10 representation is used.

`int(x)` Converts its argument `x` (a number or a string) to an integer; if `x` is a floating-point literal, decimal digits are truncated.

`float(x)` Converts its argument `x` (a number or a string) to a floating-point number.

check the type of a variable by typing `>>> type(a)`

# String Literals

There are several ways to express string literals in Python.

Single and double quotes can be used interchangeably:

```
>>> "a string" == 'a string'  
True
```

You can use the single quotes inside double-quoted strings, and viceversa:

```
>>> a = "Isn't it ok?"  
>>> b = '"Yes", he said.'
```

# String Literals II

Multi-line strings are delimited by three quote characters.

```
>>> a = """This is a string,  
... that extends over more  
... than one line.  
... """
```

In other words, you need not use the backslashes “\” at the end of the lines.

# Operators

All the usual unary and binary arithmetic operators are defined in Python: +, -, \*, /, \*\* (exponentiation), <<, >>, etc.

Logical operators are expressed using plain English words: and, or, not.

Numerical and string comparison also follows the usual notation: <, >, <=, ==, !=, ...

*Reference:*

- <http://docs.python.org/library/stdtypes.html#boolean-operations-and-or-not>
- <http://docs.python.org/library/stdtypes.html#comparisons>

# Your first exercise to compute





# Operators II

Some operators are defined for non-numeric types:

```
>>> 'U' + 'NIL'
'UNIL'
```

Some support operands of mixed type:

```
>>> "a" * 2
'aa'
>>> 2 * "a"
'aa'
```

Some do not:

```
>>> "aaa" / 3
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
TypeError: unsupported operand type(s) for /: 'str' and 'int'
```

# Operators III

The “%” operator computes the remainder of integer division.

```
>>> 9 % 2  
1
```

# Assignments

Assignment is done via the '=' statement:

```
>>> a = 1
>>> print(a)
1
```

There are a few shortcut notations:

$a += b$  short for  $a = a + b$ ,

$a -= b$  short for  $a = a - b$ ,

$a *= b$  short for  $a = a * b$ ,

etc. — one for every legal operator.

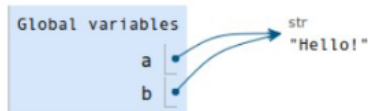
# Assignments II

**Python variables are just “names” given to values.**

This allows you to *reference* the string 'Python' by the *name* a:

```
1 a = "Hello!"  
→ 2 b = a
```

[Edit code](#)



The same object can be given many names!

# The “is” Operator

The `is` operator allows you to test whether two names refer to the same object:

```
>>> a = 1
>>> b = 1
>>> a is b
True
```

# The help Function

`help(fn)` Display help on the function named `fn`

**Q:** *What happens if you type these at the prompt?*

– `help(abs)`

– `help(max)`

# Functions

Functions are called by postfixing the function name with a parenthesized argument list.

```
>>> int("42")
42
>>> int(4.2)
4
>>> float(42)
42.0
>>> str(42)
'42'
>>> str()
''
```

**Attention — rounding towards ZERO**

# How to execute source code

example0\_hello.py

→ Store a file `hello.py` with this content:

```
print('Hello, world!')
```

→ Execute it with `$ python hello.py`

```
simon@simon-ThinkPad-T450s:~/Documents$ python hello.py
Hello, world!
simon@simon-ThinkPad-T450s:~/Documents$
```



## 2.2 Loops and Lists

example3\_while.py

- ▶ The **while loop** is used to repeat a set of statements as long as a condition is true.
  - ▶ Example: The task is to generate the rows of the table of  $C$  and  $F$  values.
  - ▶ The  $C$  value starts at -20 and is incremented by 5 as long as  $C \leq 40$ .
  - ▶ For each  $C$  value we compute the corresponding  $F$  value and write out the two temperatures.
  - ▶ In addition, we also add a line of hyphens above and below the table. We postpone to nicely format the  $C$  and  $F$  columns of numbers and perform for simplicity a plain `print(C, F)` statement inside the loop.

```
print("-----") # table heading
C = -20           # start value for C
dC = 5           # increment of C in loop
while C <= 40:    # loop heading with condition
    F = (9.0/5)*C + 32 # 1st statement inside loop
    print(C, F)        # 2nd statement inside loop
    C = C + dC         # 3rd statement inside loop
print("-----") # end of table line (after loop)
```

```
$ python example3_while.py
```

```
-----
-20 -4.0
-15 5.0
-10 14.0
-5 23.0
0 32.0
5 41.0
10 50.0
15 59.0
20 68.0
25 77.0
30 86.0
35 95.0
40 104.0
```

# Loop Implementation of a Sum

example4\_sum.py

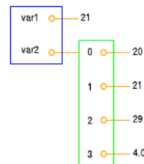
$$\sin(x) \approx x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \dots$$

```
x=1.2 # assign some value
N=25 # maximum power in sum
k=1
s=x
sign=1.0
import math
while k<N :
    sign = -sign
    k = k+2
    term = sign*x**k/math.factorial(k)
    s = s + term

print('sin(%g)=%g approximation with %d terms' % (x, s, N))
```

# Lists

- ▶ Up to now a **variable** has typically contained a single number.
- ▶ Sometimes numbers are naturally **grouped together**.
- ▶ A **Python list** can be used to represent such a group of numbers in a program.
- ▶ With a variable that refers to the list, we can **work with the whole group at once**, but we can also **access individual elements** of the group.



**Fig. 2.1** Illustration of two variables: `var1` refers to an `int` object with value 21, created by the statement `var1 = 21`, and `var2` refers to a `list` object with value `[20, 21, 29, 4.0]`, i.e., three `int` objects and one `float` object, created by the statement `var2 = [20, 21, 29, 4.0]`.

Fig. From H.P. Langtangen

- ▶ The figure illustrates the difference between an `int` object and a `list` object.
- ▶ In general, a list may contain a **sequence of arbitrary objects in a given order**. Python has great functionality for examining and manipulating such sequences of objects.

# Basic operations in Lists → type

- ▶ To **create a list** with the numbers from the first column in our table, we just put all the **numbers inside square brackets** and separate the numbers by commas:

```
>>> C = [-10, -5, 0, 5, 10, 15, 20, 25, 30] # create list
>>> C.append(35)
>>> C
[-10, -5, 0, 5, 10, 15, 20, 25, 30, 35]
```

- ▶ **Two lists can be added:**

```
>>> C = C + [40, 45]
>>> C
[-10, -5, 0, 5, 10, 15, 20, 25, 30, 35, 40, 45]
```

# Basic operations in Lists → type

- **New elements** can be inserted anywhere in the list:

```
>>> C.insert(0,-15)
>>> C
[-15, -10, -5, 0, 5, 10, 15, 20, 25, 30, 35, 40, 45]
```

- With **del C[i]** we can remove an element with index i from the list C.

```
>>> del C[2] #delete 3rd element
>>> C
[-15, -10, 0, 5, 10, 15, 20, 25, 30, 35, 40, 45]
>>> del C[2] #delete what is now the 3rd element
>>> C
[-15, -10, 5, 10, 15, 20, 25, 30, 35, 40, 45]
>>> len(C) #length of list
11
```

# How to represent Vectors

A Python program may use a **list or tuple** to represent a vector:

```
v1 = [x, y] #list of variables
v2 = (-1, 2) #list of numbers
v3 = (x1, x2, x3) #tuple of variables
from math import exp
v4 = [exp(-i*0.1) for i in range(150)]
```

# Basic operations (II) — “for loop”

- ▶ When data are collected in a list, we often want to perform the same operations on each element in the list.
- ▶ We then need to walk through all list elements. Computer languages have a special construct for doing this conveniently.
- ▶ This construct in Python and many other languages called a “for loop”.

## example5\_forloop.py

```
degrees = [0, 10, 20, 40, 100]
for C in degrees:
    print("list element:", C)
print("The degrees list has",
      len(degrees),
      "elements")
```

```
index = 0
while index < len(somelist)
element = somelist[index]
<process element>
index+=1
```

## example6\_forloop.py

```
Cdegrees = []
n = 21
C_min = -10
C_max = 40
dC = (C_max - C_min)/float(n-1)
# increment in C
for i in range(0, n):
    C = -10 + i*dC
    Cdegrees.append(C)
    Fdegrees = []

for C in Cdegrees:
    F = (9.0/5)*C + 32
    Fdegrees.append(F)

for i in range(len(Cdegrees)):
    C = Cdegrees[i]
    F = Fdegrees[i]
    print("%5.1f %5.1f" % (C, F))
```

## 2.3. Functions and Branching

The **def** statement starts a function definition.

```
def greet(name):  
    """  
    A friendly function.  
    """  
    print ("Hello,_" + name + "!")  
  
# the customary greeting  
greet("world")
```



# How to define new functions (II)

```
def greet(name):  
    """  
    A friendly function.  
    """
```

```
    print ("Hello, " + name + "!")
```

```
# the customary greeting  
greet("world")
```

## Indentation is significant

**in Python:** it is used to delimit blocks of code, like '{' and '}' in Java and C.

## How to define new functions (III)

```
def greet(name):  
    """  
    A friendly function.  
    """  
    print ("Hello,_" + name + "!")  
  
# the customary greeting  
greet("world")
```

(This is a comment. It is ignored by Python, just like blank lines.)

# How to define new functions (IV)

example7\_greet.py

This calls the function just defined.

```
def greet(name):  
    """  
    A friendly function.  
    """  
    print ("Hello,_" + name + "!")  
  
# the customary greeting  
greet("world")
```

# How to define new functions (V)

```
def greet(name):  
    """  
    A friendly function.  
    """  
    print ("Hello,_" + name + "!")  
  
# the customary greeting  
greet("world")
```

What is this? The answer  
in the next exercise!



Try this:  
>>>help(greet)

# Modules

The `import` statement reads a `.py` file, executes it, and makes its contents available to the current program.

```
>>> import hello  
Hello, world!
```

**Modules are only read once**, no matter how many times an `import` statement is issued.

# Modules II

Modules are namespaces: functions and variables defined in a module must be prefixed with the module name when used in other modules:

```
>>> hello.greet("Bob")  
Hello, Bob!
```

To import definitions into the current namespace, use the 'from *x* import *y*' form:

```
>>> from fractions import Fraction
```

# Conditionals

Conditional execution uses the `if` statement:

```
if expr:
    # indented block
elif other-expr:
    # indented block
else:
    # executed if none of the above matched
```

The `elif` can be repeated, with different conditions, or left out entirely.

Also the `else` clause is optional.

**Q:** Where's the 'end if'?

*There's no 'end if': indentation delimits blocks!*

# Branching — example “hat” function

example9\_branching.py

Branching in general

$$N(x) = \begin{cases} 0, & x < 0 \\ x, & 0 \leq x < 1 \\ 2 - x, & 1 \leq x < 2 \\ 0, & x \geq 2 \end{cases}$$

```
if condition1:
    <block of statements>
elif condition2:
    <block of statements>
elif condition3:
    <block of statements>
else:
    <block of statements>
<next statement>
```

```
def hat_function(x):
    # hat function
    if x < 0:
        return 0.0
    elif 0 <= x < 1:
        return x
    elif 1 <= x < 2:
        return 2 - x
    elif x >= 2:
        return 0.0
print(hat_function(1.4))
```



# Exercises

**Exercise A:** Type and run the code on the previous page at the interactive prompt. (Type indentation spaces, too!)

What does `help(greet)` print? What's the result of evaluating the function `greet("world")`?

**Exercise B:** Type the same code in a file named `hello.py`, then type `import hello` at the interactive prompt. What happens?

## 2.4. Input Data

```
C = 21
F = (9./5)*C + 32
print(F)
```

- ▶ In this program, *C is input data* in the sense that *C* must be known before the program can perform the calculation of *F*.
- ▶ The results produced by the program, here *F*, constitute the output data. Input data can be *hard-coded* in the program as we do above.
- ▶ We explicitly set variables to specific values  $C = 21$ .
- ▶ *This programming style may be suitable for small programs.*
- ▶ In general, however, it is considered good practice to let a user of the program *provide input data when the program is running*. → There is then no need to modify the program itself when a new set of input data is to be explored.

# Reading Keyboard Input

example10\_read.py

We may ask the user a question  $C=?$  and wait for the user to enter a number. The program can then read this number and store it in a variable  $C$ .

```
C = input('C=? ')\nC = float(C)\nF = (9./5)*C + 32\nprint(F)
```

The `raw_input` function always returns the user input as a **string object**. That is, the variable  $C$  above refers to a string object.

If we want to compute with this  $C$ , we must **convert the string to a floating-point number**:  $C = \text{float}(C)$ .

# Reading from Command Line

example11\_readsys.py

- ▶ Inside the program we can fetch the text "number" as `sys.argv[1]`. The `sys` module has a list `argv` containing all the command-line arguments to the program, i.e., all the "words" appearing after the program name when we run the program.
- ▶ Here there is only one argument and it is stored with index 1. The first element in the `sys.argv` list, `sys.argv[0]`, is always the name of the program.
- ▶ A command-line argument is treated as a text, so `sys.argv[1]` refers to a string object. Since we interpret the command-line argument as a number and want to compute with it, it is necessary to explicitly convert the string to a float object.

Run as:

\$python

example11\_readsys.py 2

```
import sys
print("This is the name of the script: ", sys.argv[0])

C = input("please write the degrees celcius outside:")

F= 9*float(C)/5 + 32
print("it is ", F , " degrees F")

print("Number of arguments: ", len(sys.argv))
print("The arguments are: " , str(sys.argv))
```

# Reading from a File

example12\_readfile.py

- ▶ We have a text file containing numbers: say `data.txt`
- ▶ We want to get first column in `a1`, second in `a2` and so on.
- ▶ Note: there are plenty of option on how to read from files → RTFM

```
1 2 3 4
5 6 7 8
9 10 11 12
13 14 15 16
```

```
a1 = []
a2 = []
a3 = []
a4 = []

with open('data.txt') as f:
    for line in f:
        data = line.split()
        a1.append(int(data[0]))
        a2.append(int(data[1]))
        a3.append(int(data[2]))
        a4.append(int(data[3]))

print(a1, a2, a3, a4)

f.close()
```

# Other things to learn about Python

The time and scope of this course is rather limited.

Here is an (incomplete) list of Python features that you might want to look up as you become more experienced in the language:

- Generators and Iterators
- Decorators
- Class-level attributes, classmethods, staticmethods
- Properties and accessors
- Metaclasses

# Do not re-invent the wheel — NumPy

**NumPy** is a package for linear algebra and advanced mathematics in Python.

It provides a *fast* implementation of multidimensional numerical arrays (C/FORTRAN like), vectors, matrices, tensors and operations on them.

*Use it if:* you long for MATLAB core features.

*See also:* <http://www.numpy.org/>

# Do not re-invent the wheel — SciPy

“**SciPy** is open-source software for mathematics, science, and engineering. [...] The SciPy library provides many user-friendly and efficient numerical routines such as routines for numerical integration and optimization.”

One of its main aim is to provide a reimplementation of the MATLAB toolboxes.

*Use it if:* you long for MATLAB toolbox features.

*See also:* <http://www.scipy.org/>



# Pandas

**Pandas** is a Python data analysis library, that provides optimized routines for analyzing 2D, 3D, 4D data.

“Pandas [...] enables you to carry out your entire data analysis workflow in Python without having to switch to a more domain specific language like R.”

*Use it if:* you need features from R, `plyr`, `reshape2`.

# Writing to a file — e.g. with numpy

example12\_writefile.py

```
import numpy as np
mat=np.matrix([[1, 2, 3],[4, 5, 6],[7, 8, 9]])
print(mat)
np.savetxt('matrix.txt',mat,fmt='%.2f')
```

# Curve Plotting

- ▶ Visualizing a function  $f(x)$  is done by drawing the curve  $y = f(x)$  in an  $x - y$  coordinate system.
- ▶ When we use a computer to do this task, we say that we plot the curve.
- ▶ Technically, we plot a curve by drawing straight lines between  $n$  points on the curve.
- ▶ The more points we use, the smoother the curve appears.
- ▶ Suppose we want to plot the function  $f(x)$  for  $a \leq x \leq b$ .

$$x_i = a + ih, \quad h = \frac{b - a}{n - 1}.$$

# Matplotlib: publication quality plotting library

**matplotlib** “is a python 2D plotting library which produces publication quality figures in a variety of hardcopy formats and interactive environments across platforms. matplotlib can be used in python scripts, the python and ipython shell (ala MATLAB® or Mathematica®), web application servers, and six graphical user interface toolkits.”

# Matplotlib: a basic example

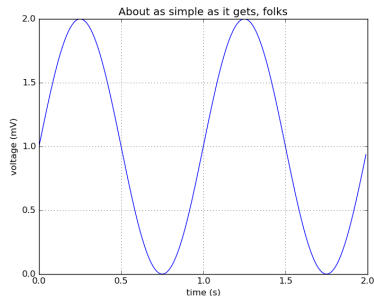
example13\_plot.py

Let us plot the curve  $s$  for values between 0 and 2 . First we generate equally spaced coordinates for  $t$ . Then we compute the corresponding  $s$  values at these points, before we call the `plot(t,s)` command to make the curve plot.

```
import matplotlib.pyplot as plt
import numpy as np

t = np.arange(0.0, 2.0, 0.01)
s = 1 + np.sin(2*np.pi*t)
plt.plot(t, s)

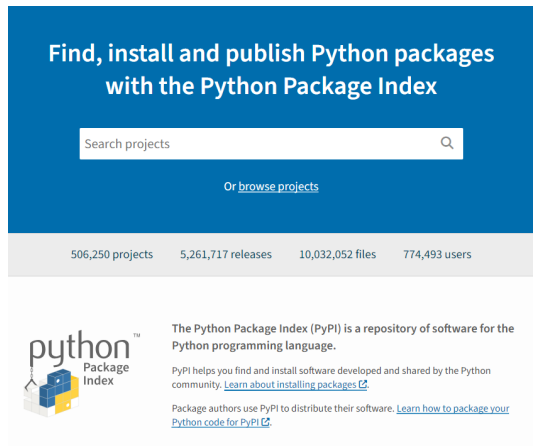
plt.xlabel('time (s)')
plt.ylabel('voltage (mV)')
plt.title('About as simple as it gets, folks')
plt.grid(True)
plt.savefig("test.png")
plt.show()
```



To include the plot in electronic documents, we need a hardcopy of the figure in PostScript, PNG, or another image format. The `savefig` function saves the plot to files in various image formats.

# Want more?

PyPI is the index of Python software packages. It currently indexes 506,250 packages, so the choice is really vast. Almost all packages can be installed with a single command by running `pip install packagename`.




The screenshot shows the PyPI homepage with a blue header and a white search bar. The header text reads "Find, install and publish Python packages with the Python Package Index". Below the search bar is a link "Or browse projects". A grey bar displays statistics: 506,250 projects, 5,261,717 releases, 10,032,052 files, and 774,493 users. The footer contains the PyPI logo and descriptive text about the index, including links to learn about installing packages and packaging code for PyPI.

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 The Python Package Index (PyPI) is a repository of software for the Python programming language.

PyPI helps you find and install software developed and shared by the Python community. [Learn about installing packages](#)

Package authors use PyPI to distribute their software. [Learn how to package your Python code for PyPI](#)

### III. Nonlinear equations & optimization.

- ▶ Our course heavily relies on solving large systems of nonlinear equations or (un-) constraint optimization problems.
- ▶ In Python, you have plenty of options, e.g.:
- ▶ SciPy.org
- ▶ PyOpt.org
- ▶ IPOPT (<https://www.coin-or.org/lpopt>;  
<https://github.com/xuy/pyipopt>)

# Constrained optimization with SciPy

The minimize function also provides an interface to several constrained minimization algorithm.

As an example, the Sequential Least Squares Programming optimization algorithm (SLSQP) will be considered here.

This algorithm allows to deal with constrained minimization problems of the form:

$$\begin{aligned} & \min F(x) \\ & \text{subject to } C_j(X) = 0, \quad j = 1, \dots, \text{MEQ} \\ & \quad \quad \quad C_j(x) \geq 0, \quad j = \text{MEQ} + 1, \dots, M \\ & \quad \quad \quad XL \leq x \leq XU, \quad l = 1, \dots, N. \end{aligned}$$



# Constrained optimization — example

As an example, let us consider the problem of optimizing the function:

$$f(x, y) = 2xy + 2x \cdot x^2 \cdot 2y^2$$

subject to an equality and an inequality constraints defined as:

$$x^3 - y = 0$$

$$y - 1 > 0$$

# Example for Optimization

```
import numpy as np
from scipy.optimize import minimize
def func(x, sign=1.0):
    """ Objective function """
    return sign*(2*x[0]*x[1] + 2*x[0] - x[0]**2 - 2*x[1]**2)
def func_deriv(x, sign=1.0):
    """ Derivative of objective function """
    dfdx0 = sign*(-2*x[0] + 2*x[1] + 2)
    dfdx1 = sign*(2*x[0] - 4*x[1])
    return np.array([ dfdx0, dfdx1 ])

"""
Note that since minimize only minimizes functions, the sign parameter is
introduced to multiply the objective function (and its derivative) by -1 in order to perform a maximization.
Then constraints are defined as a sequence of dictionaries, with keys type, fun and jac.
"""
cons = ({'type': 'eq',
        'fun' : lambda x: np.array([x[0]**3 - x[1]]),
        'jac' : lambda x: np.array([3.0*(x[0]**2.0), -1.0])},
        {'type': 'ineq',
        'fun' : lambda x: np.array([x[1] - 1]),
        'jac' : lambda x: np.array([0.0, 1.0])})

"""a constrained optimization as:"""

res = minimize(func, [-1.0,1.0], args=(-1.0,), jac=func_deriv,
               constraints=cons, method='SLSQP', options={'disp': True})

print(res.x)
```

# Root finding (nonlinear equations)

Finding a root of a set of non-linear equations can be achieved using the root function. Several methods are available, amongst which `hybr` (the default) and `lm` which respectively use the hybrid method of Powell and the LevenbergMarquardt method from MINPACK.

Consider a set of non-linear equations

$$x_0 \cos(x_1) = 4,$$

$$x_0 x_1 - x_1 = 5.$$

# Example for Nonlinear Equations

demo/python\_examples/opt\_nonlinear/example2\_nonlinear.py

```
import numpy as np
from scipy.optimize import root

def func2(x):
    f = [x[0] * np.cos(x[1]) - 4, x[1]*x[0] - x[1] - 5]
    df = np.array([[np.cos(x[1]), -x[0] * np.sin(x[1])], [x[1], x[0] - 1]])
    return f, df

sol = root(func2, [1, 1], jac=True, method='lm')
solution = sol.x

print("the solution of this nonlinear set of equations is: ", solution)
```

## IV. Pointers to tutorials and literature

There is an unlimited amount of tutorials and source codes on the web available. Here is an incomplete list:

- ▶ The Python tutorial: <http://docs.python.org/tutorial>
- ▶ [Quantecon](#)
- ▶ Books: A Primer on Scientific Programming with Python (Hans Petter Langtangen)

# Questions?

1. Advice — RTFM <https://en.wikipedia.org/wiki/RTFM>
2. Advice — <http://lmgtyfy.com/>  
<http://lmgtyfy.com/?q=introduction+to+python>

