

Programming with Python for Engineers

Release 0.0.1

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Jan 11, 2021

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Preface

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i. About this book

a. Target audience of the book

This book is intended to be an accompanying textbook for teaching programming to science and engineering students with no prior programming expertise. This endeavour requires a delicate balance between providing details on computers & programming in a complete manner and the programming needs of science and engineering disciplines. With the hopes of providing a suitable balance, the book uses Python as the programming language, since it is easy to learn and program. Moreover, for keeping the balance, the book is formed of three parts:

- **Part I: The Basics of Computers and Computing:** The book starts with what computation is, introduces both the present-day hardware and software infrastructure on which programming is performed and introduces the spectrum of programming languages.
- **Part II: Programming with Python:** The second part starts with the basic building blocks of Python programming and continues with providing the ground formation for solving a problem in to Python. Since almost all science and engineering libraries in Python are written with an object-oriented approach, a gentle introduction to this concept is also provided in this part.
- **Part III: Using Python for Science and Engineering Problems:** The last part of the book is dedicated to practical and powerful tools that are widely used by various science and engineering disciplines. These tools provide functionalities for reading and writing data from/to files, working with data (using e.g. algebraic, numerical or statistical computations) and plotting data. These tools are then utilized in example problems and applications at the end of the book.

b. How to use the book

This is an ‘interactive’ book with a rather ‘minimalist’ approach: Some details or specialized subjects are not emphasized and instead, direct interaction with examples and problems are encouraged. Therefore, rather than being a ‘complete reference manual’, this book is a ‘first things first’ and ‘hands on’ book. The pointers to skipped details will be provided by links in the book. Bearing this in mind, the reader is strongly encouraged to read and interact all contents of the book thoroughly.

The book’s interactivity is thanks to [Jupyter notebook](#)¹. Therefore, the book differs from a conventional book by providing some dynamic content. This content can appear in audio-visual form as well as some applets (small applications) embedded in the book. It is also possible that the book asks the reader to complete/write a piece of Python program, run it, and inspect the result, from time to time. The reader is encouraged to complete these minor tasks. Such tasks and interactions are of great assistance in gaining acquaintance with Python and building up a self-confidence in solving problems with Python.

Thanks to Jupyter notebook running solutions on the Internet (e.g. [Google Colab](#)², [Jupyter Notebook Viewer](#)³), there is absolutely no need to install any application on the computer. You can directly download and run the notebook on Colab or Notebook Viewer. Though, since it is faster and it provides better virtual machines, the links to all Jupyter notebooks will be served on Colab.

ii. What is computing?

Computing is the process of inferring data from data. What is going to be inferred is defined as the *task*. The original data is called the *input (data)* and the inferred one is the *output (data)*.

Let us look at some examples:

- Multiplying two numbers, X and Y , and subtracting 1 from the multiplication is a *task*. The two numbers X and Y are the *input* and the result of $X \times Y - 1$ is the *output*
- Recognizing the faces in a digital picture is a *task*. Here the *input* is the color values (3 integers) for each point (pixel) of the picture. The *output* is, as you would expect, the pixel positions that belong to faces. In other words, the output can be a set of numbers.
- The board instance of a chess game, as *input*, where black has made the last move. The task is to predict the best move for white. The best move is the *output*.
- The *input* is a set of three-tuples which look like **<Age_of_death, Height, Gender>**. The *task*, an optimization problem in essence, is to find out the curve (i.e. the function) that goes through these tuples in a 3D dimensional space spanned by Age, Height and Gender. As you have guessed already, the *output* is the parameters defining the function and an error describing how well the curve goes through the tuples.
- The *input* is a sentence to a chatbot. The *task* is to determine the sentence (the *output*) that best follows the input sentence in a conversation.

These examples suggest that computing can involve different types of data, either as input or output: Numbers, images, sets, or sentences. Although this variety might appear intimidating at first, we will see that, by using some ‘solution building blocks’, we can do computations and solve various problems with such a wide spectrum of data.

¹ <https://jupyter.org>

² <https://colab.research.google.com/>

³ <https://nbviewer.jupyter.org/>

iii. Are all ‘computing machinery’ alike?

Certainly not! This is a common mistake a layman does. There are diverse architectures based on totally different physical phenomena that can compute. A good example is the *brain* of living beings, which rely on completely different mechanisms compared to the *micro processors* sitting in our laptops, desktops, mobile phones and calculators.

The building blocks of a *brain* is the *neuron*, a cell that has several input channels, called *dendrites* and a single output channel, the *axon*, which can branch like a tree (see Fig. 1).

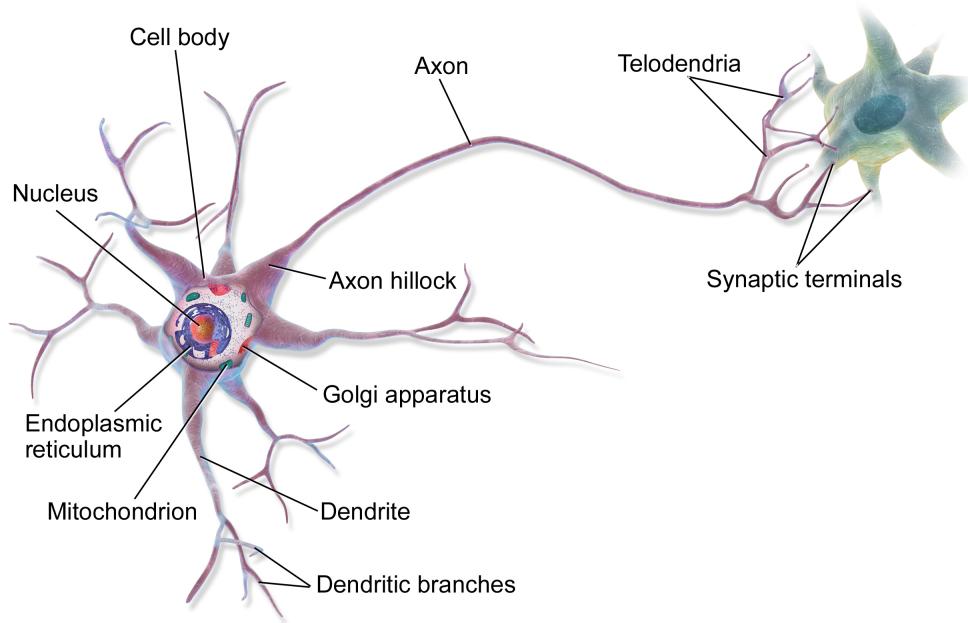


Fig. 1: Our brains are composed of simple processing units, called neurons. Neurons receive signals (information) from other neurons, process those signals and produce an output signal to other neurons. [Drawing by BruceBlaus - Own work, CC BY 3.0, <https://commons.wikimedia.org/w/index.php?curid=28761830>]

The branches of an axon, each carrying the same information, connect to other neurons' dendrites (Fig. 2). The connection with another neuron is called the *synapse*. What travels through the synapse are called *neurotransmitters*. Without going into details, one can simplify the action of neurotransmitters as messengers that cause an excitation or inhibition on the receiving end. In other words, the neurotransmitters, through a chemical process along the axon, are released into the synapse as the ‘output’ of the neuron, they ‘interact’ with the dendrite (i.e. the ‘input’) of another neuron and potentially lead to an excitation or an inhibition.

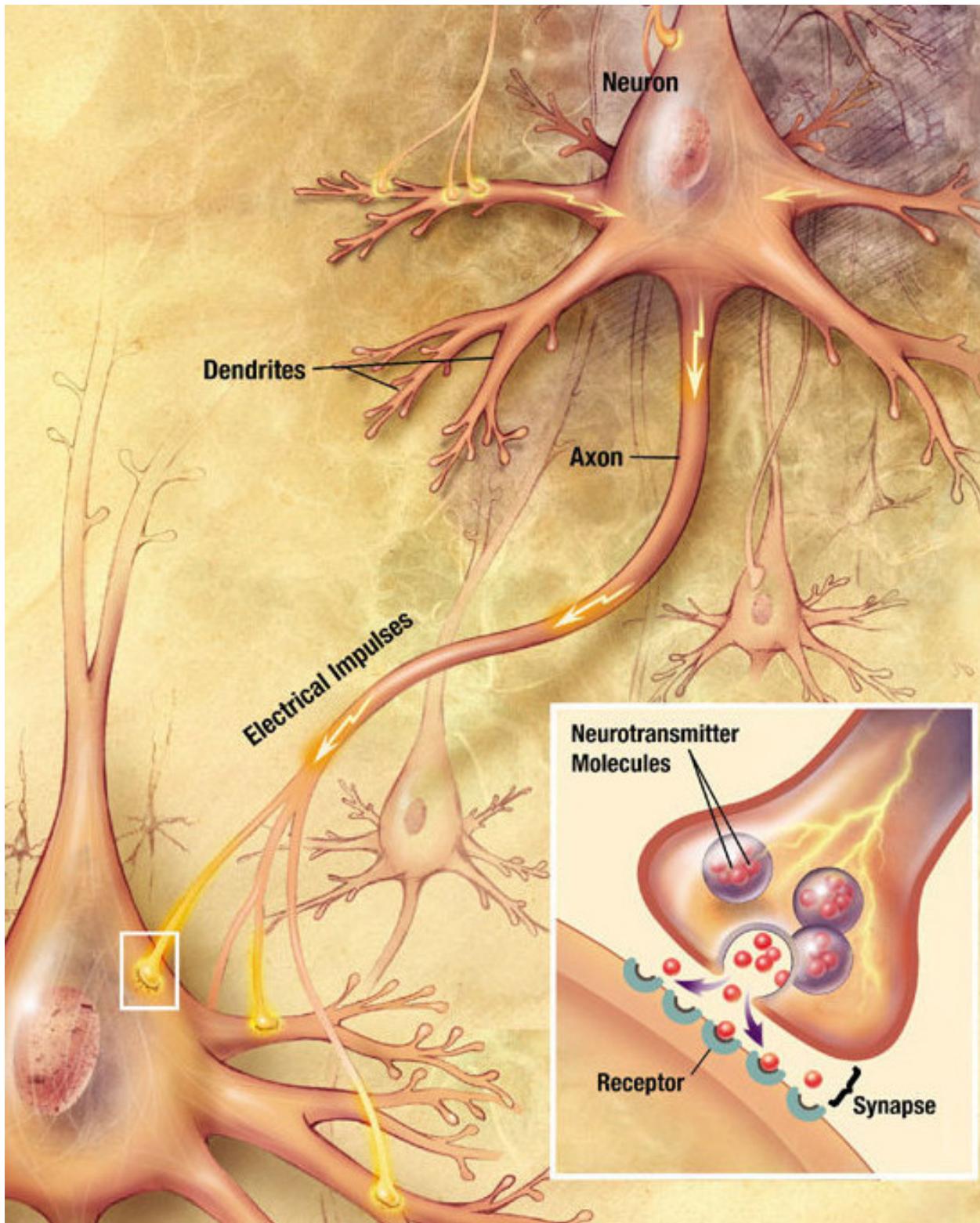


Fig. 2: Neurons ‘communicate’ with each other by transmitting neurotransmitters via synapses. [Drawing by user:Looie496 created file, US National Institutes of Health, National Institute on Aging created original - <http://www.nia.nih.gov/alzheimers/publication/alzheimers-disease-unraveling-mystery/preface>, Public Domain, <https://commons.wikimedia.org/w/index.php?curid=8882110>]

Interestingly enough, the synapse is like a valve, which reduces the neurotransmitters’ flow. We will come

to this in a second. Now, all the neurotransmitters flown in through the input channels (dendrites) have an accumulative effect on the (receiving) neuron. The neuron emits a neurotransmitter burst through its axon. This emission is not a ‘what-comes-in-goes-out’ type. It is more like the curve in Fig. 3.

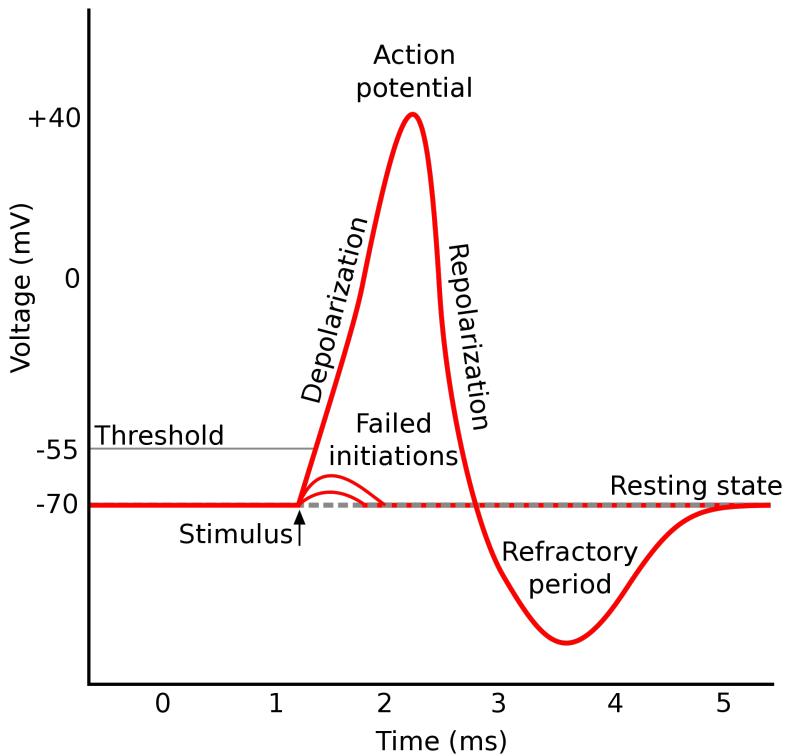


Fig. 3: When a neuron receives ‘sufficient’ amount of signals, i.e. stimulated, it emits neurotransmitters on its axon, i.e. it fires. [Plot by Original by en:User:Chris 73, updated by en:User:Diberri, converted to SVG by tiZom - Own work, CC BY-SA 3.0, <https://commons.wikimedia.org/w/index.php?curid=2241513>]

The throughput of the synapse is something that may vary with time. Most synapses have the ability to ease the flow over time if the neurotransmitter amount that entered the synapse was constantly high. High activity widens the synaptic connection. The reverse also happens: Less activity over time narrows the synaptic connection.

Some neurons are specialized in creating neurotransmitter emission under certain physical effects. Retina neurons, for example, create neurotransmitters if light falls on them. Some, on the other hand, create physical effects, like creating an electric potential that will activate a muscle cell. These specialized neurons feed the huge neural net, the brain, with inputs and receive outputs from it.

The human brain, containing about 10^{11} such neurons with each neuron being connected to 1000-5000 other neurons by the mechanism explained above, is a very unique computing ‘machine’ that inspires computational sciences.

A short video on synaptic communication between neurons

The brain never stops processing information and the functioning of each neuron is only based on signals (the neurotransmitters) it receives through its connections (dendrites). There is no common synchronization timing device for the computation: i.e. each neuron behaves on its own and functions in parallel.

An interesting phenomenon of the brain is that the information and the processing are distributed. Thanks to this feature, when a couple of neurons die (which actually happens each day) no information is lost com-

pletely.

On the contrary to the brain, which uses varying amounts of chemicals (neurotransmitters), the microprocessor based computational machinery uses the existence and absence of an electric potential. The information is stored very locally. The microprocessor consists of subunits but they are extremely specialized in function and far less in number compared to 10^{11} all alike neurons. In the brain, changes take place at a pace of 50 Hz maximum, whereas this pace is 10⁹ Hz in a microprocessor.

In Chapter 1, we will take a closer look at the microprocessor machinery which is used by today's computers. Just to make a note, there are man-made computing architectures other than the microprocessor. A few to mention would be the 'analog computer', the 'quantum computer' and the 'connection machine'.

iv. What is a 'computer'?

As you have already noticed, the word 'computer' is used in more than one context.

1. **The broader context:** Any physical entity that can do 'computation'.
2. **The most common context:** An electronic device that has a 'microprocessor' in it.

From now on, 'computer' will refer to the second meaning, namely a device that has a 'microprocessor'.

A computer...

- is based on binary (0/1) representations such that all inputs are converted to 0s and 1s and all outputs are converted from 0/1 representations to a desired form, mostly a human-readable one. The processing takes places on 0s and 1s, where 0 has the meaning of 'no electric potential' (no voltage, no signal) and 1 has the meaning of 'some fixed electric potential (usually 5 Volts, a signal).
- consists of two clearly distinct entities: The Central Processing Unit (CPU), also known as the microprocessor ($\square P$), and a *Memory*. In addition to these, the computer is connected to or incorporates other electronic units, mainly for input-output, known as 'peripherals'.
- performs a 'task' by executing a sequence of instructions, called a 'program'.
- is deterministic. That means if a 'task' is performed under the same conditions, it will produce always the same result. It is possible to include randomization in this process only by making use of a peripheral that provides electronically random inputs.

v. What is programming?

The CPU (the microprocessor - $\square P$) is able to perform several types of actions:

- Arithmetic operations on binary numbers that represent (encode) integers or decimal numbers with fractional part.
- Operations on binary representations (like shifting of digits to the left or right; inverting 0s and 1s).
- Transferring to/from memory.
- Comparing numbers (e.g. whether a number n_1 larger than n_2) and performing alternative actions based on such comparisons.
- Communicating with the peripherals.

- Alternating the course of the actions.

Each such unit action is recognized by the CPU as an *instruction*. In more technically terms, tasks are solved by a CPU by executing a sequence of instructions. Such sequences of instructions are called machine codes. Constructing machine codes for a CPU is called ‘machine code programming’.

But, programming has a broader meaning:

a series of steps to be carried out or goals to be accomplished.

And, as far as computer programming is concerned, we would certainly like these steps to be expressed in a more natural (more human readable) manner, compared to binary machine codes. Thankfully, there exist ‘machine code programs’ that read-in such ‘more natural’ programs and convert them into ‘machine code programs’ or immediately carry out those ‘naturally expressed’ steps.

Python is such a ‘more natural way’ of expressing programming steps.

Basic Computer Organization

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In this chapter, we will provide an overview of the internals of a modern computer. To do so, we will first describe a general architecture on which modern computers are based. Then, we will study the main components and the principles that allow such machines to function as general purpose “calculators”.

The von Neumann Architecture

John von Neumann

From: Oxford Reference⁴

“Hungarian-born US mathematician, creator of the theory of games and pioneer in the development of the modern computer. Born in Budapest, the son of a wealthy banker, von Neumann was educated at the universities of Berlin, Zürich, and Budapest, where he obtained his PhD in 1926. After teaching briefly at the universities of Berlin and Hamburg, von Neumann moved to the USA in 1930 to a chair in mathematical physics at Princeton. In 1933, he joined the newly formed Institute of Advanced Studies at Princeton as one of its youngest professors. By this time he had already established a formidable reputation as one of the most powerful and creative mathematicians of his day. In 1925 he had offered alternative foundations for set theory, while in his *Mathematischen Grundlagen der Quantenmechanik* (1931) he removed many of the basic doubts that had been raised against the coherence and consistency of quantum theory. In 1944, in collaboration with Oskar Morgenstern (1902–77), von Neumann published *The Theory of Games and Economic Behaviour*. A work of great originality, it is reputed to have had its origins at the poker tables of Princeton and Harvard. The basic problem was to show whether it was possible to speak of rational behaviour in situations of conflict and uncertainty as in, for example, a game of poker or wage negotiations. In 1927 von Neumann proved the important theorem that even in games that are not fully determined, safe and rational strategies exist. With entry of the USA into World War II in 1941 von Neumann, who had become an American citizen in 1937, joined the Manhattan project (for the manufacture of the atom bomb) as a consultant. In 1943 he became involved at Los Alamos on the crucial problem of how to detonate an atom bomb. Because of the enormous quantity of computations involved, von Neumann was forced to seek mechanical aid. Although the computers he had in mind could not be made in 1945, von Neumann and his colleagues began to design *Maniac I* (Mathematical analyser, numerical integrator, and computer). Von Neumann was one of the first to see the value of a flexible stored program: a program that could be changed quite easily without altering the computer’s basic circuits. He went on to consider deeper problems in the theory of logical automata and finally managed to show that self-reproducing machines were theoretically possible. Such a machine would need 200 000 cells and 29 distinct states. Having once been caught up in affairs of state von Neumann found

⁴ <https://www.oxfordreference.com/view/10.1093/oi/authority.20110803120234729>

it difficult to return to a purely academic life. Thereafter much of his time was therefore spent, to the regret of his colleagues, advising a large number of governmental and private institutions. In 1954 he was appointed to the Atomic Energy Commission. Shortly after this, cancer was diagnosed and he was forced to struggle to complete his last work, the posthumously published *The Computer and the Brain* (1958)."



Fig. 4: John von Neumann (1903 – 1957)

Components of the von Neumann Architecture

The von Neumann architecture (Fig. 5) defines the basic structure, or outline, used in most computers today. Proposed in 1945 by von Neumann, it consists of two distinct units: An *addressable memory* and a *Central Processing Unit* (CPU). All the encoded actions and data are stored together in the memory unit. The CPU, querying these actions, the so-called *instructions*, executes them one by one, sequentially (though, certain instructions may alter the course of execution order).

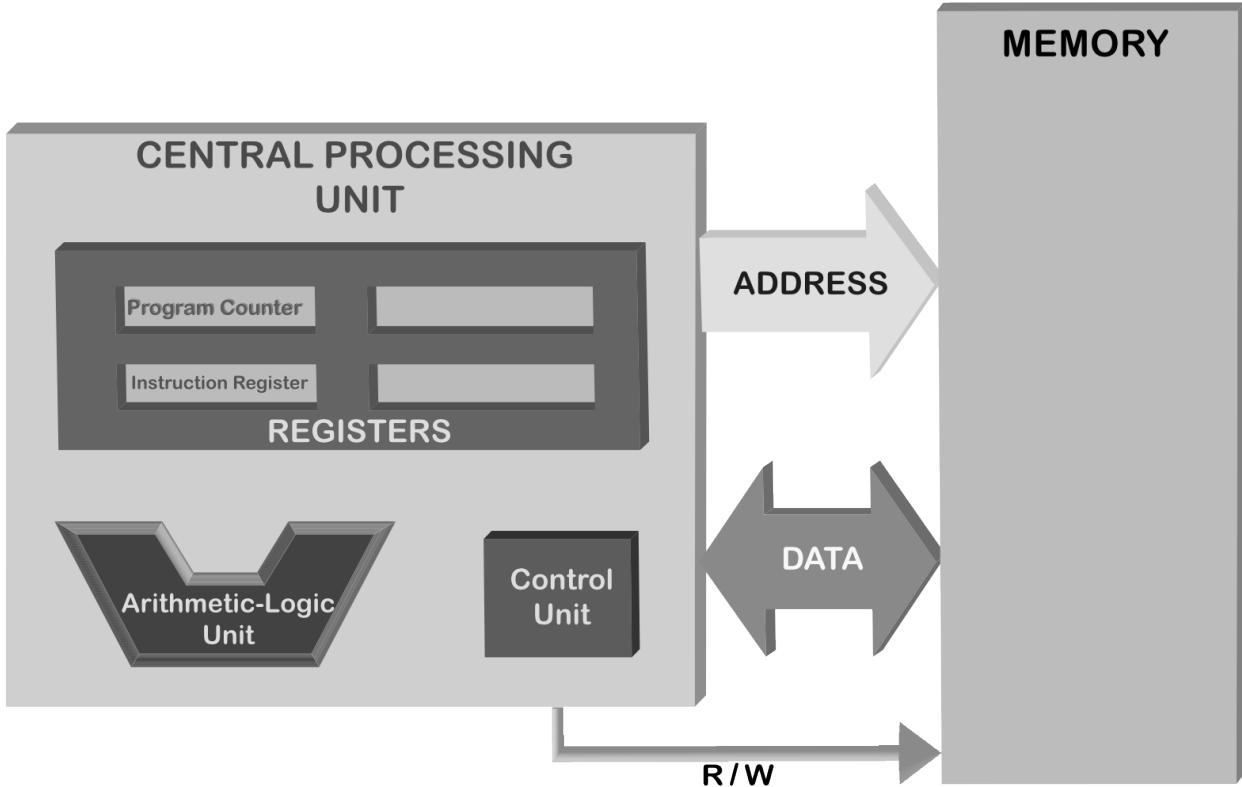


Fig. 5: A block structure view of the von Neumann Architecture.

The CPU communicates with the memory via two sets of wires, namely the *address bus* and the *data bus*, plus a single *R/W* wire (Fig. 5). These busses consist of several wires and carry binary information to/from the memory. Each wire in a bus carries one bit of the information (either a zero (0) or a one (1)). Today's von Neumann architectures are working on electricity, and therefore, these zeros and ones correspond to voltages. A one indicates usually the presence of a 5V and a zero denotes the absence of it.

The Memory

The memory can be imagined as pigeon holes organized as rows (Fig. 6). Each row has eight pigeon holes, each being able to hold a zero (0) or one (1) – in electronic terms, each pigeon hole is capable of storing a voltage (can you guess what type of an electronical component a pigeon hole is?). Each such row is named to be of the size *byte*; i.e., a byte means 8 bits.

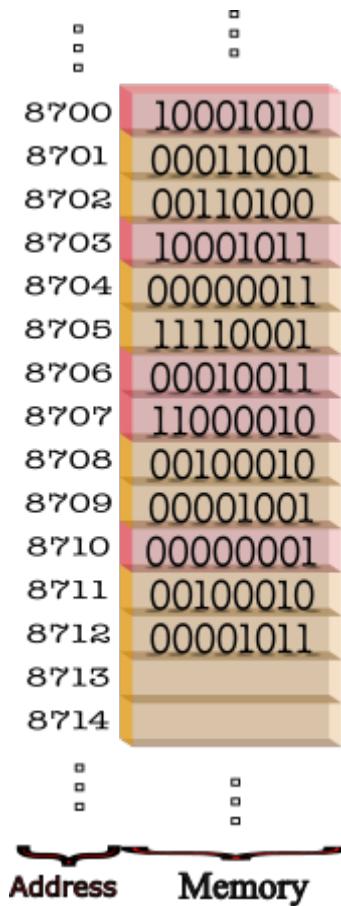


Fig. 6: The memory is organized as a stack of rows such that each row has an associated address.

Each byte of the memory has a unique address. When the address input (also called address bus – Fig. 5) of the memory is provided a binary number, the memory byte that has this number as the address becomes accessible through the data output (also called output data bus). Based on W/R wire being set to Write (1) or Read (0), the action that is carried out on the memory byte differs:

- **W/R wire is set to WRITE (1) :**

The binary content on the input data bus is copied into the 8-bit location whose address is provided on the address bus, the former content is *overwritten*.

- **W/R wire is set to READ (0) :**

The data bus is set to a copy of the content of 8-bit location whose address is provided on the address bus. The content of the accessed byte is left intact.

The information stored in this way at several addresses live in the memory happily, until the power is turned off.

The memory is also referred as Random Access Memory (RAM). Some important aspects of this type of memory have to be noted:

- Accessing any content in RAM, whether for reading or writing purposes, is *only* possible when the content's address is provided to the RAM through the address bus.
- Accessing any content takes exactly the same amount of time, irrespective of the address of the content. In todays RAMs, this access time is around 50 nanoseconds.
- When a content is overwritten, it is gone forever and it is not possible to undo this action.

An important question is who sets the address bus and communicates through the data bus (sends and receives bytes of data). As depicted in Fig. 5, the CPU does. How this is done on the CPU side will become clear in the next section.

The CPU

The Central Processing Unit, which can be considered as the ‘brain’ of a computer, consists of the following units:

- **Control Unit (CU)**, which is responsible for fetching instructions from the memory, interpreting (‘de-coding’) them and executing them. After executing an instruction finishes, the control unit continues with the next instruction in the memory. This “fetch-decode-execute” cycle is constantly executed by the control unit.
- **Arithmetic Logic Unit (ALU)**, which is responsible for performing arithmetic (addition, subtraction, multiplication, division) and logic (less-than, greater-than, equal-to etc.) operations. CU provides the necessary data to ALU and the type of operation that needs to be performed, and ALU executes the operation.
- **Registers**, which are mainly storage units on the CPU for storing the instruction being executed, the affected data, the outputs and temporary values.

The size and the quantity of the registers differ from CPU model to model. They generally have size in the range of [2-64] bytes and most registers on today’s most popular CPUs have size 64 bits (i.e. 8 bytes). Their quantity is not high and in the range of [10-20]. The registers can be broadly categorized into two: *Special Purpose Registers* and *General Purpose Registers*.

Two special purpose registers are worth mentioning to understand how a CPU’s Fetch-Decode-Execute cycle runs. The first is the so-called *Program Counter* (PC) and the second is the *Instruction Register* (IR).

- **Input/Output connections**, which connect the CPU to the other components in the computer.

The Fetch-Decide-Execute Cycle

The CPU is in fact a *state machine*, a machine that has a representation of its current *state*. The machine, being in a state, reads the next instruction and executes the instruction according to its current state. The state consists of what is stored in the registers. Until it is powered off, the CPU follows the Fetch-Decide-Execute cycle (Fig. 7) where each step of the cycle is based on its state. The *control unit* is responsible for the functioning of the cycle.

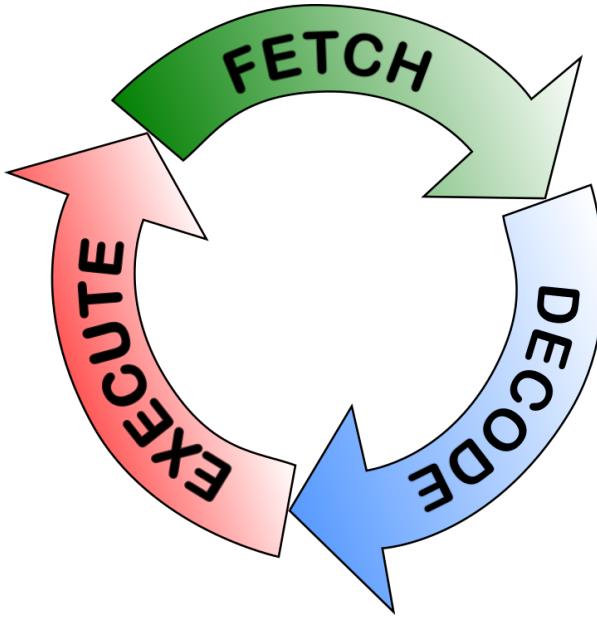


Fig. 7: The CPU constantly follows the fetch-decode-execute cycle while the computer is running a program.

1- The Fetch Phase

The cycle starts with the Fetch Phase. At the beginning of this phase, the CPU has the address (the position in the memory) of the next instruction in the PC (Program Counter) Register. During this phase, the address bus is set to this address in the PC register and the R/W wire is set to Read (0). The memory responds to this by providing the memory content at the given address on the data bus.

How many bytes are sent through the data bus is architecture dependent. Usually it is 4-8 bytes. These bytes are received into the IR (Instruction Register).

2- The Decode Phase

At the beginning of this phase, the IR is assumed to be holding the current instruction. The content of the first part of the IR electronically triggers some action. Every CPU has an electronically built-in hard-wired instruction table in which every possible atomic operation that the CPU can carry out has an associated binary code, called *operation code* (opcode in short). This table differs from CPU brand to brand.

There are three types of instructions:

- *Data manipulation*: Arithmetic/Logic operations on/among registers,
- *Data transfer*: Memory-to-Register, Register-to-Memory, Register-to-Register transfers,
- *Control flow of execution*: Instructions that stop execution, jump to a different part of the memory for next instruction, instead of the next one in the memory.

Let us assume that our instruction looks like this:

Opcode	Effect data or address
0001	0110

This is an 8-byte instruction that has the first 4 bits as representing the opcode. The designer could have designed the CPU such that the opcode 0001 denotes an instruction for reading data from the memory, writing data to the memory or adding the contents of the two registers etc. The remaining four bits then

contain the parameters of the instruction, which are the data to be operated on, the address in the memory or the codes of the registers etc.

Let us assume that this 8-bit example instruction (i.e. the opcode 0001) denotes an addition on two registers and that the remaining 4 bits encode the registers in question, with 01 denoting one register and 10 the other register. Prior to the instruction, we can assume the two registers to contain integers, and after the instruction is executed, one of the registers will be incremented by the amount of the other (by means of integer addition).

Although this was a simple and hypothetical example, it illustrates how modern CPUs can decode an instruction and decipher its elements. Though, the length of an instruction and the variety of instructions are clearly different.

3- The Execute Phase

As the name implies, the electronically activated and initialized circuitry carries out the instruction in this phase. Depending on the instruction, the registers, the memory or other components are effected. When the instruction completes, the PC is updated by one unless it was a control flow changing instruction in which case the PC is updated to the to-be-jumped address in the memory (in some designs, the PC can be updated in the fetch phase, after fetching the instruction). Not all instructions take the same amount of time to be carried out. Floating point division, for example, takes much more time compared to others.

A CPU goes through the *Fetch-Decode-Execute* cycle until it is powered off. What happens at the very beginning? The electronics of the CPU is manufactured such that, when powered up, the PC register has a very fixed content. Therefore, the first instruction is always fetched from a certain position.

An intelligent question would be “when does the CPU jump from one state to another?”. One possible answer is: whenever the previous state is completed electronically, a transition to the next state is performed. Interestingly, this is not true. The reality is that there is an external input to the CPU from which electronic pulses are fed. This input is called the *system clock* and each period of it is named as a *clock cycle*. The best performance would be that each phase of the fetch-decode-execute cycle is completed in one-and-only-one clock cycle. On modern CPUs, this is true for addition instruction, for example. But there are instructions (like floating point division) which take about 40 clock cycles.

What is length of a clock cycle? CPUs are marked with their *clock frequency*. For example, Intel’s latest processor, i9, has a maximal clock frequency of 5GHz (that is 5×10^9 pulses per second). So, since (period) = $1/(\text{frequency})$, for this processor a clock cycle is 200 pico seconds. This is such a short time that light would travel only 6 cm.

A modern CPU has many more features and functional components: *interrupts, ports, various levels of caches* are a few of them. To cover them is certainly out of the scope of this course material.

The Stored Program Concept

In order for the CPU to compute something, the corresponding instructions to do the computation have to be placed into the memory (how this is achieved will become clear in the next chapter). These instructions and data that perform a certain task are called a *Computer Program*. The idea of storing a computer program into the memory to be executed is coined as the *Stored Program Concept*.

What does a stored program look like? Below you see a real extract from the memory, a program that multiplies two integer numbers sitting in two different locations in the memory and stores the result in another memory location (to save space consecutive 8 bytes in the memory are displayed in a row, the next row displays the next 8 bytes):

```

01010101 01001000 10001001 11100101 10001011 00010101 10110010 00000011
00100000 00000000 10001011 00000101 10110000 00000011 00100000 00000000
00001111 10101111 11000010 10001001 00000101 10110111 00000011 00100000
00000000 10111000 00000000 00000000 00000000 11001001 11000011
...
11001000 00000001 00000000 00000000 00000000 00000000

```

Unless you have a magical talent, this should not be understandable to you. It is difficult because it is just a sequence of bytes. Yes, the first byte is presumably an instruction, but what is it? Furthermore, since we do not know what it is, we do not know whether it is followed by some data or not, so we cannot say where the second instruction starts. However, the CPU for which these instructions were written for would know this, hard-wired in its electronics.

When a programmer wants to write a program at this level, i.e. in terms of binary CPU instructions and binary data, s/he has to understand and know each instruction the CPU can perform, should be able to convert data to some internal format, to make a detailed memory layout on paper and then to start writing down each bit of the memory. This way of programming is an extremely painful job; though it is possible, it is impractical.

Alternatively, consider the text below:

```

main:
    pushq %rbp
    movq %rsp, %rbp
    movl alice(%rip), %edx
    movl bob(%rip), %eax
    imull %edx, %eax
    movl %eax, carol(%rip)
    movl $0, %eax
    leave
    ret
alice:
    .long 123
bob:
    .long 456

```

Though `pushq` and `moveq` are not immediately understandable, the rest of the text provides some hints. `alice` and `bob` must be some programmer's name invention, e.g. denoting variables with values 123 and 456 respectively; `imull` must have something to do with 'multiplication', since only registers can be subject to arithmetic operations; `%edx` and `%eax` must be some denotation used for registers; having uncovered this, `movls` start to make some sense: they are some commands to move around data... and so on. Even without knowing the instruction set, with a small brainstorming we can uncover the action sequence.

This text is an example *assembly* program. A human invented denotation for instructions and data. An important piece of knowledge is that each line of the assembler text corresponds to a single instruction. This assembly text is so clear that even manual conversion to the cryptic binary code above is feasible. From now on, we will call the binary code program as a *Machine Code Program* (or simply the *machine code*).

How do we automatically obtain machine codes from assembly text? We have machine code programs that convert the assembly text into machine code. They are called *Assemblers*.

Despite making programming easier for programmers, compared to machine codes, even assemblers are insufficient for efficient and fast programming. They lack some high-level constructs and tools that are necessary for solving problems easier and more practical. Therefore higher level languages that are much easier to read and write compared to assembly are invented.

We will cover the spectrum of programming languages in more detail in the next chapter.

Pros and Cons of the von Neuman Architecture

The von Neumann architecture has certain advantages and disadvantages:

Advantages

- CPU retrieves data and instruction in the same manner from a single memory device. This simplifies the design of the CPU.
- Data from input/output (I/O) devices and from memory are retrieved in the same manner. This is achieved by mapping the device communication electronically to some address in the memory.
- The programmer has a considerable control of the memory organization. So, s/he can optimize the memory usage to its full extent.

Disadvantages

- Sequential instruction processing nature makes parallel implementations difficult. Any parallelization is actually a quick sequential change in tasks.
- The famous “*Von Neumann bottleneck*” : Instructions can only be carried out one at a time and sequentially.
- Risk of an instruction being unintentionally overwritten due to an error in the program.

An alternative to the von Neumann Architecture is the [Harvard Architecture](#)⁵ which could not resist the test of time due to crucial disadvantages compared to the von Neumann architecture.

Peripherals of a computer

Though it is somewhat contrary to your expectation, any device outside of the von Neumann structure, namely the CPU and the Memory, is a *peripheral*. In this aspect, even the keyboard, the mouse and the display are peripherals. So are the USB and ethernet connections and the internal hard disk. Explaining the technical details of how those devices are connected to the von Neumann architecture is out of the scope of this book. Though, we can summarize it in a few words.

All devices are electronically listening to the busses (the address and data bus) and to a wire running out of the CPU (which is not pictured above) which is 1 or 0. This wire is called the *port_io* line and tells the memory devices as well as to any other device that listens to the busses whether the CPU is talking to the (real) memory or not. If it is talking to the memory all the other listeners keep quiet. But if the *port_io* line is 1, meaning the CPU doesn't talk to the memory but to the device which is electronically sensitive to that specific address that was put on the address bus (by the CPU), then that device jumps up and responds (through the data bus). The CPU can send as well as receive data from that particular device. A computer has some precautions to prevent address clashes, i.e. two devices responding to the same address information in *port_io*.

Another mechanism aids communication requests initiated from the peripherals. Of course it would be possible for the CPU from time to time stop and do a *port_io* on all possible devices, asking them for any data they want to send in. This technique is called *polling* and is extremely inefficient for devices that send asynchronous data (data that is send in irregular intervals): You cannot know when there will be a keyboard

⁵ https://en.wikipedia.org/wiki/Harvard_architecture

entry so, in polling, you have to ask very frequently the keyboard device for the existence of any data. Instead of dealing with the inefficiency of polling, another mechanism is built into the CPU. The interrupt mechanism is an electronic circuitry of the CPU which has inlets (wires) connected to the peripheral devices. When a device wants to communicate with (send or receive some data to/from) the CPU they send a signal (1) from that specific wire. This gets the attention of the CPU, the CPU stops what it is doing at a convenient point in time, and asks the device for a port_io. So the device gets a chance to send/receive data to/from the CPU.

The running of a computer

When you power on a computer, it first goes through a start-up process (also called booting), which, after performing some routine checks, loads a program from your disk called Operating System.

Start up Process

At the core of a computer is the von Neumann architecture. But how a machine code finds its way into the memory, gets settled there, so that the CPU starts executing it, is still unclear.

When you buy a brand new computer and turn it on for the first time, it does some actions which are traceable on its display. Therefore, there must be a machine code in a memory which, even when the power is off, does not lose its content, very much like a flash drive. It is electronically located exactly at the address where the CPU looks for its first instruction. This memory, with its content, is called Basic Input Output System, or in short BIOS. In the former days, the BIOS was manufactured as write-only-once. To change the program, a chip had to be replaced with a new one. The size of the BIOS of the first PCs was 16KB, nowadays it is about 1000 times larger, 16MB.

When you power up a PC the BIOS program will do the following in sequence:

- Power-On Self Test, abbreviated as POST, which determines whether the CPU and the memory are intact, identifies and if necessary, initializes devices like the video display card, keyboard, hard disk drive, optical disc drive and other basic hardware.
- Looking for an *operating system* (OS): The BIOS program goes through storage devices (e.g. hard disk, floppy disk, USB disk, CD-DVD drive, etc.) connected to the computer in a predefined order (this order is generally changeable by the user) and looks for and settles for the first operating system that it can find. Each storage device has a small table at the beginning part of the device, called the Master Boot Record (MBR), which contains a short machine code program to load the operating system if there is one.
- When BIOS finds such a storage device with an operating system, it loads the content of the MBR into the memory and starts executing it. This program loads the actual operating system and then runs it.

The Operating System

The operating system is a program that, after being loaded into the memory, manages resources and services like the use of memory, the CPU and the devices. It essentially hides the internal details of the hardware and makes the ugly binary machine understandable and manageable to us.

An OS has the following responsibilities:

- **Memory Management:** Refers to the management of the memory connected to the CPU. In modern computers, there is more than one machine code program loaded into the memory. Some programs are initiated by the user (like a browser, document editor, Word, music player, etc.) and some are initiated

by the operating system. The CPU switches very fast from one program (this is called a *process*) in the memory to another. The user (usually) does not feel the switching. The memory manager keeps track of the space allocated by processes in the memory. When a new program (process) is being started, it has to be placed into the memory. The memory manager decides where it is going to be placed. Of course, when a process ends, the place in the memory occupied by the process has to be reclaimed; that is the memory manager's job. It is also possible that, while running, a process demands additional space in the memory (e.g. a photoshop-like program needs more space for a newly opened JPG image file) then the process makes this demand to the memory manager, which grants it or denies it.

- **Process (Time) Management:** As said above, a modern memory generally contains more than one machine code program. An electronic mechanism forces the CPU to switch to the *Time Manager* component of the OS. At least 20 times a second, the time manager is invoked to make a decision on behalf of the CPU: Which of the processes that sit in the memory will be run during the next period? When a process gets the turn, the current state of the CPU (the contents of all registers) is saved to some secure position in the memory, in association to the last executing process. From that secure position, the last saved state information which going to take the turn is found and the CPU is set to that state. Then the CPU, for a period of time executes that process. At the end of that period, the CPU switches over to the time manager and the time manager makes a decision for the next period. Which process will get the turn? And so on. This decision making is a complex task. Still there are Ph.D. level research going on on this subject. The time manager collects some statistics about each individual process and its system resource utilization. Also there is the possibility that a process has a high priority associated due to several reasons. The time manager has to solve a kind of optimization problem under some constraints. As mentioned, this is a complex task and a hidden quality factor of an OS.
- **Device Management:** All external devices of a computer have a software plug-in to the operating system. An operating system has some standardized demands from devices and these software plug-ins implement these standardized functionality. This software is usually provided by the device manufacturer and is loaded into the operating system as a part of the device installing process. These plug-ins are named as *device drivers*.

An Operating System performs device communication by means of these drivers. It does the following activities for device management:

- Keeps tracks of all devices' status.
 - Decides which process gets access to the device when and for how long.
 - Implements some intelligent caching, if possible, for the data communication with the device.
 - De-allocates devices.
- **File Management:** A computer is basically a data processing machine. Various data are produced or used for very diverse purposes. Textual, numerical, audio-visual data are handled. Handling data also includes *storing* and *retrieving* it on some external recording device. Examples for such recording devices are hard disks, flash drives, CDs and DVDs. Data is stored on these devices as files. A *file* is a persistent piece of information that has a name, some meta data (e.g. information about the owner, the creation time, size, content type, etc.) and the data.

The organizational mechanism for how files are stored on devices is called the *file system*. There are various alternatives to do this. FAT16, FAT32, NTFS, EXT2, EXT3, ExFAT, HFS+ are a few of about a hundred (actually the most common ones). Each has its own pros and cons as far as *max allowed file size, security, robustness (repairability), extensibility, metadata, lay out policies* and some other aspects are concerned. Files are most often managed in a hierarchy. This is achieved by a concept of *directories or folders*. On the surface (as far as the user sees them), a file system usually consist of

files separated into directories where directories can contain files or other directories.

The file manager is responsible for creation & initialization of a file system, inclusion and removal of devices from this system and management of all sorts of changes in the file system: Creation, removal, copying of files and directories, dynamically assigning access rights for files and directories to processes etc.

- **Security:** This is basically for the maintenance of the computer's integrity, availability, and confidentiality. The security of a computer exists at various layers such as:

- maintaining the physical security of the computer system,
- the security of the information the system is in hold of, and
- the security of the network to which the computer is connected.

In all of these, the operating system plays a vital role in keeping the security. Especially the second item is where the operating system is involved at most. Information, as you know by now, is placed in the computer in two locations. The internal memory and the external storage devices. The internal memory is in hold of the processes and the processes should not interfere with each other (unless specifically intended). Actually in a modern day computer, there can be more than one user working at the same time on the computer. Their processes running in the memory as well as their files being on the file system must remain extremely private and separate. Even their existence has to be hidden from every other user.

Computers are connected and more and more integrated in a global network. This integration is done on a spectrum of interactions. In the extreme case, a computer can be solely controlled over the network. Of course this is done by supplying some credentials but, as you would guess, such a system is prone to malicious attacks. An operating system has to take measures to protect the computer system from such harms. Sometimes it is the case that bugs of the OS are discovered and exploited in order to breach security.

- **User Interface:** As the computer's user, when you want to do anything you do this by ordering the operating system to do it. Starting/terminating a program, exploring or modifying the file system, installing/uninstalling a new device are all done by “talking” to the operating system. For this purpose, an OS provides an interface, coined as the *user interface*. In the older days, this was done by typing some cryptic commands into a typewriter at a console device. Over the years, the first computer with a *Graphical User Interface (GUI)* emerged. A GUI is a visual interface to the user where the screen can host several windows each dedicated to a different task. Elements of the operating system (processes, files, directories, devices, network communications) and their status are symbolized by icons and the interactions are mostly via moving and clicking a pointing device which is another icon (usually a movable arrow) on the screen. The *Xerox Alto*⁶ introduced on March 1973 was the first computer that had a GUI. The first personal computer with a GUI was *Apple Lisa*⁷, introduced in 1983 with a price of \$10,000. Almost three years later, by the end of 1985, Microsoft released its first OS with a GUI: Windows 1.0. The archaic console typing still exists, in the form a type-able window, called terminal, which is still very much favoured among programming professionals because it provides more control for the OS.

⁶ <https://github.com/sinankalkan/CENG240/blob/master/figures/XeroxAlto.jpg?raw=true>

⁷ <https://github.com/sinankalkan/CENG240/blob/master/figures/AppleLisa.jpg?raw=true>

Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- The von Neumann Architecture.
- The interaction between the CPU and the memory via address, R/W and data bus lines.
- The crucial components on the CPU: The control unit, the arithmetic logic unit and the registers.
- The fetch-decode-execute cycle.
- The stored program concept.
- Operating system and its responsibilities.

Further Reading

- Computer Architectures:
 - Von Neumann Architecture: http://en.wikipedia.org/wiki/Von_Neumann_architecture
 - Harvard Architecture: http://en.wikipedia.org/wiki/Harvard_architecture
 - Harvard vs. Von Neumann Architecture: http://www.pic24micro.com/harvard_vs_von_neumann.html
 - Quantum Computer: http://en.wikipedia.org/wiki/Quantum_computer
 - Chemical Computer: http://en.wikipedia.org/wiki/Chemical_computer
 - Non-Uniform Memory Access Computer: http://en.wikipedia.org/wiki/Non-Uniform_Memory_Access
- Running a computer:
 - Booting a computer: <https://en.wikipedia.org/wiki/Booting>
 - History of operating systems: https://en.wikipedia.org/wiki/History_of_operating_systems
 - Operating systems: https://en.wikipedia.org/wiki/Operating_system

Exercises

- To gain more insight, play around with the von Neumann machine simulator at <http://vnsimulator.altervista.org>
- Using Google and the manufacturer's web site, find the following information for your desktop/laptop:
 - Memory (RAM) size
 - CPU type and Clock frequency
 - Data bus size
 - Address bus size
 - Size of the general purpose registers of the CPU

- Harddisk or SSD size and random access time

Opcode	Affected address
0001	0100

- Assume that we have a CPU that can execute instructions with the format and size given above.
 - What is the number of different instructions that this CPU can decode?
 - What is the maximum number of rows in the memory that can be addressed by this CPU?

A Broad Look at Programming and Programming Languages

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The previous chapter provided a closer look at how a modern computer works. In this chapter, we will first look at how we generally solve problems with such computers. Then, we will see that a programmer does not have to control a computer using the binary machine code instructions we introduced in the previous chapter: We can use human-readable instructions and languages to make things easy for programming.

How do we solve problems with programs?

The von Neumann machine, on which computers' design is based, makes a clear distinction between instruction and data (do not get confused by the machine code holding both data and instructions: The data field in such instructions are generally addresses of the data to be manipulated and therefore, data and instructions exist as different entities in memory). Due to this clear distinction between data and instruction, the solutions to world problems were approached and handled with this distinction in mind (Fig. 8):

"For solving world problems, the first task of the programmer is to identify the information to be processed to solve the problem. This information is called data. Then, the programmer has to find an action schema that will act upon this data, carry out those actions according to the plan, and produce a solution to the problem. This well-defined action schema is called an algorithm."

[From: G. Üçoluk, S. Kalkan, Introduction to Programming Concepts with Case Studies in Python, Springer, 2012⁸]

⁸ <https://link.springer.com/book/10.1007/978-3-7091-1343-1>

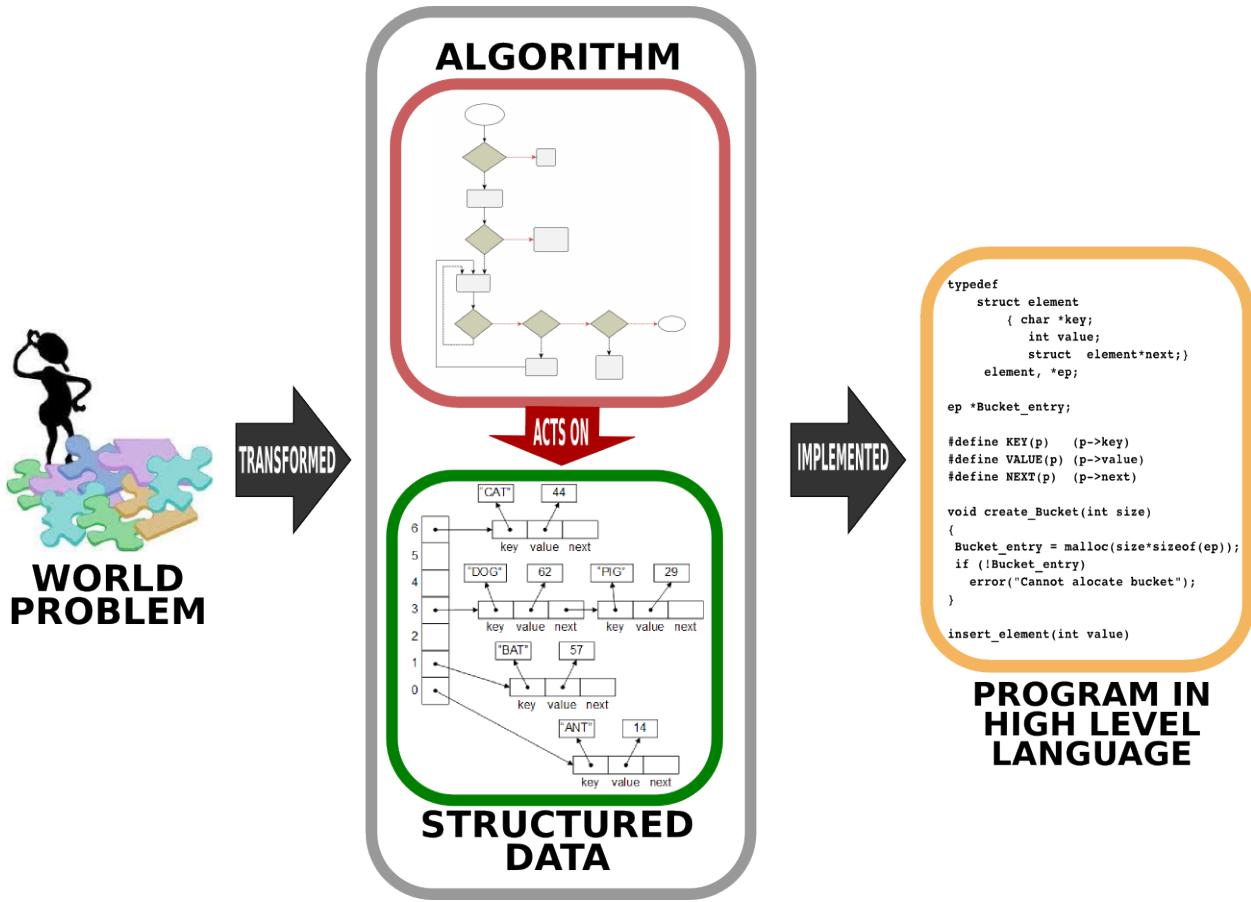


Fig. 8: Solving a world problem with a computer requires first designing how the data is going to be represented and specifying the steps which yield the solution when executed on the data. This design of the solution is then written (implemented) in a programming language to be executed as a program such that, when executed, the program outputs the solution for the world problem. [From: G. Üçoluk, S. Kalkan, *Introduction to Programming Concepts with Case Studies in Python*, Springer, 2012⁹]

Algorithm

An algorithm is a step-by-step procedure that, when executed, leads to an output for the input we provided. If the procedure was correct, we expect the output to be the desired output, i.e. the solution we wanted for the algorithm to compute.

Algorithms can be thought of as recipes for cooking. This analogy makes sense since we would define a recipe as a step-by-step procedure for cooking something: Each step performs a little action (cutting, slicing, stirring etc.) that brings us closer to the outcome, the meal.

This is exactly the case in algorithms as well: At each step, we make a small progress towards the solution by performing a small computation (e.g. adding numbers, finding the minimum of a set of real numbers etc.). The only difference with cooking is that each step needs to be *understandable* by the computer; otherwise, it is not an algorithm.

The origins of the word ‘algorithm’ The word ‘algorithm’ comes from the Latin word *algorithmi*, which is the Latinized name of Al-Khwarizmi. Al-Khwarizmi was a Persian Scientist who has written a book on al-

⁹ <https://link.springer.com/book/10.1007/978-3-7091-1343-1>

gebra titled “The Compendious Book on Calculation by Completion and Balancing” during 813–833 which presented the first systematic solution of linear and quadratic equations. His contributions established algebra, which stems from his method of “al-jabr” (meaning “completion” or “rejoining”). The reason the world algorithm is attributed to Al-Khwarizmi is because he proposed systematic methods for solving equations using sequences of well-defined instructions (e.g. “take all variables to the right. divide the coefficients by the coefficient of x ...”) – i.e. using what we call today as algorithms.



Fig. 9: Muhammad ibn Musa al-Khwarizmi (c. 780 – c. 850)

** Are algorithms the same thing as programs? **

It is very natural to confuse algorithms with programs as they are both step-by-step procedures. However, algorithms can be studied and they were invented long before there were computers or programming languages. We can design and study algorithms without using computers with just a pen and paper. A program, on the other hand, is just an implementation of an algorithm in a programming language. In other words, algorithms are designs and programs are the written forms of these designs in programming languages.

How to write algorithms

As we have discussed above, before programming our solution, we first need to design it. While designing an algorithm, we generally use two mechanisms:

1. **Pseudo-codes.** Pseudo-codes are natural language descriptions of the steps that need to be followed in the algorithm. It is not as specific or restricted as a programming language but it is not as free as the language we use for communicating with other humans: A pseudo-code should be composed of precise and feasible steps and avoid ambiguous descriptions.

Here is an example pseudo-code:

Algorithm 1. Calculate the average of numbers provided by the user.

Input: N -- the count of numbers

Output: The average of N numbers to be provided

Step 1: Get how many numbers will be provided **and** store that **in** N

Step 2: Create a variable named Result **with** initial value 0

Step 3: Execute the following step N times:

(continues on next page)

Step 4: Get the **next** number **and** add it to Result

Step 5: Divide Result by N to obtain the average

2. **Flowcharts.** As an alternative to pseudocodes, we can use flowcharts while designing algorithms. Flowcharts are diagrams composed of small computational elements that describe the steps of the algorithm. An example in Fig. 10 illustrates what kind of elements are used and how they are brought together to describe an algorithm.

Flowcharts can be more intuitive to work with. However, for complex algorithms, flowcharts can get very large and prohibitive to work with.

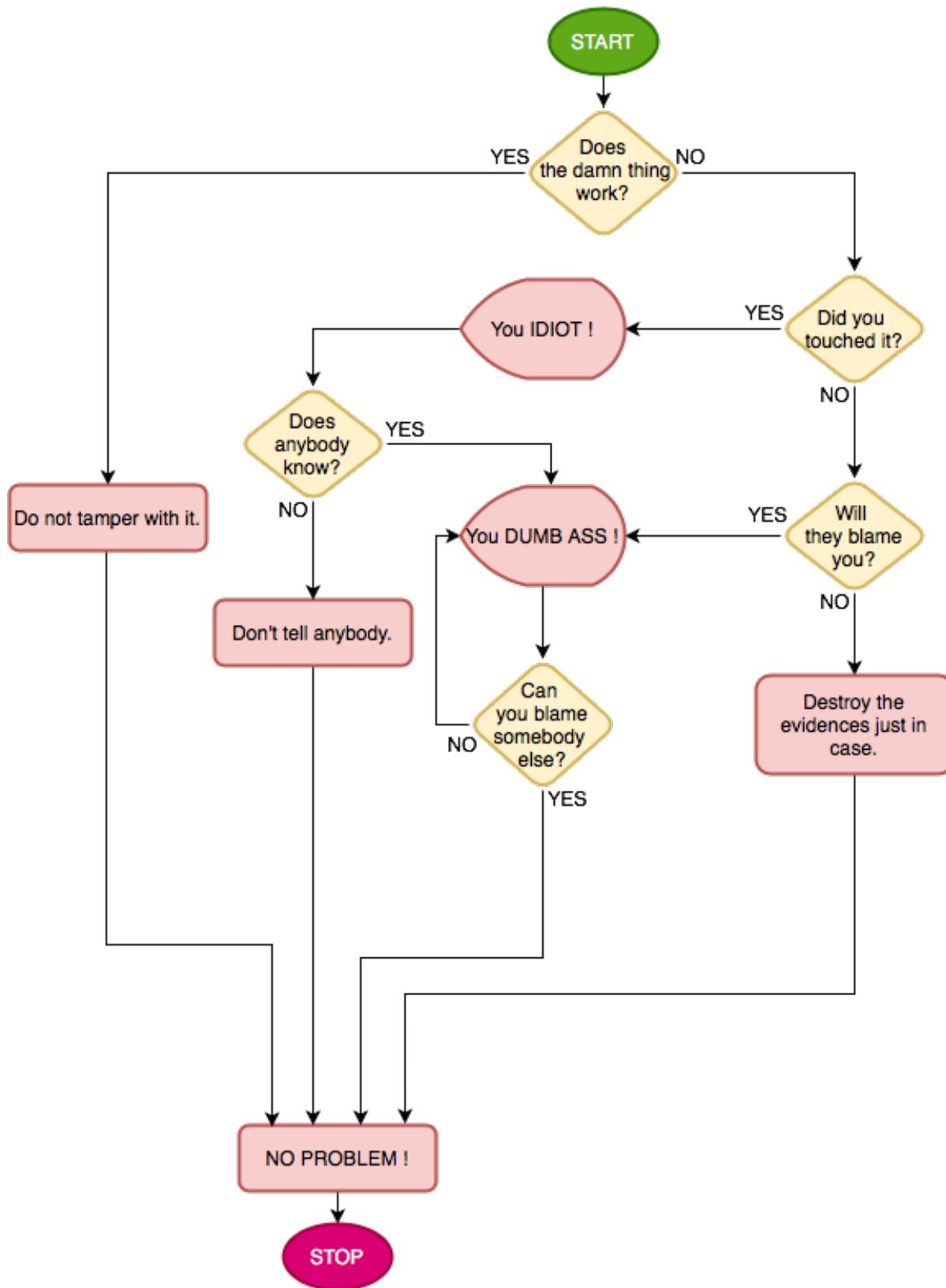


Fig. 10: Flowcharts describe relationships by using basic geometric symbols and arrows. The program start or end is depicted with an oval. A rectangular box denotes a simple action or status. Decision making is represented by a diamond and a parallelogram of the Input/Output process. A silhouette of a TV tube means displaying a message. The Internet is portrayed as a cloud.

How to compare algorithms

If two algorithms find the same solution, are they of the same quality? For a second, recall a game we used to play when we were in primary school: “Guess My Number”.

The rule is as follows: There is a setter and a guesser. The setter sets a number from 1 to 1000 which s/he does not tell. The guesser has to find this number. At each turn of the game, the guesser can propose any number from 1 to 1000. The setter answers by one of following:

- **HIT:** The guesser found the number.
- **LESSER:** The hidden number is less than the proposed one.
- **GREATER:** The hidden number is greater than the proposed one.

In how many turns the number is found is recorded. The guesser and the setter switch. This goes on for some agreed count of rounds. Whoever has a lower total count of turns wins.

Many of you have played this game and certainly have observed that there are three categories of children:

1. *Random guessers*: Worst category. Usually they cannot keep track of the answers and just based on the last answer, they randomly utter a number that comes to their mind. Quite possibly they repeat themselves.
2. Sweepers: They start at either 1 or 1000, and then systematically increase or decrease their proposal, e.g.:
 - -is it 1000? Answer: LESSER
 - -is it 999? Answer: LESSER
 - -is it 998? Answer: LESSER... and so on. Certainly at some point such players do get a HIT. There is a group which decreases the number by two or three as well. With a first GREATER reply, they start to increment by one.

3. *Middle seekers*: Keeping a possible lower and a possible upper value based on the reply they got, at every stage they propose the number just in the middle of lower and upper values, e.g.:

- -is it 500? Answer: LESSER
- -is it 250? Answer: LESSER
- -is it 125? Answer: GREATER
- -is it 187? (which was $(125+250)/2$) Answer: GREATER
- ... and so on.

All three categories actually adopt different algorithms, which will find the answer in the end. However, as you may have realised even as you were a child, the first group performs the worst, then comes the second group. The third group, if they do not make mistakes, is unbeatable.

In other words, algorithms that aim to solve the same problem may not be of the same “quality”: Some perform better. This is the case for all algorithms and one of the challenges in Computer Science is to find “better” algorithms. But, what is “better”? Is there a quantitative measure for “better”ness? The answer is yes.

Let us look at this in the child game described above. First consider the last group’s algorithm (the middle seekers). At every turn, this kind of seeker narrows down the search space by a factor of 1/2. Starting with 1000 numbers, the search space is reduced as follows: 1000, $1000/2$, $1000/2^2$, ... So, in the worst case,

it will take m turns until $1000/2^m$ gets down to 1 (the one remaining number, which has to be the hidden number). In other words, in the worst case, $1000/2^m = 1$ and from this we can derive $m = \log_2(1000)$. For 1000, this means approximately $m = 10$ turns. If we double the range, m would change only by 1 (yes, think about it, only 11 turns).

We call such an algorithm of “order $\log(n)$ ” or more technically, $\mathcal{O}(\log(\cdot))$. In our case 1000 determines the ‘size’ of the problem. This is symbolized with n . $\mathcal{O}(\log(\cdot))$ is the quantitative information about the algorithm which signifies that the solution time is proportional to $\log(n)$. This information about an algorithm is named as *complexity*.

What about the sweepers algorithm for the problem above? In the worst case, the sweeper would ask a question 1000 times (the correct number is at the other end of the sequence). If the size (1000 in our case) is symbolized with n , then it will take a time proportional to n to reach the solution. In other words this algorithm’s complexity is $\mathcal{O}(n)$.

Certainly the algorithm that has $\mathcal{O}(\log(\cdot))$ is better than the one with $\mathcal{O}(n)$, which is illustrated in Fig. 11. In other words, an $\mathcal{O}(\log(\cdot))$ algorithm requires less number of steps and is likely to run faster than the one with $\mathcal{O}(n)$ complexity.

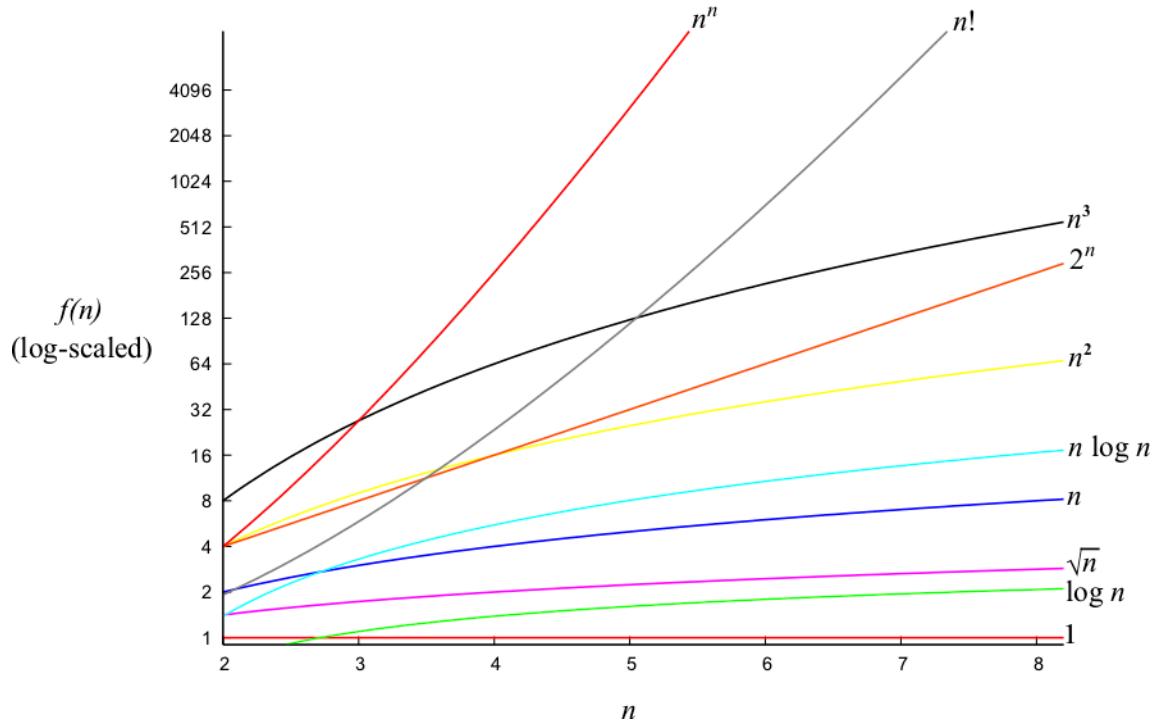


Fig. 11: A plot of various complexities.

Data Representation

The other crucial component of our solutions to world problems is the data representation, which deals with encoding the information regarding the problem in a form that is most suitable for our algorithm.

If our problem is the calculation of the average of grades in a class, then before implementing our solution, we need to determine how we are going to represent (encode) the grades of students. This is what we are going to determine in the ‘data representation’ part of our solution and to discuss in Chapter 3.

The World of Programming Languages

Since the advent of computers, many programming languages have been developed with different designs and levels of complexity. In fact, there are about 700 programming languages - see, e.g. [the list of programming languages¹⁰](#) - that offer different abstraction levels (hiding the low-level details from the programmer) and computational benefits (e.g. providing built-in rule-search engine).

In this section, we will give a flavour of programming languages in terms of abstraction levels (low-level vs. high-level – see Fig. 12) as well as the computational benefits they provide.

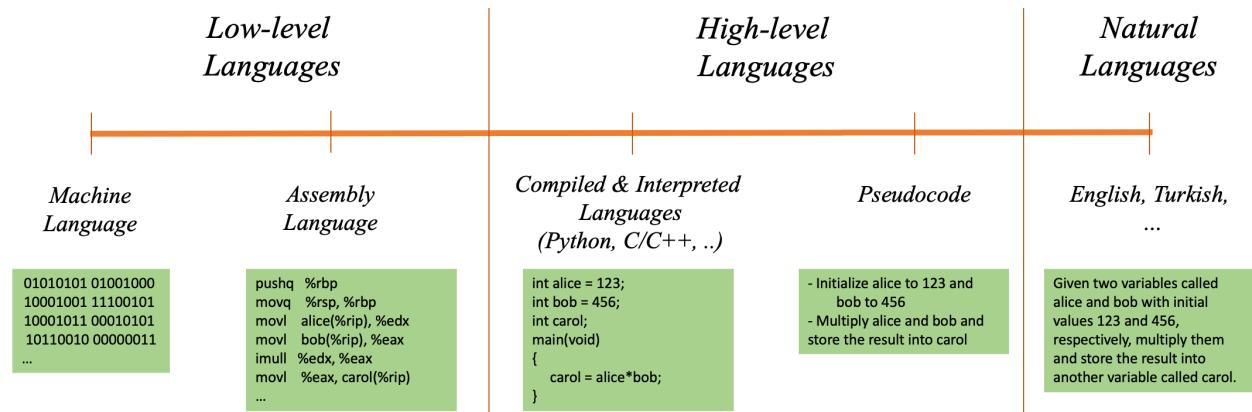


Fig. 12: The spectrum of programming languages, ranging from low-level languages to high-level languages and natural languages.

Low-level Languages

In the previous chapter, we introduced the concept of machine code program. A machine code program is an aggregate of instructions and data, all being represented in terms of zeros (0) and ones (1). A machine code is practically unreadable and very burdensome to create, as we have seen before and illustrated below:

```
01010101 01001000 10001001 11100101 10001011 00010101 10110010 00000011  
00100000 00000000 10001011 00000101 10110000 00000011 00100000 00000000  
00001111 10101111 11000010 10001001 00000101 10111011 00000011 00100000  
00000000 10111000 00000000 00000000 00000000 00000000 11001001 11000011  
...  
11001000 00000001 00000000 00000000 00000000 00000000
```

To overcome this, *assembly* language and assemblers were invented. An assembler is a machine code program that serves as a translator from some relatively more readable text, the assembly program, into machine code. The key feature of an assembler is that each line of an assembly program corresponds exactly to a single machine code instruction. As an example, the binary machine code above can be written in an assembly language as follows:

```
main:  
pushq %rbp  
movq %rsp, %rbp  
movl alice(%rip), %edx  
movl bob(%rip), %eax
```

(continues on next page)

¹⁰ https://en.wikipedia.org/wiki/List_of_programming_languages_by_type

```

imull %edx, %eax
movl %eax, carol(%rip)
movl $0, %eax
leave
ret
alice:
.long 123
bob:
.long 456

```

Pros of assembly:

- Instructions and registers have human recognizable mnemonic words associated. Like integer addition instruction being ADDI, for example.
- Numerical constants can be written down in human readable, base-10 format, the assembler does the conversion to internal format.
- Implements naming of memory positions that hold data. In other words, assembly has a primitive implementation of the variable concept.

Cons of assembly:

- No arithmetic or logical expressions.
- No concept of functions.
- No concept of statement grouping.
- No concept of data containers.

High-level Languages

To overcome the limitations of binary machine codes and the assembly language, more capable *Programming Languages* were developed. We call these languages *High-level languages*. These languages hide the low-level details of the computer (and the CPU) and allow a programmer to write code in a more human-readable form.

A high-level programming language (or an assembly language) is defined, similar to a natural language, by syntax (a set of grammar rules governing how to bring together words) and semantics (the meaning – i.e. what is meant by the sequences of words in the syntax) associated for the syntax. The syntax is based on keywords from a human language (due to historical reasons, English). Using human-readable keywords ease comprehension.

The following example is a program expressed in Python that asks for a Fahrenheit value and prints its conversion into Celsius:

```

Fahrenheit = input("Please Enter Fahrenheit value:")
print("Celsius equivalent is:", (Fahrenheit - 32) * 5/9)

```

Here input and print are keywords of the language. Their semantics is self explanatory. Fahrenheit is a naming we have chosen for a variable that will hold the input value.

High-level languages (*HL-languages* from now on) implement many concepts which are not present at the machine code programming level. Most outstanding features are:

- human readable form of numbers and strings (*like decimal, octal, hexadecimal representations for numbers*),
- containers (*automatic allocation for places in the memory to hold, access and name data*),
- expressions (*calculation formulas based on operators which have precedences the way we are used to from mathematics*),
- constructs for repetitive execution (*conditional re-execution of code parts*),
- functions,
- facilities for data organization (*ability to define new data types based on the primitive ones, organizing them in the memory in certain layouts*).

Implementing with a High-level Language: Interpreter vs. Compiler

We can implement our solution in a high-level programming language in two manners:

1. **Compilative Approach.** In this approach, a translator, called *compiler*, takes a high-level programming language program as input and converts all actions in the program into a machine code program (Fig. 13). The outcome is a machine code program that can be run any time (by asking the OS to do so) and does the job described in the high-level language program.

Conceptually this is correct, but actually, this schema has another step in-the-loop. The compiler produces an almost complete machine code with some holes in it. These holes are about the parts of the code which is not actually coded by the programmer, but filled in from a pre-created machine code library (it is actually named as *library*). A program, named *linker* fills those holes. The linker knows about the library and patches in the parts of the code that are referenced by the programmer.

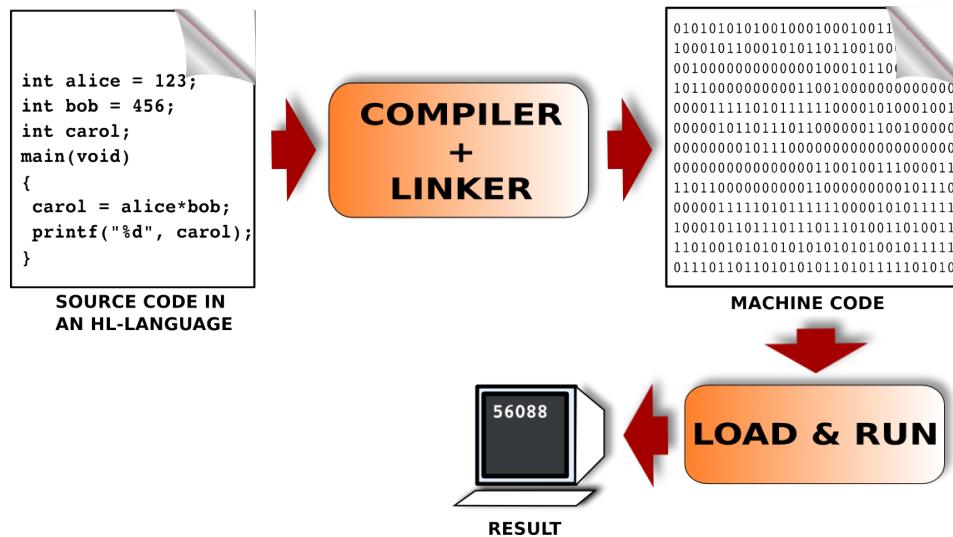


Fig. 13: A program code in a high-level language is first translated into machine understandable binary code (machine code) which is then loaded and executed on the machine to obtain the result. [From: G. Üçoluk, S. Kalkan, Introduction to Programming Concepts with Case Studies in Python, Springer, 2012¹¹]

2. **Interpretive Approach.** In this approach, a machine code program, named as *interpreter*, when run, inputs and processes the high-level program line by line (Fig. 14). After taking a line as input, the

¹¹ <https://link.springer.com/book/10.1007/978-3-7091-1343-1>

actions described in the line are *immediately* executed; if the action is printing some value, the output is printed right away; if it is an evaluation of a mathematical expression, all values are substituted and at that very point-in-time, the expression is evaluated to calculate the result. In other words, any action is carried out immediately when the interpreter comes to its line in the program. In practice, it is always possible to write down the program lines into a file, and make the interpreter read the program lines one by one from that file as well.

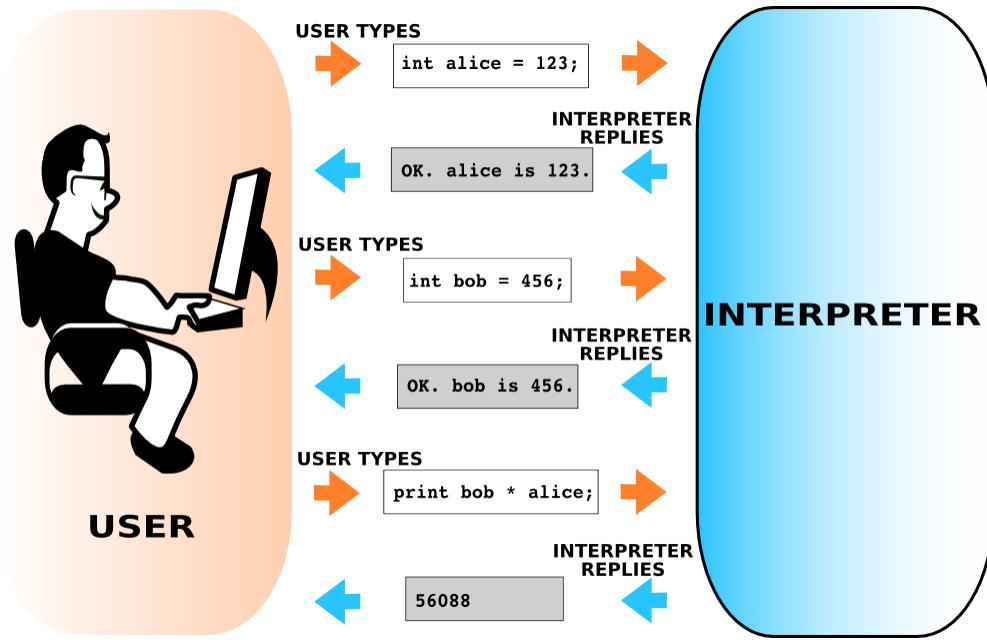


Fig. 14: Interpreted languages (e.g. Python) come with interpreters that process and evaluate each action (statement) from the user on the run and returns an answer. [From: G. Üçoluk, S. Kalkan, Introduction to Programming Concepts with Case Studies in Python, Springer, 2012¹²]

Which approach is better?

Both approaches have their benefits. When a specific task is considered, compilers generate fast executing machine codes compared to the same task being carried out by an interpreter. On the other hand compilers are unpleasant when trial-and-errors are possible while developing the solution. Interpreters, on the other hand, allow making small changes and the programmer receives immediate responses, which makes it easier to observe intermediate results and adjust the algorithm accordingly. However, interpreters are slower since they involve an interpretation component while running the code. Sometimes this slowness is by a factor of 20. Therefore, the interpretive approach is good for quick implementations whereas using a compiler is good for computation-intense big projects or time-tight tasks.

¹² <https://link.springer.com/book/10.1007/978-3-7091-1343-1>

Programming-language Paradigms

As we mentioned before, there are more than 700 programming languages. Certainly some are for academic purposes and some did not gain any popularity. But there are about 20 programming languages which are commonly used for writing programs. How do we choose one when implementing our solution?

Picking a particular programming language is not just a matter of taste. During the course of the evolution of the programming languages, different strategies or world views about programming have also developed. These world views are reflected in the programming languages.

For example, one world view regards the programming task as transforming some initial data (the initial information that defines the problem) into a final form (the data that is the answer to that problem) by applying a sequence of functions. From this perspective, writing a program consists of defining some functions which are then used in a functional composition; a composition which, when applied to some initial data, yields the answer to the problem.

This concept of world views are coined as *programming paradigms*. The Oxford dictionary defines the word paradigm as follows:

paradigm |'pa:rə,dɪm|

noun

A world view underlying the theories and methodology of a particular scientific subject.

Below is a list of some major paradigms:

- **Imperative:** Is a paradigm where programming statements and their composition directly map to the machine code segments, so that the whole machine code is covered.
- **Functional:** In this paradigm, solving a programming task is to construct a group of functions so that their ‘functional composition’ acting on the initial data produces the solution.
- **Object oriented:** In this paradigm the compulsory separation (due to the von Neumann architecture) of algorithm from data is lifted, and algorithm and data are reunited under an artificial computational entity: *the object*. An object has algorithmic properties as well as data properties.
- **Logical-declarative:** This is the most contrasting view compared to the imperative paradigm. The idea is to represent logical and mathematical relations among entities (as rules) and then ask an inference engine for a solution that satisfies all rules. The inference engine is a kind of ‘prover’, i.e. a program, that is constructed by the inventor of the logical-declarative programming language.
- **Concurrent:** A paradigm where independent computational entities work towards the solution of a problem. For problems that can be solved by a divide-and-conquer strategy, this paradigm is very suitable.
- **Event driven:** This paradigm introduces the concept of events into programming. Events are assumed to be asynchronous and they have ‘handlers’, i.e. programs that carry out the actions associated with a particular event. Programming graphical user interfaces (GUIs) is usually performed using event-driven languages: An event in a GUI is generated e.g. when the user clicks the “Close” button, which triggers the execution of a handler function that performs the associated closing action.

In contrary to the layman programmers’ assumption, these paradigms are not mutually exclusive. Many paradigms can very well co-exist in a programming language together. At a meta level, we can call them ‘orthogonal’ to each other. This is why we have so many programming languages around. A language can provide imperative as well as functional and object-oriented constructs. Then it is up to the programmer to blend them in his or her particular program. As it is with many ‘world views’ among humans, in the field

of programming, fanaticism exists too. You can meet individuals that do only functional programming or object-oriented programming. We better consider them outliers.

Python, the subject language of this book, supports strongly the imperative, functional and object-oriented paradigms. It also provides some functionality in other paradigms by some modules.

Introducing Python

After having provided background on the world of programming, let us introduce Python: Although it is widely known to be a recent programming language, Python's design, by [Guido van Rossum](#)¹³, dates back to 1980s, as a successor of the ABC programming language. The first version was released in 1991 and with the second version released in 2000, it started gaining a wider interest from the community. After it was chosen by some big IT companies as the main programming language, Python became one of the most popular programming languages.

An important reason for Python's wide acceptance and use is its design principles. By design, Python is a programming language that is easier to understand and to write but at the same time powerful, functional, practical and fun. This has deep roots in its design philosophy (a.k.a. [The Zen of Python](#)¹⁴):

“Beautiful is better than ugly. Explicit is better than implicit. Simple is better than complex.
Complex is better than complicated. Readability counts. [...] *there are 14 more*”

Python is multi-paradigm programming language, supporting imperative, functional and object-oriented paradigms, although the last one is not one of its strong suits, as we will see in Chapter 7. Thanks to its wide acceptance especially in the open-source communities, Python comes with or can be extended with an ocean of libraries for practically solving any kind of task.

The word ‘python’ was chosen as the name for the programming language not because of the snake species python but because of the comedy group [Monty Python](#)¹⁵. While van Rossum was developing Python, he read the scripts of Monty Python’s Flying Circus and thought ‘python’ was “short, unique and mysterious”¹⁶ for the new language. To make Python more fun to learn, earlier releases heavily used phrases from Monty Python in example programming codes.

With version 3.9 being released in October 2020 as the latest version, Python is one of the most popular programming languages in a wide spectrum of disciplines and domains. With an active support from the open-source community and big IT companies, this is not likely to change in the near future. Therefore, it is in your best interest to get familiar with Python if not excel in it.

This is how the Python interpreter looks like at a Unix terminal:

```
$ python3
Python 3.8.5 (default, Jul 21 2020, 10:48:26)
[Clang 11.0.3 (clang-1103.0.32.62)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>>
```

The three symbols >>> indicate that the interpreter is ready to collect our computational demands, e.g.:

¹³ https://en.wikipedia.org/wiki/Guido_van_Rossum

¹⁴ https://en.wikipedia.org/wiki/Zen_of_Python

¹⁵ https://en.wikipedia.org/wiki/Monty_Python

¹⁶ <https://docs.python.org/2/faq/general.html#why-is-it-called-python>

where we asked what was 21+21 and Python responded with 42, which is one small step for a man but one giant leap for mankind.

Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- How we solve problems using computers.
- Algorithms: What they are, how we write them and how we compare them.
- The spectrum of programming languages.
- Pros and cons of low-level and high-level languages.
- Interpretive vs. compilative approach to programming.
- Programming paradigms.

Further Reading

- The World of Programming chapter available at: https://link.springer.com/chapter/10.1007/978-3-7091-1343-1_1
- Programming Languages:
 - For a list of programming languages: http://en.wikipedia.org/wiki/Comparison_of_programming_languages
 - For a comparison of programming languages: http://en.wikipedia.org/wiki/Comparison_of_programming_languages
 - For more details: Daniel P. Friedman, Mitchell Wand, Christopher Thomas Haynes: Essentials of Programming Languages, The MIT Press 2001.
- Programming Paradigms:
 - Introduction: http://en.wikipedia.org/wiki/Programming_paradigm
 - For a detailed discussion and taxonomy of the paradigms: P. Van Roy, Programming Paradigm for Dummies: What Every Programmer Should Know, New Computational Paradigms for Computer Music, G. Assayag and A. Gerzso (eds.), IRCAM/Delatour France, 2009 <http://www.info.ucl.ac.be/~pvr/VanRoyChapter.pdf>
 - Comparison between Paradigms: http://en.wikipedia.org/wiki/Comparison_of_programming_paradigms

Exercise

- Draw the flowchart for the following algorithm:

Step 1: Get a list of N numbers in a variable named Numbers
Step 2: Create a variable named Sum with initial value 0
Step 3: For each number i in Numbers, execute the following line:
Step 4: if $i > 0$: Add i to Sum
Step 5: if $i < 0$: Add the square of i to Sum
Step 5: Divide Sum by N

- What is the complexity of Algorithm 1 (in Section 2.2)?
- What is the complexity of the following algorithm?

Step 1: Get a list of N numbers in a variable named Numbers
Step 2: Create a variable named Mean with initial value 0
Step 3: For each number i in Numbers, execute the following line:
Step 4: Add i to Mean
Step 5: Divide Mean by N
Step 6: Initialize a variable named Std with value 0
Step 7: For each number i in Numbers, execute the following line:
Step 8: Add the square of (i-Mean) to Std
Step 9: Divide Std by N and take its square root

- Assuming that a step of an algorithm takes 1 second, fill in the following table for different algorithms for different input sizes (n):

Input Size

$\mathcal{O}(\log \sqrt{n})$

$\mathcal{O}(\sqrt{n})$

$\mathcal{O}(\sqrt{n} \log \sqrt{n})$

$\mathcal{O}(\sqrt{n}^\epsilon)$

$\mathcal{O}(\sqrt{n}^{\beta})$

$\mathcal{O}(n^\epsilon)$

$\mathcal{O}(n^{\frac{1}{2}})$

$n = 10^2$

$n = 10^3$

$n = 10^4$

$n = 10^5$

- Assume that we have a parser than can process and parse natural language descriptions (without any syntactic restrictions) for programming a computer. Given such a parser, do you think we would use natural language to program computers? If no, why not?
- For each situation below, try to identify which paradigm is more suitable compared to the others:
- Writing a program which should take an image as input, an RGB color value and find all pixels in the image that match the given color.

- Writing a theorem proving program.
- Writing the auto pilot program flying an airplane.
- Writing a document editing program as an alternative to Microsoft Word.

1 | Representation of Data

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As we discussed in detail in Chapter 2, when we want to solve a world problem using a computer, we have to find what data is involved in this problem and how we can process this data (i.e. determine the algorithm) towards the solution of the problem – let us recall this with Fig. 1.1 from Chapter 2.

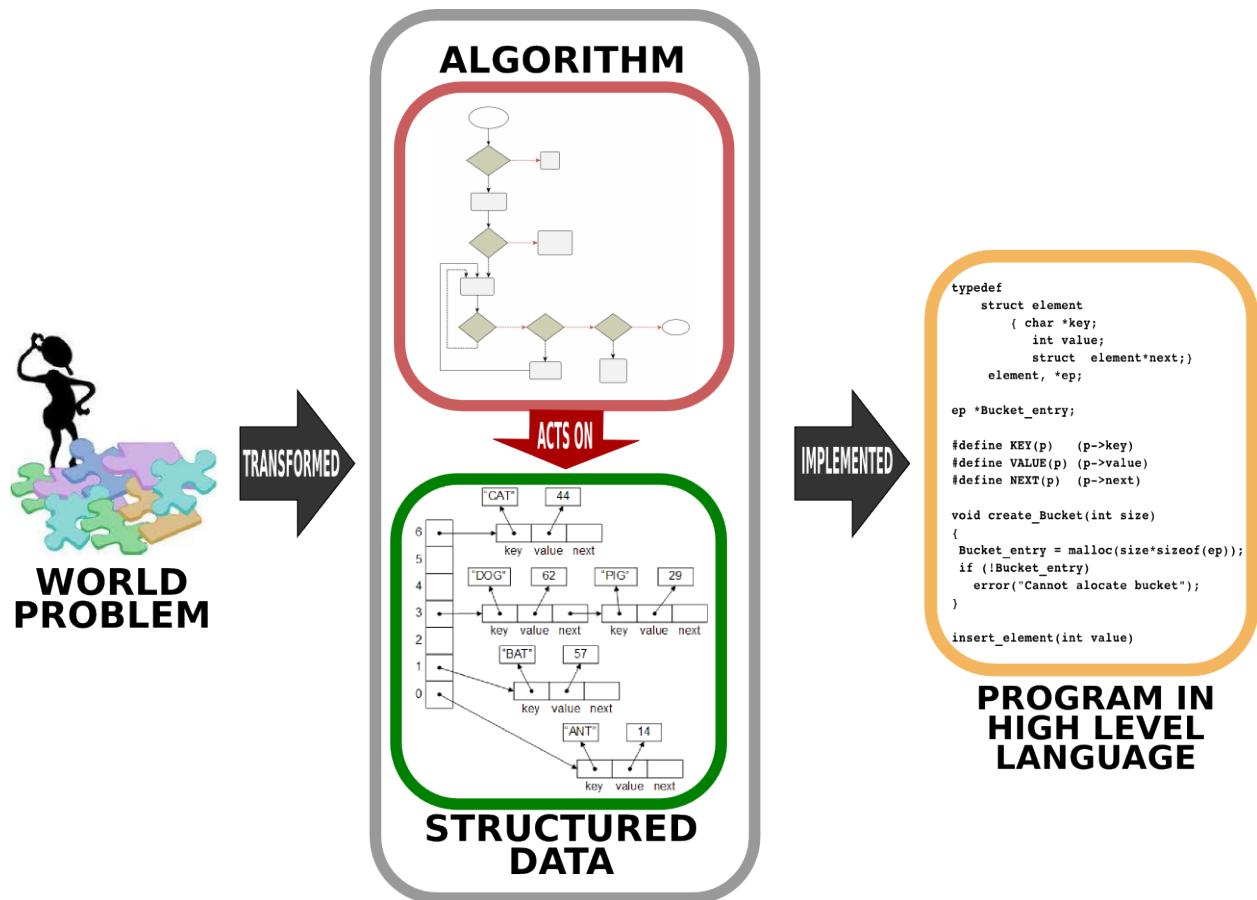


Fig. 1.1: Solving a world problem with a computer requires first designing how the data is going to be represented and specifying the steps which yield the solution when executed on the data. This design of the solution is then written (implemented) in a programming language to be executed as a program such that, when executed, the program outputs the solution for the world problem. [From: G. Üçoluk, S. Kalkan, *Introduction to Programming Concepts with Case Studies in Python*, Springer, 2012¹⁷]

At this stage, you may be wondering what ‘structured data’ is and how it differs from ‘data’. As we already know, data is stored in the memory. Let us illustrate this with an example: Assume that we have a table full of rows such that each row holds an angle value and its cosine value (both expressed as decimal numbers). How would you organize the storing of these rows in the memory? Two straightforward options are:

- a) Row-by-row:

$$\begin{aligned} & \text{Anglevalue}_1 \\ & \text{Cosinevalue}_1 \\ & \text{Anglevalue}_2 \\ & \text{Cosinevalue}_2 \\ & \vdots \\ & \text{Anglevalue}_n \\ & \text{Cosinevalue}_n \end{aligned}$$

- b) Column-by-Column:

$$\begin{aligned} & \text{Anglevalue}_1 \\ & \text{Anglevalue}_2 \\ & \vdots \\ & \text{Anglevalue}_n \\ & \text{Cosinevalue}_1 \\ & \text{Cosinevalue}_2 \\ & \vdots \\ & \text{Cosinevalue}_n \end{aligned}$$

Apart from this ordering, there is the issue of whether we should sort the values. If yes by which one: the angle or the cosine values? In a descending order or ascending order? All these questions are what we try to determine in a structured data.

There are other ways to organize data even for the example data as simple as the above example table. Unfortunately, these are beyond the scope of this book.

Now, we will look into the atomic structure of data representation: i.e. how integers, floating points and characters are represented.

The electronic architecture used for the von Neumann machine, namely the CPU and the memory, is based on the presence and absence of a fixed voltage. We conceptualize this absence and presence by ‘0’ and ‘1’. This means that any data that is going to be processed on this architecture has to be converted to a representation of ‘0’s and ‘1’s. We, though, keep in mind, that any ‘1’ (or ‘0’) in our representation is actually the presence (or absence) of a voltage in a specific point of the electronic circuitry.

1.1 Representing integers

Mathematics already has a solution for representing integers in binary via base-2 calculation or representation. The idea behind base-2 representation is the same as representing base-10 (decimal) integers. Namely, we have a sequence of digits, each of which can be either 0 or 1. Counting starts from the right-most digit. A ‘1’ in a position k means “additively include a value of 2^k ”:

$$\begin{array}{llllll} \text{Position :} & n & n-1 & \dots & 2 & 1 & 0 \\ \text{Meaning :} & 2^n & 2^{n-1} & \dots & 2^2 & 2^1 & 2^0 \end{array}$$

The following is an example for expressing the integer **181** in base-2:

¹⁷ <https://link.springer.com/book/10.1007/978-3-7091-1343-1>

Position

$$\begin{array}{cccccccc}
 & 7 & 6 & 5 & 4 & 3 & 2 & 1 & 0 \\
 \boxed{1} & 0 & 1 & 1 & 0 & 1 & 0 & 1 \\
 \downarrow & \downarrow \\
 2^7 + & 2^5 + 2^4 + & 2^2 + & 2^0 & & & & \\
 = & 181 & & & & & &
 \end{array}$$

In other words, $(181)_{10} = (10110101)_2$.

Converting a decimal number into binary

A decimal number can be easily converted into binary by repeatedly dividing the number by 2, as shown in Fig. 1.1.1. At each step, the quotient of the previous step is divided by two. This division is repeated until the quotient is zero. At this point, the binary sequence of remainders is the representation of the decimal number.

Having doubts? You can easily cross-check your calculation by multiplying each bit by its value (2^i if the bit is at position i) and sum up the values (like we did above).

	Dividend	Divisor	Quotient	Reminder
Step 1	19	÷ 2	= 9	1
Step 2	9	÷ 2	= 4	1
Step 3	4	÷ 2	= 2	0
Step 4	2	÷ 2	= 1	0
Step 5	1	÷ 2	= 0	1

Continue until quotient is zero The result:

1	0	0	1	1
---	---	---	---	---

Fig. 1.1.1: The division method for converting a decimal number into binary.

This looks easy. However, this is just a partial solution to the ‘binary representation of integers’ problem: It does not answer how we can represent negative integers.

1.1.1 Sign-Magnitude Notation

Decimal arithmetics provide the minus sign (-) for representing negativity. However, electronics of the von Neumann machinery requires that the minus is also represented by either a ‘1’ or ‘0’. We can reserve a bit, for example the left-most digit, for this purpose. If we do this, when the left-most digit is a ‘1’, the rest of the digits are encoding the magnitude of the ‘negative’ integer. One point to be mentioned is that this requires a fixed size (a fixed number of digits) for the ‘integer representation’. In this way, the electronics can recognize the sign bit and the magnitude part. This is called *the sign-magnitude notation*.

Sadly, this notation has certain disadvantages:

1. Addition and subtraction

Consider adding two integers. Based on their signs, we have the following possibilities:

- *positive + positive*
- *negative + positive*
- *positive + negative*
- *negative + negative*

Then, to be able to perform addition, the electronics must do the following:

- if both integers are *positive* then the result is *positive*, obtained by adding the magnitudes (and not setting the sign bit).
- if both integers are negative, then the result is negative, obtained by adding the magnitudes and setting the sign bit to *negative*.
- otherwise, if one is *negative* and the other is *positive* then:
 1. find the bigger magnitude,
 2. subtract the smaller magnitude from the bigger one, obtain the result,
 3. if the bigger magnitude integer was negative the result is negative (set the sign bit) else don’t set the sign bit in result.

This was only for the case of addition, a similar electronic circuitry is needed for subtracting two integers.

This technique has the following drawbacks: * Requires separate electronics for subtraction. * Requires electronics for magnitude-based comparison and an algorithm implementation for setting the sign bit. * Electronically, it has to differentiate among addition and subtraction.

2. Representing number zero

Another limitation of the sign-magnitude notation is that number zero (0)₁₀ has two different representations, e.g. in a 4-bit representation:

- $(1\ 000)_2 ==> (-0)_{10}$
- $(0\ 000)_2 ==> (+0)_{10}$

In modern computers, we use a method that does not have these drawbacks.

1.1.2 Two's Complement Representation

Two's complement representation can be considered as an extension of the sign-magnitude notation:

- The positive integers are represented by their base-2 representation.
- For negative integers, we need a one-to-one mapping for all negative integers bounded by value to a binary representation (also bounded by value), so that :
 1. The sign bit is set to 1, and
 2. When the whole binary representation (including the sign bit) is treated as a single binary number it operates correctly under addition. When the result, obtained purely by addition, produces a sign bit, this means the result is the encoding of a negative integer.

There are two alternatives for this mapping: One's-complement and two's complement. In this section, we will introduce the more popular one, namely the two's complement representation:

If we are given n binary digits to be used (for a 32-bit computer, $n = 32$; for a 64-bit computer, it is 64), then we are able to represent integer values in the range $[-2^{n-1}, 2^{n-1}-1]$. Then, two's complement representation of an integer can be obtained as follows:

- If the integer is positive simply, convert it to base-2.
- If it is negative: Let the magnitude (its absolute value) be p , then
 1. convert p to base-2
 2. negate this base-2 representation by flipping all 1s to 0s and all 0s to 1s: $1 \leftrightarrow 0$.
 3. add 1 to the result of the negation.

Here are some examples for 8-bit numbers (note that the valid decimal range is $[-128, 127]$):

Integer	2's complement	Pos./Neg.	Action:Binary Result
0	00000000	—	Direct base-2 encoding:
1	00000001	Positive	Direct base-2 encoding:
-1	11111111	Negative	<i>magnitude</i> :00000001 <i>inverse</i> :11111110 +1:11111111
-2	11111110	Negative	<i>magnitude</i> :00000010 <i>inverse</i> :11111101 +1:11111110
18	00010010	Positive	Direct base-2 encoding:
-18	11101110	Negative	<i>magnitude</i> :00010010 <i>inverse</i> :11101101 +1:11101101
-47	11010001	Negative	<i>magnitude</i> :00101111 <i>inverse</i> :11010000 +1:11010001
-111	10010001	Negative	<i>magnitude</i> :01101111 <i>inverse</i> :10010000 +1:10010001
111	01101111	Positive	Direct base-2 encoding:
112	01110000	Positive	Direct base-2 encoding:
-128	10000000	Negative	<i>magnitude</i> :10000000 <i>inverse</i> :01111111 +1:10000000
-129	Not Calculated	Negative	(Out of valid range):
128	Not Calculated	Positive	(Out of valid range):

(1.1.1)

1.1.3 Why does Two's Complement work?

The Two's Complement method may sound arbitrary at first. However, there are solid reasons for why it works. To be able to explain why it works, let us first revisit our basic computer organization from Chapter 1:

The CPUs can only understand and work with fixed-length representations: Assume that our computer is an 8-bit computer such that registers in the CPU holding data and the arithmetic-logic unit can only work with 8 bits. The fixed-length design of the CPU has a severe implication. Consider the following 8-bit number (which is $2^8 - 1$) in a register in the CPU:

1	1	1	1	1	1	1	1
---	---	---	---	---	---	---	---

If you add 1 to this number, the result would be:

0	0	0	0	0	0	0	0
---	---	---	---	---	---	---	---

In other words, we lose the 9th bit since the CPU cannot fit that into the 8-bit representation. Mathematically, this arithmetic corresponds to *modular arithmetic*: For our example, the modulo value is 2^8 and the addition that we just performed can be written mathematically as:

$$(2^8 - 1) + 1 \equiv 0 \pmod{2^8} \quad (1.1.2)$$

What does this have to do with the Two's Complement method? Consider taking the negative of a number a in a 2^n -modulo system:

$$-(a) \equiv 0 - a \equiv 2^n - a \pmod{2^n} \quad (1.1.3)$$

Now let us rewrite this in a form that will seem familiar to us:

$$2^n - a \equiv 2^n - 1 + 1 - a \equiv \underbrace{(2^n - 1 - a)}_{\text{Invert the bits of } a} + \underbrace{1}_{\text{Add 1 to the inverted bits}} \pmod{2^n} \quad (1.1.4)$$

In other words, Two's Complement representation uses the negative value of a number relying on the modular arithmetic, i.e. the fixed-length representation of the CPUs. This technique is not new and was used in mechanical calculators long before there were computers.

1.1.4 Benefits of the Two's Complement Representation

Let us revisit the limitations of the sign-magnitude representation:

- **Addition and subtraction:** With the two's complement method, we do not need to check the signs of the numbers and perform addition and subtraction using just an addition circuitry. E.g. $(+2)_{10} + (-3)_{10}$ is just equal to $(-1)_{10}$ without doing anything extra other than plain addition (for a 4-bit representation):

	$(0010)_2$		$(+2)_{10}$
	$(1101)_2$		$(-3)_{10}$
+			
	$(1111)_2$		$(-1)_{10}$

(1.1.5)

- **Representation of +0 and -0:** Another issue with the sign-magnitude representation was that $+0$ and -0 had different representations. In the Two's Complement representation, we see that this is resolved – for example (for a 4-bit representation):
 - $(+0)_{10} = (0000)_2$
 - $(-0)_{10} = -(0000)_2 = (1111)_2 + (1)_2 = (0000)_2$, where we used Two's Complement to convert $-(0000)_2$ into $(1111)_2 + (1)_2$ by flipping the bits and adding 1.

The fifth bit is lost because we have only four bits for representation.

1.1.5 PRACTICE TIME

Please follow the Colab link at the top of the page to have a practical session on Two's Complement representation.

1.2 Representing real numbers

Floating point is the data type used to represent non-integer real numbers. On today's computers, all non-integer real numbers are represented using the floating point data type. Since all integers are real numbers, we could represent integers also using the floating point data type. Although you could do so, this is usually not preferred, since floating point operations are more time consuming compared to integer operations. Also, there is the danger of precision loss, which we will discuss later.

Almost all processors have adopted the IEEE 754 binary floating point standard for binary representation of floating point numbers. The standard allocates 32 bits for the representation, although there is a recent 64-bit definition which is based on the same layout idea just with some more bits.

Let us see how we represent a floating point number with an example. Let us consider a decimal number with fraction: 12263.921875. This number can be represented in binary as two binary numbers: the whole part in binary and the fractional part in binary. Then, we can join them with a period.

To see this, let us first dissect decimal (base-10) 12263.921875:

$$\begin{array}{cccccccccccccccccc} 10^4 & 10^3 & 10^2 & 10^1 & 10^0 & . & 10^{-1} & 10^{-2} & 10^{-3} & 10^{-4} & 10^{-5} & 10^{-6} \\ \hline 1 & 2 & 2 & 6 & 3 & . & 9 & 2 & 1 & 8 & 7 & 5 \end{array} \quad (1.2.1)$$

Keeping the denotational similarity, but switching to (base-2), in other words to binary, we can express the same number as:

$$\begin{array}{cccccccccccccccccc} 2^{13} & 2^{12} & 2^{11} & 2^{10} & 2^9 & 2^8 & 2^7 & 2^6 & 2^5 & 2^4 & 2^3 & 2^2 & 2^1 & 2^0 & . & 2^{-1} & 2^{-2} & 2^{-3} & 2^{-4} & 2^{-5} & 2^{-6} \\ \hline 1 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 & . & 1 & 1 & 1 & 0 & 1 & 1 \end{array} \quad (1.2.2)$$

How did we obtain the fractional part? By multiplying the fractional by two until we obtain zero for the fraction part, as illustrated in Fig. 1.2.1. This is in certain ways the reverse of what we did for converting the whole part into binary, in the previous section.

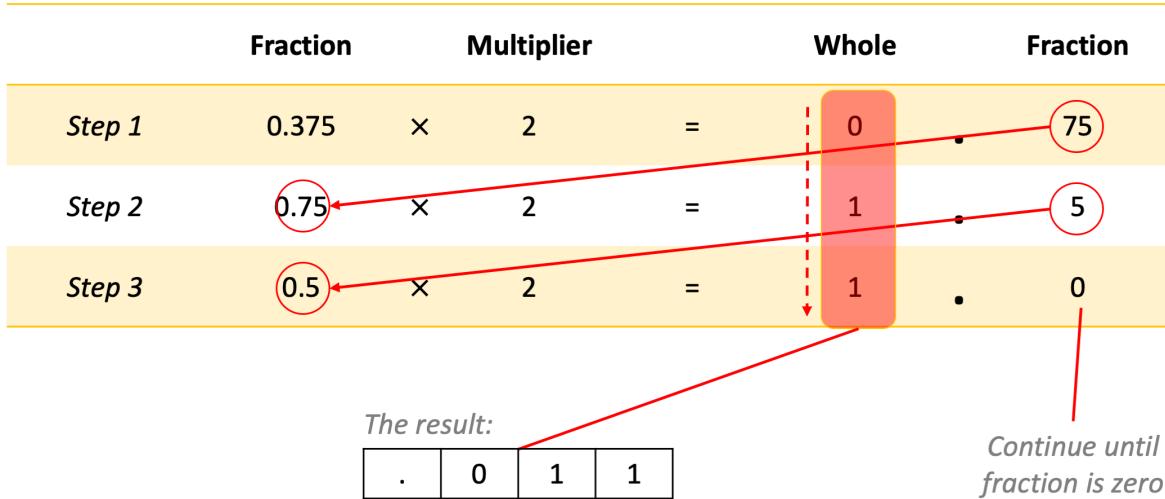


Fig. 1.2.1: The multiplication method for converting a fractional number into binary.

At this stage, it is worth mentioning that it is not always possible to convert the fractional part into binary with finite number of bits. In other words, it is quite possible to have a finite number of fractional digits in one base, and infinitely many in another base for the same value. We will come back to this point later.

Depending on the size of the whole part, the period could be anywhere. Therefore, the next step towards obtaining the IEEE 754 representation is to reposition the period that separates the whole part from the fraction, to be placed just after the leftmost ‘1’. To be able to do this without changing the value of the number, a multiplicative factor of 2^n has to be introduced, where n is how many bits the period is moved. If it is moved to the left, it has a positive value, otherwise it is negative. This factor is important, because it will contribute to the representation.

For our example, the period has to be moved left by 13 digits. Therefore, the multiplicative factor (to keep

the value the same) is $\times 2^{+13}$. At this stage our representation has become:

2^0	.	2^{-1}	2^{-2}	2^{-3}	2^{-4}	2^{-5}	2^{-6}	2^{-7}	2^{-8}	2^{-9}	2^{-10}	2^{-11}	2^{-12}	2^{-13}	2^{-14}	2^{-15}	2^{-16}
$2^{+13} \times$	1	.	0	1	1	1	1	1	1	0	0	1	1	1	1	1	0

(1.2.3)

Since this is doable for all values (except 0.0, which will be dealt with with an exception), there is no need to keep a record of the whole part, i.e. the only remaining '1' value to the left of the period. Also, the period is always there, so we can simply drop it. The *mantissa* part of the representation is obtained by keeping exactly the first 23 bits of what is left. This leads to the following 23 bits for our example (note the extra zeros at the end, added to fill complete the representation to 23 bits):

0	1	1	1	1	1	1	1	0	0	1	1	1	1	1	1	0	1	1	0	0	0	0
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

1.2.1 The IEEE754 Representation

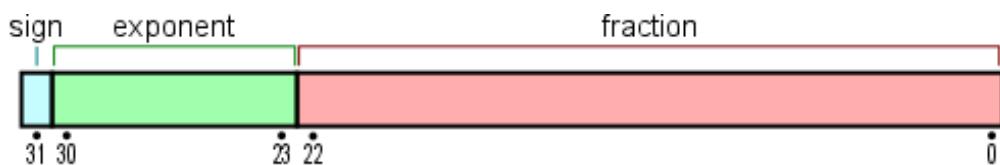


Fig. 1.2.2: The 32-bit IEEE754 floating point representation.

The exponent of the multiplicative factor, namely n (which can be negative) in 2^n , becomes a part of the representation – see Fig. 1.2.2. To get rid of the minus sign problem, a constant value, 127, is added to n . This value becomes the *exponent* part of the representation.

Adding a constant value to a number to be able to represent positive and negative numbers in binary is called the excess representation, or k -excess representation, with k being the constant number that is added, e.g. $k = 127$. Why we use k -excess representation is going to be clear when we compare it with two's complement representation in Table 1.2.1. You should see from the table that if the binary representation of a decimal number is larger, the decimal number is also larger with the k -excess representation; however, this is not the case for the two's complement representation. This is important for comparing two floating point numbers: Without decoding the whole floating point representation, which is expensive, we can just look at the k -excess representation of the exponents and the fractional parts to compare numbers.

Table 1.2.1: A comparison between the k-excess representation and the two's complement representation.

Decimal number	k-excess ($k = 8$)	Two's complement
7	1111	0111
6	1110	0110
5	1101	0101
4	1100	0100
3	1011	0011
2	1010	0010
1	1001	0001
0	1000	0000
-1	0111	1111
-2	0110	1110
-3	0101	1101
-4	0100	1100
-5	0011	1011
-6	0010	1010
-7	0001	1001
-8	0000	1000

In our example the factor was 2^{13} . Adding $k = 127$ yields $13 + 127 = 140$, which has an 8-bit representation of 10001100. This will become the exponent portion (the 8 green bits in Figure 3.4) of the IEEE754 representation.

It is possible that the value that is going to be represented is a negative value. This information is stored as a ‘1’ in the first bit of the representation. For a positive value, a ‘0’ bit is used.

Finally, our example gets a IEEE754 representation as:

0	1	0	0	0	1	1	0	0	0	1	1	1	1	1	1	1	0	0	1	1	1	1	1	1	0	1	1	0	0	0	0
---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---	---

How is real number ‘0.0’ represented?

Floating point number zero is represented as all zero bits in the positional range [1-31]. The zeroth bit, namely the sign bit, can be either ‘0’ or ‘1’.

1.2.2 Information loss in floating-point representations

The condition for a floating point number to be represented “exactly” by the IEEE754 standard is for the number to be equal to:

$$f = \sum_{k=n}^m digit_k \times 2^k, \quad (1.2.4)$$

where m and n are two integers so that $|m - n| \leq 24$ (it is fine if the equation is not very clear – we will show some examples below). In addition to this, there is the constraint that $|n| \leq 127$ (think about why). Nothing can be done about the second constraint, but as far as the first constraint is concerned, practically we can approximate the number leaving off (truncating) the less significant bits (those to the right, or mathematically those with a smaller k value in the sum above), so that $|m - n| \leq 24$ is satisfied.

Actually, many rational numbers, even, are not expressible in the form of the sum above: As an example, try deriving the representation of 4.1 and see whether you can represent it in binary with finite number of bits.

In addition, we have infinitely many irrational numbers which do not have finite fractions: e.g. $\sqrt{2}$, $\sqrt{3}$, π , e . To be able to use all these numbers in computers, we approximate them. Do not worry, it is something quite common in applied sciences.

Approximation comes with some dangers: When you subtract two truncated numbers which are close to each other, then the result you obtain has a high imprecision. This also is the case with multiplication and division of relatively big numbers.

Though we have not started working with Python yet, we will display some self explanatory examples and comment on them:

- `>>> 0.9375 - 0.9`
0.0374999999999998

The first line is some input that we typed in, to be carried out, and the following line is what the Python interpreter returned as the result. Surprise! (Actually a bad one!) In contrary to our expectation, the result is not 0.0375. The reason is that 0.9375 is one of the rare numbers that could be represented as a finite sum $\sum_{k=1}^N (digit_k \cdot 2^{-k})$, $digit_k \in 0, 1$ such that N stays in the IEEE representation limit. Actually for 0.9375, $digit = [1, 1, 1, 1]$ and $N = 4$.

On the other hand, quite unexpectedly, 0.9 is not so. It cannot be expressed as a similar sum where N stays in the IEEE representation limit. Actually, N extends to $+\infty$ for 0.9. Hence the $digit_n$ sequence has to be truncated before it can be stored in the IEEE representation. The bits that do not fit into the representation are simply ignored: In other words, the number loses its precision.

This is combined with a similar representation problem of 0.0375, which leads to another loss and we arrive at 0.0374999999999998. Bottom line: many numbers cannot exactly be represented in the IEEE754 format, and this causes precision loss.

- Things can get even worse. Consider:

```
>>> 2000.0041 - 2000.0871
-0.082999999998563

>>> 2.0041 - 2.0871
-0.082999999999974
```

Actually both results should have been -0.0830. Despite having an imprecision, the imprecision is not consistent. This is because the loss in the first example (the one where the whole part is 2000) is bigger than the loss in the second one since 2000 needs more bits to be represented compared to 2.

- Pi (π) is a transcendental number. The fractional part never stops, in any base. Let us give it a shot on the Python interpreter:

```
>>> PI = 3.141592653589793238462643383279502884197169399375105820974944592307816406286
>>> print(PI)
3.141592653589793
```

Ok, from this we understand that the IEEE representation could only accommodate so many bits for the 15 places in the fractional part. That looks quite precise, but let us take a look at the sin and cos values:

```
>>> sin(PI)
1.2246467991473532e-16
>>> cos(PI)
-1.0
```

Interestingly, we received a slight error for the sine value, which is different from 0.0. But when it comes to the cosine value, we were lucky that imprecision somewhat cancelled out and gave us the correct result.

- We are thought since primary school that addition is associative. Hence $A + (B + C)$ is the same as $(A + B) + C$. In floating point arithmetic, this may not be so:

```
>>> A = 1234.567
>>> B = 45.67834
>>> C = 0.0004
>>> AB = A + B
>>> BC = B + C
>>> print(AB+C)
1280.245739999998

>>> print(A+BC)
1280.245740000001
```

This is again a combination of the precision loss phenomena introduced above. Most of the intermediate steps of a calculation have precision losses of their own.

As a final word about using floating point numbers, it is worth stressing a common mistake commonly made but has nothing to do with the precision loss mentioned. Let us assume you provide your program the Pi number to be 3.1415. You do your calculations and obtain floating point numbers with 14-15 digit fractional parts. Knowing about the precision loss, you assume that maybe a couple of the last digits are wrong but at least 10 digits after the decimal point are correct. However, this is a mistake: You made an approximation in the 5th digit after the decimal point in number Pi which will propagate through your calculation. It can get worse (for example if you subtract two very close numbers and use it in the denominator), but can never get better. Your best chance is to get a correct result in the 4th digit after the decimal point. The following digits, as far as precision is concerned, are bogus.

So, what can we do? Here are some rules of thumb about using floating point numbers:

- It is in your best interest to refrain from using floating points. If it is possible transform the problem to the integer domain.
- Use the most precise type of floating point provided by your high-level language, some languages provide you with 64 bit or even 128 bit floats, use them.
- Use less precision floating points only when you are in short of memory.
- Subtracting two floating points close in value has a potential danger.
- If you add or subtract two numbers which are magnitude-wise not comparable (one very big the other very small), it is likely that you will lose the proper contribution of the smaller one. Especially when you iterate the operation (repeat it many times), the error will accumulate.
- You are strongly advised to use well-known, commonly used scientific computing libraries instead of coding floating point algorithms by yourself.

1.2.3 PRACTICE TIME

Please follow the Colab link at the top of the page to have a practical session on the IEEE754 floating point representation.

1.3 Numbers in Python

Python provides the following representations for numbers:

- **Integers:** You can use integers as you are used to from your math classes. Interestingly Python adopts a seamless internal representation so that integers can effectively have any number of digits. The internal mechanism of Python switches from the CPU-imposed fixed-size integers to some elaborated big-integer representation silently when needed. You do not have to worry about it. Furthermore, bear in mind that “73.” is **not** an integer in Python. It is a floating point number (73.0). An integer cannot have a decimal point as part of it.
- **Floating point numbers (float in short):** In Python, numbers which have decimal point are taken and represented as floating point numbers. For example, 1.45, 0.26, and -99.0 are float but 102 and -8 are not. We can also use the scientific notation ($a \times 10^b$) to write floating point numbers. For example, float 0.000000436 can be written in scientific notation as 4.36×10^{-8} and in Python as 4.36E-8 or 4.36e-8.
- **Complex numbers:** In Python, complex numbers can be created by using j after a floating point number (or integer) to denote the imaginary part: e.g. 1.5-2.6j for the complex number $(1.5 + 2.6i)$. The j symbol (or i) represents $\sqrt{-1}$. There are other ways to create complex numbers, but this is the most natural way, considering your previous knowledge from high school.

1.4 Representing text

As we said in the first lines of this chapter, programming is mostly about a world problem which generally includes human related or interpretable data to be processed. These data do not consist of numbers only but can include more sophisticated data such as text, sound signals and pictures. We leave the processing of sound and pictures out of this book’s scope. Text, though, is something we have to study.

1.4.1 Characters

Written natural languages consist of basic units called graphemes. Alphabetic letters, Chinese-Japanese-Korean characters, punctuation marks, numeric digits are all graphemes. There are also some basic actions that go commonly hand in hand with textual data entry. “Make newline”, “Make a beep sound”, “Tab”, “Enter” are some examples. These are called “unprintables”.

How can we represent graphemes and unprintables in binary? Graphemes are heavily culture dependent. The shapes do not have a numerical foundation. As far as computer science is concerned, the only way to represent such information in numbers is to make a table and build this table into electronic input/output devices. Such a table will have two columns: The graphemes and unprintables in one column and the assigned binary code in the other, e.g.:

Grapheme or Unprintable	Binary Code
:	:

Throughout the history of computers, there has been several such tables, mainly constructed by computer manufacturers. In time, most of them vanished and only one survived: The ASCII (American Standard Code for Information Interchange) table which was developed by the American National Standards Institute (ANSI). This American code, developed by Americans, is naturally quite ‘American’. It incorporates all characters of the American-English alphabet, including, for example, the dollar sign, but stops there. The table does not contain a single character from another culture (for example, even the pound sign ‘£’ is not in the table).

The ASCII table has 128 lines. It maps 128 American graphemes and unprintables to 7-bit long codes. Since the 7-bit long code can be interpreted also as a number, for convenience, this number is also displayed in the ASCII table – see Fig. 1.4.1.

Dec	Bin	Char	Dec	Bin	Char	Dec	Bin	Char	Dec	Bin	Char
0	0000 0000	[NUL]	32	0010 0000	space	64	0100 0000	@	96	0110 0000	`
1	0000 0001	[SOH]	33	0010 0001	!	65	0100 0001	A	97	0110 0001	a
2	0000 0010	[STX]	34	0010 0010	"	66	0100 0010	B	98	0110 0010	b
3	0000 0011	[ETX]	35	0010 0011	#	67	0100 0011	C	99	0110 0011	c
4	0000 0100	[EOT]	36	0010 0100	\$	68	0100 0100	D	100	0110 0100	d
5	0000 0101	[ENQ]	37	0010 0101	%	69	0100 0101	E	101	0110 0101	e
6	0000 0110	[ACK]	38	0010 0110	&	70	0100 0110	F	102	0110 0110	f
7	0000 0111	[BEL]	39	0010 0111	'	71	0100 0111	G	103	0110 0111	g
8	0000 1000	[BS]	40	0010 1000	(72	0100 1000	H	104	0110 1000	h
9	0000 1001	[TAB]	41	0010 1001)	73	0100 1001	I	105	0110 1001	i
10	0000 1010	[LF]	42	0010 1010	*	74	0100 1010	J	106	0110 1010	j
11	0000 1011	[VT]	43	0010 1011	+	75	0100 1011	K	107	0110 1011	k
12	0000 1100	[FF]	44	0010 1100	,	76	0100 1100	L	108	0110 1100	l
13	0000 1101	[CR]	45	0010 1101	-	77	0100 1101	M	109	0110 1101	m
14	0000 1110	[SO]	46	0010 1110	.	78	0100 1110	N	110	0110 1110	n
15	0000 1111	[SI]	47	0010 1111	/	79	0100 1111	O	111	0110 1111	o
16	0001 0000	[DLE]	48	0011 0000	0	80	0101 0000	P	112	0111 0000	p
17	0001 0001	[DC1]	49	0011 0001	1	81	0101 0001	Q	113	0111 0001	q
18	0001 0010	[DC2]	50	0011 0010	2	82	0101 0010	R	114	0111 0010	r
19	0001 0011	[DC3]	51	0011 0011	3	83	0101 0011	S	115	0111 0011	s
20	0001 0100	[DC4]	52	0011 0100	4	84	0101 0100	T	116	0111 0100	t
21	0001 0101	[NAK]	53	0011 0101	5	85	0101 0101	U	117	0111 0101	u
22	0001 0110	[SYN]	54	0011 0110	6	86	0101 0110	V	118	0111 0110	v
23	0001 0111	[ETB]	55	0011 0111	7	87	0101 0111	W	119	0111 0111	w
24	0001 1000	[CAN]	56	0011 1000	8	88	0101 1000	X	120	0111 1000	x
25	0001 1001	[EM]	57	0011 1001	9	89	0101 1001	Y	121	0111 1001	y
26	0001 1010	[SUB]	58	0011 1010	:	90	0101 1010	Z	122	0111 1010	z
27	0001 1011	[ESC]	59	0011 1011	;	91	0101 1011	[123	0111 1011	{
28	0001 1100	[FS]	60	0011 1100	<	92	0101 1100	\	124	0111 1100	
29	0001 1101	[GS]	61	0011 1101	=	93	0101 1101]	125	0111 1101	}
30	0001 1110	[RS]	62	0011 1110	>	94	0101 1110	^	126	0111 1110	~
31	0001 1111	[US]	63	0011 1111	?	95	0101 1111	_	127	0111 1111	[DEL]

Fig. 1.4.1: The ASCII table.

Do not worry, you do not have to memorize it, even professional computer programmers do not. However, some properties of this table has to be understood and kept in mind:

- The general layout of the ASCII table:

Dec. Range	Property
0-31	Unprintables
32	Space char.
33-47	Punctuations
48-57	Digits 0-9
58-64	Punctuations
65-90	Upper case letters
91-96	Punctuations
97-122	Lower case letters
123-127	Punctuations

- There is no logic in the distribution of the punctuations.
- It is based on the English alphabet, characters of other languages are simply not there. Moreover, there is no mechanism for diacritics.
- Letters are ordered and uppercase letters come first in the table (have a lower decimal value)
- Digits are also ordered but are not represented by their numerical values. To obtain the numerical value for a digit, you have to subtract 48 from its ASCII value.
- The table is only and only about 128 characters, neither more nor less. There is nothing like Turkish-ASCII, French-ASCII. The extensions, where the 8th bit is set has nothing to do with the ASCII table.
- Python makes use of ASCII character representation.

The frustrating discrepancies and shortcomings of the ASCII table have led the programming society to seek a solution. A non-profit group, the Unicode Consortium, was founded in the late 80s with the goal of providing a substitute for the current character tables, which is also compliant (backward compatible) with them. The Unicode Transformation Format (UTF) is their suggested representation scheme.

This UTF representation scheme has variable length and may include components of 1-to-4 8-bit wide (in the case of UTF-8) or 16-bit wide components of 1-to-2 (in the case of UTF-16). UTF is now becoming part of many recent high-level language implementations, including Python, Java, Perl, TCL, Ada95 and C#, gaining wide popularity.

1.4.2 Strings

Text is as vital a data as numbers are. Text is expressed as character sequences. These sequences are named as strings. But we have here a problem. As introduced, numbers (integers and floating points) have a niche in the CPU. There are instructions designed for them: we can store and retrieve them to/from the memory; we can perform arithmetical operations among them. A character data can be represented and processed as well because they are mapped to one byte integers. But when it comes to strings, the CPU does not have any facility for them.

The only reasonable way is to store the codes of each character that make up a string into the memory in consecutive bytes. Does this solve the problem of ‘representation’? Unfortunately no. The trouble is determining how to know where the string ends. Two methods come to mind:

1. Prior to the string characters, store the length (the number of characters in the string) as an integer of fixed number of bytes.
2. Store a special byte value, which is not used to represent any other character, at the end of the string characters.

1.5 Containers

The representation of a string is maybe the most simple representation of a data that is not directly supported by the CPU. However, it gives an idea for what can be done in similar cases. The key concept is to find a layout that is a mapping from the space of the data to an organization in the memory.

Also notice that whatever is placed in the memory has an ‘address’ and the value of the address can also become a part the organization. As far as the string is concerned, the usage of the ‘address concept’ was simple: A single address marks the start of the string. When we want to process the string, we go to this address and then start to process the character codes sequentially.

It is possible to have data organizations which include addresses of other data organizations. In other words, it is possible to jump from one group of data to some other in the memory. This type of organizations are name *Data Structures* in Computer Science. So, string is a data structure. As far as Python is concerned, there are several other data structures. They are coined in Python as *containers*. In addition to strings Python provide lists, tuples, sets and dictionaries as containers. Except strings, which is introduced above, the others have more complex data structures which will not be covered, because it falls outside of the scope of this book.

1.6 Representing truth values (Booleans)

Boolean is another data type that has its roots in the very structure of the CPU. Answers to all questions asked to the CPU are either *true* or *false*. The logic of a CPU is strictly based on binary evaluation system. This logic system is coined as *Boolean logic*. It was introduced by George Boole in his book “The Mathematical Analysis of Logic” (1847).

It is tightly connected to the binary 0 and 1 concepts. In all CPUs, falsity is represented with a 0 whereas truth is represented with a 1 and on some with any value which is not 0.

1.7 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- Sign-magnitude notation and two’s complement representation for representing integers.
- The IEEE754 standard for representing real numbers.
- Precision loss in representing floating point numbers.
- Representing characters with the ASCII table.
- Representing truth values.

1.8 Further Reading

- Two's Complement: http://en.wikipedia.org/wiki/Two%27s_complement
- The Method of Complements: https://en.wikipedia.org/wiki/Method_of_complements
- Excess-k Representation: https://en.wikipedia.org/wiki/Offset_binary
- IEEE 754 Floating Point Standard: http://en.wikipedia.org/wiki/IEEE_754-2008
- ASCII: <http://en.wikipedia.org/wiki/ASCII>
- UTF—UCS Transformation Format: <http://en.wikipedia.org/wiki=UTF-8>

Exercises

- By hand, find the 5-bit Two's Complement representation of the following numbers: 4, -5, 1, -0, 11.
- Represent 6 and (-7) in a 5-bit sign-magnitude notation and add them up in binary, without looking at their signs.
- Find the IEEE 754 32-bit representation of the following floating point numbers: 3.3, 3.37, 3.375.

2 | Dive into Python

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After having covered some background on how a computer works, how we solve problems with computers and how we can represent data in binary, we are ready to interact with Python and to learn representing data and performing actions in Python.

The Python interpreter that we introduced in Chapter 2 waits for our computational demands if not executing something already. Those demands that describe an algorithm have to be expressed in Python as a sequence of ‘actions’ where each action can serve two broad purposes:

- **Creating or modifying data:** These actions take in data, perform sequential, conditional or repetitive execution on the data, and produce other data. Computations that form the bases for our solutions are going to be these kinds of actions.
- **Interacting with the environment:** Our solutions will usually involve interacting with the user or the peripherals of the computer to take in (input) data or take out (output) data.

Irrespective of its purpose, an action can be of two types:

- **Expression:** An expression (e.g. $3 + 4 * 5$) specifies a calculation, which, when evaluated (performed), yields some data as a result. An expression can consist of:
 - basic data (integer, floating point, boolean etc.) or container data (e.g. string, list, set etc.).
 - expressions involving operations among data and other expressions.
 - functions acting on expressions.
- **Statement:** Unlike an expression, a statement does *not* return data as a result and can be either basic or compound:
 - **Basic statement:** A basic statement can be e.g. for storing the result of an expression in a memory location (an assignment statement for further use (in following actions), deleting an item from a collection of data etc. Each statement has its special syntax that generally involves a special keyword.
 - **Compound statement:** Compound statements are composed of other statements and executing the compound statement means executing the statements in the compound.

Naming and Printing Data

For better illustrations and examples, we will use two concepts in the first part of the chapter before they are introduced. Let us briefly describe them and leave the coverage of the details to their individual sections:

- **Variables:** In programming languages, we can give a name to data and use that name to access it, e.g.:

```
>>> a = 3  
>>> 10 + a  
13
```

We call such names variables and the action `a = 3` is called an assignment. We defer a more detailed coverage until Section 4.4.

- Printing data: Python provides the `print()` function to display data items on screen:

```
print(item1, item2, ..., itemN)
```

For example:

```
>>> print('Python', 'is', 'so', 'fun')  
Python is so fun
```

2.1 Basic Data

Let us remember what basic data types we had:

- Numbers
 - Integers
 - Floating points
 - Complex numbers
- Booleans

Python is a language in which all arithmetic operations among the same type of numbers are provided very much as expected from our math knowledge. Furthermore, mixed type operations (e.g. subtracting a floating point number from an integer) are also defined.

In programming, being able to ask questions about data is of vital importance. The atomic structures for asking questions are the *comparison operations* (e.g. “is a value equal to another value”, or “is a value greater than another value”, etc.). Operators that serve these purposes do exist in Python and provide resulting values that are True or False (Booleans). It is also possible to combine such questions under *logical operations*. The and, or and not operators stand for conjunction, disjunction and negation, correspondingly. Needless to say, these operators also return Boolean values.

2.1.1 Numbers in Python

Python provides the following representations for numbers (the following is an essential reminder from the previous chapter):

- **Integers:** You can use integers as you are used to from your math classes. Interestingly Python adopts a seamless internal representation so that integers can effectively have any number of digits. The internal mechanism of Python switches from the CPU-imposed fixed-size integers to some elaborated big-integer representation silently when needed. You do not have to worry about it. Furthermore, bear in mind that “73.” is **not** an integer in Python. It is a floating point number (73.0). An integer cannot have a decimal point as part of it.

- **Floating point numbers (float in short):** In Python, numbers which have decimal point are taken and represented as floating point numbers. For example, 1.45, 0.26, and -99.0 are float but 102 and -8 are not. We can also use the scientific notation ($a \times 10^b$) to write floating point numbers. For example, float 0.000000436 can be written in scientific notation as 4.36×10^{-8} and in Python as 4.36E-8 or 4.36e-8.
- **Complex numbers:** In Python, complex numbers can be created by using j after a floating point number (or integer) to denote the imaginary part: e.g. 1.5-2.6j for the complex number $(1.5 - 2.6i)$. The j symbol (or i) represents $\sqrt{-1}$. There are other ways to create complex numbers, but this is the most natural way, considering your previous knowledge from highschool.

More on Integers and Floating Point Numbers

Python provides int data type for integers and float data type for floating point numbers. You can easily play around with int and float numbers and check their type as follows:

```
>>> 3+4
7
>>> type(3+4)
<class 'int'>
>>> type(4.1+3.4)
<class 'float'>
```

where <class 'int'> indicates type int.

In Python version 3, integers do not have fixed-size representation and their size is only limited by your available memory. In Python version 2, there were two integer types: int, which used the fixed length representation supported by the CPU, and long type, which was unbounded. Since this book is based on Python version 3, we will assume that int refers to an unbounded representation.

As for the float type, Python uses the 64-bit IEEE754 standard, which allows representing numbers in the range [2.2250738585072014E-308, 1.7976931348623157E+308].

Useful Operations:

The following operations can be useful while working with numbers:

- abs(<Number>): Takes the absolute value of the number.
- pow(<Number1>, <Number2>): Takes the power of <Number1>, i.e. $<\text{Number1}>^{<\text{Number2}>}$
- round(<FloatNumber>): Rounds the floating point number to the *closest* integer.
- Functions from the math library: sqrt(), sin(), cos(), log(), etc (see [the Python documentation¹⁸](#) for a full list). This requires *importing* from the built-in math library first as follows:

```
>>> from math import *
>>> sqrt(10)
3.1622776601683795
>>> log10(3.1622776601683795)
0.5
```

¹⁸ <https://docs.python.org/3/library/math.html>

2.1.2 Boolean Values

Python provides the bool data type which allows only two values: True and False. For example:

```
>>> type(True)
<class 'bool'>
>>> 3 < 4
True
>>> type(3 < 4)
<class 'bool'>
```

Also due to decades of programming experience, Python converts several instances of other data types to some certain boolean values, if used in place of a boolean value. For example,

- 0 (the integer zero)
- 0.0 (the floating point zero)
- "" (the empty string)
- [] (the empty list)
- {} (the empty dictionary or set)

are interpreted as False. All other values of similar kinds are interpreted as True.

Useful Operations:

With boolean values, we can use not (negation or inverse), and and or operations:

```
>>> True and False
False
>>> 3 > 4 or 4 < 3
False
>>> not(3 > 4)
True
```

and returns a True value only if both of its operands are True, otherwise it returns False. or returns True if any or both of its operands are True. The following table gives result of the boolean operations for the given operand pair:

a	b	a and b	a or b
True	True	True	True
True	False	False	True
False	True	False	True
False	False	False	False

2.2 Container data (str, tuple, list, dict, set)

Up to this point we have seen the basic data types. They are certainly needed for computation but many world problems for which we seek computerized solutions need more elaborate data. Just to mention a few:

- Vectors
- Matrices
- Ordered and unordered sets
- Graphs
- Trees

Vectors and matrices are used in almost all simulations/problems of the physical world; sets are used to keep any property information as well as orders of items, equivalences; graphs are necessary for many spatial problems; trees are vital to representing hierarchical relational structures, action logics, organizing data for a quick search.

Python provides five container types for these:

1. **String (`str`)**: A string can hold a sequence of characters or only a single character. A string cannot be modified after creation.
2. **List (`list`)**: A list can hold ordered sets of all data types in Python (including another list). A list's elements can be modified after creation.
3. **Tuple (`tuple`)**: The tuple type is very similar to the list type but the elements cannot be modified after creation (similar to strings).
4. **Dictionary (`dict`)**: A very efficient method to form a mapping from a set of numbers, booleans, strings and tuples to any set of data in Python. Dictionaries are easily modifiable and extendable. Querying the mapping of an element to the ‘target’ data is performed in almost constant time (regardless of how many elements the dictionary has). In Computer Science terms, it is a *hash table*.
5. **Set (`set`)**: The set type is equivalent to sets in mathematics. The element order is undefined. (*We deemphasize the use of set*).

The first three, namely String, List and Tuple are called *sequential containers*. They consist of consecutive elements indexed by integer values starting at 0. Dictionary is not sequential, element indexes are arbitrary. For simplicity we will abbreviate sequential containers as *s-containers*.

All these containers have external representations which are used in inputting and outputting them (with all their content). Below we will walk through some examples to explain them.

Mutability vs. Immutability

Some container types are created ‘frozen’. After creating them you can wholly destroy them but you cannot change or delete their individual elements. This is called *immutability*. Strings and tuples are immutable whereas lists, dictionaries and sets are *mutable*. With a mutable container, adding new elements and changing or deleting existing ones is possible.

2.2.1 Accessing elements in sequential containers

All containers except set reveal their individual elements by an indexing mechanism with brackets:

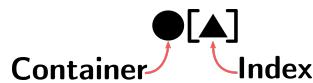


Fig. 2.2.1: How elements of a container are accessed

For the s-containers, the index is an ordinal number where counting starts with zero. For dictionaries, the index is a Python data item from the source (domain) set. A *negative index* (usable only on s-containers) has a meaning that the (counting) value is relative to the end. A negative index can be converted to a positive index by adding to the negative value the length of the container. It is nothing but index obtained by adding the length of the container.

Below we have an s-container that has a length of $(n + 1)$
(careful: indexing started at 0!):

\square_0	\square_1	\dots	\square_{n-1}	\square_n	(2.2.1)
[0]	[1]	\dots	[$n - 1$]	[n]	
$[-(n + 1)]$	$[-n]$	\dots	$[-2]$	$[-1]$	

As you surely have observed, when you add $(n + 1)$ to the negative index you obtain the positive one.

Slicing

s-containers provide a rich mechanism, called slicing, that allows accessing multiple elements at once. Thanks to this mechanism, you can define a start and end index and obtain the portion that lies in between (Fig. 2.2.2):

- The element at the start index is the first to be accessed.
- The end index is where accessing stops (the element at the end index is **not** accessed – i.e. the end index is not inclusive).
- It is also possible to optionally define an increment (jump amount) between indexes. After the element at [start] is accessed first, [start + increment] is accessed next. This goes on until the accessed position is equal or greater than the end index. For negative indexing, a negative increment has to work from the bigger index towards the lesser, so (*start index > end index*) is expected.

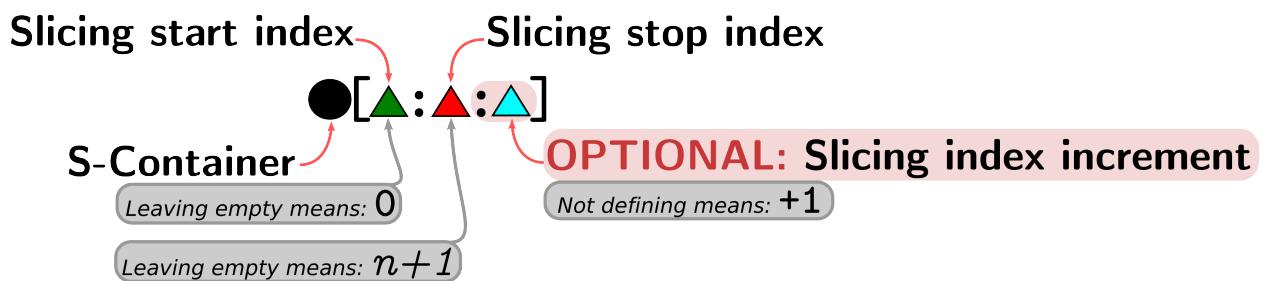


Fig. 2.2.2: Accessing multiple elements of an s-container is possible via the slicing mechanism, which specifies a starting index, an ending index and an index increment between elements.

Below, with the introduction of strings, we will have extensive examples on slicing.

If the s-container is immutable (e.g. string and tuple containers) then slicing creates a copy of the sliced data. Otherwise, i.e. if the s-container is mutable (i.e. the ‘list’ container) then slicing provides direct access to the original elements and therefore, they can be updated, which updates the original s-container.

2.2.2 Useful operations common to containers

The following operations are common to all or a subset of containers:

1- Number of elements:

For all containers len() is a built-in function that returns the count of elements in the container that is given as argument to it, e.g.:

```
>>> len("Five")
4
```

2- Concatenation:

String, tuple and list data types can be combined using ‘+’ operation:

```
<Container1> + <Container2>
```

where the containers need to be of the same type. For example:

```
>>> "Hell" + "o"
'Hello'
```

3- Repetition:

String, tuple and list data types can be repeated using “**” operation:

```
<Container1> * <Number>
```

where the container is copied “” many times. For example:

```
>>> "Yes No " * 3
'Yes No Yes No Yes No '
```

4- Membership:

All containers can be checked for whether they contain a certain item as an element using in and not in operations:

```
<item> in <Container>
```

or

```
<item> not in <Container>
```

Of course, the result is either True or False. For dictionaries in tests if the domain set contains the element, for others it simply tests if element is a member.

2.2.3 String

As was explained in the previous chapter, a string is used to hold a sequence of characters. Actually, it is a container where each element is a character. However, Python does not have a special representation for a single character. Characters are represented externally as strings containing a single character only.

Writing strings in Python

In Python a string is denoted by enclosing the character sequence between a pair of quotes ('') or double quotes (""). A string surrounded with triple double quotes (""" ... """") allows you to have any combination of quotes and line breaks within a sequence, and Python will still view it as a single entity.

Here are some examples:

- "Hello World!"
- 'Hello World!'
- 'He said: "Hello World!" and walked towards the house.'
- "A"
- """ Andrew said: "Come here, doggy". The dog barked in reply: 'woof """

The backslash (\) is a special character in Python strings, also known as the *escape character*. It is used in representing certain, the so called, unprintable characters: (\t) is a tab, (\n) is a newline, and (\r) is a carriage return. [Table 2.2.1](#) provides the full list.

Table 2.2.1: The list of escape characters in Python.

Escape Sequence	Meaning
\\	Backslash ()
\'	Single quote ()
\"	Double quote ()
\a	ASCII Bell (BEL)
\b	ASCII Backspace (BS)
\f	ASCII Formfeed (FF)
\n	ASCII Linefeed (LF)
\r	ASCII Carriage Return (CR)
\t	ASCII Horizontal Tab (TAB)
\v	ASCII Vertical Tab (VT)
\ooo	ASCII character with octal value <i>ooo</i>
\xhh	ASCII character with hex value <i>hh</i>
\uhhhh	UNICODE character with hex value <i>hhhh</i>

Conversely, prefixing a special character with (\) turns it into an ordinary character. This is called *escaping*. For example, (\') is the single quote character. 'It\'s raining' therefore is a valid string and equivalent to "It's raining". Likewise, (") can be escaped: "\"hello\" is a string that begins and ends with the literal double quote character. Finally, (\) can be used to escape itself: (\\\) is the literal backslash character. For '\nnn', *nnn* is a number in base 8, for '\xnn' *nn* is a number in base 16 (including letters from A to F as digits for values 10 to 15).

In Python v3, all strings use the Unicode representation where all international symbols are possible, e.g.:

```
>>> a = "Fıstıkçı şahap"  
>>> a  
'Fıstıkçı şahap'
```

Examples with strings

Let us look at some examples to see what strings are in Python and what we can do with them:

```
>>> "This is a string"  
"This is a string"  
>>> "This is a string"[0]  
'T'  
>>> s = "This is a string"  
>>> print(s[0])  
T  
>>> print(s[0],s[1],s[8],s[14],s[15])  

```

Since strings are immutable an attempt to change a character in a string will badly fail:

```
>>> s = "This is a string"  
>>> print(s)  
This is a string  
>>> s[2] = "u"  
Traceback (most recent call last):  
  File "<stdin>", line 1, in <module>  
TypeError: 'str' object does not support item assignment
```

Bottom line: You cannot change a character in a created string.

Let us go through a sequence of examples. We encourage you to run the following examples in the Colab version of this chapter. Feel free to change the text and rerun the examples.

```
my_beautiful_string = "The quick brown fox jumps over the lazy dog"  
print("THE STRING:", my_beautiful_string, len(my_beautiful_string), "CHARACTERS")
```

THE STRING: The quick brown fox jumps over the lazy dog 43 CHARACTERS

```
my_beautiful_string[0]
```

```
'T'
```

```
my_beautiful_string[4]
```

```
'q'
```

```
my_beautiful_string[0:4]
```

```
'The '
```

```
my_beautiful_string[:4]
```

```
'The '
```

```
my_beautiful_string[4:]
```

```
'quick brown fox jumps over the lazy dog'
```

```
my_beautiful_string[10:15]
```

```
'brown'
```

```
my_beautiful_string[:-5]
```

```
'The quick brown fox jumps over the laz'
```

```
my_beautiful_string[-8:-5]
```

```
'laz'
```

```
my_beautiful_string[:]
```

```
'The quick brown fox jumps over the lazy dog'
```

```
my_beautiful_string[::-1]
```

```
'god yzal eht revo spmuj xof nworb kciuq ehT'
```

```
my_beautiful_string[-6:-9:-1]
```

```
'zal'
```

```
my_beautiful_string[0:15:2]
```

```
'Teqikbon'
```

Strings are used to represent non-mathematical textual information. Common places where strings are used are:

- Textual communication in natural language with the user of the program.
- Understandable labeling of parts of data: City names, names of individuals, addresses, tags, labels.
- Denotation needs of human-to-human interactions.

Useful operations with strings:

- String creation: In addition to using quotes for string creation, the str() function can be used to create a string from its argument, e.g.:

```
>>> str(4)
'4'
>>> str(4.578)
'4.578'
```

- Concatenation, repetition and membership:

```
>>> 'Programming' + ' ' + 'with ' + 'Python is' + ' fun!'
'Programming with Python is fun!'
>>> 'really fun ' * 10
'really fun really fun '
>>> 'fun' in 'Python'
False
>>> 'on' in 'Python'
True
```

- Evaluate a string: If you have a string that is an expression describing a computation, you can use the eval() function to evaluate the computation and get the result, e.g.:

```
>>> s = '3 + 4'
>>> eval(s)
7
```

Deletion and Insertion from/to strings

Since strings are immutable, this is not possible. The only way is to create a new string, making use of slicing and concatenation operation (using +), then replacing the new created string in same place of the former one. For example:

```
>>> a = 'Python'
>>> a[0] = 'S'
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
TypeError: 'str' object does not support item assignment
>>> b = 'S' + a[1:]
>>> b
'Sython'
```

2.2.4 List and tuple

Both list and tuple data types have a very similar structure on the surface: They are sequential containers that can contain any other data type (including other tuples or lists) as elements. The only difference concerning the programmer is that tuples are immutable whereas lists are mutable. As previously said, being immutable means that, after being created, it is not possible to change, delete or insert any element in a tuple.

Lists are created by enclosing elements into a pair of brackets and separating them with commas, e.g. ["this", "is", "a", "list"]. Tuples are created by enclosing elements into a pair of parentheses, e.g. ("this", "is", "a", "tuple"). There is no restriction on the elements: They can be any data (basic or container).

Let us look at some examples for lists:

- [9,3,1,-1,6]
- []
- [2020]
- [3.1415, 2.718281828]
- [{"pi":3.1415}, {"e":2.718281828}, 1.41421356]
- ['the', 'quick', 'brown', 'fox', 'jumped', 'over', 'the', 'lazy', 'dog']
- [10, [5, [3, [[30, [], []], []], []], [8, [], []], [30, [], []]]]
- [[1,-1,0],[2,-3.5,1.1]]

and some examples for tuples:

- ('north','east','south','west')
- ()
- ('only',)
- ('A',65,"1000001","0x41")
- ("abx",[1.32,-5.12],-0.11)

Of course, tuples can become list members as well, or vice versa:

- [("ahmet","akhunlar",("deceased", 1991)), ("huri","huriyegil","not born")]
- [("ahmet","akhunlar",("deceased", 1991)], ["huri","huriyegil","not born"])]

Programmers generally prefer using lists over tuples since they allow changing elements, which is often a useful facility in many problems.

Lists (and tuples) are used whenever there is a need for an ordered set. Here are a few usecases for lists and tuples:

- Vectors.
- Matrices.
- Graphs.
- Board game states.
- Student records, address book, any inventory.

Useful operations with lists and tuples

1- Deletion from lists

As far as deletion is concerned, you can use two methods:

- Assigning an empty list to the slice that is going to be removed:

```
>>> L = [111,222,333,444,555,666]
>>> L[1:5] = []
>>> print(L)
[111, 666]
```

- Using the `del` statement on the slice that is going to be removed:

```
>>> L = [111,222,333,444,555,666]
>>> del L[1:5]
>>> print(L)
[111, 666]
```

2- Insertion into lists

For insertion, you can use three methods:

- Using assignment with a degenerate use of slicing:

```
>>> L = [111,222,333,444,555,666]
>>> L[2:2] = [888,999]
>>> print(L)
[111, 222, 888, 999, 333, 444, 555, 666]
```

- The second method can insert only one element at a time, and requires object-oriented features, which will be covered in Chapter 7.

```
>>> L = [111,222,333,444,555,666]
>>> L.insert(2, 999)
>>> print(L)
[111, 222, 999, 333, 444, 555, 666]
```

where the `insert` function takes two parameters: The first parameter is the index where the item will be inserted and the second parameter is the item to be inserted.

- The third method uses the `append()` method to insert an element only to the end or `extend()` to append more than one element to the end:

```
>>> L = [111,222,333,444,555]
>>> L.append(666)
>>> print(L)
[111, 222, 333, 444, 555, 666]
>>> L.extend([777, 888])
>>> print(L)
[111, 222, 333, 444, 555, 666, 777, 888]
```

3- Data creation with ``tuple()`` and ``str()`` functions: Similar to other data types, tuple and list data types provide two functions for creating data from other data types.

4- Concatenation and repetition with lists and tuples: Similar to strings, `+` and `*` can be used respectively to concatenate two tuples/lists and to repeat a tuple/list many times.

5- Membership: Similar to strings, `in` and `not in` operations can be used to check whether a tuple/list contains an element.

Here is an example that illustrates the last three items:

```
>>> a = ([3] + [5])*4
>>> a.append([3, 5])
>>> print(a)
[3, 5, 3, 5, 3, 5, 3, 5, [3, 5]]
>>> a.extend([3, 5])
```

(continues on next page)

```

>>> print(a)
[3, 5, 3, 5, 3, 5, 3, 5, [3, 5], 3, 5]
>>> b = tuple(a)
>>> print(b)
(3, 5, 3, 5, 3, 5, 3, 5, [3, 5], 3, 5)
>>> [3, 5] not in b
False
>>> [5, 3] not in b
True      # test for single element, not subsequence

```

As you have recognized, the examples with some containers included two types of constructs which were not covered yet: One is the use of ‘functions’ on containers, e.g. the use of `len()`. Due to your high school background, this is certainly easy to understand. The second construct is something new. It appears that we can use some functions suffixed by a dot to a container (e.g. the `append` and `insert` usages in the examples above). This construct is an internal function call of data structure called *object*. Containers are actually objects and in addition to their data containment property, they also have some defined action associations. These actions are named as *member functions*, and called (applied) on that object (in our case -the container-) by means of this dot notation:

$$\bullet.f(\square) \text{ has the conceptual meaning of } f(\bullet, \square) \quad (2.2.2)$$

(Don’t try this explicitly, it will not work. The equivalence is just ‘conceptual’: meaning the function receives the object internally, as a ‘hidden’ argument). All these will be covered in details in Chapter 7. Till then, for sake of completeness, from time to time we will referring to this notation. Till then simply interpret it based on the equivalence depicted above.

Example: Matrices as Nested Lists

In many real-world problems, we often end up with a set of values that share certain semantics or functionality, and benefit from representing them in a regular grid structure that we call matrix:

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \ddots & & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mn} \end{pmatrix}, \quad (2.2.3)$$

which has n columns and m rows, and we generally shorten this as $m \times n$ and say that matrix A has size $m \times n$. The following set of equations describe relations among a set of variables and called system of equations:

$$\begin{aligned} 3x + 4y + z &= 4, \\ -3x + 3y + 5 &= 3, \\ x + y + z &= 0, \end{aligned} \quad (2.2.4)$$

which can be represented with matrices as:

$$\begin{pmatrix} 3 & 4 & 1 \\ -3 & 3 & 5 \\ 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 4 \\ 3 \\ 0 \end{pmatrix}, \quad (2.2.5)$$

which defines the same problems in terms of matrices and matrix multiplication. It is okay if you are not familiar with matrix multiplication – we will briefly explain it and use it as an example in the next chapter.

Writing a problem in a matrix form like we did above allows us to group the related aspects of the problem together and focus on these groups for solving a problem. In our example, we grouped coefficients in a

matrix and this allows us to analyze and manipulate the coefficients matrix to check whether for this system of equations there is a solution, whether the solution is unique or what the solution is. All these are questions that are studied in Linear Algebra and beyond the scope of our book.

Now let us see how we can represent matrices in Python. A very straightforward approach that would also allow changing elements of the matrix later on is to use lists in a nested form, as follows:

```
>>> A = [[3, 4, 1],  
... [-3, 3, 5],  
... [1, 1, 1]]  
>>> A  
[[3, 4, 1], [-3, 3, 5], [1, 1, 1]]
```

where each row is represented as a list and a member of the outer list. This would allow us to access entries like this:

```
>>> A[1]  
[-3, 3, 5]  
>>> A[1][0]  
-3
```

Although we can represent matrices like this, there are very advanced libraries that make representing and working with matrices more practical, as we will see in Chapter 10. For an extended coverage on matrices and matrix operations, we refer to [Matrix algebra for beginners](#)¹⁹ (by Jeremy Gunawardena) or [Chapter 2.2 of “Mathematics for Machine Learning”](#)²⁰ (by Marc Peter Deisenroth, A. Aldo Faisal and Cheng Soon Ong).

2.2.5 Dictionary

Dictionary is a container data type where accessing items can be performed with indexes that are not numerical; in fact, in dictionaries, indexes are called keys. A list, tuple, or string data type stores a certain element at each numerical index (key). Similarly, a dictionary stores an element (value) for each key. In other words, a dictionary is just a mapping from keys to values (Fig. 2.2.3).

The keys can be only immutable data types, i.e., numbers, strings, or tuples (with only immutable elements) – some other immutable types that we do not cover in the book are also possible. Since lists and dictionaries are mutable, they cannot be used for keys for indexing. As for values, there is no limitation on the data type.

A dictionary is a discrete mapping from a set of Python elements to another set of Python elements. Itself, as well as its individual elements, are mutable (you can replace them). Moreover, it is possible to add and remove items from the mapping.

¹⁹ <http://vcp.med.harvard.edu/papers/matrices-1.pdf>

²⁰ <https://mml-book.github.io/book/mml-book.pdf>

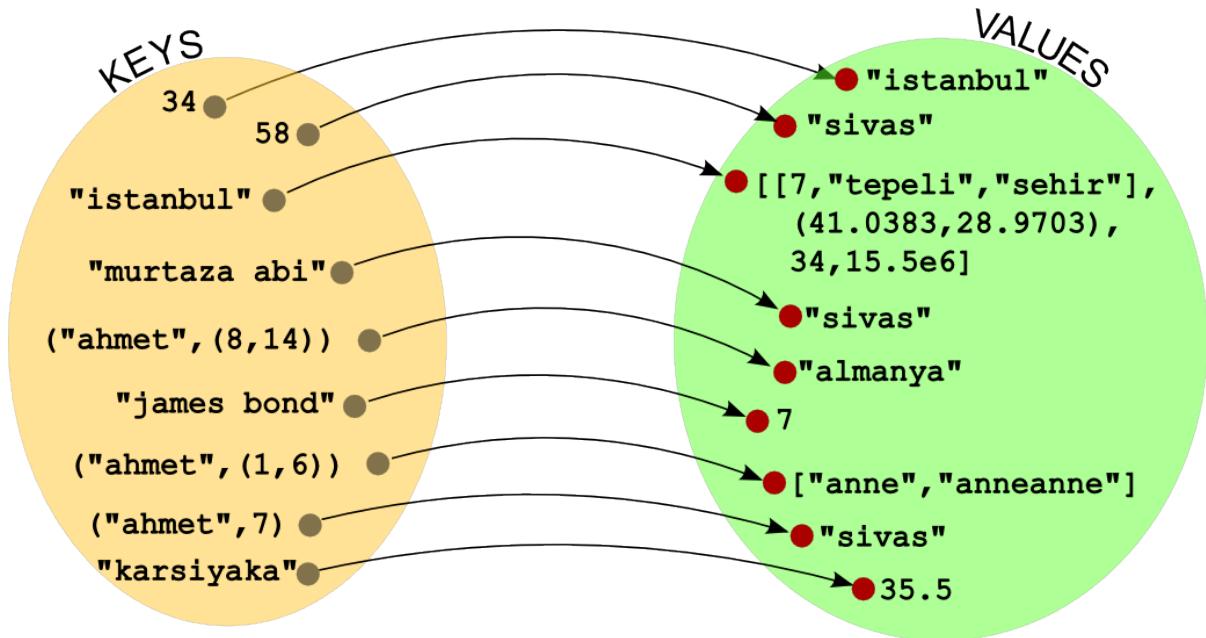


Fig. 2.2.3: A dictionary provides a mapping from keys to values.

A dictionary is represented as key-value pairs, each separated by a colon sign (:) and all enclosed in a pair of curly braces. The dictionary in Fig. 2.2.3 would be denoted as:

```
{34:"istanbul",
58:"sivas",
"istanbul":[[7,"tepeli","sehir"],(41.0383,28.9703),34,15.5e6],
"murtaza abi":"sivas",
("ahmet", (8,14)):"almanya", "james bond":7,
("ahmet", (1,6)):["anne", "anneanne"],
("ahmet", 7):"sivas",
"karsiyaka":35.5}
```

Similar to other containers, we usually store containers under a variable. Let us assume the dictionary above was assigned to a variable with the name conno and look at some examples:

```
conno = {34:"istanbul", 58:"sivas", "istanbul":[[7,"tepeli","sehir"],(41.0383,28.9703),34,15.5e6], "murtaza abi":  
    ↪ "sivas", ("ahmet", (8,14)):"almanya", "james bond":7, ("ahmet", (1,6)):["anne", "anneanne"], ("ahmet", 7):"sivas", □  
    ↪ "karsiyaka":35.5}  
print(conno["murtaza abi"])  
print(conno["istanbul"])
```

```
sivas  
[[7, 'tepeli', 'sehir'], (41.0383, 28.9703), 34, 15500000.0]
```

Let us ask for something that does not exist in the dictionary:

```
>>> print(conno["ankara"])
KeyError: 'ankara'
```

Ups, that was bad. Though we have a decent method to test for the existence of a key in a dictionary, namely the use of in:

```
print("ankara" in conno)
```

False

It is also possible to remove/insert mappings from/to a dictionary:

```
print("conno has this many keys:", len(conno))
conno["ankara"] = ["baskent", "anitkabir", 6]
print("conno has this many keys now:", len(conno))
print(conno["ankara"])
print(conno["murtaza abi"])
del conno["murtaza abi"]
print("murtaza abi" in conno)
print("After murtaza abi is deleted we have this many keys:", len(conno))
```

```
conno has this many keys: 9
conno has this many keys now: 10
['baskent', 'anitkabir', 6]
sivas
False
After murtaza abi is deleted we have this many keys: 9
```

The benefit of using a dictionary is ‘timewise’. The functionality of a dictionary could be attained by using (key, value) tuples inserted into a list. Then, when you need the value of a certain key, you can search one-by-one each (key, value)-tuple element of the list until you find your key in the first position of a tuple element. However, this will consume a time proportional to the length of the list (worst case). On the contrary, in a dictionary, this time is almost constant.

Moreover, a dictionary is more practical to use since it already provides accessing elements in a key-based fashion.

Useful Operations with Dictionaries

Dictionaries support `len()` and membership (`in` and `not in`) operations that we have seen above. You can also use `<dictionary>.values()` and `<dictionary>.keys()` to obtain lists of values and keys respectively.

2.2.6 Set

Sets are created by enclosing elements into a pair of curly-braces and separating them with commas. Any immutable data type, namely a number, a string or a tuple, can be an element of a set. Mutable data types (lists, dictionaries) cannot be elements of a set. Being mutable, sets **cannot** be elements of a sets.

Here is a small example with sets:

```
a = {1,2,3,4}
b = {4,3,4,1,2,1,1,1}
print(a == b)
a.add(9)
a.remove(1)
print(a)
```

True

{2, 3, 4, 9}

The most functionalities of sets can be undertaken by lists. Furthermore, lists do not possess the restrictions sets do. On the other hand, especially membership tests are much faster with sets, since member repetition is avoided.

Frozenset

Python provides an immutable version of the set type, called frozenset. A frozenset can be constructed using the frozenset() function as follows:

```
>>> s = frozenset({1, 2, 3})
>>> print(s)
frozenset({1, 2, 3})
```

Being immutable, frozensets can be a member of a set or a frozenset.

Useful Operations with Sets

Apart from the common container operations (len(), in and not in), sets and frozensets support the following operators:

- $S_1 \leq S_2$: True if S_1 is a subset of S_2 .
- $S_1 \geq S_2$: True if S_1 is a superset of S_2 .
- $S_1 | S_2$: Union of the sets (equivalent to $S_1.union(S_2)$).
- $S_1 & S_2$: Intersection of the sets (equivalent to $S_1.intersection(S_2)$).
- $S_1 - S_2$: Set difference (equivalent to $S_1.difference(S_2)$).

The following are only applicable with sets (and not with frozensets) as they require a mutable container:

- $S.add(element)$: Add a new element to the set.
- $S.remove(element)$: Remove element from the set.
- $S.pop()$: Remove an arbitrary element from the set.

2.3 Expressions

Expressions such as $3 + 4$ describe calculation of an operation among data. When an expression is *evaluated*, the operations in the expression are applied on the data specified in the expression and a resulting value is provided.

Operations can be graphically illustrated as follows:

$$\square_1 \odot \square_2 \quad (2.3.1)$$

where \odot is called the operator, and \square_1 and \square_2 are called operands. This was a binary operator; i.e. it acted on two operands.

We can also have unary operators:

$$\odot \square \quad (2.3.2)$$

or operators that have more than two operands (see chained comparison operators below).

Before we can cover how such operations are evaluated, let us look at commonly used operations (operators) in Python.

2.3.1 Arithmetic, Logic, Container and Comparison Operations

Python provides the operators in Table 2.3.1 for arithmetic (addition, subtraction, multiplication, division, exponentiation), logic (and, or, not), container (indexing, membership) and comparison (less, less-than, equality, not-equality, greater, greater-than) operations.

Note that operators such as + and * have different meanings on different data types. For numerical data, they mean addition and multiplication whereas for container data, they mean concatenation and repetition.

Table 2.3.1: Arithmetic, Logic, Container and Comparison operators in Python.

Operator	Operation	Result Type
[]	Indexing	Any data type
**	Exponentiation	Numeric
*	Multiplication or Repetition	Numeric or container
/	Division	Numeric (floating point)
//	Integer Division	Numeric (integer)
+	Addition or concatenation	Numeric or container
-	Subtraction	Numeric
<	Less than	Boolean
<=	Less than or equal to	Boolean
>	Greater than	Boolean
>=	Greater than or equal to	Boolean
==	is equal to	Boolean
!=	is not equal to	Boolean
in	is a member	Boolean
not in	is not a member	Boolean
not	logical negation	Boolean
and	logical and	Boolean
or	logical or	Boolean

Below are some illustrations:

```
S1 = "Four"
S2 = "Five"
B1 = len(S1) < len(S2)
print("B1 is: ", B1)
B2 = S1 != S2
print("B2 is: ", B2)
B3 = B1 or B2
print("B3 is: ", B3)
```

```
B1 is: False
B2 is: True
B3 is: True
```

Exercise

Give one example for each row in [Table 2.3.1](#). Please complete this exercise in the Colab version of the chapter.

2.3.2 Evaluating Expressions

In the previous section, we have seen simple use of operators in an expression. In many cases, we combine several operators for brevity and readability, e.g. $2.3 + 3.4 * 4.5$. This expression can be evaluated in two different ways:

- $(2.3 + 3.4) * 4.5$, which would yield 25.65.
- $2.3 + (3.4 * 4.5)$, which would yield 17.59999999999998 in Python.

Since the results are very different, it is very important for a programmer to know in which order operators are evaluated when they are combined. There are two rules that govern this:

1. Precedence: Each operator has an associated precedence (priority) based on which we can determine which operator is going to be evaluated first. E.g. multiplication has higher precedence than addition, and therefore, $2.3 + 3.4 * 4.5$ would be evaluated as $2.3 + (3.4 * 4.5)$ in Python.
2. Associativity: If two operators have the same precedence, evaluation order is determined based on associativity. Associativity can be from left to right or from right to left.

For the operators, the complete associativity and precedence information are listed in [Table 2.3.2](#).

Table 2.3.2: Precedence and associativity for the operators in [Table 2.3.1](#).

Operator	Precedence	Associativity
[]	1.	Left-to-right
**	2.	Right-to-left
*, /, //, %	3.	Left-to-right
+, -	4.	Left-to-right
<, <=, >, >=, ==, !=, in, not in	5.	Special
not	6.	Unary
and	7.	Left-to-right (with short-cut)
or	8.	Left-to-right (with short-cut)

Therefore, according to Table 2.3.2, a sophisticated expression such as $2**3**4*5-2//2-1$ is equivalent to $2**81*5-1-1$ which is equivalent to 12089258196146291747061760-2 which is 12089258196146291747061758.

Below are some notes and explanations regarding expression evaluation:

- (i) The *Special* keyword in Table 2.3.2 means some treatment which is common to mathematics but not programming. In that sense Python is unique among commonly used programming languages. If \odot_i is any boolean comparison operator and \square_j is any numerical expression, the sequence of

$$\square_1 \odot_1 \square_2 \odot_2 \square_3 \odot_3 \square_4 \dots \square_{n-1} \odot_{n-1} \square_n \quad (2.3.3)$$

is interpreted as:

$$\square_1 \odot_1 \square_2 \text{ and } \square_2 \odot_2 \square_3 \text{ and } \square_3 \odot_3 \square_4 \dots \square_{n-1} \odot_{n-1} \square_n \quad (2.3.4)$$

- (ii) It is **always** possible to override the precedence by making use of parenthesis. We are familiar with this since our primary school days.
- (iii) If two numeric operands are of the same type, then the result is of that type unless the operator is / (for which the result is always a floating point number). Also comparison operators return bool typed values.
- (iv) If two numeric operands that enter an operation are of different types, then a computation occurs according to the following rules:
 - **if one operand is integer and the other is floating point:** The integer is converted to floating point.
 - **if one operand is complex:** The complex arithmetic is carried out according to the rules of mathematics among the real/imaginary part coefficients (which are either integers or floating points). Each of the two resulting coefficients are separately checked for having zero (.0) fractional part. If so, that one is converted to integer.
- (v) Except for the two logical operators and and or, all operators have an evaluation scheme which is coined as *eager evaluation*. Eager evaluation is the strategy where all operands are evaluated first and then the semantics of the operators kicks in, providing the result. Here is an example: Consider mathematical expression of: $0*(2**150-3**95)$ As a human being, our immediate reaction would be: Anything multiplied with 0 (zero) is 0, therefore we do not have to compute the two huge exponentiations (the second operand). This is taking a *short-cut* in evaluation and is certainly **far from** eager evaluation. Eager evaluation would evaluate the internals of the parenthesis, obtain - 69364745433935423843323618063349607247325483 and then multiply this with 0 to obtain 0. Yes, Python would go this ‘less intelligent’ way and do eager evaluation. The logical operators and and or, though, **do not** adopt eager evaluation. On the contrary, they use *shortcuts* (this is known as *based-on-need evaluation* in computer science).

In a conjunctive expression like:

$$\square_1 \text{ and } \square_2 \text{ and } \square_3 \text{ and } \dots \text{ and } \square_n \quad (2.3.5)$$

The evaluation proceeds as follows:

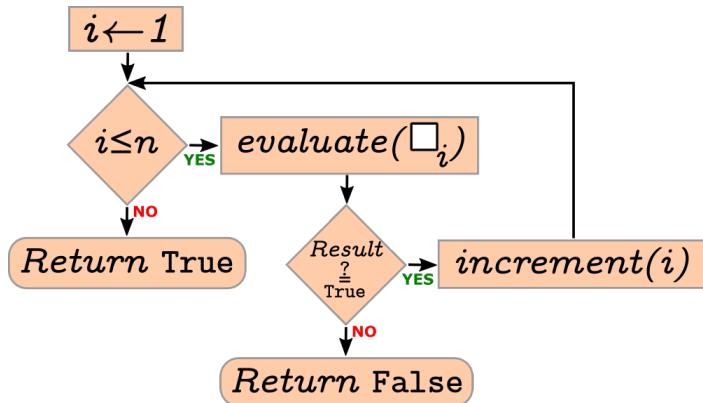


Fig. 2.3.1: Logical AND evaluation scheme

Similarly, a disjunctive expression:

$$\square_1 \text{ or } \square_2 \text{ or } \square_3 \text{ or } \dots \text{ or } \square_n \quad (2.3.6)$$

has the following evaluation scheme:

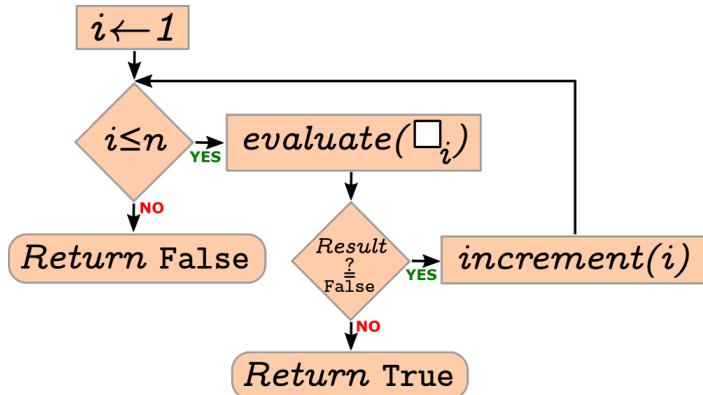


Fig. 2.3.2: Logical OR evaluation scheme

Although high-level languages provide mechanisms for evaluating expressions involving multiple operators, it is not a good programming practice to leave multiple operators without parentheses. A programmer should do his/her best to write code that is readable and understandable by other programmers and that does not include any ambiguity whatsoever. This includes expressions.

2.3.3 Implicit and Explicit Type Conversion

In Python, when you apply a binary operator on items of two different data types, it tries to convert one data to another one if possible. This is called *implicit type conversion*. For example,

```

>>> 3+4.5
7.5
>>> 3 + True
4
>>> 3 + False
3

```

which illustrates that an integer is converted to a float, True is converted to integer 1, and False is converted to integer zero.

Although Python can do such conversions, it is a good programming practice to make these conversions explicit and make the intention clear to the reader. Explicit type conversion, also called as *type casting*, can be performed using the keyword for the target type as a function. For example:

```
>>> 1.1*(7.1+int(2.5*5))  
21.01
```

Not all conversions are possible, of course. Implicit conversions are allowed only for the basic data types as illustrated below:

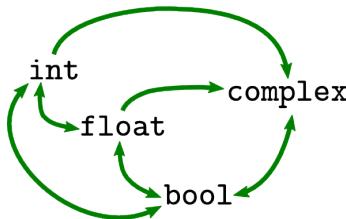


Fig. 2.3.3: Type casting among numeric and Boolean

Type casting can accommodate conversion between a wider spectrum of data types, including containers:

```
>>> str(34)  
'34'  
>>> list('34')  
['3', '4']
```

2.4 Basic Statements

Now, let us continue with actions that do not provide (return) us data as a result.

2.4.1 Assignment Statement and Variables

When we perform computation in Python, we either print the result and/or keep the result for further computations that we are going to perform. *Variables* help us here as named memory positions in which we can store data. You can imagine them as pigeonholes that are able to hold a **single** data item.

There are two methods to create and store some data into a variable. Here we will mention the overwhelmingly used one, the second is more implicit and will be introduced when we deal with functions.

A variable receives data for storage by the use of the *assignment statement*. It has the following form:

Variable = **Expression**

Although the equal sign resembles an operator that is placed between two operands, it is not an operator: Operators return a value, and in Python, the assignment is not an operator and it does not return a value (this can be different in other programming languages).

The action semantics of the assignment statement is simple:

1. The *Expression* is evaluated.
2. If the *Variable* does not exist, it is created.
3. The evaluation result is stored into the *Variable* (by doing so, any former value, if existing, is purged).

After assignment, the value can be repetitively used. To use the value in a computation, we can use the name of the variable. Here is an example:

```
>>> a = 3
>>> b = a + 1
>>> (a-b+b**2)/2
7.5
```

It is quite common to use a variable on both sides of the assignment statement. For example:

```
>>> a = 3
>>> b = a + 1
>>> a = a + 1
>>> (a-b+b**2)/2
8.0
```

The expression on the second line uses the 3 value for a. In the next line, namely the third line, again 3 is used for a in the expression (a+1). Then, the result of the evaluation (3+1) which is a 4 is stored in variable a. The variable a had a previous value of 3; that value is purged and replaced by 4. The former value is not kept anywhere and cannot be recovered.

Multiple assignments

It is possible to have multiple variables assigned to the same value, e.g.:

```
>>> a = b = 4
```

assigns an integer value of 4 to both a and b. After the multi-assignment above, if you change b to some other value, the value of a will still remain to be 4.

Multiple assignment with different values Python provides a powerful mechanism for providing different values to different variables in assignment:

```
>>> a, b = 3, 4
>>> a
3
>>> b
4
```

This is internally handled by Python with tuples and equivalent to:

```
>>> (a,b) = (3, 4)
>>> a
3
>>> b
4
```

This is called *tuple matching* and would also work with lists (i.e. [a, b] = [3, 4]).

Swapping values of variables Tuple matching has a very practical benefit: Let us say you want to swap the values in variables. Normally, this requires the use of a temporary variable:

```
>>> print(a,b)
3 4
>>> temp = a
>>> a = b
>>> b = temp
>>> print(a,b)
4 3
```

With tuple matching, we can do this in one line:

```
>>> print(a,b)
3 4
>>> a,b = b,a
>>> print(a,b)
4 3
```

Frequently-asked questions about assignments

- **QUESTION:** Considering the example below, one may have doubts about the value in b: Is it updated? On the fourth line, there is an expression using b: Which value is it referring to? 4 or 5? When we use b in a following expression, will the ‘definition’ be retrieved and recalculated?

```
>>> a = 3
>>> b = a + 1
>>> a = a + 1
>>> (a-b+b**2)/2
8.0
```

- **ANSWER:** No. Statements are executed only once: the moment they are entered (it is possible to repetitively execute a statement but here it is not used). Each assignment in the example above is executed only once. No reevaluation is performed, the use of a variable in an expression, the ‘‘a’’ and those ‘‘b’’s, refer solely to the last calculated and stored values: In the evaluation of ‘‘(a-b+b**2)/2’’, ‘‘a’’ is 4 and ‘‘b’’ is 4.
- **QUESTION:** We had variables in math, especially in middle school and high school. So, this is very similar to that right? But I am confused having seen a line like $a = a + 1$. What’s happening? The a cancel out and we are left with $0 = 1$?
- **ANSWER:** The use of the equality sign (=) is confusing to some extent. It does not stand for a balance among the left-hand-side and the right-hand-side. Do not interpret it as an ‘equality of mathematics’. It has a absolutely different semantics. As said, it only means:
 1. First calculate the right-hand side,
 2. then store the result into an (electronic) pigeon hole which has the name label given to the left-hand-side of the equal sign.
- **QUESTION:** I typed in the following lines:

```
>>> x = 5
>>> y = 3
>>> x = y
>>> y = x
>>> print x,y
3 3
```

However, it should have been 3 5, right? Or am I doing something wrong?

- **ANSWER:** You are somehow missing the time flow. Statements are executed in order:

1. **First:** ``x`` is set to 5.
2. **Second:** ``y`` is set to 3.
3. **Third:** ``x`` is set to the value stored in ``y`` which is 3. ``x`` now holds 3.
4. **Fourth:** ``y`` is set to the value stored in ``x`` which is 3 (just look to the 3. item which right above this one). ``y`` now holds 3.
5. **Fifth:** print both the values ``x`` and ``y``. Both are ``3`` and they got printed.

2.4.2 Variables & Aliasing

There is something peculiar about lists that we need to be careful while assigning them to variables. First consider the following code:

“The first example”

```
print("address of 5: ", id(5))
a = 5
print("address of a: ", id(a))
b = a
print("address of b: ", id(b))
a = 3
print("address of a: ", id(a))
print("b is: ", b)
```

```
address of 5: 4380465840
address of a: 4380465840
address of b: 4380465840
address of a: 4380465776
b is: 5
```

Here, we used the `id()` function to display the address of variables in the memory to help us understand what happens in those assignments: * The second line creates 5 in memory and links that with a. * The fourth line links the content of a with variable b. So, they are two different names for the same content. * The sixth line creates a new content, 3, and assigns it to a. Now, a points to a different memory location than b. * b still points to 5, which is printed.

Now keep the task the same but change the data from integer to a list:

“The second example”

```
a = [5,1,7]
b = a
print("addresses of a and b: ", id(a), id(b))
print("b is: ", b)
a = [3,-1]
print("addresses of a and b: ", id(a), id(b))
print("b is: ", b)
```

```
addresses of a and b: 4411372864 4411372864
```

```
b is: [5, 1, 7]
```

```
addresses of a and b: 4414271936 4411372864
```

```
b is: [5, 1, 7]
```

In other words, this works similar to the first example, as expected. But now, consider the following slightly different example:

“The third example”

```
a = [5,1,7]
b = a
print("addresses of a and b: ", id(a), id(b))
print("b is: ", b)
a[0] = 3
print("addresses of a and b: ", id(a), id(b))
print("b is: ", b)
```

```
addresses of a and b: 4414272384 4414272384
```

```
b is: [5, 1, 7]
```

```
addresses of a and b: 4414272384 4414272384
```

```
b is: [3, 1, 7]
```

To our surprise, the first element’s replacement of a got also reflected in b. This should not be surprising since both a and b point to the same memory location and since a list is mutable, when we change an element in that memory location, it affects both a and b that are just names for that memory location.

Although the examples above used lists for illustration purposes, aliasing pertains to all mutable data types.

Aliasing is a powerful concept that can be hazardous and beneficial depending on the content:

- If you carelessly assign mutable variable to another variable, changes on one variable is going to reflect the other one. If this was not intended and the location in the code where the aliasing was initiated could not be identified, you may lose hours or days trying to identify what the problem is with your code.
- Aliasing can be beneficial especially when we want our changes on one variable to be reflected on another. This will be useful for passing data to functions and getting the results from functions.

2.4.3 Naming variables

Programmers usually select names for variables so that it indicates what the content will be. Variable names may be arbitrarily long. They may contain letters (from the English alphabet) as well as numbers and underscores, but they must start with a letter or an underscore. While using upper case letters is allowed, bear in mind that programmers reserve starting with an upper case to differentiate a property (scope) of the variable which you will learn later (when we introduce functions).

Here are a few examples for variable names (all are different):

y	y1	Y	Y_1	_1
te mperature	temperat ure_today	Tempera tureToday	C umulative	coo rdinate_x
alb145c	a 1_b1_45_c	s_s_	_	___

As you might have recognized, though they are perfectly valid, the five examples in the last line do not make much sense. Here is a short list that you should prefer to follow in variable naming:

- Name variables in the context of the value they are going to store. For example

```
>>> a = b * c
```

is syntactically correct, but its purpose is not evident. Contrast this with:

```
>>> salary = hours_worked * hourly_pay_rate
```

- Use different variables for different data, a.k.a. the ‘Single Responsibility Principle’. For example, even if you could use the same variable in a statement for counting and in another statement, for holding the largest grade, this is not recommended: Do not economise with variables. Devise two different variables where each of which will reflect the semantics and the context, uniquely.
- Variable names should be pronounceable, which makes them easier to remember.
- Do not use variable names which could misguide you or whoever look into your code.
- Use i,j,k,m,n for counting only: Programmers implicitly recognize them as integer holding (the historical reason for this dates to 60 years ago).
- Use x,y,z for coordinate values or multi-variate function arguments.
- Do not use single character variable l as it can be easily confused with 1 (one).
- If you are going to use multiple words for a variable, choose one of these:
 - Put all words into lowercase, affix them using _ as separator (e.g. highest_midterm_grade, shortest_path_distance_up_to_now).
 - Put all words but the first into first-capitalized-case, put the first one into lowercase, affix them without using any separator (e.g.highestMidtermGrade, shortestPathDistanceUpToNow).

Reserved names

The following keywords are being used by Python already and therefore, you cannot use them to name your variables.

and	def	exec	if	not	return
assert	del	finally	import	or	try
break	elif	for	in	pass	while
class	else	from	is	print	yield
continue	except	global	lambda	raise	

2.4.4 Other Basic Statements

Python has other basic statements listed below:

pass, del, return, yield, raise, break, continue, import, future, global, nonlocal.

Among these, we have seen del and we will see some others in the rest of the book.

print used to be a statement in version 2, which however changed in version 3: print is a function in version 3 and therefore, it has a value (which we will see later).

2.5 Compound Statements

Like other high-level languages, Python provides statements combining many statements as their parts. Two examples are:

- Conditional statements where different statements are executed based on the truth value of a condition, e.g.:

```
if <boolean-expression>:  
    statement-true-1  
    statement-true-2  
    ...  
else:  
    statement-false-1  
    statement-false-2  
    ...
```

- Repetitive statements where some statements are executed more than once depending on a condition or for a fixed number of times, e.g.:

```
while <boolean-condition>:  
    statement-true-1  
    statement-true-2  
    ...
```

which executes the statements while the condition is true.

We will see these and other forms of compound statements in the rest of the book.

2.6 Basic actions for interacting with the environment

In our programs, we frequently require obtaining some input from the user or displaying some data to the user. We can use the following for these purposes.

2.6.1 Actions for input

In Python, you can use the `input()` function for obtaining input from the user, e.g.:

```
>>> s = input("Now enter your text: ")  
Now enter your text: This is the text I entered  
>>> print(s)  
This is the text I entered
```

If you expect the user to enter an expression, you can evaluate it using the `eval()` function as we explained in Section 4.2.3.

2.6.2 Actions for output

For displaying data to the screen, Python provides the print() function:

```
print(item1, item2, ..., itemN)
```

For example:

```
>>> print('Python', 'is', 'so', 'fun')
Python is so fun
```

In many cases, we end up with strings that have placeholders for data items which we can fill in using a formatting function as follows:

```
>>> print("I am {0} tall, {1} years old and have {2} eyes".format(1.86, 20, "brown"))
I am 1.86 tall, 20 years old and have brown eyes
```

Alternatively, instead of using integers for the placeholders, we can give names to the placeholders:

```
>>> print("I am {height} tall, {age} years old and have {eyes} eyes. Did I tell you that I was {age}?" .format(age=20,
    ↴ eyes="brown", height=1.86))
I am 1.86 tall, 20 years old and have brown eyes. Did I tell you that I was 20?
```

The format() function provides much more functionalities than the ones we have illustrated. However, this extent should be sufficient for general uses and this book. The reader interested in a complete coverage is referred to the [Python's documentation on string formatting²¹](#).

We can also ask Python to directly take in the values of the variables for which we provide the names:

```
>>> age = 20
>>> height = 1.70
>>> eye_color = "brown"
>>> print(f'I am {height} tall, {age} years old and have {eye_color} eyes')
I am 1.7 tall, 20 years old and have brown eyes
```

2.7 Actions that are ignored

In Python, we have two actions that are ignored by the interpreter:

2.7.1 Comments

Like other high-level languages, Python provides programmers mechanisms for writing comments on their programs:

- Comments with #: When Python encounters # in your code, it ignores the rest of the line, assumes the current line is finished, evaluates & runs the current line and continues interpretation with the next line. For example:

²¹ <https://docs.python.org/3/library/string.html>

```
>>> 3 + 4 # We are adding two numbers here
```

```
7
```

- Multi-line comments with triple-quotes: If you wish to provide comments longer than one line, you can use triple quotes:

```
"""
This is a multi-line comment.
We are flexible with the number of lines &
characters,
spacing. Python
will ignore them.
"""
```

Triple-quote comments are generally used by programmers to write documentation-level explanations and descriptions for their codes. There are document-generation tools that process triple-quotes for automatically generating documents for codes.

As we have seen before, the triple-quote comments are actually strings in Python. Therefore, if you use triple-quotes for providing a comment, it should not overlap with an expression or statement line in your code.

2.7.2 Pass statements

Python provides the pass statement that is ignored by the interpreter. The pass statement is generally used in incomplete function implementations or compound statements to place a dummy holder (some instruction) such that the interpreter does not complain about a statement being missing. For example:

```
if <condition>:
    pass #@TODO fill this part
else:
    statement-1
    statement-2
    ...
```

2.8 Actions and data packaged in libraries

Many high-level programming languages like Python provide a wide spectrum of actions and data predefined and organized in ‘packages’ that we call libraries. For example, there is a library for mathematical functions and constant definitions which you can access using from math import * as follows:

```
>>> pi
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
NameError: name 'pi' is not defined
>>> sin(pi)
Traceback (most recent call last):
  File "<stdin>", line 1, in <module>
NameError: name 'sin' is not defined
>>> from math import *
```

(continues on next page)

```
>>> pi
3.141592653589793
>>> sin(pi)
1.2246467991473532e-16
```

Below is a short list of libraries that might be useful:

Library	Description
math	Mathematical functions and definitions
cmath	Mathematical functions and definitions for complex numbers
fractions	Rational numbers and arithmetic
random	Random number generation
statistics	Statistical functions
os	Operating system functionalities
time	Time access and conversion functionalities

Of course, the list is too wide and it is not practical to list and explain all libraries here. The interested reader is direct to to check [the comprehensive list at Python docs](#)²².

The import statement that we used above loads the library and makes its contents directly accessible to us by directly using their names (e.g. sin(pi)). Alternatively, we can do the following:

```
>>> import math
>>> math.sin(math.pi)
1.2246467991473532e-16
```

which requires us to specify the name math everytime we need to access something from it. We could also change the name:

```
>>> import math as m
>>> m.sin(m.pi)
1.2246467991473532e-16
```

However, we discourage this way of using libraries until Chapter 7 where we introduce the concept of objects and object-oriented programming.

However, to be able to learn what is available in a library, you can use this form (with dir() function):

```
>>> import math
>>> dir(math)
['__doc__', '__file__', '__loader__', '__name__', '__package__', '__spec__', 'acos', 'acosh', 'asin', 'asinh', 'atan', 'atan2',
 'atanh', 'ceil', 'comb', 'copysign', 'cos', 'cosh', 'degrees', 'dist', 'e', 'erf', 'erfc', 'exp', 'expm1', 'fabs', 'factorial', 'floor',
 'fmod', 'frexp', 'fsum', 'gamma', 'gcd', 'hypot', 'inf', 'isclose', 'isfinite', 'isinf', 'isnan', 'isqrt', 'ldexp', 'lgamma', 'log',
 'log10', 'log1p', 'log2', 'modf', 'nan', 'perm', 'pi', 'pow', 'prod', 'radians', 'remainder', 'sin', 'sinh', 'sqrt', 'tan', 'tanh', 'tau',
 'trunc']
```

²² <https://docs.python.org/3/library/>

2.9 Providing your actions to the interpreter

Python provides different mechanisms for you to provide your actions and get them executed.

2.9.1 Directly interacting with the interpreter

As we have seen up to now, we can interact with the interpreter directly by typing our actions to the interpreter. When you are done with the interpreter, you can quit using quit() or exit() functions or by pressing CTRL-D. E.g.:

```
$ python3
Python 3.8.5 (default, Jul 21 2020, 10:48:26)
[Clang 11.0.3 (clang-1103.0.32.62)] on darwin
Type "help", "copyright", "credits" or "license" for more information.
>>> print("Python is fun")
Python is fun
>>> print("Now I am done")
Now I am done
>>> quit()
$
```

where we see that after quitting the interpreter, we are back at the terminal shell.

Although this way of coding is simple and very interactive, when your code gets longer and more complicated, it becomes difficult to manage your code. Moreover, when you exit the interpreter, all your actions are lost and to be able to run them again, you need to type them again, from scratch. This can be tedious, redundant, impractical and inefficient.

2.9.2 Writing actions in a file (script)

Alternatively, we can place our actions in a file with an .py extension in the filename as follows:

```
print("This is a Python program that reads two numbers from the user, adds the numbers and prints the result\n\n")
[a, b] = input("Enter two numbers: ")
print("You have provided: ", a, b)
result = a + b
print("The sum is: ", result)
```

Assuming that you save these lines into a file named test.py, you can execute those statements from a terminal window as follows:

```
$ cat test.py
print("This is a Python program that reads two numbers from the user, adds the numbers and prints the result\n\n")
s = input("Enter a list of two numbers [a, b]: ")
[a, b] = eval(s)
print("You have provided: ", a, b)
result = a + b
print("The sum is: ", result)
$ python3 test.py
This is a Python program that reads two numbers from the user, adds the numbers and prints the result
```

(continues on next page)

```
Enter a list of two numbers [a, b]: [3, 4]
You have provided: 3 4
The sum is: 7
```

It is possible to provide command-line arguments to your script and use the provided values in your script (named test.py):

```
from sys import argv

print("The arguments of this script are:\n", argv)

exec(argv[1]) # Get a
exec(argv[2]) # Get b

print("The sum of a and b is: ", a+b)
```

which can be run as follows:

```
$ python3 test.py a=10 b=20
The arguments of this script are:
['test.py', 'a=10', 'b=20']
The sum of a and b is: 30
```

Note that this example used the function `exec()`, which executes the statement provided to the function as a string argument. Compare this with the `eval()` function that we have introduced before: `eval()` takes an expression whereas `exec()` takes a statement.

2.9.3 Writing your actions as libraries (modules)

Another mechanism for executing your actions is to place them into libraries (modules) and provide them to Python using `import` statement, as we have illustrated in Section 4.7. For example, if you have a `test.py` file with the following content:

```
a = 10
b = 8
sum = a + b
print("a + b with a =", a, " and b =", b, " is: ", sum)
```

In another Python script or in the interpreter, you can directly type:

```
>>> from test import *
a + b with a = 10 and b = 8 is: 18
>>> a
10
>>> b
8
```

In other words, what you have defined in `test.py` becomes accessible after being imported.

2.10 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter (all related to Python):

- Basic data types.
- Basic operations and expression evaluation.
- Precedence and associativity.
- Variables and how to name them.
- Aliasing problem.
- Container types.
- Accessing elements of a container type (indexing, negative indexing, slicing).
- Basic I/O.
- Commenting your codes.
- Using libraries.

2.11 Further Reading

- A detailed history of Python and its versions: https://en.wikipedia.org/wiki/History_of_Python
- The concept of aliasing: http://en.wikipedia.org/wiki/Aliasing_%28computing%29

Exercises

- Without using Python, determine the results of the following expressions and validate your answers with Python:
 - $2 - 3^{**} 4 / 8 + 2 * 4^{**} 5 * 1^{**} 8$
 - $4 + 2 - 10 / 2 * 4^{**} 2$
 - $3 / 3^{**} 3 * 3$
- Assuming that a is True, b is True and c is False, what would be the values of the following expressions?
 - (a) $\text{not } a == b + d < \text{not } a$
 - (b) $a == b <= c == \text{True}$
 - (c) $\text{True} <= \text{False} == b + c$
 - (d) $c / a / b$
- The Euclidean distance between two points (a, b) and (c, d) is defined as: $\sqrt{(a-c)^2 + (b-d)^2}$. Write a Python code that reads a, b, c, d from the user, calculates the Euclidean distance and prints the result.

3 | Conditional and Repetitive Execution

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Many circumstances require the execution to change its flow based on the truth value of a condition or to repeat a set of steps for a number of items or until a condition is not true any more. These two kinds of actions are very crucial components of programming solutions and Python provides several alternatives for them. As we are going to see in this chapter, some of these alternatives are compound statements, i.e. they include other statements as part of the statement, whereas others are expressions.

3.1 Conditional execution

Asking (mostly) mathematical questions that have Boolean type answers and taking some actions (or not) based on the Boolean answers are crucial tools in designing algorithms. This is so vital that there is no single programming language that does not provide conditional execution.

3.1.1 if statement

The syntax of the conditional (if) statement is

if *Boolean expression* : *Statement*

The semantics is obvious. If the *Boolean expression* evaluates to True, then the *Statement* is carried out; otherwise *Statement* is not executed.

```
>>> if 5 > 2: print("Hurray")
Hurray
>>> if 2 > 5: print("No I will not believe that !")
```

We observe that the Boolean expression in the last example evaluates to False and hence the statement with the print function is not carried out.

How to group statements?

It is quite often that we want to do more than one action instead of executing a single statement. As a general syntax rule of Python:

- switch to a new line,
- indent by one tab,
- write your first statement to be executed,

- switch to the next line,
- indent the same amount (usually your Python-aware editor will do it for you)
- write your second statement to be executed,
- and so on...
- To finish this writing task, and presumably enter a statement which is *not* part of the group action, just do not intend.

It is very very important that the statements that are part of the if part have the same amount and type of whitespace. E.g. if the first statement has 4 spaces, all following statements in the if statement need to start with 4 spaces. If it is a tab character, all following statements in the if statement need to start with a tab character. Since these whitespaces are not visible, it is very easy to make mistakes and get annoying errors from the interpreter. To avoid this, we strongly recommend you to choose a style of indentation (e.g. 4 whitespaces or a single tab) and stick to it as a programming style.

Here is an example:

```
>>> if 5 > 2:
...     print(7*6)
...     print("Hurray")
...     x = 6
42
Hurray
>>> print(x)
6
```

The >>> as well as ... prompts appear when you sit in front of the interpreter. When you type your programs into a file and then run them, of course they will not show up. If you type in these small programs (we call them *snippets*) just ignore the >>> and ... from the examples, as follows:

```
if 5 > 2:
    print(7*6)
    print("Hurray")
    x = 6
print(x)
```

```
42
Hurray
6
```

As you continue practicing programming, you will soon come across a need to be able to define actions that should be carried out in case a Boolean expression turns out to be False. If it were not provided, we would have to ask the same question again, but this time negated:

```
>>> if x == 6: print("still it is six")
>>> if not (x == 6): print("it is no more six")
```

One of them will certainly fire (be true). Although this is a feasible solution, there is a more convenient way: We can combine the two parts into one if-else statement with the following syntax:

if *Boolean expression* : *Statement*

else : **Statement**

Making use of the else part, the last example would be written as:

```
>>> if x == 6: print("still it is six")
... else: print("it is no more six")
```

Of course, using multiple statements in the if part or the else part is possible by indenting them to the same level.

Exercise

In the following code cell, you are expected to insert a couple of lines so that the output is always the absolute value of N (try the program for various values of N by altering the right-hand side of the assignment):

```
N = -100 # Feel free to change this to any numerical value #
# @TODO type in your code that changes the content of N to its absolute value, below this line
# @TODO print the result
```

3.1.2 Nested if statements

It is quite possible to nest if-else statements: i.e. combine multiple if-else statements within each other. There is no practical limit to the depth of nesting. This enables us to code a structure, called a *decision tree*. A decision tree is a set of binary questions & answers where at every case of an answer either a new question is asked or an action is carried out. Fig. 3.1.1 displays such a decision tree for *forecasting rain* based on the temperature, wind and air pressure values.

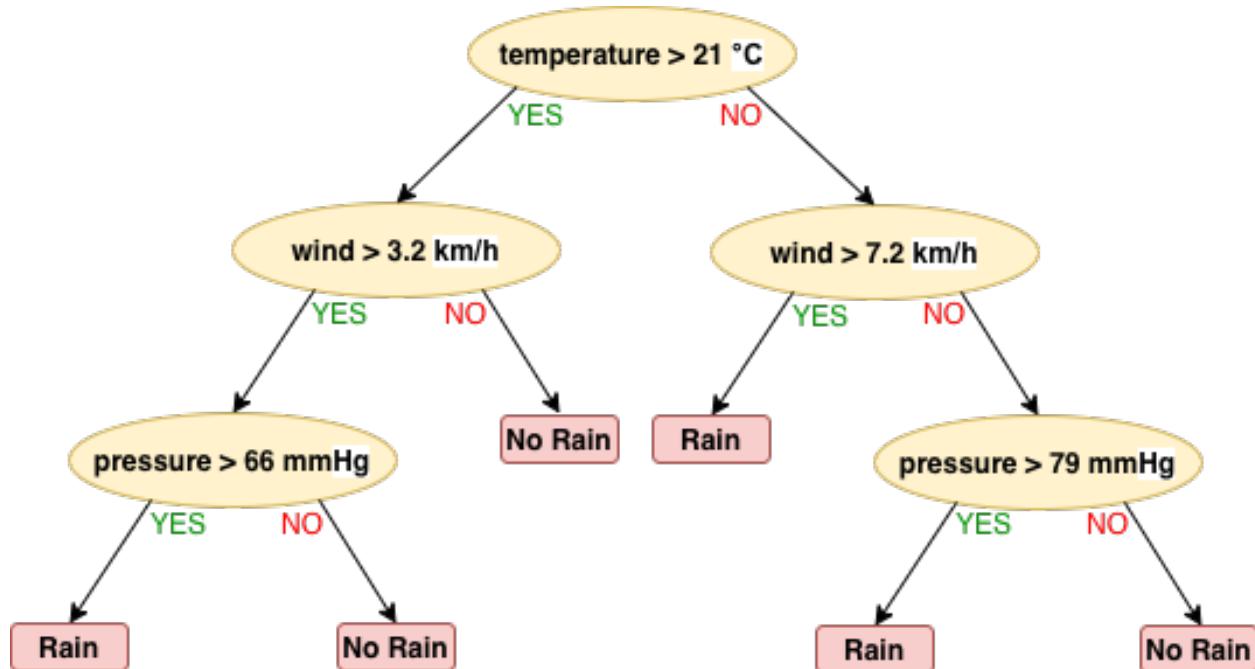


Fig. 3.1.1: An example decision tree.

The tree in Fig. 3.1.1 can be coded as nested if-else statements:

```
if temperature > 21:  
    if wind > 3.2:  
        if pressure > 66: rain = True  
        else: rain = False  
    else: rain = False  
else:  
    if wind > 7.2: rain = True  
    else:  
        if pressure > 79: rain = True  
        else: rain = False
```

Sometimes the else case contains another if which has an else of its own. And this ladder goes on. For such a case, elif serves as a combined keyword for the else if action, as follows:

```
if Boolean expression1 : Statement1  
elif Boolean expression2 : Statement2  
:  
elif Boolean expressionn : Statementn  
else : Statementotherwise
```

The flowchart in Fig. 3.1.2 explains the semantics of the if-elif-else combination.

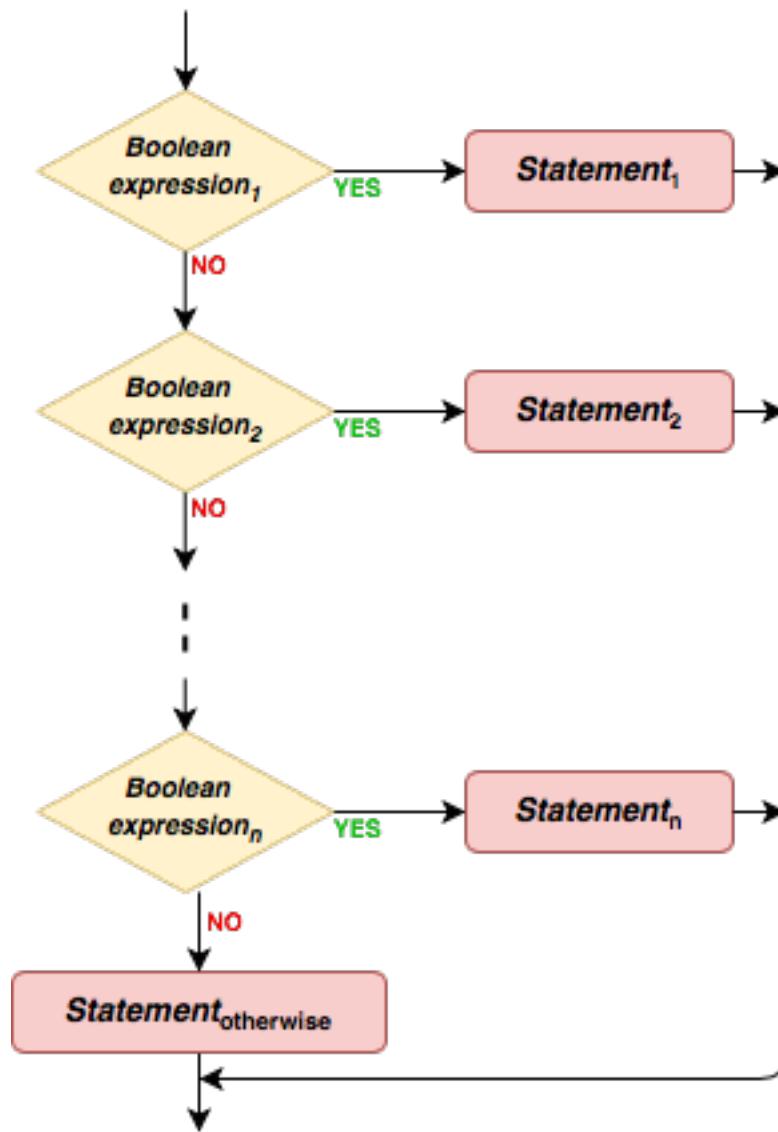


Fig. 3.1.2: The semantics of the if-elif-else combination.

There is no restriction on how many `elif` statements are used. Furthermore, the presence of the last statement (the `else`) is optional.

3.1.3 Practice

Let us assume that you have a value assigned to a variable x. Based on this value, a variable s is going to be set as:

$$s = \begin{cases} (x+1)^2, & x < 1 \\ x - 0.5, & 1 \leq x < 10 \\ \sqrt{x+0.5}, & 10 \leq x < 100 \\ 0, & otherwise \end{cases} \quad (3.1.1)$$

It is convenient to make use of an if-elif-else structure:

```
#@TODO Assign a value to x
```

```
x = 10
```

```
if x < 1: s = (x+1)**2
elif x < 10: s = x-0.5
elif x < 100: s = (x+0.5)**0.5
else: s = 0

print("s is: ", s)
```

```
s is: 3.24037034920393
```

3.1.4 Conditional expression

The if statement does not return a value. As said, that is so for all statements. They do not have a value of their own. A non-statement alternative that has a return value is the *conditional expression*.

It also uses the if and else keywords. This time if is not at the start of a statement, but following a value. Here is the syntax:

```
[expressionYES] if [Boolean expression] else [expressionNO]
```

This whole structure is an expression. It yields a value. So, it can be used in any place an expression is allowed to be used. It is evaluated as follows:

- First the *Boolean expression* is evaluated.
- If the outcome is True then *expression_{YES}* is evaluated and used as value (*expression_{NO}* is left untouched).
- If the outcome is False then *expression_{NO}* is evaluated and used as value (*expression_{YES}* is left untouched).

Though it is not compulsory, it is wise to use conditional expression enclosed in parenthesis to prevent wrong sub-expression groupings.

Let us look at an example:

```
>>> x = -34.1905
>>> y = (x if x > 0 else -x)**0.5
>>> print(y)
5.84726431761
```

As you have observed, y is assigned the value $\sqrt{|x|}$. For code readability, it is strongly advisable not to nest conditional expressions. Instead, restructure your coding into nested if-else statements (by making use of intermediate variables).

3.2 Repetitive execution

Repeating a sequence of instructions over-and-over is a programming ingredient which is used frequently. This action is called *iteration* or *loop*.

We use iteration

to systematically deal with all possible cases or all elements of a collection, or

to jump from one case to another as a function of the previous case.

The repetition of a sequence of instructions is carried out either for a known number of times or until a criterion is met.

Iteration examples:

- Computing letter grades of a class (Type I, for all students).
- Finding the shortest path from city A to city B in a map (Type II).
- Root finding by Newton-Raphson method (Type II).
- Finding darkest and brightest point(s) in a image (Type I, for all pixels).
- Computing a function value using Taylor's expansion (Type I).
- Computing the next move in a chess game (Type II).
- Obtaining the letter frequency of a text (Type I, for all letters).

Python provides two statements for iteration. Namely, while and for. for is used mostly for (Type I) iterations whereas while is used for both types.

3.2.1 while statement

The syntax of while resembles the synax of the if statement:

while *Boolean expression* : *Statement*

It is certainly possible to have a statement group subject to the while, as it was with the if statement. The semantics can be expressed as the flowchart in Fig. 3.2.1:

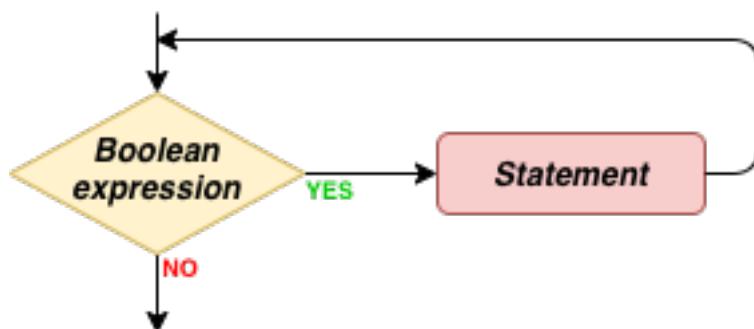


Fig. 3.2.1: The flowchart illustrating how a while statement is executed.

Later in this chapter, when we have introduced the for statement as well, we will consider some special statements (break and continue) that are allowed only under the scope of a while or for and are capable of altering the execution flow (to some limited extent).

Since a while statement is a statement, it can be part of another while statement (or any other compound statement):

```
while <condition-1>:  
    statement-1  
    statement-2  
    ...  
    while <condition-2>:  
        statement-inner-1  
        statement-inner-2  
        ...  
        statement-inner-M  
        ... # statements after the second while  
    statement-N
```

Of course, there is no practical limit on the nesting level.

Let us look at several examples below to illustrate these concepts.

3.2.2 Examples with while statement

Example 1: Finding Average of Numbers in a List

Let's say we have a list of numbers and we are asked to find their average. To make things easier to follow, let us start with the mathematical definition:

$$\text{avg}(L) = \frac{1}{N} \sum_{i=1}^N L_i, \quad (3.2.1)$$

where L_i is the i th number in the list which contains N numbers.

Let us see the algorithm before implementing a solution in Python (note that, in the equation, indexing started with 1 – compare this with the following):

Input: A **list** L that includes N numbers
Output: avg, which holds the average of numbers **in** L

Step 1: Initialize a **sum** variable **with** value 0
Step 2: Initialize an index variable, i, **with** value 0
Step 3: While i **is** less than N, Execute Steps 4-5
Step 4: sum = sum + L[i]
Step 5: i = i + 1
Step 6: avg = sum/N

Before we proceed with the Python implementation, make sure that you have understood the algorithm. The best way to make sure that is to take a pen & paper and go through each step while keeping a track of the variables, as if you are the computer.

Here is the implementation in Python:

```

# L: the list of numbers
#@TODO: Change the list and check if the code works
L = [10, -4, 4873, -18]
N = len(L)

sum = 0      # Step 1
i = 0       # Step 2

while i < N:    # Step 3
    sum = sum + L[i] # Step 4
    i = i + 1      # Step 5

avg = sum / N    # Step 6
print(avg)

```

1215.25

Have you noticed how close the Python code is to the algorithm? Python's principles for keeping things simple makes it so much easier to write that it can be very close to the pseudo-code.

Example 2: Standard Deviation

Now, let us look at a highly related problem, that of calculating the standard deviation. Standard deviation can be formally defined as follows:

$$\text{std}(L) = \sqrt{\frac{1}{N} \sum_{i=1}^N (L_i - \text{avg}(L))^2}. \quad (3.2.2)$$

The extension of the previous example is rather straightforward therefore but we will write it down nonetheless since these are your first iterative examples.

```

L = [10, 20, 30, 40]
N = len(L)

# CALCULATE THE AVG FIRST (COPY-PASTE FROM THE FIRST EXAMPLE)
sum = 0
i = 0

while i < N:
    sum = sum + L[i]
    i = i + 1

avg = sum / N

# CALCULATE THE STD NOW
sum = 0
i = 0

while i < N:
    sum = sum + (L[i] - avg)**2
    i = i + 1

std = (sum / N)**0.5

print("Avg & Std of the list are: ", avg, std)

```

Exercise

Write down the algorithm that we used in this Python code as a pseudo-code.

Example 3: Factorial Factorial of a number, denoted by $n!$, is an important mathematical construct that we frequently use while formulating our solutions. $n!$ can be defined formally as:

$$n! = \begin{cases} n \times (n - 1) \times \dots \times 2 \times 1, & \text{if } n > 0 \\ 1, & \text{if } n = 0. \end{cases} \quad (3.2.3)$$

Let us first write down the algorithm:

Input: n
Output: n_factorial

Step 1: If n is negative, n_factorial is 1. Return n_factorial and exit
 Step 2: Initialize n_factorial with 1
 Step 3: Initialize an index variable, i, with 1
 Step 4: While i \leq n, Execute Steps 4 an 5:
 Step 5: n_factorial = n_factorial * i
 Step 6: i = i + 1
 Step 7: The result is n_factorial

which can be implemented in Python as follows:

```
# Let us choose an n value:
n = 5

if n < 0: n_factorial = 1 # Step 1
elif n > 0:                # Steps 2-6
    n_factorial = 1         # Step 2
    i = 1                  # Step 3
    while i <= n:          # Step 4
        n_factorial *= i   # Step 5
        i += 1               # Step 6

print("n! is ", n_factorial)
```

n! is 120

Exercise

Modify our factorial implementation such that variable i starts from n.

Example 3: Computing Sine with Taylor Expansion

Let us assume we want to compute $\sin(x)$, for a given value of x , up to a given precision. This is just for the sake of having an understandable example. Actually today's CPUs have embedded math coprocessors that do this at microcode level. We will not use this convenience and do the computation ourselves.

The computation of many analytic functions are performed using the Taylor series expansion. The Taylor series expansion of $\sin(x)$ around zero is:

$$\sin(x) \approx x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} \dots, \quad (3.2.4)$$

which could also be written as:

$$\sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)!} x^{2k+1}. \quad (3.2.5)$$

Let us implement this. We will use the factorial example as a nested iteration. The outer iteration runs over the terms in the summation, and continues until a term becomes too small ($|term| < \epsilon$, where ϵ is a small value, e.g. 10^{-12}).

```
epsilon = 1.0E-12
x = 3.14159265359/4.0 # i.e. pi/4 (45 degrees in radians)
result = 0.0
k = 0
term = 2*epsilon #just a trick to bypass the first test
while abs(term) > epsilon:
    # Calculate the denominator - i.e. (2k+1)!
    factorial = 1
    while i <= 2*k+1:
        factorial *= i
        i += 1

    # Now calculate the term
    term = (((-1)**k) / factorial) * (x**((2*k)+1))

    result += term
    k += 1
```

This is a readable but at the same time quite an inefficient code:

- * $2*k+1$ is computed several times. Actually, do we need $2*k+1$ at all? *
- * It uses factorial computation which does not make use of its preceding computations. For example $9!$ is actually $9 \times 8 \times 7!$. But it is computed as $2 \times 3 \times 4 \times 5 \times 6 \times 7 \times 8 \times 9$. Therefore, there is significant inefficiency regarding the use of factorial in the nested iteration.
- * Similar to the inefficiency with the factorial computation, the computation of $x^{(n+2)}$ does not make use of the already computed x^n value.
- * Do we need to compute $(-1)^k$ to get an alternating sign? Can there be a simpler way to program this?

Let us investigate the proportionality of two consecutive terms ($k = n$) and ($k = n + 1$):

$$\frac{term_{n+1}}{term_n} = \frac{(-1)^{(n+1)} x^{2(n+1)+1}}{(2(n+1)+1)!} \times \frac{(2n+1)!}{(-1)^n x^{2n+1}} = \frac{-x^2}{(2n+2)(2n+3)}. \quad (3.2.6)$$

This is interesting because it suggests us a relatively faster way to compute the next term in the series. We do not have to compute x^n for each new term that we are going to add. We also discover that there is nothing magical about $(2n+1)$. It can simply be called as ($d \equiv 2n+1$) which increments by 2 for each consecutive term. Then we have

$$\frac{term_{n+1}}{term_n} = \frac{-x^2}{(d+1)(d+2)} \quad (3.2.7)$$

Now, let us see the more efficient implementation in action:

```

epsilon = 1.0E-12
x = 3.14159265359/4.0 # i.e. pi/4 (45 degrees in radians)
x_square = x*x
term = term
result = term
d = 1 # 2*n+1
while abs(term) > epsilon:
    term *= -x_square/((d+1)*(d+2))
    result += term
    d += 2

print("sin(x) [Ours] is: ", result)

# Compare this with the CPU-implemented version
from math import *
print("sin(x) [CPU ] is: ", sin(x))

```

```

sin(x) [Ours] is: 0.707106781186584
sin(x) [CPU ] is: 0.7071067811865841

```

3.2.3 for statement

The syntax of the for statement is:

for **Variable** in **Iterator** : **Statement**

An *iterator* is an object that provides a countable number of values on demand. It has an internal mechanism that responds to three requests:

1. Reset (initialize) it to the start.
2. Respond to the “Are we at the end?” question.
3. Provide the next value in line.

The for statement is a mechanism that allows traversing all values provided by an *Iterator*, one-by-one assigning them to a *Variable* and then executing a given *Statement*.

The semantics of the for statement is displayed in Fig. 3.2.2:

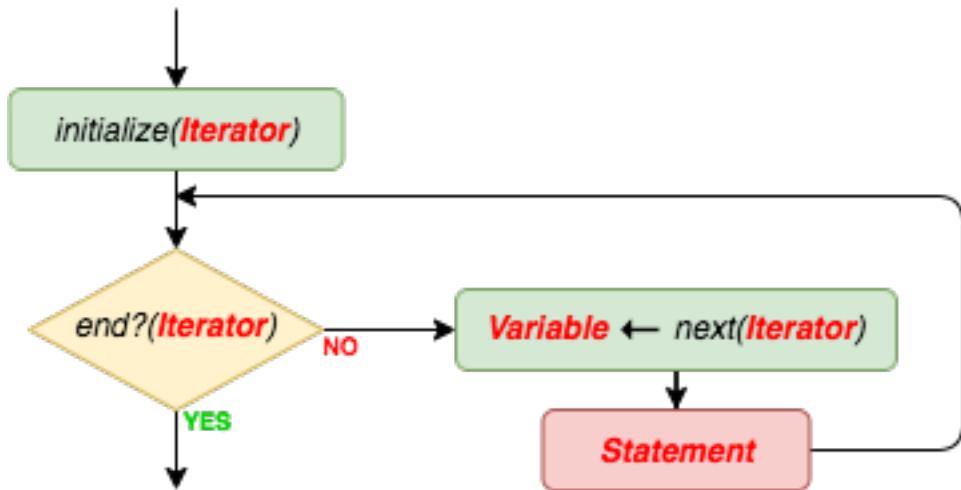


Fig. 3.2.2: The flowchart illustrating how a for statement is executed.

What iterators do we have?

1. All containers are also iterators (strings, lists, dictionaries, sets).
2. The built-in function range returns an iterator that generates a sequence of integers, starting from 0 (default), and increments by 1 (default), and stops before a given number:

`range(start, stop, step)`

Parameter	Opt./Req.	Default	Description
start	Optional	0	An integer specifying the start value.
stop	Required		An integer specifying the stop value (stop value will not be taken)
step	Optional	1	An integer specifying the incrementation.

3. A user-defined iterator. Since this is an introductory book, we will not cover how this is done.

3.2.4 Examples with for statement

Example 1: Words Starting with Vowels and Consonants

Let us split a list of words into two lists: those that start with a vowel and those that start with a consonant.

```

mixed = ["lorem", "ipsum", "dolor", "sit", "amet", "consectetur", "adipiscing", "elit", "sed", "do", "eiusmod", "tempor",
        "incididunt", "ut", "labore", "et", "dolore", "magna", "aliqua"]
vowels = []
consonants = []
for word in mixed:
    if word[0] in ['a', 'e', 'i', 'o', 'u']:
        vowels += [word]
    else:
        consonants += [word]

print("Starting with consonant:", consonants)
print("Starting with vowel:", vowels)

```

Starting with consonant: ['lorem', 'dolor', 'sit', 'consectetur', 'sed', 'do', 'tempor', 'labore', 'dolore', 'magna']
 Starting with vowel: ['ipsum', 'amet', 'adipiscing', 'elit', 'eiusmod', 'incididunt', 'ut', 'et', 'aliqua']

Exercise

Write this solution in pseudo-code.

Example 2: Run-length Encoding

Run-length encoding is a compression technique for data that repeats itself contiguously. Images bear such data: For example, a clear sky portion is actually rows of ‘blue’. In the example below, we investigate a string for consequent character occurrences: If found, repetitions are coded as a list of [character, repetition count].

So, a text of "aaaaaaxxxmyyyaaaasssssssttuivvvv" gets encoded as:

`[['a',6],['x',4],['m',1],['y',3],['a',4],['s',9],['t',3],['u',1],['v',4]].`

```
text = "aaaaaaxxxmyyyaaaasssssssttuivvvv"
code_list = []
last_character = text[0]
count = 1

# Go over each character except for the first
for curr_character in text[1:]:
    # If curr_character is equal to last_character, we found a duplicate
    if last_character == curr_character:
        count += 1
    else:
        # We have finished a sequence of same characters: Save the count and
        # reinitialize last_character and count accordingly
        code_list += [last_character if count==1 else [last_character, count]]
        count = 1
        last_character = curr_character

# handle the last_character here:
code_list += [last_character if count==1 else [last_character, count]]

print(code_list)
```

`[['a', 6], ['x', 4], 'm', ['y', 3], ['a', 4], ['s', 9], ['t', 3], 'u', 'i', ['v', 4]]`

Exercise

Modify this code such that it removes consecutive duplicate characters. In other words, "aaaabbbcd" should be reduced to "abcd".

Example 3: Permutations

Permutations are keys to shuffling a sequence of data. Permutations can be denoted in various forms. One way is to give an order list: The i^{th} element of the list stores the old position where the i^{th} element of the new sequence will come from. In our implementation counting starts from 0 (zero).

```
word_list = ["he", "came", "home", "late", "yesterday"]
permutation = [4,3,2,0,1]
length = len(permutation)
new_list = [None]*length
```

(continues on next page)

```

for i in range(length):
    new_list[i] = word_list[permutation[i]]

print(new_list)

```

```
[yesterday, 'late', 'home', 'he', 'came']
```

Example 4: List Split

In the example below the first element of the list is taken and the rest is split into two lists: Those that are smaller than the first element, and those that are not.

```

list_to_split = [42, 59, 53, 84, 43, 8, 75, 34, 40, 89, 29, 15, 51, 6, 90, 32, 58, 77, 4, 24]
list_smaller = []
list_not_smaller = []

for x in list_to_split[1:]:
    if x < list_to_split[0]: list_smaller += [x]
    else: list_not_smaller += [x]

print("list head was.      :", list_to_split[0])
print("smaller than head  :", list_smaller)
print("not smaller than head:", list_not_smaller)

```

```

list head was.      : 42
smaller than head  : [8, 34, 40, 29, 15, 6, 32, 4, 24]
not smaller than head : [59, 53, 84, 43, 75, 89, 51, 90, 58, 77]

```

Example 5: Dot Product

A frequently used operation with vectors is the dot product between two vectors, e.g. \mathbf{u} and \mathbf{v} :

$$\mathbf{u} \cdot \mathbf{v} = \sum_{i=1}^n u_i v_i, \quad (3.2.8)$$

where the vectors have n elements each. Let us implement this in Python:

```

# Define the vectors (as lists)
u = [1, 2, 4, 10]
v = [10, 4, 2, 1]
n = len(u)
dot_prod = 0

if n != len(v): print("Sizes don't match!")
else:
    for i in range(n):
        dot_prod += u[i] * v[i]
    print("u . v is: ", dot_prod)

```

```
u . v is: 36
```

Exercise

Implement dot product between two vectors using a while statement.

Example 6: Angle between Two Vectors

The angle between two vectors \mathbf{u} and \mathbf{v} is closely related to their dot product:

$$\mathbf{u} \cdot \mathbf{v} = \|\mathbf{u}\| \|\mathbf{v}\| \cos(\theta), \quad (3.2.9)$$

where θ is the angle between the vectors, and $\|\cdot\|$ denotes the norm of a vector:

$$\|\mathbf{u}\| = \sqrt{\mathbf{u} \cdot \mathbf{u}} = \sqrt{\sum_{i=1}^n u_i^2}. \quad (3.2.10)$$

The angle can be derived from these as follows:

$$\theta = \arccos \left(\frac{\mathbf{u} \cdot \mathbf{v}}{\|\mathbf{u}\| \|\mathbf{v}\|} \right). \quad (3.2.11)$$

Let us implement this:

```
from math import sqrt, acos

# Define two vectors that have 90deg (pi/2) between them
u = [1, 0, 0]
v = [0, 1, 0]
n = len(u)

if n != len(v):
    print("Sizes don't match!")

else:
    # Calculate dot product & norms
    dot_prod = u_norm_sum = v_norm_sum = 0
    for i in range(n):
        dot_prod += u[i] * v[i]
        u_norm_sum += u[i]**2
        v_norm_sum += v[i]**2

    u_norm = sqrt(u_norm_sum)
    v_norm = sqrt(v_norm_sum)

    theta = acos(dot_prod / u_norm * v_norm)

    print("angle between u and v is: ", theta)
```

angle between u and v is: 1.5707963267948966

Example 7: Matrix Multiplication

Our last example is matrix multiplication. As you know, a matrix A can be multiplied with the matrix B if the column-count (m) of A is equal to the row-count of B . The product matrix is of a size where row-count equals that of A and the column-count equals that of B .

$$(A \cdot B)_{ij} = \sum_{k=0}^{m-1} A_{ik} \cdot B_{kj}. \quad (3.2.12)$$

As we discussed in the previous chapter, since Python provides no two dimensional containers, but a very flexible list container, matrices are mostly represented as lists of lists each of which represent a row. For example, a 3×4 matrix:

$$\begin{pmatrix} -2 & 3 & 5 & -1 \\ 0 & 3 & 10 & -7 \\ 11 & 0 & 0 & -8 \end{pmatrix} \quad (3.2.13)$$

can be represented as:

```
A = [[-2,3,5,-1], [0,3,10,-7], [11,0,0,-8]]
```

This representation is also coherent with the indexing of matrices: A_{ij} is accessible in Python as $A[i][j]$. The code below multiplies two matrices, given in this representation, and prints the result.

```
A = [[-2,3,5,-1], [0,3,10,-7], [11,0,0,-8]]
B = [[2,1], [-1,1], [0,4], [8,0]]

# C = A*B

# Create a result matrix with entries filled with 0 (zeros)
C = []
for i in range(len(A)):
    C += [[0] * len(B[0])] # This is done to overcome the aliasing problem

for i in range(len(C)):
    for j in range(len(C[0])):
        for k in range(len(B)):
            C[i][j] += A[i][k]*B[k][j]

print(C)
```

```
[[[-15, 21], [-59, 43], [-42, 11]]]
```

3.2.5 continue and break statements

It is possible to alter the flow of execution in a while or for repetition. This is almost always used in combination with statement grouping, where a group of statements is subject to the while or for.

Let's assume you are executing a sequence of statements by means of statement grouping. Somewhere in the process, without waiting for the terminating condition to become False in a while statement or exhausting all items in the iterator in a for statement, you decide to terminate looping. The break statement does exactly serve this purpose: The while (or for) is stopped immediately and the execution continues with the statement after the while (or for).

Similarly, somewhere in the process you decide not to execute the rest of the statements in the grouping and straight away continue with the test. This is achieved by a continue statement usage. See Fig. 3.2.3 and Fig. 3.2.4 for how the continue statement changes the flow of execution.

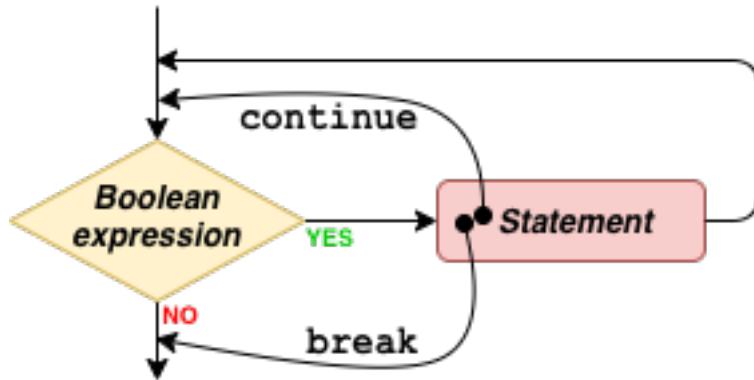


Fig. 3.2.3: How continue and break statements change execution in a while statement.

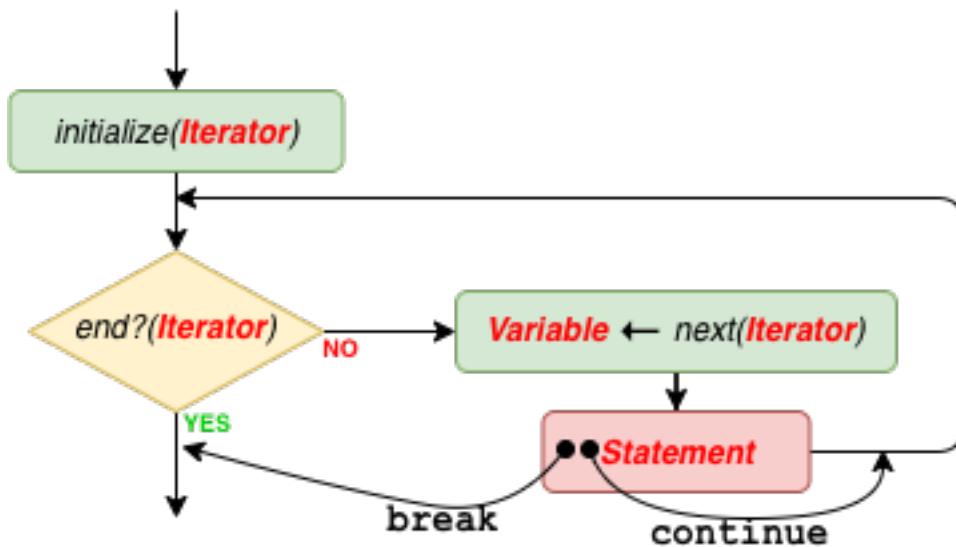


Fig. 3.2.4: How continue and break statements change execution in a while statement.

3.2.6 Set and list comprehension

A well-known and extensively-used notation to describe a set in mathematics is the so-called ‘set-builder notation’. This is also known as *set comprehension*. This notation has three parts (from left-to-right):

1. an expression in terms of a variable,
2. a colon or vertical bar separator, and
3. a logical predicate.

Something like this:

$$\{x^3 \mid x \in \{0, 1, \dots, 7\}\} \quad (3.2.14)$$

which defines the set:

$$\{0, 1, 8, 27, 64, 125, 216, 343\} \quad (3.2.15)$$

or as something more elaborate:

$$\{x^3 \mid x \in \{0, 1, \dots, 7\} \wedge (x \bmod 2) = 1\} \quad (3.2.16)$$

defining

$$\{1, 27, 125, 343\} \quad (3.2.17)$$

There exists a Python notation with the same semantics both for sets and lists:

```
>>> [x**3 for x in range(8)]
[0, 1, 8, 27, 64, 125, 216, 343]
>>> {x**3 for x in range(8)}
{0, 1, 64, 8, 343, 216, 27, 125}
```

The second example, which imposes a constraint on x to be an odd number, would be coded as:

```
>>> [x**3 for x in range(8) if x%2 == 1]
[1, 27, 125, 343]
>>> {x**3 for x in range(8) if x%2 == 1}
{1, 27, 125, 343}
```

Certainly the condition (following the if keyword) could have been constructed as a more complex boolean expression.

The expression that can appear to the left of the for keyword can be any Python expression and container. Here are a couple of more examples on matrices.

```
print( [[0 for i in range(3)] for j in range(4)] )
print( [[1 if i==j else 0 for i in range(3)] for j in range(3)] )
print( [[(i,j) for i in range(3)] for j in range(4)] )
print( [[(i+j)%2 for i in range(3)] for j in range(4)] )
print( [[i+3*j for i in range(3)] for j in range(4)] )
```

```
[[0, 0, 0], [0, 0, 0], [0, 0, 0], [0, 0, 0]]
[[1, 0, 0], [0, 1, 0], [0, 0, 1]]
[((0, 0), (1, 0), (2, 0)), ((0, 1), (1, 1), (2, 1)), ((0, 2), (1, 2), (2, 2)), ((0, 3), (1, 3), (2, 3))]
[[0, 1, 0], [1, 0, 1], [0, 1, 0], [1, 0, 1]]
[[0, 1, 2], [3, 4, 5], [6, 7, 8], [9, 10, 11]]
```

3.3 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- Conditional execution with if, if-else, if-elif-else statements.
- Nested if statements.
- Conditional expression as a form of conditional computation in an expression.
- Repetitive execution with while and for statements.
- Changing the flow of iterations with break and continue statements.
- Set and list comprehension as a form of iterative computation in an expression.

3.4 Further Reading

- “Managing the size of a problem”, Chapter 4 of “Introduction to Programming Concepts with Case Studies in Python”: https://link.springer.com/chapter/10.1007/978-3-7091-1343-1_4

Exercises

We have provided many exercises throughout the chapter, please study and answer them as well.

- Implement the while statement examples in Section 5.2.2 using for statement:
- Calculating the average of a list of numbers.
- Calculating the standard deviation of a list of numbers.
- Calculating the factorial of a number.
- Taylor series expansion of $\sin(x)$.
- Implement the for statement examples in Section 5.2.4 using while statement:
- Words with vowels and consonants.
- Run-length encoding.
- Permutation.
- List split.
- Matrix multiplication.
- What does the variable `c` hold after executing the following Python code?

```
c = list("address")
for i in range(0, 6):
    if c[i] == c[i+1]:
        for j in range(i, 6):
            c[j] = c[j+1]
```

- Write a Python code that removes duplicate items in a list. E.g. [12, 3, 4, 12] should be changed to [12, 3, 4]. The order of items should not change.
- Write a Python code that replaces a nested list of numbers with the average of the numbers. E.g. [[1, 3], [4, 5, 6], 7, [10, 20]] should yield [2, 5, 7, 15].
- Write a Python code that finds all integers dividing a given integer without a remainder. E.g. for number 21, your code should compute [1, 3, 7].
- Write a Python code that converts an integer (less than 128) into binary string using a for/while statement. E.g. 21 should be represented as 00010101.
- Write a Python code that converts a binary string like 00010101 into integer.

4 | Functions

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A *function* (or sometimes synonymously referred to as subroutine, procedure or sub-program) is a grouping of actions under a given name that performs a specific task. `len()`, `print()`, `abs()`, `type()` are functions that we have seen before. Python adopts a syntax that resembles mathematical functions.

A function, i.e. ‘named’ pieces of code, can receive parameters. These parameters are variables that carry information from the “calling point” (e.g. when you write `N = len("The number of chars")`) to the callee, i.e. the piece of code that *defined* the function (`len()` in our example). The life span of these variables (parameters) is as long as the function is active (for that call).

4.1 Why define functions?

There are four main reasons for using functions while developing solutions with a programming language:

1- Reusability

A function is defined at a single point in a program but it can be called from several different points. Assume you need to calculate the run-length encoding of a string (the example code from the previous chapter) in your program for n different strings in different positions of your code. In a programming language without functions, you would have to copy-paste that code piece in n different places. Thanks to functions, we can place the code piece in a function once (named `encodeRunLen` for example) and use it in n places via simple function calls like `enc = encodeRunLen(inpstr)`.

If functions would not be present, even if we would have the piece of code that does the actions of the function, how would we return to the different calling points after the actions are completed? Something, that is theoretically possible but extremely painful.

2- Maintenance

Using functions makes it easier to make updates to the algorithm. Let us explain this with the run-length encoding example: Assume that we found a bug in our calculation or we have discovered a better algorithm than the one we are using. Without functions, you would need to go through all your code, find the locations where your run-length encoding algorithm is implemented, and update each and every one of them. This is impractical and very tedious. With functions, it is sufficient if you just change the function that implements the run-length encoding.

3- Structuredness

Let us have a look at a perfectly valid Python expression:

```
(b if b<c else c) if (a if a<b else b)<(b if b<c else c) else (a if a<b else b)
```

which certainly takes some time to parse and understand but it just performs the following:

```
max(min(a,b), min(b,c))
```

Assume instead of the long expression above, the one with min and max are used. Even if the definition of max and min are not given yet, still one can grasp what the expression is up to. It is not only because the expression is smaller, but because function naming can depict the meaning for the actions.

4- Benefits of the functional programming paradigm

If a programmer sticks to the functional paradigm, then he or she has to plot a functional decomposition so that the solution of the problem is obtained by means of functional composition, something that is well-known and understood through Mathematics. This type of a solution does not suffer from unexpected side effects or variable alterations; therefore, testing and debugging are easier. Another benefit of the functional paradigm is recursion: In other words, while defining a function, we can call the function that is being defined – we will cover this seemingly confusing concept below. Moreover, we can define higher-order functions that take functions as input and apply them to a sequence of data. All these benefits come free with using functions, as we will illustrate below.

Even when we do not limit ourselves to ‘functional programming’, it is essential to use functions in professional programming. General algorithms that are coded as functions are becoming very valuable because they can be reused again and again in new programs. Collections formed by such general purpose functions are called *libraries*. For almost all application areas libraries have been created over decades.

4.2 Defining functions

For defining a function, Python adopts the following syntax:

```
def FunctionName (Parameter1, Parameter2, ...): Statement
```

The *Statement*, which can be replaced by multiple statements like we did with other compound statements, can make use of the *Parameter_i*s to obtain the actual arguments sent to the function at call-time. If the function is going to give a value in return to the call, this value is provided by a return statement.

FunctionName is the name of the function being defined. Python follows the same naming rules and conventions used for naming variables – if you do not remember them, we recommend you to go back and check the restrictions for naming variables in Chapter 4.

Here is a straightforward example. Let us assume that we want to implement the following function:

$$F_{\text{gravity}}(m_1, m_2, r) = G \frac{m_1 m_2}{r^2}. \quad (4.2.1)$$

The following is the one-line Python code that defines it:

```
def F_gravity(m_1, m_2, r): return G * m_1 * m_2 / (r * r)
```

This function, *F_gravity*, returns a value. This is provided by the return statement. As you may have observed, the values *m₁*, *m₂* and *r* are provided as the first, the second and the third parameters, named as *m₁*, *m₂* and *r*, respectively.

But what about G? It is not provided in the arguments and used in the return expression for its value. If the definition were a multi-statement definition (indented multi-statements following the def line), then Python would seek for a defined value for G among them. But this is not even the case, so the last alternative is to seek a value in the global environment, the environment in which F_gravity is called.

Therefore, before we call F_gravity, we must make sure that a value for a global variable G (which apparently is the *Gravitational Constant*) is set. In the **Scope of Variables** section, we will be handling the rules of this to a greater extent.

```
def F_gravity(m1, m2, r): return G * m1 * m2 / (r * r)
```

```
G = 6.67408E-11
print(F_gravity(1000, 20, 0.5), "Newton")
```

```
5.339264000000006e-06 Newton
```

4.3 Passing parameters to functions

When a function is called, first its arguments are evaluated. The function will receive the results of these evaluations. The parameter variables used in the definition are created, and set to the result of the argument evaluations. Then the statement that follows the column (:) after the argument parenthesis is executed. Certainly this statement can and will make use of the parameter variables (which are set to the result of the argument evaluations).

Let us look at an example:

```
def F_gravity(m_1, m_2, r): return G * m_1 * m_2 / (r * r)
```

```
G = 6.67408E-11
```

```
S = 100
```

```
Q = 2000
```

```
print(F_gravity(Q+S, Q-S, ((504.3-66.1)**2+(351.1-7.7)**2)**0.5))
```

```
8.59177215925003e-10
```

This is a legitimate piece of code that performs the following in order:

- Defines the function F_gravity.
- Sets the value of the global variable G and S and Q
- Calls the (internally defined) print function which receives one argument. This argument is a function call to F_gravity. So, in order to have a value to print, this function call has to be performed.
- A call to F_gravity is prepared: It has three arguments, each has to be evaluated and boiled down to a value. So, in a left-to-right order the arguments are evaluated:
 - Q+S is evaluated, and the result is stored into m_1.
 - Q-S is evaluated, and the result is stored into m_2.
 - Euclidean distance, $\sqrt{(504.3-66.1)^2+(351.1-7.7)^2}$, is evaluated and the result is stored into r.

- Since all arguments are evaluated, the statement defining the function `F_gravity` can be executed.
- This statement is return $G * m_1 * m_2 / (r * r)$, which requires the expression following the `return` keyword to be evaluated and the result to be returned as the result of the function call.
- Now the `print` function has got its parameter evaluated. The defining action of the `print` function can be carried out (This is an internally defined function, i.e. we cannot see its definition, but the documents defining the language explain it).

The bottom line is: Before the function is called, there is a preparation phase where all arguments are evaluated and hence converted to a value. This has a name in computer science and is coined as *Call-by-value*.

4.3.1 Default Parameters

While defining a function, we can provide default values to parameters as follows:

```
def FunctionName (Parameter1 = Exp1, Parameter2 = Exp2, ...): Statement
```

where *Exp_i* is an expression. When calling the function, we may omit providing the parameters for which the function has default values.

Let us have a look at a simple example:

```
def norm(x1, x2, norm_type="L1", verbose=True):
    result = None
    if norm_type == "L1": result = abs(x1) + abs(x2)
    elif norm_type == "L2": result = (x1**2 + x2**2)**0.5
    elif verbose: print("Norm not known:", norm_type)

    if verbose: print(f"The {norm_type} norm of", [x1, x2], "is:", result)
    return result

norm(3, 4)                      # CASE 1
norm(3, 4, "L2")                # CASE 2
norm(3, 4, norm_type="L2")       # CASE 3
norm(3, 4, verbose=False)        # CASE 4: Does not print the value
norm(3, 4, verbose=True, norm_type="L1")  # CASE 5
norm(x2=3, x1=4, verbose=True, norm_type="L1") # CASE 6
```

```
The L1 norm of [3, 4] is: 7
The L2 norm of [3, 4] is: 5.0
The L2 norm of [3, 4] is: 5.0
The L1 norm of [3, 4] is: 7
The L1 norm of [4, 3] is: 7
```

7

```
# Let us look at some cases that lead to errors:
>>> norm(3, 4, norm_type="L1", True)      # CASE 7
File "<ipython-input-19-128dc3e43256>", line 2
    norm(3, 4, norm_type="L1", True)      # CASE 7
                                         ^
SyntaxError: positional argument follows keyword argument
```

In this example, you should notice the following crucial points:

- We can call a function without providing any value for the parameters that have default values (CASE 1, .., CASE 5).
- We can swap the order of default parameters when we are calling the function (CASE 5 and CASE 6).
- When calling a function, we can give values to non-default parameters by using their names (CASE 6).
- The parameters after the default parameters need to be given names as well, both while defining the function and calling the function (CASE 7).

4.4 Scope of variables

We extensively use variables while programming our solutions. Not all variables are accessible from everywhere. There is a governing set of rules for that determine which parts of a code can access a variable. The code part from which a variable is accessible is called its *scope*.

In Python, there are four categories of scopes. As will be explained shortly, they are abbreviated with their initials , which then combine to form the rule mnemonic LEGB standing for:

[*L*ocal < *E*nclosing < *G*lobal < *B*uilt-in]

1- Local Scope

Defining a variable in a function in Python makes it local.

Local variables are the most ‘private’ ones. Any code which is external to that function cannot see it. If you make an assignment anywhere in the function to a variable, it is registered as a local variable. If you attempt to refer to such a local variable prior to the assignment, Python will generate a run-time error.

The local variables are created each time the function is called (it is activated) and are annihilated (destructed) the moment the function returns (finishes).

2- Enclosing Scope

As we mentioned before, it is possible to define functions inside functions. They are coined as *local functions* and can refer (but not change) to the values of the local variables of its parent function (the function in which the local function is defined). The scope of the outer function is the enclosing scope for the inner function. Though the parent function’s variables are visible to the local function, the converse is not true. The parent function cannot access its local function’s local variables. Therefore, the accessibility is from inward to outward and for referring purposes only.

3- Global Scope

If a variable is not defined in a function then it is a *global variable*. It can be accessed outside as well as inside of any function. If a global variable is accessed inside a function, it cannot be altered there. If it is altered anywhere in the function, this is recognised at the declaration-time and that variable is declared (created) as a local variable. A local variable that has the same name with a global variable conceals the global variable.

If you want to change the value of a global variable inside a function, then you have to explicitly declare it as a global variable by a statement:

global *Variable*

Then an assignment to *Variable* will not register it as a local variable but merely refer to the global *Variable*. As said, since the system will recognize them automatically, there is no need to use the global statement for global variables which are referred to for their values only. However, it is a good programming habit to do so in order to enhance readability and prevent accidental local variable creations (due to careless assignments to global variables).

4- Built-in Scope

Built-in scope is a special Python scope that is created or loaded whenever you run a script or open an interactive session. This is actually the scope in which the Python interpreter starts. It contains names such as keywords, built-in functions, exceptions, and some other attributes. Entities in this scope are also available from everywhere in your code.

An Interactive Example for Scope

Please follow the Colab link at the top of the page for an interactive demo on scope of variables.

A variable occurrence has different meanings for different positions in the program:

1. First time occurrence of the variable at the left-hand side of an assignment:

This tells Python to declare a variable in the current scope, the current function or the global scope. If there is a variable with the same name in an outer scope, it is hidden as long as the new variable is active. This declaration will be active for the scope it is created in including statements preceding it.

2. Second and later occurrences of the variable at the left-hand side of an assignment:

They simply update the previously declared variable.

3. Occurrences of the variable at the right-hand side of an assignment or any other place in an expression:

Python places value (content) of the variable in the expression position. Variable is searched in all scopes from inner to outer (local, then enclosing, then global, then built-in) and the first found variable is used. If the declaration of the variable is after its reference in current scope, Python will raise the error 'Reference before assignment'.

Note that global declaration changes the behaviour above. It makes all occurrences to refer to the global variable and does not declare a variable in the current scope with the globally defined names.

4.5 Higher-order functions

Python provides several flavours of the functional paradigm, one of the most powerful of which is the ability to easily pass functions as parameters to other functions. No special syntax or rule is used for this: If you use a parameter as if it is a function and when calling the higher-order function, pass a function name as a parameter, Python will handle the rest.

Python provides two very practical higher-order functions for us:

- **map** function: The map function has the following syntax:

```
map(function, Iterator)
```

which yields an iterator where each element is function being applied on the corresponding element in Iterator. Here is a simple example:

```
>>> abs_it = map(abs, [10, -4, 20, -100])
>>> for x in abs_it: print(x)
10
4
20
100
```

- **filter** function: The filter function has a similar syntax to the map function:
`filter(predicate, Iterator)`
where predicate is a function with a boolean return value. The filter function applies predicate to each element of the Iterator and only keeps the ones for which predicate returns True. For example:

```
>>> def positive(x): return x > 0
>>> for x in filter(positive, [10, -4, 20, -100]): print(x)
10
20
```

Of course, the functional capabilities of Python is more diverse than we can cover in this introductory textbook. The reader is referred to [Python docs²³](#). The curious reader is especially recommended to look at *lambda expressions* and the *reduce* function.

4.6 Functions in programming vs. functions in Mathematics

It is to be noted that functions have a differentiated meaning compared to functions in Mathematics.

- In Mathematics, a function is a mapping from a domain to a range (target); a function returns a value.
In Python: Functions may not return a value at all. If so, they are intended to code a parametrized action. A few examples to this are:
 - Drawing a *red* line from (x_0, y_0) to (x_1, y_1) .
 - Printing a separating line made of n ‘minus’ signs.
 - Turning off the lights.
 - Sending a digital initialization string to a device connected through the USB port.
- In Mathematics, a function definition is global. You do not have function definitions local to some function.
In Python: Since a function definition is done by a Python *Statement* (or a group of statements – grouped by indentation), it is quite possible to have another definition as part of the defining statements. Such a function can only be usable in the *Statement* group that defines the outer function and access its local variables and parameters. Outside of the function, this interior function (called a *local function*) will not be visible nor usable.
- In Mathematics, an element from the domain is mapped to one and only one target element by the function. The mapping does not change. Moreover, a mathematical function returns a value that only depends on the arguments. Hence, for the same arguments, the result is the same.

²³ <https://docs.python.org/3/howto/functional.html>

In Python: Even if such a mapping exists (i.e. a function returns a value), it is possible that the function acts differently due to different settings of the variables (outside of the function) that can be accessed in the functions. Consider the F_gravity function above: A different setting for the G (the Gravitational Constant) will yield a different F_gravity result even when the parameters are the same.

- In Mathematics, a function's operation is reflected on the value it returns: It does not have side effects. In other words, a mathematical function does not change the mathematical environment that is external to it (variables or the ways other functions are evaluated).

In Python: This may not be true. Consider the G value of the F_gravity function above. Hypothetically, it is possible that, at each call of F_gravity, the G value is increased slightly (1% for example):

```
>>> def F_gravity(m1, m2, r):
...     global G      # since we alter it
...     G = 1.01 * G
...     return G * m1 * m2 / (r * r)

>>> G = 6.67408E-11

>>> print(F_gravity(1000, 20, 0.5), "Newton")
5.39265664e-06 Newton

>>> print(F_gravity(1000, 20, 0.5), "Newton")
5.4465832064e-06 Newton

>>> print(F_gravity(1000, 20, 0.5), "Newton")
5.501049038464e-06 Newton
```

In these aspects, a function defined in Python has a greater freedom. As previously stated, there are paradigms of programming. One of these paradigms, the *functional paradigm*, promotes the function's usage to be restricted to the mathematical sense. In other words, the *functional paradigm* followers deliberately renounce the additional freedom programming languages like Python provides in function definitions and usages with respect to the mathematical sense. As a rule-of-thumb we can say that deviating from the mathematical sense makes your programming error prone.

4.7 Recursion

Recursion is a function definition technique in which the definition makes use of calls to the function being defined. Although it is difficult to grasp, it allows compact and more readable code for recursive algorithms, relations or mathematical functions.

It is customary to give the infamous example of the recursive definition of factorial. First, let us put it down in mathematical terms:

$$\begin{aligned} N! &= (N - 1)! \times N, & \text{for } N \in \mathbb{N}, \quad N > 0 \\ 0! &= 1, \end{aligned}$$

Based on this, we can realize that:

- 6! is $6 \times 5!$
- 5! is $5 \times 4!$
- 4! is $4 \times 3!$
- 3! is $3 \times 2!$

- $2!$ is $2 \times 1!$
- $1!$ is $1 \times 0!$
- $0!$ is 1

Substituting any factorial value, based on this rule, one ends up with

$$6! = 6 \times 5 \times 4 \times 3 \times 2 \times 1 \times 1. \quad (4.7.1)$$

Making use of $(N - 1)!$ while we are defining $N!$ is making a recursive definition. The Python equivalent of the above given recursive mathematical definition of the factorial would be:

```
def factorial(N):
    if N == 0: return 1
    else: return N * factorial(N-1)
```

High-level languages are designed so that each call to the factorial function does not remember any previous call(s) even if they are still active (unfinished). For every new call, fresh positions for all local variables are created in the memory without forgetting the former values of variables for the unfinished calls.

From the programmers point of view, the only concern is the algorithmic answer to the question:

“Having the recursive call returned the correct answer to the smaller problem, how can I cook up the answer to the actual problem?”

It requires a kind of ‘stop thinking’ (leap of faith) action: ‘Stop thinking how the recursive call comes up with the correct answer’. Just concentrate on the next step paraphrased in the quotation above.

Not to get into an infinite, non-stopping recursive loop, you should be careful about two aspects:

1. The recursive call should be made with a decrescent (getting smaller) argument. In the factorial example, calculation of $N!$ recursively called $(N - 1)!$, i.e. a smaller value than $N!$.
2. The function definition must start with a test for the smallest possible argument case (in the factorial example, this was 0 (zero)) where a value for this case is directly returned (in the factorial example this was 1 (one)). This is called the termination or base condition.

Let us consider another example: We have a list of unordered numbers. Nothing is pre-known about the magnitude of the numbers. The problem is to find the maximum of the numbers in that list.

Let us say you are given a list of, say, 900 numbers. For a second, assume that you have a very loving grandpa. Your grandpa has a rule of his own: not to corrupt you, he will not solve the problem for you but, if you reduce the problem slightly, his heart softens and provides the answer for the smaller problem.

Presumably, the simplest ‘reduction’ that you can do on a 900-element list is removing an element from it and making it a list of 899 numbers. As far as Python lists are concerned, the simplest of the simple is to remove the first element: If L is your list, $L[0]$ is the first element and $L[1:]$ is the list of remaining elements. So, the trick is to remove the first element, take $L[1:]$ to your grandpa (that is making the recursive call), and ask for the solution. Your grandpa is very cooperative and gives you the solution (the biggest number) for the list ($L[1:]$) you passed to him.

However, we are not finished: On one hand you have what your grandpa returned to you as the biggest number of the slightly reduced list ($L[1:]$), and on the other hand, you have the removed (first) element $L[0]$. Now, which one will you return as the solution of the 900 number list? Think about it!

Here is the solution in Python:

```

def find_max(L):
    if len(L) == 1: return L[0] # Terminating condition
    else:
        grandpa_result = find_max(L[1:]) #recursion is on L with the 0th element removed
        if grandpa_result > L[0]: return grandpa_result
        else: return L[0]

# Let's try with a simple list -- try changing M and check the result
M = [-100, 10, -10, 100]
print("The maximum element of M is:", find_max(M))

```

The maximum element of M is: 100

As you may have recognized, the definition started with testing for the smallest case. That is a single element list for which the result (the biggest number in the list) is that single number itself.

Recursion helps writing elegant functions. However, it does not come for free. The price is in the time and memory overhead spent on creating a new function call. Time may be something tolerable but memory is limited. For functions that make thousands of recursive calls, you should better seek algorithmic solutions that do not lean on recursion. Python has a default for recursion depth, which is set to 1000. This can be altered. As said, it is better to seek a non-recursive solution unless you know very well of what you are doing.

Any recursive function can be implemented using iterations. The reverse is also true: Any iterative function can be implemented using recursion. The definition of the problem or the algorithm generally provides hints for whether recursion or iteration is better for implementing your solution.

4.8 Function Examples

Example 1: Computing average and standard-deviation

In the previous chapter, we provided iterative definitions for calculating the average and the standard-deviation of a list of numbers. Let us look at these definitions again with functions. For the sake of ease, the mathematical definitions are provided again. Moreover, we will use this opportunity to talk more about iterations as well.

Average of a set (S) of numbers is calculated by dividing the sum of the values in the set by their number. So, if we have a set S :

$$avg(S) = \frac{1}{|S|} \sum_{x \in S} x, \quad (4.8.1)$$

which can be coded as:

```

def avg(S):
    sum = 0.0
    for x in S: sum += x
    return sum/len(S)

S = [11, 2, 9, 6]
print("The avg of S:", avg(S))

```

The avg of S: 7.0

This is quite elegant. As you see it works at a higher abstraction level. This can be done because the `in` operator comes in very handy and when used as an iterator, it iterates over the elements of the list.

Sometimes it is more desirable to work with the indices to reach out to each element. Remember that indexing of container elements start at zero. So, a more index-based formulation of the same formula would be:

$$\text{avg}(S) = \frac{1}{|S|} \sum_{i=0}^{|S|-1} S_i \quad (4.8.2)$$

The following implements this definition:

```
def avg(S):
    sum = 0.0
    for i in range(0, len(S)):
        sum += S[i]
    return sum/len(S)

S = [11, 2, 9, 6]
print("The avg of S:", avg(S))
```

This is almost okay but not perfect. `len` is a built-in function that returns the element count of any container (string, list, tuple). As you have observed `len(S)` is calculated twice. This is inefficient. Function calls have a price, time-wise and space-wise and unnecessary calls should be avoided. To fix this, we change the code to do computation once and store the result for further usages.

```
def avg(S):
    sum = 0.0
    length = len(S)
    for i in range(0, length):
        sum += S[i]
    return sum/length

S = [11, 2, 9, 6]
print("The avg of S:", avg(S))
```

The avg of S: 7.0

`sum`, `length`, `i` and the parameter `S` are all local variables of the function `avg`. In contrary to many other programming languages, in Python we do not have to declare locals. They are automatically recognized. This comes in very handy.

One point to note about the code is that the $|S| - 1$ is missing. It is not necessary because the range iterator excludes the end value, as we discussed in the previous chapter.

Now let us also introduce the code for standard deviation. First the mathematical definition:

$$\text{std}(S) = \sqrt{\frac{1}{|S|} \sum_{i=0}^{|S|-1} (S_i - \text{avg}(S))^2} \quad (4.8.3)$$

This time we bear in mind that unnecessary function calls should be avoided:

```
def avg(S):
    sum = 0.0
    length = len(S)
    for i in range(0, length): sum += S[i]
    return sum/length

def std(S):
    sum = 0.0
    length = len(S)
    average = avg(S)
    for i in range(0, length): sum += (S[i] - average)**2
    return (sum/length)**0.5

S = [11, 2, 9, 6]
print("The avg of S:", avg(S))
print("The std of S:", std(S))
```

```
The avg of S: 7.0
The std of S: 3.391164991562634
```

We gave the solution in terms of explicit indexing. As given below this particular problem can be coded without an iteration over indices. Such problems are rare. Problems that require operations over vectors and matrices or problems that aim optimizations usually require explicit index iterations.

For sake of completeness we state the index-less solution of the average and standard-deviation problem:

```
def avg(S):
    sum = 0.0
    length = len(S)
    for x in S: sum += x
    return sum/length

def std(S):
    sum = 0.0
    length = len(S)
    average = avg(S)
    for x in S: sum += (x - average)**2
    return (sum/length)**0.5

S = [11, 2, 9, 6]
print("The avg of S:", avg(S))
print("The std of S:", std(S))
```

```
The avg of S: 7.0
The std of S: 3.391164991562634
```

Example 2: Computing check digit

A Standard Definition from Wikipedia²⁴:

“A *check digit* is a form of redundancy check used for error detection on identification numbers, such as bank account numbers, which are used in an application where they will at least

²⁴ https://en.wikipedia.org/wiki/Check_digit

sometimes be input manually. It consists of one or more digits computed by an algorithm from the other digits (or letters) in the sequence input.

With a check digit, one can detect simple errors in the input of a series of characters (usually digits) such as a single mistyped digit or some permutations of two successive digits.”

Middle East Technical University, our university, also implements a check digit algorithm for student numbers. A student number has exactly six digits. The algorithm to generate the checkdigit is as follows:

- $sum \leftarrow 0$
- For each digit in the student number (the leftmost digit is the named as the ‘first’) that has an odd position (first, third, fifth), take the digit and add it to the sum .
- For each digit in the student number that has an even position (second, forth, sixth) take twice the digit. If this result of doubling is a two digit number, then add each of these digits to the sum , otherwise add the result of the doubling (which is a single digit number itself) to the sum .
- The one digit number, which when added to the sum results in a multiple of 10, is the check digit.

Take as example the student number **167912**:

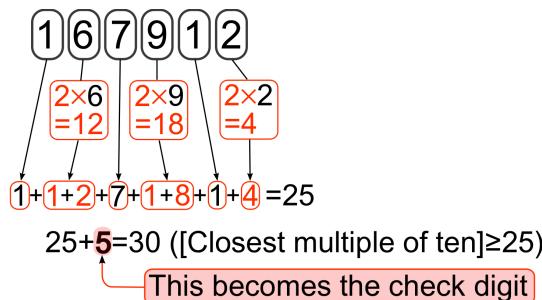


Fig. 4.8.1: How checksum is calculated for a student number.

The check digit of the student number **167912** is found to be **5**. As you all well know, this is written as **167912-5**. That is called the *student-id*.

Below you will find the code that computes the checkdigit for a student number, given as a string. We encourage you to investigate it. A very good technique to understand how a code progresses when it runs is to insert print statements to points of interest. You can start by inserting:

```
print(digit, sum)
```

right after the line of else: (left-aligned with the else).

```
def checksum(S):
    sum = 0
    for i in range(0, len(S)):
        digit = int(S[i])
        if i%2 == 0: sum += digit
        else: sum += (9 if digit==9 else (2*digit) % 9)
    n = sum % 10
    return 0 if n == 0 else 10 - n

print(checksum("167912"))
```

A few notes about the code:

- Remember indexing starts in Python at zero. One group of digits, namely (first, third, fifth) are actually at S[0], S[2] and S[4]. Their indices are **even**. Or in mathematical terms, they are (modulo 2) zero.
- Summing the digits of a number is a trick we learned in primary school. It is actually nothing else but a quick way to do (modulo 9). So, we are actually taking the (modulo 9) of the doubled digit. With one exception: If the digit is 9, the double is 18 where we have to add a $1+8=9$ to the sum. But $(18 \% 9)$ would give us zero (not 9). So, here we have to insert an exception: For all digits except 9, we can use $(2*\text{digit}) \% 9$. For 9, we ought to add a 9 to the sum.
- The rule of constructing the check digit from the sum has a similar exception case for sum being a multiple of 10 (i.e. $n \pmod{10} = 0$). In that case we would have a checkdigit of 10 (because $10-0 = 10$) which is not a digit, but two digits. The designers decided to use a zero as the checkdigit for this particular case.

Now let us see how the checkdigit can be used to recover a missing digit of the student id.

Let us assume you have a student ID as: 1□9503-7. Now, can we discover what the (□) digit is?

For this purpose we will write a function `find_q_mark()` that will take a string as an argument, in which the missing digit is indicated by a (?) (question mark). We are expecting that a call of `find_q_mark("1?9503-7")` will recover the missing digit and return the demystified string: "169503-7".

(The ``checksum()`` definition of above is still effective)

```
# places digit in the place of '?' in the string S
def replace_q_mark(S, digit):
    new_S =""
    for c in S: new_S += str(digit) if c=="?" else c
    return new_S

# finds the value for the position with '?'
def find_q_mark(MissingStdID):      # MissingStdID is something like "1?7912-5"
    six_digit_string = MissingStdID[:6] # "1?7912"
    checksum_digit = int(MissingStdID[7])
    for missing_digit in range(0, 10):
        candidate = replace_q_mark(six_digit_string, missing_digit)
        if checksum(candidate) == checksum_digit: return candidate + MissingStdID[6:]

print(find_q_mark("1?7912-5"))
```

167912-5

A few notes about the code: * `replace_q_mark()` function is called by `find_q_mark()`. It is only called once, therefore its actions could have been migrated into `find_q_mark()`. Efficiency-wise there would be no change. But separating it out, making it into a function and naming it accordingly makes the code more readable.

- The first two lines that define `find_q_mark()` actions are merely dissecting the string into a student-id and a checkdigit part.
- What we do in the for loop in `find_q_mark()` (on Lines 11-13) is coined in Computer Science as *brute force*. Practically, it is trying every possible case for being a solution. In this problem, the (?) mark

can be any digit in the range [0,9]. The for loop tries each of these possibilities out until the computed checksum becomes the same as the checkdigit appearing in the input string.

Example 3: Sequential Search

Searching an item in a list or any other container is a frequently performed operation required while solving world problems. For the sake of simplicity, let us just focus on situations where only numbers are involved; i.e. the searched item is a number and the list includes only numbers. Extension to other data types is trivial.

In a search problem, we have a query item (let's call it x) and a list of items (let's call it L). If x is a member of L , then we want the search algorithm to return True, optionally by returning its index in L . If x is not a member of L , we expect the algorithm to return False.

Consider the example list below:

109	-48	25	4	-13
-----	-----	----	---	-----

(4.8.4)

If x is 4, the search algorithm should return True. If it is 5, the answer should be False.

Let us start with the simplest algorithm we can use: Sequential Search. In sequential search, we start with the beginning of the list, go over each item in the list and check if the query is equal to any item that we go over. Here is the algorithm:

Algorithm: Sequential Search **with** While Iterations

Input: x -- the query number

L -- the list of numbers

Output: **True (if x is in L) or False (if x is not in L)**

Step 1: Create a variable named Index **with** initial value 0

Step 2: Create a variable named N **with** value length(L)

Step 3: While Index < N **is True**, execute Steps 3 and 4:

Step 4: If x **is** equal to $L[Index]$, then **return True** as the result

Step 5: Index = Index + 1

Step 6: Return **False** as the result

Let us implement this simple algorithm in Python:

```
# Sequential Search with while statement
def seq_search(x, L):
    index = 0          # Step 1
    N = len(L)         # Step 2
    while index < N:   # Step 3
        if x == L[index]: return True # Step 4
        index = index + 1      # Step 5
    return False        # Step 6

# Now let us test the function with examples:
L = [109, -48, 25, 4, -13]
x = 4
print(f"seq_search({x}, {L}): ", seq_search(x, L))
x = 5
print(f"seq_search({x}, {L}): ", seq_search(x, L))
x = 5
L = []
print(f"seq_search({x}, {L}): ", seq_search(x, L))
```

```

seq_search(4, [109, -48, 25, 4, -13]): True
seq_search(5, [109, -48, 25, 4, -13]): False
seq_search(5, []): False

```

That looks nice. However, we can have a more compact solution using for loops:

```

# Sequential Search with for statement
def seq_search(x, L):
    for y in L:
        if x == y: return True
    return False

# Now let us test the function with examples:
L = [109, -48, 25, 4, -13]
x = 4
print(f"seq_search({x}, {L}): ", seq_search(x, L))
x = 5
print(f"seq_search({x}, {L}): ", seq_search(x, L))
x = 5
L = []
print(f"seq_search({x}, {L}): ", seq_search(x, L))

```

```

seq_search(4, [109, -48, 25, 4, -13]): True
seq_search(5, [109, -48, 25, 4, -13]): False
seq_search(5, []): False

```

That's the beauty of Python. These two are iterative solutions. Let us have a look at a recursive solution. First, let us have a look at the algorithm. The idea is essentially the same: We compare with the first item and return True if they match. Otherwise, we continue our search with the remaining items.

Algorithm: Sequential Search **with** Recursion

Input: x -- the query number
 L -- the list of numbers
 Output: **True** (**if x is in L**) or **False** (**if x is not in L**)

Step 1: If L is empty, **return False**
 Step 2: If x is equal to the first item of L (L[0]), **return True**
 Step 3: Make a recursive call on L[1:N], **and return** its answer

And here is the implementation in Python:

```

# Sequential Search with recursion
def seq_search(x, L):
    if L == []: return False    # Step 1: We have exhausted the list, x was not found
    if x == L[0]: return True    # Step 2: x was at the beginning of the list, yay!
    return seq_search(x, L[1:]) # Step 3: Search in the remaining items since x != L[0]

# Now let us test the function with examples:
L = [109, -48, 25, 4, -13]
x = 4
print(f"seq_search({x}, {L}): ", seq_search(x, L))
x = 5

```

(continues on next page)

```
print(f"seq_search({x}, {L}): ", seq_search(x, L))
x = 5
L = []
print(f"seq_search({x}, {L}): ", seq_search(x, L))
```

```
seq_search(4, [109, -48, 25, 4, -13]): True
seq_search(5, [109, -48, 25, 4, -13]): False
seq_search(5, []): False
```

Exercise

Write down the pseudocode for the Python function `seq_search` with `for` statement.

Exercise

Extend the *recursive* implementation of `seq_search` to search for an item `x` in a list `L` in cases where `L` can be nested. In other words, the extended search algorithm shoud return True for:

```
seq_search_nested(5, [10, [4, [5]], -84, [3]])
```

and False for:

```
seq_search_nested(8, [10, [4, [5]], -84, [3]])
```

Example 4: Binary Search

If the list of items (numbers in our case) is not sorted, sequential search is the only option for searching for an item. If, however, the numbers are sorted (in an increasing or decreasing order), then we have a much more efficient algorithm called binary search.

Assuming that `L`, our list of numbers, is sorted in an increasing order: In binary search, we make our first comparison with the number that is at the center (middle) of the list. If the middle number is equal to `x`, then we obviously return True. Otherwise, we compare `x` with the middle number: If `x` is smaller, then it has to be to the left of the middle number – we can continue our search on the left part of `L`. If, on the other hand, `x` is larger than the middle number, it has to be on the right side of the middle number – we can continue our search on the right part of `L`. This is illustrated in the following figure.

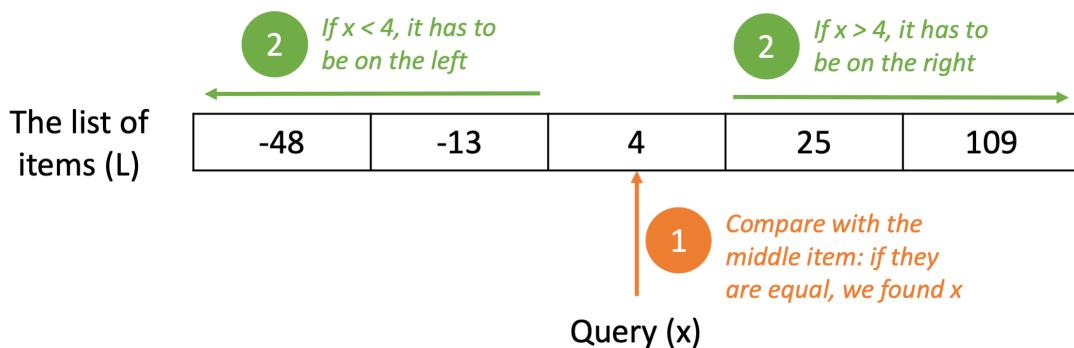


Fig. 4.8.2: Binary search algorithm.

Here is the pseudocode that describes this algorithm:

Algorithm: Binary Search **with** Recursion

Input: x -- the query number

L -- the list of numbers

Output: **True** (if x is in L) or **False** (if x is not in L)

Step 1: If $\text{length}(L)$ is zero then **return False** since the list is empty

Step 2: Create a variable Mid_index with value $\text{length}(L)/2$

Step 3: If $\text{length}(L)$ is 1 then **return False** since the only item in L is not equal to x

Step 4: If $x < L[\text{Mid_index}]$ then make recursive call with $L[0:\text{Mid_index}]$ and return its answer

Step 5: Otherwise ($x > L[\text{Mid_index}]$) then make a recursive call with $L[\text{Mid_index}+1:]$ and return its answer

The following is the implementation in Python:

```
# Binary search with recursion
def bin_search(x, L):
    if len(L) == 0: return False # Step 1: Terminating condition
    Mid_index = len(L) // 2 # Step 2: Uses integer division
    if x == L[Mid_index]: return True # Step 3
    if x < L[Mid_index]: return bin_search(x, L[0:Mid_index]) # Step 4
    if x > L[Mid_index]: return bin_search(x, L[Mid_index+1:]) # Step 5: Can drop if statement

# Now let us test the function with examples:
L = [-48, -13, 4, 25, 109]
x = 4
print(f"bin_search({x}, {L}): ", bin_search(x, L))
x = 5
print(f"bin_search({x}, {L}): ", bin_search(x, L))
x = []
print(f"bin_search({x}, {L}): ", bin_search(x, L))
```

```
bin_search(4, [-48, -13, 4, 25, 109]): True
bin_search(5, [-48, -13, 4, 25, 109]): False
bin_search([], []): False
```

Exercise

Implement binary search using while statements.

Exercise

Identify the complexity of sequential search and binary search in the following cases:

- Best case: When the item that we are making our first comparison with is the one we were looking for.
- Worst case: The item we are looking for is the last item with which we performed the comparison.
- Average case.

Example 5: Sorting

Sorting pertains to ordering a list of items (L) so that each item in L satisfies the following constraint:

$$L_i < L_{i+1}, \quad (4.8.5)$$

which leads to an ascending (increasing) order of items in L and this is called *ascending sort*. If the order of the constraint is changed to $L_i > L_{i+1}$, the outcome is a descending (decreasing) order of items in L and this is called *descending sort*.

An algorithm that can perform ascending sort can easily be changed to descending sort; therefore, we will just focus on one of them, namely, ascending sort. Moreover, we will focus on sorting a list of numbers; however, the same algorithms can be applied on other data types as long as an ordering constraint ($<$ or $>$) can be defined.

Bubble Sort

Let us have a look at a very simple though inefficient sorting algorithm, called *Bubble Sort*. In Bubble Sort, we start from the beginning of the list and check whether the constraint $L_i < L_{i+1}$ is violated for an i value. If it is, we swap L_i with L_{i+1} . When we hit the end of the list, we start from the beginning of the list again and continue checking the constraint $L_i < L_{i+1}$. Once at the end of the list, we again go back to the beginning and continue checking the constraint for each i . This continues until no i value violates the constraint $L_i < L_{i+1}$, which means that the numbers are sorted.

Therefore, in Bubble Sort, we have two loops, one outer loop that continues until all numbers are sorted and an inner loop that goes through the list and checks the constraint. Here is a pseudo-code for this:

Algorithm: Bubble Sort

Input: L -- the list of numbers (not sorted)

Output: L -- the sorted list of numbers (ascending order)

Step 1: Create a variable Is_sorted with value **False**

Step 2: Create a variable N with value $\text{length}(L)$

Step 3: Create a variable Index

Step 4: While Is_sorted is **False**, repeat Steps 5-11:

Step 5: Set Is_sorted to **True**

Step 6: Set Index to zero

Step 7: While $\text{Index} < (N-1)$, repeat Steps 8-11

Step 8: If $L[\text{Index}] > L[\text{Index}+1]$, then execute Steps 9 & 10:

Step 9: Swap $L[\text{Index}]$ and $L[\text{Index}+1]$

Step 10: Set Is_sorted to **False**

Step 11: $\text{Index} = \text{Index} + 1$

Step 12: **return** L

One outer iteration of the algorithm is illustrated on a small list of numbers below:

1

The first iteration of the outer loop: start from the beginning and check the constraint at every position

1

109	-13	25	-48	25
-----	-----	----	-----	----

Index=0

*Constraint not satisfied:
Swap 109 and -13;
Increment Index*

2

-13	109	25	-48	25
-----	-----	----	-----	----

Index=1

*Constraint not satisfied:
Swap 109 and 25;
Increment Index*

3

-13	25	109	-48	25
-----	----	-----	-----	----

Index=2

*Constraint not satisfied:
Swap 109 and -48;
Increment Index*

4

-13	25	-48	109	25
-----	----	-----	-----	----

Index=3

*Constraint not satisfied:
Swap 109 and 25;
Increment Index*

*The condition $\text{Index} < (N-1)$ is not True anymore, the inner loop finishes.
Execution continues with the outer loop.*

2

The second iteration of the outer loop: start from the beginning and check the constraint at every position

1

-13	25	-48	25	109
-----	----	-----	----	-----

Index=0

...

...

Fig. 4.8.3: One outer iteration of the Bubble Sort algorithm.

With one outer iteration, the list appears to be one step closer to a sorted list. In the example above, the largest number has found its correct place after one outer iteration. With a second one, the second largest number will find its place. With a third iteration, the third largest number will find its place etc.

And here is the implementation in Python:

```
# Bubble Sort

def bubble_sort(L):
    Is_sorted = False                      # Step 1
    N = len(L)                            # Step 2
    Index = 0                             # Step 3: Can be removed in Python

    while Is_sorted is False:              # Step 4
        Is_sorted = True                  # Step 5
        Index = 0                         # Step 6
        while Index < (N-1):             # Step 7
            if L[Index] > L[Index+1]:      # Step 8
                (L[Index], L[Index+1]) = (L[Index+1], L[Index]) # Step 9
            Is_sorted = False            # Step 10
            Index = Index + 1           # Step 11
    return L                             # Step 12

# Let us test our implementation with some sample lists
L = [109, -13, 4, -48, 25]
print(f"bubble_sort({L}): ", bubble_sort(L))

L = [-48, -13, 4, 25, 109]
print(f"bubble_sort({L}): ", bubble_sort(L))

L = []
print(f"bubble_sort({L}): ", bubble_sort(L))
```

```
bubble_sort([109, -13, 4, -48, 25]): [-48, -13, 4, 25, 109]
bubble_sort([-48, -13, 4, 25, 109]): [-48, -13, 4, 25, 109]
bubble_sort([]): []
```

4.9 Programming Style

With the topics covered in this chapter, we started working with longer and more elaborated Python codes. Up to now, we have introduced crucial aspects that can be arranged differently among programmers:

- Naming variables and functions.
- Indentation.
- Function definition.
- Commenting.

Longing for brevity and readability, the creators of Python have defined some guidelines of style for those interested: [Python Style Guide²⁵](https://www.python.org/dev/peps/pep-0008/).

²⁵ <https://www.python.org/dev/peps/pep-0008/>

There are alternative styles and we strongly recommend you to choose one and stick to it as a programming style.

4.10 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter (all related to Python):

- Defining functions.
- Function parameters and how to pass values to functions.
- Default parameters.
- Scopes of variables.
- Local, enclosing, global and built-in scopes.
- Higher-order functions.
- Differences of functions between programming and Mathematics.
- Recursion.

4.11 Further Reading

- Functional tools of Python: <https://docs.python.org/3/howto/functional.html>
- A more comprehensive coverage on recursion: https://link.springer.com/chapter/10.1007/978-3-7091-1343-1_4
- Python style guide: <https://www.python.org/dev/peps/pep-0008/>

Exercises

- Write a Python function named `only_numbers()` that removes items in a list that are not numbers. E.g. `only_numbers([10, "ali", [20], True, 4])` should return `[10, 4]`. Implement two versions: One using iteration and another using recursion.
- Write a Python function named `flatten()` that removes nesting in a nested list and lists all elements in a single non-nested list. E.g. `flatten([1, [4, 5, [6]], [["test"]]])` should return `[1, 4, 5, 6, "test"]`.
- Write a Python function named `reverse()` that reverses the order of elements in a list. E.g. `reverse([10, 5, 0])` should return `[0, 5, 10]`. Implement two versions: One using iteration and another using recursion.
- Write a Python function named `greatest_divisor()` that finds the greatest divisor of an integer. The greatest divisor of an integer n is an integer $x < n$ that satisfies $n = k \cdot x$ for some integer k . E.g. `greatest_divisor(12)` should return `6`.

5 | A Gentle Introduction to Object-Oriented Programming

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At this stage of programming, you must have realized that programming possesses some idiosyncrasies:

- Unless a randomization is explicitly build in, all computations are deterministic; i.e., the result is always the same for the same input.
- The logic involved is binary; i.e., two truth values exist: True and False.
- There is a clear distinction of *actions* and *data*. Actions are coded into expressions, statements and functions. Data is coded into integers, floating points and containers (strings, tuples and lists).

The first two can be dealt with in a controlled manner. Furthermore, mostly it is very much preferred to have a crisp and deterministic outcome. But, the third is not so natural. The world we live in is not made of data and independent actions acting on that data. This is merely an abstraction. The need for this abstraction stems from the very nature of the computing device mankind has manufactured, the von Neumann Machine. What you store in the *memory* is either some data (integer or floating point) or some instruction. The *processor* processes the data based on a series of instructions. Therefore, we have a clear separation of data and action in computers.

But when we look around, we don't see such a distinction. We see *objects*. We see a tree, a house, a table, a computer, a notebook, a pencil, a lecturer and a student. Objects have some properties which would be quantified as data, but they also have some capabilities that would correspond to some actions. What about reuniting data and action under the natural concept of "object"? *Object Oriented Programming*, abbreviated as OOP, is the answer to this question.

5.1 Properties of Object-Oriented Programming

OOP is a paradigm that comes with some properties:

- *Encapsulation*: Combining data and functions that manipulate that data under a concept that we name as 'object' so that a rule of "need-to-know" and "maximal-privacy" is satisfied.
- *Inheritance*: Defining an object and then using it to create "descendant" objects so that the descendant objects inherit all functions and data of their ancestors.
- *Polymorphism*: A mechanism allowing a descendant object to appear and function like its ancestor object when necessary.

5.1.1 Encapsulation

Encapsulation is the property that data and actions are glued together in a data-action structure called ‘object’ that conforms to a rule of “need-to-know” and “maximal-privacy”. In other words, an object should provide access only to data and actions that are needed by other objects and other data & actions that are not needed should be hidden and used by the object itself for its own merit.

This is important especially to keep implementation modular and manageable: An object stores some data and implements certain actions. Some of these are private and hidden from other objects whereas others are *public* to other objects so that they can access such public data and actions to suit their needs.

The public data and actions function as the interface of the object to the outside world. In this way, objects interact with each other’s interfaces by accessing public data and actions. This can be considered as a message passing mechanism: Object1 calls Object2’s action f, which calls Object3’s function g, which returns a message (a value) back to Object2, which, after some calculation returns another value to Object 1. As a realistic example of a university registration system, assume Student object calls register action of a Course object and it calls checkPrerequisite action of a Curriculum object. checkPrerequisite checks if course can be taken by student and returns the result. register action does additional controls and returns the success status of the registration to the Student.

In this modular approach, Object1 does not need to know how Object2 implements its actions or how it stores data. All Object1 needs to know is the public interface via which ‘messages’ are passed to compute the solution.

Assume you need to implement a simple weather forecasting system. This hypothetical system gets a set of meteorological sensor data like humidity, pressure, temperature from various levels of atmosphere and try to estimate the weather conditions for the next couple of days. The data of such a system may have a time series of sensor values. The actions of such system would be a group of functions adding sensor data as they are measured and forecasting functions for getting the future estimate of weather conditions. For example:

```
sensors = [{"datetime":'20201011 10:00','temperature':12.3,
    'humidity': 32.2, 'pressure':1.2,
    'altitute':1010.0},
    {"datetime":'20201011 12:00','temperature':14.2,
    'humidity': 31.2, 'pressure':1.22,
    'altitute':1010.0},
    ...]

def addSensorData(sensorarr, temp, hum, press, alt):
    """Add sensor data to sensor array with
    current time and date"""

    ...

def estimate(sensorarr, offset):
    """return whether forecast for given
    offset days in future"""

    ...

addSensorData(sensors, 20.3, 15.4, 0.82, 10000)
...
print(estimate(sensors, 1))
..."
```

In the implementation above, the data and actions are separated. The programmer should maintain the list containing the data and make sure actions are available and called as needed with the correct data. This

approach has a couple of disadvantages:

1. There is no way to make sure actions are called with the correct sensor data format and values (i.e. estimate('Hello world', 1,1,1,1)).
2. addSensorData can make sure that sensor list contains correct data, however, since sensors data can be directly modified, its integrity can be violated later on (i.e. sensors[0]='Hello World').
3. When you need to have forecast of more than one location, you need to duplicate all data and maintain them separately. Keeping track of which list contains which location requires extra special care.
4. When you need to improve your code and change data representation like storing each sensor type on a separate sorted list by time, you need to change the action functions. However, if some code directly accesses the sensor data, it may conflict with the changes you made on data representation. For example, if the new data representation is as follows:

```
sensors = {'temperature': [('202010101000', 23), ...],  
          'humidity': [('2020101000', 45.3), ...],  
          'pressure': [('2020100243', 1.02), ...]}
```

Any access to sensors[0] as a dictionary directly by code segments will be incorrect.

With encapsulation, sensor data and actions are put into the same body of definition so that the only way to interact with the data would be through the actions. In this way:

1. Data and actions maintained together. Encapsulation mechanism guarantees that data exists and it has correct format and values.
2. Multiple instances can be created for forecasting for multiple locations, and each location is maintained in its object as if it was a simple variable.
3. Since no code part accesses the data directly but calls the actions, changing internal representation and implementation of functions will not cause any problem.

The following is an example OOP implementation for the problem at hand:

```
class WhetherForecast:  
    # Data  
    __sensors = None  
  
    # Actions acting on the data  
    def __init__(self):  
        self.__sensors = [] # this will create initial sensor data  
  
    def addSensorData(self, temp, hum, press, alt):  
        ....  
  
    def estimate(self, offset):  
        ....  
        return {'lowest':elow, 'highest':ehigh,...}  
  
ankara = WhetherForecast() # Create an instance for location Ankara  
ankara.addSensorData(...)  
....  
  
izmir = WhetherForecast() # Create an instance for location Izmir
```

(continues on next page)

```

izmir.addSensordata(...)

....
```

```

print(ankara.estimate(1)) # Work with the data for Ankara
print(izmir.estimate(2)) # Work with the data for Izmir
```

The above syntax will be more clear in the following sections; however, please note how the newly created objects ankara and izmir behave. They contain their sensor data internally, and the programmer does not need to care about their internals. The resulting object will syntactically behave like a built-in data type of Python.

5.1.2 Inheritance

In many applications, the objects we are going to work with are going to be related. For example, in a drawing program, we are going to work with shapes such as rectangles, circles, triangles which have some common data and actions, e.g.:

- Data:
 - Position
 - Area
 - Color
 - Circumference
- and actions:
 - draw()
 - move()
 - rotate()

What kind of data structure we use for these data and how we implement the actions are important. For example, if one shape is using Cartesian coordinates (x, y) for position and another is using Polar coordinates (r, θ) , a programmer can easily make a mistake by providing (x, y) to a shape using Polar coordinates.

As for actions, implementing such overlapping actions in each shape from scratch is redundant and inefficient. In the case of separate implementations of overlapping actions in each shape, we would have to update all overlapping actions if we want to correct an error in our implementation or switch to a more efficient algorithm for the overlapping actions. Therefore, it makes sense to implement the common functionalities in another object and reuse them whenever needed.

These two issues are handled in OOP via inheritance. We place common data and functionalities into an ancestor object (e.g. Shape object for our example) and other objects (Rectangle, Triangle, Circle) can inherit (reuse) these data and definitions in their definitions as if those data and actions were defined in their object definitions.

In real life entities, you can observe many similar relations. For example:

- A Student is a Person and an Instructor is a Person. Updating personal records of a Student is no different than that of an Instructor.

- An DC Engine, a Diesel Engine, and a Stream Engine are all Engines. They have the same characteristic features like horse power, torque etc. However, DC Engine has power consumption in units of Watt whereas Diesel Engine consumption can be measured as litres per km.
- In a transportation problem, a Ship, a Cargo Plane and a Truck are all Vehicles. They have the same behaviour of carrying a load; however, they have different capacities, speeds, costs and ranges.

Assume we like to improve the forecasting accuracy through adding radar information in our WhetherForecast example above. We need to get our traditional estimate and combine it with the radar image data. Instead of duplicating the traditional estimator, it is wiser to use existing implementation and *extend* its functionality with the newly introduced features. This way, we avoid code duplication and when we improve our traditional estimator, our new estimator will automatically use it.

Inheritance is a very useful and important concept in OOP. Together with encapsulation, it improves reusability, maintenance, and reduces redundancy.

5.1.3 Polymorphism

Polymorphism is a property that enables a programmer to write functions that can operate on different data types uniformly. For example, calculating the sum of elements of a list is actually the same for a list of integers, a list of floats and a list of complex numbers. As long as the addition operation is defined among the members of the list, the summation operation would be the same. If we can implement a polymorphic sum function, it will be able to calculate the summation of distinct datatypes, hence it will be polymorphic.

In OOP, all descendants of a parent object can act as objects of more than one types. Consider our example on shapes above: The Rectangle object that inherits from the Shape object can also be used as a Shape object since it bears data and actions defined in a Shape object. In other words, a Rectangle object can be assumed to have two data types: Rectangle and Shape. We can exploit this for writing polymorphic functions. If we write functions or classes that operate on Shape with well-defined actions, they can operate on all descendants of it including, Rectangle, Circle, and all objects inheriting Shape. Similarly, actions of a parent object can operate on all its descendants if it uses a well-defined interface.

Polymorphism improves modularity, code reusability and expandability of a program.

5.2 Basic OOP in Python

The way Python implements OOP is not to the full extent in terms of the properties listed in the previous section. Encapsulation, for example, is not implemented strongly. But inheritance and polymorphism are there. Also, operator overloading, a feature that is much demanded in OOP, is present.

In the last decade, Python started to become a standard for Science and Engineering computation. For various computational purposes, software packages were already there. Packages to do numerical computations, statistical computations, symbolic computations, computational chemistry, computational physics, all sorts of simulations were developed over four decades. Now many such packages, free or proprietary, are *wrapped* to be called through Python. This packaging is done mostly in an OOP manner. Therefore, it is vital to know some basics of OOP in Python.

5.2.1 The Class Syntax

In Python, an object is a code structure that is like in Fig. 5.2.1:

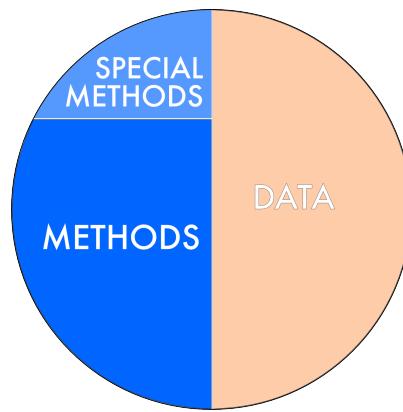


Fig. 5.2.1: An object includes both data and actions (methods and special methods) as one data item.

First, a piece of jargon:

- **Class:** A prescription that defines a particular object. The blueprint of an object.
- **Class Instance** ;
Object: A computational structure that has functions and data fields built according the blueprint, namely the class. Similar to the construction of buildings according to an architectural blueprint, in Python we can create *objects* (more than one) conforming to a class definition. Each of these objects will have their own data space and in some cases customized functions. Objects are equivalently called *Class instances*. Each object provides the following:
 - **Methods:** Functions that belong to the object.
 - **Sending a message to an object:** Calling a method of the object.
 - **Member:** Any data or method that is defined in the class.

So, as you would guess, we start with a structural plan, using the jargon, the ‘class definition’. In Python this is done by the keyword `class`:

```
class ClassName :  
    Statement block
```

Here is an example:

```
class shape:  
    color = None  
    x = None  
    y = None  
  
    def set_color(self, red, green, blue):  
        self.color = (red, green, blue)  
  
    def move_to(self, x, y):  
        self.x = x  
        self.y = y
```

This blueprint tells Python that:

1. The name of this class is shape.
2. Any object that will be created according to this blueprint has three data fields, named color, x and y. At the moment of creation, these fields are set to None (a special value of Python indicating that there is a variable here but no value is assigned yet).
3. Two member functions, the so-called methods, are defined: set_color and move_to. The first takes four arguments, constructs a tuple of the last three values and stores it into the color data field of the object. The second, move_to, takes three arguments and assign the last two of them to the x and y data_fields, respectively.

The peculiar keyword self in the blueprint refers to the particular instance (when an object is created based on this blueprint). The first argument to all methods (the member functions) have to be coded as self. That is a rule. The Python system will fill it out when that function is activated.

To refer to any function or any data field of an object, we use the (.) dot notation. Inside the class definition, it is self.□. Outside of the object, the object is certainly stored somewhere (a variable or a container). The way (syntax) to access the stored object is followed. Then, this syntax is appended by the (.) dot which is then followed by the data field name or the method name.

For our example shape class, let us create two objects and assign them to two global variables p and s, respectively:

```
p = shape()  
s = shape()  
p.move_to(22, 55)  
p.set_color(255, 0, 0)  
s.move_to(49, 71)  
s.set_color(0, 127, 0)
```

The object creation is triggered by calling the class name as if it is a function (i.e. shape()). This creates an *instance* of the class. Each instance has its private data space. In the example, two shape objects are created and stored in the variables p and s. As said, the object stored in p has its private data space and so does s. We can verify this by:

```
print(p.x, p.y)  
print(s.x, s.y)
```

When a class is defined, there are a bunch of methods, which are automatically created, and they serve the integration of the object with the Python language. For example, what if we issue a print statement on the object? What will

```
print(s)
```

```
print?
```

These default methods can be overwritten (redefined). Let us do it for two of them: `__str__` is the method that is automatically activated when a print function has an object to be printed. The built-in print function sends to the object an `__str__` message (that was the OOP jargon, i.e. calls the `__str__` member function (method)). All objects, when created, have some *special methods* predefined. Many of them are out of the scope of this course, but `__str__` and `__init__` are among these special methods.

It is possible that the programmer, in the class definition, overwrites (redefines) these predefinitions. `__str__` is set to a default definition so that when an object is printed such an internal location information is printed:

```
<__main__.shape object at 0x7f295325a6a0>
```

Not very informative, is it? We will overwrite this function to output the color and coordinate information, which will look like:

```
shape object: color=(0,127,0) coordinates=(47,71)
```

The second special method that we will overwrite is the `__init__` method. `__init__` is the method that is automatically activated when the object is first created. As default, it will do nothing, but can also be overwritten. Observe the following statement in the code above:

```
s = shape()
```

The object creation is triggered by calling the class name as if it is a function. Python (and many other OOP languages) adopt this syntax for object creation. What is done is that the arguments passed to the class name is sent ‘internally’ to the special member function `__init__`. We will overwrite it to take two arguments at object creation, and these arguments will become the initial values for the `x` and `y` coordinates.

Now, let us switch to the real interpreter and give it a go:

```
class shape:  
    color = None  
    x = None  
    y = None  
  
    def set_color(self, red, green, blue):  
        self.color = (red, green, blue)  
  
    def move_to(self, x, y):  
        self.x = x  
        self.y = y  
  
    def __str__(self):  
        return "shape object: color=%s coordinates=%s" % (self.color, (self.x,self.y))  
  
    def __init__(self, x, y):  
        self.x = x  
        self.y = y  
  
    def __lt__(self, other):  
        return self.x + self.y < other.x + other.y  
  
p = shape(22,55)  
s = shape(12,124)  
p.set_color(255,0,0)  
s.set_color(0,127,0)  
  
print(s)  
s.move_to(49,71)  
print(s)  
  
print(p.__lt__(s))  
print(p < s) #just the same as above but now infix
```

(continues on next page)

```
print(s.__dir__())
```

```
shape object: color=(0, 127, 0) coordinates=(12, 124)
shape object: color=(0, 127, 0) coordinates=(49, 71)
```

```
True
```

```
True
```

```
[x', 'y', 'color', '__module__', 'set_color', 'move_to', '__str__', '__init__', '__lt__', '__dict__', '__weakref__', '__doc__', '__repr__', '__hash__', '__getattribute__', '__setattr__', '__delattr__', '__le__', '__eq__', '__ne__', '__gt__', '__ge__', '__new__', '__reduce_ex__', '__reduce__', '__subclasshook__', '__init_subclass__', '__format__', '__sizeof__', '__dir__', '__class__']
```

5.2.2 Special Methods/Operator Overloading

There are many more special methods than the ones we described above. For a complete reference, we refer you to “[Section 3.3 of the Python Language Reference](#)”²⁶.

Last, but not least, a special method to mention is the magnitude comparison for an object. In other words, if you have an object, how will it behave under comparison? For example, the following rich comparisons are possible:

- $x < y$ calls `x.__lt__(y)`,
- $x \leq y$ calls `x.__le__(y)`,
- $x == y$ calls `x.__eq__(y)`,
- $x \neq y$ calls `x.__ne__(y)`,
- $x > y$ calls `x.__gt__(y)`, and
- $x \geq y$ calls `x.__ge__(y)`.

Having learned this, please copy-and-paste the following definition to the class definition of `shape` above in to the code box. Now, you have the ($<$) comparison operator available.

```
def __lt__(self, other):
    return self.x + self.y < other.x + other.y
```

As you can see, the comparison result is based on the *Manhattan distance* from the origin. You can give it a test right away and compare the two objects `s` and `p` as follows:

```
print(s < p)
```

How would you modify the comparison method so that it compares the Euclidean distances from the origin?

As we have created our first object in Python, we strongly advise that the ‘encapsulation’ property of OOP is followed by the programmer, i.e. you. This property is that the data of an object is private to the object and not open to modification (or not even to inspection if ‘encapsulation’ is taken extremely strictly) by a piece of code external to the object. Only member functions, the so-called methods, of that object can do this. Therefore, if you want to update the color value, for example, of an `shape` object, though you can do it ‘brutally’ by e.g.:

²⁶ <https://docs.python.org/3/reference/>

```
p.color = (127,64,5)
```

However, you should not do so. In contrary to some other OOP programming languages, Python does not forbid this by a brutal force. Therefore, it is not a **you cannot** but a **you should not** type of action. All data access should be done through messages (functions).

5.2.3 Example 1: Counter

Now, let us implement a very simple object called Counter. Counter has two important restrictions: it starts with zero and it can only be incremented. If you use a simple integer variable instead of Counter, its value can be initialized to any value and it can directly be assigned to an arbitrary value. Implementing a Python class for a Counter will let you enforce those restrictions since you define the initialization and the actions.

```
class Counter:  
    def __init__(self):  
        self.value = 0 # this is the initialization  
  
    def increment(self):  
        "increment the inner counter"  
        self.value += 1  
  
    def get(self):  
        "return the counter as value"  
        return self.value  
  
    def __str__(self):  
        "define how your counter is displayed"  
        return 'Counter:{}'.format(self.value)  
  
stcnt = Counter() # create the counter  
stcnt.increment()  
stcnt.increment()  
print("# of students", stcnt)  
  
sheep = Counter()  
while sheep.get() < 1000:  
    sheep.increment()  
  
print("# of sheep",sheep)
```

```
# of students Counter:2  
# of sheep Counter:1000
```

5.2.4 Example 2: Rational Number

As our next example, let us try to define a new data type, **Rational Number**, as a Python class. Representing a rational number simply as a tuple of integers as (numerator, denominator) is possible. However, this representation has a couple of issues. First, the denominator can be 0, which leads to an invalid value. Second, many distinct tuples represent practically the same value and they need to be interpreted in a special way in operators like comparison. We need to either normalize all into their simplest form or implement comparison operators to respect the values they represent. In the following implementation, we choose the first approach: We find greatest common divisor of numerator and denominator and normalize them.

```
import math

class Rational:
    def __init__(self, n, d):
        """initialize from numerator and denominator values"""
        if d == 0:
            raise ZeroDivisionError # raise an error. Explained in following chapters
        self.num = n
        self.den = d
        self.simplify()

    def simplify(self):
        if self.num == 0:
            self.den = 1
            return
        gcd = math.gcd(self.num, self.den)
        if self.den < 0:      # flip their signs if denominator is negative
            self.den *= -1
            self.num *= -1
        self.num = self.num // gcd
        self.den = self.den // gcd # normalize them by dividing by greatest common divisor

    def __str__(self):
        return '{}/{}'.format(self.num, self.den)

    def __mul__(self, rhs):      # this special method is called when * operator is used
        """(a/b)*(c/d) -> a*c/b*d in a new object """
        retval = Rational(self.num * rhs.num, self.den * rhs.den) # create a new object
        return retval

    def __add__(self, rhs):      # this special method is called when + operator is used
        """(a/b)+(c/d) -> a*d+b*c/d*b in a new object """
        retval = Rational(self.num * rhs.den + rhs.num * self.den,
                          self.den * rhs.den) # create a new object with sum
        return retval

    # -, /, and other operators left as exercise

    def __eq__(self, rhs):      # called when == operator is used
        """a*d == b*c """
        return self.num*rhs.den == self.den*rhs.num

    def __lt__(self, rhs):      # called when < operator is used
        """a*d < b*c """
        return self.num*rhs.den < self.den*rhs.num
```

(continues on next page)

```
# rest can be defined in terms of the first two
def __ne__(self, rhs): return not self == rhs

def __le__(self, rhs): return self < rhs or self == rhs

def __gt__(self, rhs): return not self <= rhs

def __ge__(self, rhs): return not self < rhs
```

Let us play with our Rational class

```
a = Rational(3, 9)
b = Rational(16, 24)
print(a, b, a*b+b*a)
print(a < b, a+b == Rational(1, 1))
```

1/3 2/3 4/9

True True

This class definition only implements *, +, and comparison operators. The remaining operators are left as an exercise. Our new class Rational behaves like a built-in data type in Python, thanks to the special methods implemented. User-defined data types implementing integrity restrictions through encapsulation are called **Abstract Data Types**.

5.2.5 Inheritance with Python

Now let's have a look on the second property on OOP, namely ‘inheritance’, in Python. We will do that by extending our shape example.

A shape is relatively a general term. We have many types of shapes: Triangles, circles, ovals, rectangles, even polygons. If we incorporated them into a software, for example, a simple drawing and painting application for children, each of them would have a position on the screen and a color. This would be common to all shapes. But then, a circle would be identified (additionally) by a radius; a triangle by two additional corner coordinates etc.

Therefore, a triangle object should inherit all the properties and member functions of a shape object plus some other.

Starting to define a triangle object, for example, with all properties and member functions copied from shape is done by a first line:

```
class triangle(shape):
```

following the general syntax below:

```
class ClassName (BaseClass1, BaseClass2, .., ):
```

Statement block

Though multiple inheritance (inheriting form more than one class) is possible, it is seldom used and is not

preferred. It has elaborated rules for resolving member function name clashes, which is beyond the scope of an introductory book. We will continue with an example that does inheritance from a single base class.

5.2.6 Interactive Example: A Simple Shape Drawing Program

Below, you see a simple object-oriented Python code that draws a red circle and a green rectangle, and then moves the green rectangle towards the circle. When you hover your mouse over the code below, a popup window will explain that line of code.

Following this interactive code display, you can find a code box, the one with a small triangle on the left, which is the same code. So, you can run it, and observe the code live, running. In the exercise part, you will be asked to modify the code.

The dark brownish sections in the code contain calls to a drawing library (named calysto) which is also object oriented but has nothing to do with you. Not to distract the reader intentionally, we have darkened it out.

Our object-oriented programming (OOP) intention in this example is to define a general class that we will name shape. shape contains all the properties and functions that a drawable geometric object (circle, rectangle, triangle, ...) possesses. All of them are drawn on an imaginary canvas at a certain coordinate with some color. So, all shapes have a coordinate at which they are drawn and a color. The first lines of the class shape definition starts with these variables.

[You can get additional information by hovering your mouse over any piece of code.]

In this example, we implement just two geometric shapes, the circle and the rectangle. This piece of code with the green background is the definition of the circle class. It is *derived* from the *base* class shape. So, it *inherits* all the definitions of shape (but these definitions can be overwritten, in other words, can be redefined). As you observe, it defines a radius variable (in addition to the color, x, y variables that were inherited form the base class). Also, it defines, for the first time, a draw member function which has the duty to draw a circle on the canvas, based on the parameters x, y, radius and color using some functions of the library calysto. The details of this drawing implementation is not the reader's concern (therefore it is darkened out).

[You can get additional information by hovering your mouse over any piece of code.]

The second geometric shape, which is implemented, is the rectangle. The orange backgrounded code defines this class. Again, it is a *descendent* of the base class shape. Hence, it *inherits* all the definitions of shape (just as circle did). This time, it does not add a radius but a width and a height variables to the class. In addition to the redefinition of the initializer `__init__`, which is activated the moment an instance is created, this class has its own definition of the draw member function.

[You can get additional information by hovering your mouse over any piece of code.]

Now, for an instance, return to the class shape definition (the yellow box). There, you will see a displace member function being defined. It is a function that displaces a geometric shape by an amount of $(\Delta x, \Delta y)$. Please inspect the function now. You will discover that the function:

- memorizes the color of the shape,
- changes the color to white,
- calls the draw member function and draws a white shape exactly on top of the old one,
- restores the drawing color (from white to the memorized color),
- changes the x, y values by amounts `delta_x` and `delta_y`, respectively,
- calls the draw member function and draws at the new x,y coordinates the shape with the original color.

Now we have an interesting phenomenon. `draw` is even not defined in `shape`. It will be defined differently for each class that is derived from the `shape` base class. How can a function of `shape` make a reference to a function which does not exist for `shape` and will only be defined in classes that are descendants of this base class? Also note that the each of the descendant classes (`circle` and `rectangle`) are going to define it (the `draw` function) their own way. This is called forward-referencing and polymorphism, a nice and powerful feature of OOP.

Note that the class definitions (class `shape`, class `circle`, class `rectangle`) are merely blueprints. They do not create any data. They define how they will be created and which functions will act how. The actual creation (based on these blueprints) are done in the code in the last (turquoise colored) box.

In summary, the code below performs the following:

- An instance of the `circle` class is created (by calling its initializer) at coordinates (100,100) with a radius of 50. This instance is stored into the variable `mycircle`.
- The color of this freshly created object is changed to the brightest red.
- The object's `draw` function is called (in OOP jargon: a `draw` message is sent to the object stored in `mycircle`)
- Similarly, an instance of `rectangle` class is created at coordinates (200,100) and with `width=50`, `height=80`. This instance is stored into the variable `myrectangle`.
- The color of the rectangle is changed to the brightest green.
- The rectangles `draw` function is called.
- The program pauses (waits) for 1 second.
- Finally, it calls the `displace` function of the rectangle. Though it was defined in the base class, `displace` locates the correct `draw` (the `draw` of the rectangle) and performs the job.

Please use the Colab link at the top to see the interactive demo.

5.2.7 Useful Short Notes on Python's OOP

These notes are provided for completeness and a possible need in your further studies. These are out of the introductory scope of the book.

- It is possible that the derived class overrides the base class's member function. But, still want to access the (former) definition in the base class. One can access that definition by prefixing the function call by `super()`. (no space after the dot).
- There is no proper destructor in Python. This is because the Python engine does all the memory allocation and book-keeping. Though entirely under the control of Python, sometimes the so-called *Garbage Collection* is carried out. At that moment, all unused object instances are wiped out of the memory. Before that, a special member function `__del__` is called. If you want to do a special treatment of an object before it is wiped forever, you can define the `__del__` function. The concept of garbage collection is complex and it is wrong to assume that `__del__` will right away be called even if an object instance is deleted by the `del` statement (`del` will mark the object as unused but it will not necessarily trigger a garbage collection phase).
- Infix operators have special, associated member functions (those that start and end with double underscores). If you want your objects to participate in infix expressions, then you have to define those. For example '+' has the associated special member function `__add__`. For a complete list and how-to-do's, search for "special functions of Python" and "operator overloading".

- You can restrict the accessibility of variables defined in a class. There are three types of accessibility modifications you can perform: public, private, and protected. The default is public.
 - Public access variables can be accessed anywhere inside or outside the class.
 - Private variables can only be accessed inside the class definitions. A variable which starts with two underscores is recognized by programmers as private.
 - Protected variables can be accessed within the same package (file). A variable which starts with a single underscore is recognized by programmers as protected.

5.3 Widely-used Member Functions of Containers

Being acquainted with the OOP concepts, it is time to reveal the ‘object’ properties of some Python components. In Python, every data is an object. However, here we will look at the OOP components of containers.

Strings

Assume S is a string. In the table below, you will find some of the very frequently used member functions of strings (in the **Operation** column, anything in square brackets denotes that the content is optional – if you enter the optional content, do no type in the square brackets):

Operation	Result
S.capitalize()	Returns a copy of S with its first character capitalized, and the rest of the characters lowercased.
S .count(sub [, start [, end]])	Returns the number of occurrences of substring sub in string S.
`` S.find(sub [, start [, end]])``	Returns the lowest index in S where substring sub is found. Returns -1 if sub is not found.
S.isalnum()	Returns True if all characters in S are alphanumeric, False otherwise.
S.isalpha()	Returns True if all characters in S are alphabetic, False otherwise.
S.isdigit()	Returns True if all characters in S are digit characters, False otherwise.
S.islower()	Returns True if all characters in S are lowercase, False otherwise.
S.isspace()	Returns True if all characters in S are whitespace characters, False otherwise.
S.isupper()	Returns True if all characters in S are uppercase, False otherwise.
separator.join(seq)	Returns a concatenation of the strings in the sequence seq, separated by string separator, e.g.: "#".join(["a","bb","ccc"]) returns "a#bb#ccc"
S.ljust/rjust/c enter(width [, fillChar=''])	Returns S, left/right justified/centered in a string of length width. surrounded by the appropriate number of fillChar characters.
S.lower()	Returns a copy of S converted to lowercase.
S.lstrip([chars])	Returns a copy of S with leading chars (default: blank chars) removed.
S.partition(separ)	Searches for the separator separ in S, and returns a tuple (head, sep, tail) containing the part before it, the separator itself, and the part after it.
S.replace(old, new [, maxCount = -1])	Returns a copy of S with the first maxCount (-1: unlimited) occurrences of substring old replaced by new.
S.split([separator [, maxsplit]])	Returns a list of the words in S, using separator as the delimiter string.
S.splitlines([keepends])	Returns a list of the lines in S, breaking at line boundaries.
S.startswith(prefix [, start [, end]])	Returns True if S starts with the specified prefix, otherwise returns False. Negative numbers may be used for start and end. Prefix can also be a tuple of strings to try.
S.strip([chars])	Returns a copy of S with leading and trailing chars (default: blank chars) removed.
S.swapcase()	Returns a copy of S with uppercase characters converted to lowercase and vice versa.
S.upper()	Returns a copy of S converted to uppercase.

Lists

Assume **L** is a list. In the table below, you will find some of the very frequently used member functions of lists (in the **Operation** column, anything in square brackets denotes that the content is optional – if you enter the optional content, do no type in the square brackets):

Operation	Result
L.append(x)	same as L[len(L) : len(L)] = [x]
L.extend(x)	same as L[len(L) : len(L)] = x
L.count(x)	returns number of i's for which L[i] == x
`L.index(x [, start [, stop]])`	returns smallest i such that L[i] == x. start and stop limit search to only part of the list.
L.insert(i, x)	same as L[i:i] = [x] if i ≥ 0. if i < -1, inserts before the last element.
L.remove(x)	same as del L[L.index(x)]
L.pop([i])	same as x = L[i]; del L[i]; return x
L.reverse()	reverses the items of L in place
L.sort([cmp]) OR L.sort([cmp=cmpFct] [, key=keyGetter] [, reverse=bool])	sorts the items of L in place

Dictionaries

Assume **D** is a dictionary. In the table below, you will find some of the very frequently used member functions of dictionaries (in the **Operation** column anything in square brackets denotes that the content is optional – if you enter the optional content, do no type in the square brackets):

Operation	Result
D.from_keys(iterable, value=None)	Class method to create a dictionary with keys provided by iterator, and all values set to value
D.clear()	Removes all items from D
D.copy()	A shallow copy of D
D.has_key(k) OR k in D	True if D has key k, else False
D.items()	A copy of D's list of (key, item) pairs
D.keys()	A copy of D's list of keys
D1.update(D2)	for k, v in D2.items(): D2[k] = v
D.values()	A copy of D's list of values
D.get(k, defaultval)	The item of D with key k
D.setdefault(k [, defaultval])	D[k] if k in D, else defaultval (also setting it)
D.iteritems()	Returns an iterator over (key, value) pairs
D.iterkeys()	Returns an iterator over the mapping's keys
D.itervalues()	Returns an iterator over the mapping's values.
D.pop(k [, default])	Removes key k and returns the corresponding value. If key is not found, default is returned if given, otherwise KeyError is raised.
D.popitem()	Removes and returns an arbitrary (key, value) pair from D

Sets

Assume **T, T1, T2** are sets (unless otherwise stated). In the table below you will find some of the very frequently used member functions of sets (in the **Operation** column anything in square brackets denotes that the content is optional – if you enter the optional content, do no type in the square brackets):

Operation	Result
T1.issubset(T2)	True if every element in T1 is in iterable T2
T1.issuperset(T2)	True if every element in T2 is in iterable T1
T.add(elt)	Adds element elt to set T (if it doesn't already exist)
T.remove(elt)	Removes element elt from set T. KeyError if element not found
T.discard(elt)	Removes element elt from set T if present
T.pop()	Removes and returns an arbitrary element from set T; raises KeyError if empty
T.clear()	Removes all elements from this set
T1.intersection(T2 [, T3 ...])	Synonym to (T1 & T2). Returns a new Set with elements common to all sets (in the method T2, T3, ... can be any iterable)
T1.union(T2 [, T3 . ..])	Synonym to (T1 T2). Returns a new Set with elements from either set (in the method T2, T3, ... can be any iterable)
`` T1.difference(T2 [, T3 ...])``	Synonym to (T1 - T2). Returns a new Set with elements in T1 but not in any of T2, T3, .. (in the method T2, T3, ... can be any iterable)
` ` T1.symmetric_difference(T2)` `	Synonym to (T1 ^ T2). Returns a new Set with elements from either of two sets but not their intersection
T.copy()	Returns a shallow copy of set T

5.4 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- Encapsulation, inheritance and polymorphism.
- Benefits of the Object-Oriented Paradigm.
- Concepts such as class, instance, object, member, method, message passing.
- Concepts such as base class, ancestor, descendant.

5.5 Further Reading

- Special Methods in Python: <https://docs.python.org/3/reference/datamodel.html#special-method-names>
- Object-oriented Programming chapter: https://link.springer.com/chapter/10.1007/978-3-7091-1343-1_7

Exercises

Go to the interactive example and modify it as follows:

1. Add a triangle class. It should take, at creation time, (x,y,dx2,dy2,dx3,dy3) as parameter, where x,y are the coordinates of one of the corners of the triangle on the canvas, and dx2,dy2 are the increments relative to x1,y1 to reach the second corner of the triangle (so, the absolute coordinate on the canvas of the second corner becomes (x+dx2,y+dy2)), dx3,dy3 have a similar meaning to reach the third corner.

You are expected to define all member functions present in circle or rectangle, this time for triangle. For the draw member function, you can investigate the content of the draw of the rectangle class.

2. Implement a move_on_line(x_fin, y_fin, count_of_steps) that will work for all geometric shapes and displace a geometric shape starting from its current position on the canvas and ending at (x_fin,y_fin) coordinate in count_of_steps many displacements.
3. Create a class car, which is a child-drawing style car, that consists of a rectangle and two circles below it. It should implement all member functions of circle or rectangle. Make use of the existing rectangle and circle classes.

6 | File Handling

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All variables used in a program are kept in the main memory and they are **volatile**, i.e., their values are lost when the program ends. Even if you write a program running forever, your data will be lost in case of a shutdown or a power failure.

Another drawback of the main memory is the capacity limitation. In the extreme case, when you need more than a couple of gigabytes for your variables, it will be difficult to keep all of them in the main memory. Especially, infrequently required variables are better kept on an external storage device instead of the main memory.

Files provide a mechanism for storing data **persistently** in hard drives which provide significantly larger storage than the main memory. These devices are also called *secondary storage* devices. The data you put in a file will stay on the hard drive until someone overwrites or deletes the file (or when the hard drive fails, which is a sad but rare case).

A **File** is a sequence of bytes stored on the secondary storage, typically hard drive (alternative secondary storage devices include CD, DVD, USB disk, tape drive). Data on a file has the following differences from data in memory (variables):

1. A file is just a sequence of bytes. Therefore, data in a file is unorganized, there is no data type, no variable boundaries.
2. Data needs to be accessed indirectly, using I/O functions. E.g. updating a value in a file requires reading it in memory, updating in memory, then writing it into the file back.
3. Accessing and updating data is significantly slower since it is on an external device.

Keeping data on a file instead of the main memory has the following use cases:

1. Data needs to be persistent. Data will be in the file when you restart your program, reboot your machine or when you find your ancient laptop in the basement 30 years later (Probably it will not be there when a 3000BC archeologist finds your laptop on an excavation site. Hard disks are not that durable. So, persistency is bounded).
2. You need to exchange data with another program. Examples:
 - You download data from web and your program gets it as input.
 - You like to generate data in your program and put it on a spreadsheet for further processing.
3. You have large amount of data which does not fit in the main memory. In this case, you will probably use a library or software like a database management system to access data in a faster and organized way. Files are the most primitive, basic way of achieving it.

In this chapter, we will talk about simple file access so that you will learn about simple file operations like open, close, read, write. The examples of the chapter will create and modify files when run – we strongly encourage you to check the contents of the created files using the file access mechanism at the left-hand side.

6.1 First Example

Let us quickly look at a simple example to get a feeling for the different steps involved in working with files.

```
fpointer = open('firstexample.txt', "w")
fpointer.write("hello\n")
fpointer.write("how are\n")
fpointer.write("you?\n")
fpointer.close()
```

The program above will create a file in the current directory with filename firstexample.txt. You can open it with your favourite text editor (there are plenty of text editors for operating systems: notepad, wordpad, textedit, nano, vim) to see and edit it. The content will look like this:

```
hello
how are
you?
```

First line of the program is `fpointer = open('firstexample.txt', "w")`. This line opens the file named firstexample.txt for writing to it. If the file exists, its content will be erased (it will be an empty file afterwards). The result of `open()` is a file object that we will use in the following lines. This object is assigned to variable `fpointer`.

In the following lines, all functions we call with this file object `fpointer` will work on this file (i.e. firstexample.txt). This special *dot* notation helps us with calling functions in scope of the file. `fpointer.functionname()` will call the `functionname` function for this file. `write(string)` function will write the string content to the file. Each call to `write(string)` will append the string to the file and the file will grow. At the end, when we are done, we call `close()` to finish accessing the file so that your operating system will know and do necessary actions about it. All open files will be closed when your program terminates. However, calling `close()` after finishing writing is a good programming practice.

Now, let us read this file:

```
fp = open("firstexample.txt", "r")
content = fp.read()
fp.close()
print(content)
```

```
hello
how are
you?
```

In this case, we called `open()` with argument "r" which tells that we are going to read the file (or use it as an input source). If you skip the second argument in `open()`, it is assumed to be "r", so `open("firstexample.txt")` will be equivalent. The `read()` call gets an optional argument, which is the number of bytes to read. If you skip it, it will read the whole file content and return it as a string. Therefore, after the call, the content variable will be a string with the file content.

6.2 Files and Sequential Access

A file consists of bytes and read/write operations access those bytes **sequentially**. In sequential access, the current I/O operation updates the file state so that next I/O operation will resume from the end of the current I/O operation.

Assume you have an old MP3 player that supports only *play me next 10 seconds* operation on a button. Pressing it will play the next 10 seconds of the song. When you press again, it will resume from where it is left and play another 10 seconds. This follows until the song is over. The sequential access is like this. A *file pointer* keeps the current offset of the file and each I/O operation advances it so that next call will read or write from this new offset – see Fig. 6.2.1.

Sequential Read of a File

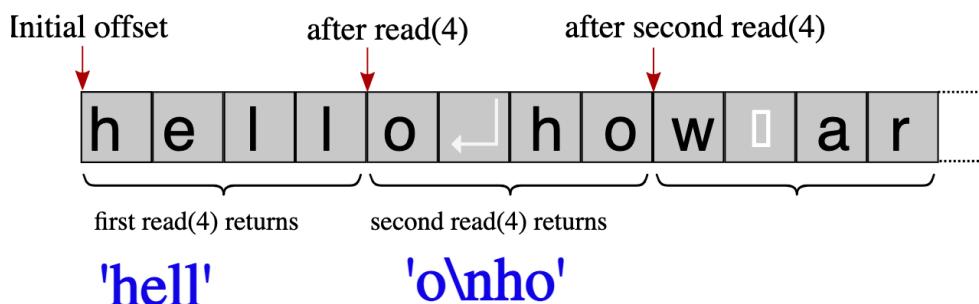


Fig. 6.2.1: Sequential reading of a file.

The following is a sample program illustrating sequential access:

```
fp = open("firstexample.txt", "r") # the example file we created above

for i in range(3):      # repeat 3 times
    content = fp.read(4)  # read 4 bytes in each step
    print("> ", content) # output 4 bytes preceded by >

fp.close()
```

```
> hell
> o
ho
> w ar
```

The text in the file was:

```
hello
how are
you?
```

The first read() reads 'hell', the second reads 'o\nho' (note that \n stands for a new line so that ho is printed on a new line), and the third reads 'w ar'. After these operations, the file offset is left at a position so that the following reads will resume from content 'e\nyou\n'.

We provided the example with 4-byte read operations. However, for text files, the typical scenario is reading characters line by line instead of fixed size strings.

6.3 Data Conversion and Parsing

A file, specifically a text file, consists of strings. However, especially in engineering and science, we work with numbers. A number is represented in a text file as a sequence of characters including digits, a sign prefix ('-' and '+') and at most one occurrence of a dot ('.'). That means in your Python program, you may use π as 3.1416 however, in the text file, you store '3.1416', which is a string consisting of chars '3','.','1','4','1','6'.

```
pi = 3.1416
pistr = '3.1416'
print(pi+pi, pi * 3)
print(pistr+pistr, pistr *3)
```

```
6.2832 : 9.4248
3.14163.1416 : 3.14163.14163.1416
```

Funny, the second line of output above is a result of Python interpreting + operator as string concatenation, and * as adjoining multiple copies of a string. If we need to treat numbers as numbers, we need to convert them from string. There are two handy functions for this: int() and float() convert a string into an integer and a floating point value, respectively. Here is an illustration:

```
pistr = ' 0.31416E01 '
nstr = '47'

# Convert numbers in the strings into numerical data types:
piflt = float(pistr)
nint = int(nstr)

print(piflt*2, nint*2)
```

```
6.2832 94
```

Note that we cannot call int('3.1416') since the string is not a valid integer. That brings us another challenge of making sure that strings we need to convert are actually numbers. Obviously int('hello') and float('one point five') will not work. The ways of dealing with such errors are left for the next chapter. In this chapter, we assume that we have our data carefully created and all conversions work without any error.

Our next challenge is having multiple numbers on a string separated by special characters or simply spaces as '10.0 5.0 5.0'. In this case, we need to decompose a string into string pieces representing numbers, so that we will have '10.0','5.0','5.0' for the above string. The next step will be converting them into numbers:

'10.0 5.0 5.0' $\xrightarrow{\text{Step 1}}$ ['10.0','5.0','5.0'] $\xrightarrow{\text{Step 2}}$ [10.0, 5.0, 5.0]

For the first step, we will use the split() method of a string. String, or the variable containing the string, is followed by .split(delimiter), which returns a list of strings separated by the given delimiters. The delimiters are removed and all values in between are put in the list – for example:

```
print('a:b:c'.split(':'))
print('hello darkness, my old friend'.split(','))
print('a <=> b <=> c'.split('<=> '))
print('multiple    spaces    are    tricky'.split(' '))
a = '10.0 5.0 5.0'
print(a.split(' '))
```

```
[a', 'b', 'c']
['hello', 'darkness', 'my', 'old', 'friend']
[a', 'b', 'c']
['multiple', " ", " ", " ", " ", 'spaces', " ", " ", " ", " ", " ", 'are', " ", " ", " ", " ", " ", "tricky"]
['10.0', '5.0', '5.0']
```

For the second step, we will use the float() function on a list (or the int() function if you have a list of integers). We have couple of options for this. One is to start from an empty list and append the converted value at each step:

```
instr = '10.0 5.0 5.0'
outlst = []

# Go over each substring
for substr in instr.split(' '):
    outlst += [float(substr)] # Convert each element to float and append it to the list

print(outlst)
```

```
[10.0, 5.0, 5.0]
```

A more practical and faster version will be list comprehension, which is the compact version of mapping a value into another as:

```
instr = '10.0 5.0 5.0'

outlst = [ float(substr) for substr in instr.split(' ')]

print(outlst)
```

```
[10.0, 5.0, 5.0]
```

As we have explained in Chapter 3, the syntax is similar to set/list notation in Math:

$\{ \text{float}(s) \mid s \in S \}$ vs. [float(s) for s in S]

If you need to have multiple spaces within the values, you can use import re and call re.split(' +', inputstr) instead of inputstr.split(' '). This will split the 'multiple spaces are tricky' example above into 4 words without spaces. How it works is beyond the scope of the book. Curious readers can refer to re and parse modules for more advanced forms of input parsing. These are not trivial modules for beginners.

Now, let us consider the reverse of the operation: Assume we have a list of integers and we like to convert that into string that can be written in a file:

$[10.0, 5.0, 5.0] \xrightarrow{\text{Step 1}} ['10.0', '5.0', '5.0'] \xrightarrow{\text{Step 2}} '10.0 5.0 5.0'$

The first step will be handled with the str() function which converts any Python value into a human readable string:

```
inlst = [10.0, 5.0, 5.0]

outlst = [str(num) for num in inlst]
```

(continues on next page)

```
print(outlst)
```

```
['10.0', '5.0', '5.0']
```

The next step is to join those elements with a delimiter, which is reverse of the split() operation. Not by accident, name of this operation is join(). join() is a method of the delimiter string and list is the argument of it. ':'.join(['hello','how','are','you?']) returns 'hello:how:are:you?'.

```
inlst = [10.0, 5.0, 5.0]
```

```
outlst = [str(num) for num in inlst]
```

```
print(' '.join(outlst))
```

```
10.0 5.0 5.0
```

A more advanced way of converting values into strings is called *formatted output* and briefly introduced in a section below.

6.4 Accessing Text Files Line by Line

Files consisting of human readable strings are called **text files**. Text files consist of strings separated by the *end of line* character '\n', also known as *new line*. The sequence of characters in a file contains the end-of-line characters so that a text editor will end the current line and show following characters on a new line. We use end-of-line characters so that logically relevant data is on the same line. For example:

```
4
10.0 20.0
15.5 22.2
3 44
10 10.5
```

Let us assume the integer value 4 on the first line denotes how many lines will follow. Assume also that each of the following 4 lines have two real values denoting x and y values of a point. In this way, we can represent our input separated by end-of-line characters for each point and by space character for each value in a line.

Let us create such a text file from a Python list. Please note that the file read function returns a string, the write function expects a string argument. I.e., calling write(3.14) will fail. In order to make the conversion, we use the str() function for numeric values and call write(str(3.14)) instead. Another tricky point is that write() does not put end of line character automatically. You need to put it in the output string or call an extra write("\n").

```
pointlist = [(0,0), (10,0), (10,10), (0,10)]
fp = open("pointlist.txt", "w")      # open file for writing
fp.write(str(len(pointlist)))       # write list length
```

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```

fp.write('\n')

# Go over each point in the list
for (x,y) in pointlist:      #for each x,y value in the list
    fp.write(str(x))        # write x
    fp.write(' ')           # space as number separator
    fp.write(str(y))        # write y
    fp.write('\n')          # \n as line separator

fp.close()

# let us read the content to verify what we wrote
fp = open("pointlist.txt")    # open for reading
content = fp.read()
print(content)
fp.close()

```

```

4
0 0
10 0
10 10
0 10

```

Using `read()` will get the whole content of the file; if the file is large, your program would use too much memory and processing the data will be difficult. Instead of that, we can access a text file line by line using the `readline()` function.

Let us write a program to read and output the content of a text file. We need a loop to read the file line by line and output. But, when we are going to stop is another problem. Python's `read()` and `readline()` functions return an empty string "" when there is nothing left to read. We can use this to stop reading:

```

fp = open("pointlist.txt")      # open file for reading

nextline = fp.readline()        # read the first line
while nextline != "":          # while read is successful
    print(nextline)            # output the line
    nextline = fp.readline()    # read the nextline

fp.close()                     # when nextline == "" loop terminates

```

```

4

0 0

10 0

10 10

0 10

```

Please note the empty lines between the each output line. This is due to '\n' character at the end of the string that `readline()` returns. In other words, `readline()` keeps the new line character it reads. `print()` puts an end of line after the output (this can be suppressed by adding an `end=" "` argument). As a result, we have extra

end-of-line at the end of each line. In order to avoid it, you can call `rstrip("\n")` on the returned string to remove end of line. The new code will be:

```
fp = open("pointlist.txt")      # open file for reading

nextline = fp.readline()        # read the first line
while nextline != "":           # while read is successful
    nextline = nextline.rstrip("\n")  # remove occurrences of '\n' at the end
    print(nextline)                # output the line
    nextline = fp.readline()       # read the nextline

fp.close()
```

```
4
0 0
10 0
10 10
0 10
```

Converting this file into the initial Python list `[(0,0), (10,0), (10,10), (0,10)]` is our next challenge. This requires conversion of a string as "0 0\n" into (0,0). The first one is of type str whereas the second is a tuple of numeric values. We can use `int()` or `float()` functions to convert strings into numbers. Note that the string should contain a valid representation of a Python numeric value: `int("hello")` will raise an error.

The second issue is separating two numbers in the same string. We can use `split()` function followed by the separator string as in `nextline.split(' ')`. This call will return a sequence of strings from a string. If the separator does not occur in the string, it will return a list with one element, if there is one separator, it will return two elements. For n occurrences of the separator, it will return a list with $n - 1$ elements.

Here is the solution in Python:

```
fp = open("pointlist.txt")      # open file for reading

pointlist = []                  # start with empty list

nextline = fp.readline()        # read the first line
n = int(nextline)               # find number of lines to read

for i in range(n):              # repeat n times
    nextline = fp.readline()    # read the nextline
    nextline = nextline.rstrip("\n")  # remove occurrences of '\n' at the end
    (x, y) = nextline.split(' ')  # get x and y (note that they are still strings)
    x = float(x)                 # convert them into real values
    y = float(y)
    pointlist.append( (x,y) )    # add tuple at the end

fp.close()
print(pointlist)                # output the resulting list
```

```
[(0.0, 0.0), (10.0, 0.0), (10.0, 10.0), (0.0, 10.0)]
```

6.5 Termination of Input

There are two ways to stop reading input:

1. By reading a definite number of items.
2. By the end of the file.

In our previous examples, we read an integer that told us how many lines followed in the file. Then, we called readline() in a for loop with the given number of lines. This is an example of the first case which provides a definite number of items.

The alternative is to read lines in a while loop until a termination condition arises. The termination condition is usually the **end of file**, the case where functions like read() and readline() return an empty string "".

```
fp = open("pointlist.txt")      # open file for reading

pointlist = []                  # start with empty list
nextline = fp.readline()        # skip the first line (4) since we don't need it

nextline = fp.readline()        # read the first line
while nextline != "":           # until end of file
    nextline = nextline.rstrip("\n") # remove occurrences of '\n' at the end
    (x, y) = nextline.split(' ')   # get x and y (note that they are still strings)
    x = float(x)                 # convert them into real values
    y = float(y)
    pointlist.append( (x,y) )     # add tuple at the end
    nextline = fp.readline()      # read the nextline

fp.close()
print(pointlist)
```

```
[(0.0, 0.0), (10.0, 0.0), (10.0, 10.0), (0.0, 10.0)]
```

Note that the example above skips (reads and throws away) the first line so that the integer on the first line is ignored. When your input does not contain such an unnecessary value, you can delete this line.

Sometimes termination can be marked explicitly by a *sentinel value* which is a value marking the end of values. This is especially useful when you have multiple objects to read:

```
# First, create a file named `twopointlists.txt`
fp = open("twopointlists.txt", "w")
fp.write("3 0
3.4 2.1
5.1 3.2
EOLIST
1 1.5
2.0 2.5")
fp.close()
```

This will create a sample file content as:

```
3 0
3.4 2.1
5.1 3.2
```

(continues on next page)

EOLIST
1 1.5
2.0 2.5

```

fp = open("twopointlists.txt")
pntlst1 = []           # start with empty list
pntlst2 = []           # start with empty list

nextline = fp.readline()      # read the first line
while nextline != 'EOLIST\n':    # sentinel value
    nextline = nextline.rstrip('\n')  # remove occurrences of '\n' at the end
    (x, y) = nextline.split(' ')    # get x and y (note that they are still strings)
    x = float(x)                  # convert them into real values
    y = float(y)
    pntlst1.append( (x,y) )        # add tuple at the end
    nextline = fp.readline()       # read the nextline

#first list has been read, now continue with the second list from the same file
nextline = fp.readline()
while nextline != "":          # until end of file
    nextline = nextline.rstrip('\n')  # remove occurrences of '\n' at the end
    (x, y) = nextline.split(' ')    # get x and y (note that they are still strings)
    x = float(x)                  # convert them into real values
    y = float(y)
    pntlst2.append( (x,y) )        # add tuple at the end
    nextline = fp.readline()

fp.close()
print('List 1:', pntlst1)
print('List 2:', pntlst2)

```

List 1: [(3.0, 0.0), (3.4, 2.1), (5.1, 3.2)]
List 2: [(1.0, 1.5), (2.0, 2.5)]

The output will be:

List 1: [(3.0, 0.0), (3.4, 2.1), (5.1, 3.2)]
List 2: [(1.0, 1.5), (2.0, 2.5)]

6.6 Example: Processing CSV Files

CSV stands for *Comma Separated Value*; it is a text-based format for exporting/importing spreadsheet (i.e. Excel) data. Each row in a CSV file is separated by newlines and each column is separated by a comma ,. Actually, the format is more complex but for the time being, let us ignore comma that might be appearing in strings and focus on a simple form as follows:

Name,Surname,Grade
Han,Solo,80
Luke,Skywalker,90
Obi,Van Kenobi,88

(continues on next page)

Leya,Skywalker,91
Anakin,Skywalker,55

Usually first line is the names of the columns in a spreadsheet. Now, let us create this file:

```
content = "Name,Surname,Grade
Han,Solo,80
Luke,Skywalker,90
Obi,Van Kenobi,88
Leya,Skywalker,91
Anakin,Skywalker,55
"
fp = open("first.csv", "w") # open for writing
fp.write(content)          # write in a single operation, practical for small files
fp.close()
```

Our next task is to read this file in memory as a list of dictionary form, as: `[{"Name": "Han", "Surname": "Solo", "Grade": "80"}, ...]`

We need to read the file line by line, extract the components using the `split()` function, then create the dictionary. Then, we can append it to resulting list. For example:

```
fp = open("first.csv", "r")           # open for reading

line = fp.readline()                 # read column names
line = line.rstrip('\n')             # get rid of new line
colnames = line.split(',')          # list of column names

result = []                         # resulting list of dictionaries
line = fp.readline()
while line != "":
    line = line.rstrip('\n')
    entry = {}                      # start with empty dictionary
    c = 0                           # a counter to address column number
    for v in line.split(','):
        entry[colnames[c]] = v      # in a loop process each column of the row
        c += 1
    result.append(entry)
    line = fp.readline()            # add dictionary to result
                                    # read next line

fp.close()
print(type(result))
print(result)
```

```
<class 'list'>
[{'Name': 'Han', 'Surname': 'Solo', 'Grade': '80'}, {'Name': 'Luke', 'Surname': 'Skywalker', 'Grade': '90'}, {'Name': 'Obi', 'Surname': 'Van Kenobi', 'Grade': '88'}, {'Name': 'Leya', 'Surname': 'Skywalker', 'Grade': '91'}, {'Name': 'Anakin', 'Surname': 'Skywalker', 'Grade': '55'}]
```

Let us improve this example by adding a column as a result of a computation. Let us calculate the grade average and show the difference from the average as a new column. We need to go over all grade values in the list, convert to them real values (so that we can do arithmetic on them), calculate the average, then go over all rows to add a new column. Then, go over the list again to export/write it into a new CSV file.

```

n = 0

# Calculate the average
sum = 0
for entry in result:
    sum += float(entry['Grade'])
    n += 1
average = sum / n

# Calculate the difference of each grade from the average
for entry in result:
    entry['Avgdiff'] = str(float(entry['Grade']) - average)

# Write the updated content into another CSV file
fp = open('second.csv', 'w')
colnames = entry.keys()          # this returns the keys (column names) of the CSV file
fp.write(','.join(colnames) + '\n') # write this as the first line with comma separated values
for entry in result: # Go over each row
    vals = []
    for key in colnames: # Write each column on this row
        vals.append(entry[key])      # extract values of entry, entry.values() is a short version of this
    fp.write(','.join(vals) + '\n')

# Finished, close the file
fp.close()

```

```
%cat second.csv
```

Name	Surname	Grade	Avgdiff
Han	Solo	80	-0.799999999999972
Luke	Skywalker	90	9.200000000000003
Obi	Van Kenobi	88	7.200000000000003
Leya	Skywalker	91	10.200000000000003
Anakin	Skywalker	55	-25.799999999999997

6.7 Formatting Files

Sometimes readability is important for text files, especially if data is in a tabular form. For example, seeing all related data in a column start at the same position can improve readability significantly. The following shows the unformatted and formatted versions of the same data side by side:

Name,Surname,Grade,Avgdiff	Name , Surname , Grade, Avgdiff
Han,Solo,80,-0.799999999999972	Han , Solo , 80, -0.800
Luke,Skywalker,90,9.200000000000003	Luke , Skywalker , 90, 9.200
Obi,Van Kenobi,88,7.200000000000003	Obi , Van Kenobi , 88, 7.200
Leya,Skywalker,91,10.200000000000003	Leya , Skywalker , 91, 10.200
Anakin,Skywalker,55,-25.799999999999997	Anakin , Skywalker , 55,-25.800

In order to achieve this, you can use the `format()` method of a template string as in

```
'{:10}, {:20}, {:3d}, {:f7.3}'.format('Han', 'Solo', 80, -0.2)'.
```

Each {} in the template matches a data value in the arguments. The value after : denotes the (minimum) width of the data. If data fits in a smaller number of characters, spaces are inserted on the right to make it have exactly given size (left-aligned). For integers, the number is followed by a d to format it as a decimal value spaced padded on the left (right aligned). For floating point values, this value can be followed by a ‘.’ and another number and an f. The second number denotes the size of the fraction, f marks this value as a float, and the fraction part is rounded to given number of digits.

The detailed description of format() is out of the scope of this course and the document. For detailed description, please refer to Python reference manuals.

Let us rewrite the output part of the code using formatted output:

```
template = '{:10}, {:20}, {:5d}, {:.7f}\n'
fp = open('third.csv', 'w')
colnames = entry.keys()                                     # this returns the keys of the CSV file
fp.write('{:10}, {:20}, {:5}, {:.7}\n'.format(*colnames))      # write this as the first line with comma
                                                               # separated values
for entry in result:
    fp.write(template.format(entry['Name'], entry['Surname'],           # convert strings to numbers to respect
                                                               # number formatting
                                                               int(entry['Grade']), float(entry['Avgdiff'])))
fp.close()
```

```
# Let us display the content of the file after formatting:
%cat third.csv
```

Name	,	Surname	,	Grade	Avgdiff
Han	,	Solo	,	80	-0.800
Luke	,	Skywalker	,	90	9.200
Obi	,	Van Kenobi	,	88	7.200
Leya	,	Skywalker	,	91	10.200
Anakin	,	Skywalker	,	55	-25.800

6.8 Binary Files

So far, we have only looked at text files where all values are represented as human readable text where all numerical values are represented as decimal strings. However, if you remember our early chapters, computers do not store and process numbers as decimal digit sequences. They store variables in binary format like Two's Complement and the IEEE754 floating point standard. In order to process, read and write decimal data in text, programming language and libraries convert data. Even though you won't notice the time spent in conversion, if you read 10 millions of numbers, you start spending significant amount of CPU time for converting data.

Binary files, on the other hand, store numbers as they are stored in computer's memory. They are still sequences of bytes, but in a more structured way. For example, a 4-byte integer is kept as a sequence of 4 bytes, each byte is a part of the number in Two's Complement form. Reading a binary file is simply copying data to memory, either no conversion is performed or only the order of bytes is changed.

A floating point number 0 takes 1 byte in a text file, but the number 3.1415926535897932384626433832795028 takes 34 bytes. In a binary file, the total size of a number is fixed as the size of IEEE 754 format, i.e. 4 bytes on a 32-bit computer. Both 0 and the π are stored in 4 bytes for single precision, 8 bytes for double precision, in a binary file.

Keeping values in binary files has the following advantages:

1. It is more compact: Data occupies less space in the file.
2. No decimal to binary conversion is required. More efficient in terms of CPU usage.
3. Since sizes are fixed, randomly jumping to a location and reading relevant data is possible. In a text file, you have to start from the beginning and read all lines up to the relevant data. This kind of usage is a more advanced case and harder to understand for beginners.

On the other hand, using text files has the following advantages:

1. Files are human readable and editable. User can change data using a standard editor. In binary files, special software should be used.
2. File format is more flexible, using variablename: value patterns in the file, data can be stored in any order in a flexible way. This is why text files are often used as configuration files.

Most of the special formats with .exe, .xls, .zip, .pdf extensions are binary file formats.

Note: Binary files are kept out of scope of this book. The following paragraphs give couple of pointers for curious readers.

In order to use binary files:

1. You need to add 'b' character in the second argument of open() method as: open('test.bin','rb') or open('test.bin','wb').
2. Binary I/O requires bytes typed values instead of str typed values. bytes is a sequence of bytes. Elements of a byte sequence are not printable in contrast to str.
3. Python has struct module for converting any value into bytes value. struct.pack(format, values) converts values into bytes. However, this conversion is much more cheaper computationally than decimal to binary conversion.
4. struct.unpack(format, bytesval) can be used to convert bytes value into Python values. It is much cheaper than binary to decimal conversion.
5. read(), write() can be used as usual. In read(nbytes), data size should be given. struct.calcsize(format) can be used to calculate data size from format.

The following is an example of binary I/O. Assume the binary file contains an integer N , for the number of points, and followed by $2 \times N$ floating point values. Let us write and then read this data:

```
import struct

points = [(1,1), (2.5, 3.4), (5.4,3.3), (2.2, 1.121)]

# 1- Open and write the binary file
fp = open("points.bin", "wb")
fp.write(struct.pack('i', len(points))) # 'i' denotes a single integer value is converted into bytes

for (x,y) in points:
    fp.write(struct.pack('dd', x, y)) # 'dd' denotes two double precision floating point values are converted into bytes

fp.close()

# 2- Open and read the binary file
fp = open("points.bin", "rb") # open same file for reading
```

(continues on next page)

```

content = fp.read(struct.calcsize('i')) # read binary data with length sizeof integer bytes
(n,) = struct.unpack('i', content)      # unpack returns a tuple, 1tuple in this case

newpoints = []
for i in range(n):                  # n times
    content = fp.read(struct.calcsize('dd'))
    (x,y) = struct.unpack('dd', content) # read two double precision floats
    newpoints += [(x,y)]             # append value at the end

fp.close()

# 3- Print the read and converted values
print("The read & converted points are:", newpoints)

print("This is what binary data looks like:")
fp = open("points.bin", "rb")
print(fp.read())
fp.close()

```

The read & converted points are: [(1.0, 1.0), (2.5, 3.4), (5.4, 3.3), (2.2, 1.121)]

This is what binary data looks like:

```
b'x04x00x00x00x00x00x00x00x00xf0?x00x00x00x00x00xf0?x00x00x00x00x00x00x04@333333x0b@x9ax99x99
xb2x9dxeefx1?'
```

6.9 Note on Files, Directory Organization and Paths

Files are organized under directories so that you can put relevant files under same category together. Operating systems provide a **filesystem hierarchy** consisting of directories (some prefer word **folder** instead) and regular files.

Directories can be arbitrarily nested. You may need to traverse N levels of directories to find your file. For example, your program can be in the Homeworks directory under the Desktop directory under the user directory under the Desktop Users directory under the root directory (/), which is the topmost level on your filesystem. The top-level directory and the separator is backslash, \ in MS Windows operating systems. However, / works in Python for Windows too.

In order to address a file, we use a **path** which is a sequence of directory names separated by /, ended by the name of the file. For example, "/Desktop Users/user/Desktop/Homeworks/homework1.py" is a path for the file named "homework1.py".

A path can be either **full** (absolute) or **relative**. In the former case, it starts with a slash (/). In the relative case, it is considered relative to the current working directory, i.e. the directory where you started your program. Full paths ignore your current directory whereas relative paths depend on it. For example, if you are currently in the Desktop directory, the path "Homeworks/homework1.py" will address the same full path above.

6.10 List of File Class Member Functions

For completeness, below you can find commonly used member functions of the file class.

Assume **F** is a file. In the table below you will find some of the very frequently used member functions of files (in the **Operation** column anything in square brackets denotes that the content is optional – if you enter the optional content, do no type in the square brackets):

Operation	Result
F .seek(*offset[, whence=0*])	Set file F 's position, like stdio's fseek(). <i>whence</i> \square 0 then use absolute indexing (using <i>offset</i>). <i>whence</i> \square 1 then <i>offset</i> relative to current pos. <i>whence</i> \square 2 then <i>offset</i> relative to file end.
F.tell()	Return file F 's current position (byte offset).
F.truncate([size])	Truncate F 's size. If <i>size</i> is present, F is truncated to (at most) that size, otherwise F is truncated at current position (which remains unchanged).
F .write(`str`)	Write string <i>str</i> to file F .
F.writelines(list)	Write <i>list</i> of strings to file F . No EOL are added.
F.close()	Close file F .
F.fileno()	Get fileno (fd) for file F .
F.flush()	Flush file F 's internal buffer.
F.isatty()	1 if file F is connected to a tty-like dev, else 0.
F.next()	Returns the next input line of file F , or raises StopIteration when EOF is hit.
F.read([size])	Read at most <i>size</i> bytes from file F and return as a string object. If <i>size</i> omitted, read to EOF.
F.readline()	Read one entire line from file F . The returned line has a trailing \n, except possibly at EOF. Return "" on EOF.
F.readlines()	Read until EOF with readline() and return a list of lines read.

6.11 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- Sequential access. File access.
- Text files. Reading and writing text files. Parsing a text file.
- End of file, new line.
- Formatting files.
- Binary files and binary file access.

6.12 Further Reading

- String formatting in Python: <https://docs.python.org/3.4/library/string.html#format-spec>
- Working with binary data and files in Python: <https://docs.python.org/3/library/binary.html>
- Comma-Separated Values (CSV) file format: https://en.wikipedia.org/wiki/Comma-separated_values

Exercises

- Write a function that reads a text file with the following format (ignore characters following #):

```
N      # Number of students
      # Empty line
Name Surname # First student
M      # Number of courses that the student has taken
Coursename1: Grade # Grade is a real number
Coursename2: Grade
Coursename3: Grade
...
CoursenameM: Grade

      # Empty line
Name Surname # Second student
P      # Number of courses that the student has taken
Coursename1: Grade # Grade is a real number
Coursename2: Grade
Coursename3: Grade
...
CoursenameP: Grade
...
...
...
      # Empty line
Name Surname # Last student
Z      # Number of courses that the student has taken
Coursename1: Grade # Grade is a real number
Coursename2: Grade
Coursename3: Grade
...
CoursenameZ: Grade
```

- Write a function that writes a list of dictionaries that have the following format into a text file. You may choose to write the number of elements at the top of the file.

```
{ "city": "Ankara",
  "plate code": "06",
  "max temperature (C)": 40,
  "min temperature (C)": -20,
  "population": 5700000
}
```

- Write a function that reads a list of dictionaries from a file that you have written in the previous question.

- Write a function that read the text file given below, represent the same content in binary, save it in a binary file and read it back.

3 0 3.4 2.1 5.1 3.2 EOLIST 1 1.5 2.0 2.5

7 | Error Handling and Debugging

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As Turkish song says “*There is no servant without fault, love me with the faults I have*”, we all make mistakes and programming is far from being an exception to this. It is a highly technical, error-intolerant task requiring full attention from the programmer. Even a single letter you mistype can produce in complete opposite of what you aim to get. The history of computing is full of examples on large of amounts of money wasted on small programming mistakes (banks losing millions due to penny roundings, satellites turning into most expensive fireworks, robots bricked on Mars surface etc). Even worse, lives of some people can depend on proper functioning of a program.

For this reason, writing programs as error free as possible is an important challenge and responsibility for a programmer. Programming errors can be classified in three groups:

1. Syntax errors
2. Run-time errors
3. Logical errors

7.1 Types of Errors

7.1.1 Syntax Errors

Syntax errors are due to strict wellformedness requirements of programming languages. In a natural language essay, we can use no punctuation at all, we can use silly abbreviations, mix the ordering of words, make typing mistakes and still it will make sense to a reader (though your English teacher might reduce some points).

Computer programs are entirely different. When a programming language specification tells you to define blocks based on indentation, to match parentheses properly, to follow certain statements with some certain punctuation (i.e. loops and functions and :), you have to obey that. Because our compilers and interpreters cannot convert a program with syntax errors into a machine understandable form.

The first step of the Python interpreter reading your program is to break it up into parts and construct a machine-readable structure out of it. If it fails, you will get a syntax error, for example:

```
>>> for i in range(10)
...     print(i)
```

File "<ipython-input-1-12d72cac235a>", line 1

(continues on next page)

```
for i in range(10)
^
SyntaxError: invalid syntax
```

```
>>> x = float(input())
>>> a = ((x+5)*12+4
File "<ipython-input-2-dead5b360d91>", line 2
    a = ((x+5)*12+4
^
SyntaxError: invalid syntax
```

```
>>> s = 0
>>> for i in range(10):
...     s += i
...     print(i)
File "<ipython-input-3-c3ef5d622e47>", line 4
    print(i)
^
IndentationError: unexpected indent
```

```
>>> while x = 4:
...     s += x
File "<ipython-input-4-befcf7769cec>", line 1
    while x = 4:
^
SyntaxError: invalid syntax
```

In the examples above, syntax errors are:

1. `:` is missing at the end of the for loop.
2. The first parenthesis does not have a matching closing parenthesis.
3. Different indentation levels are used in the loop body.
4. `while` expects a boolean expression but an assignment is given (`=` is used instead of `==`).

These are only a small sample of large number of possible syntax errors one can do.

Syntax errors are the most innocent errors since you are notified of the error immediately when you start running your program. Running your program once will give you the exact spot (though, sometimes parentheses and quote matching can be non-trivial) in the error output. If you have learnt the syntax of your language, you can fix it with a small effort.

7.1.2 Type errors

Python is an interpreted language and it does not make strict type checks like a compiler would check type compatibility at compile time. Though, when it comes to performing an operation that is not compatible with the current type of a variable/data, Python will complain. For example, when you try to override a string element with an integer value, use an integer on a string context, select an element out of a float variables etc., you will get an error:

```
astr = 'hello'  
bflt = 4.56  
cdict = {'a':4, 'b':5}  
  
print(astr ** 3)      # second power of a string  
print(bflt[1])       # select first member of a float  
print(cdict * 2)     # multiply a dictionary by two  
cdict < astr        # compare a dictionary with a string
```

These will lead to the following errors:

```
>>> print(astr ** 3)  
Traceback (most recent call last):  
  File "<stdin>", line 1, in <module>  
TypeError: unsupported operand type(s) for ** or pow(): 'str' and 'int'  
>>> print(bflt[1])  
Traceback (most recent call last):  
  File "<stdin>", line 1, in <module>  
TypeError: 'float' object is not subscriptable  
>>> print(cdict * 2)  
Traceback (most recent call last):  
  File "<stdin>", line 1, in <module>  
TypeError: unsupported operand type(s) for *: 'dict' and 'int'  
>>> cdict < astr  
Traceback (most recent call last):  
  File "<stdin>", line 1, in <module>  
TypeError: '<' not supported between instances of 'dict' and 'str'
```

Compiled languages and some interpreters enforce type compatibility at compile time and treat all such errors as if they are syntax errors, providing a safer programming experience at run time. However, Python and most other interpreters wait until command is first executed and raise the error at the execution time, causing a **run-time error**.

7.1.3 Run-Time Errors

Run-time errors are more sneaky compared to syntax and other compile-time errors. Your program starts to execute silently, visit many loops and functions without an error, produce some intermediate output, and suddenly, in the most unexpected moment, it raises an error and you get a disappointing error text instead of the decent result output that you expected.

The following example gets an input value and counts how many of the integers in the range [1, 1000] are divisible by the input value.

```
def divisible(m, n):  
    return m % n == 0
```

(continues on next page)

```

def count(m):
    sum = 0
    for i in range(1,1000):
        if divisible(i, m):
            sum += 1

    return sum

value = int(input())
print('input value is:', value)
print(value, ' divides ', count(value), ' many integers in range [1, 1000]')

```

It works without any problem for non-zero input values. However if you enter 0, it outputs:

```

input value is: 0
-----
ZeroDivisionError                                     Traceback (most recent call last)

  in ()
      12 value = int(input())
      13 print('input value is:', value)
-> 14 print(value, ' divides ', count(value), ' many integers in range [1, 1000'])

  in count(m)
      5     sum = 0
      6     for i in range(1,1000):
-> 7         if divisible(i,m):
      8             sum += 1
      9

  in divisible(m, n)
      1 def divisible(m, n):
-> 2     return m % n == 0
      3
      4 def count(m):
      5     sum = 0

ZeroDivisionError: integer division or modulo by zero

```

Fig. 7.1.1: A traceback example.

This output is called error **Traceback**. When a run-time error occurs, you will get one of these and the execution of the program will be terminated. Depending on the settings, the output may be more brief but you will get line numbers and the line leading to the error.

The reason for this example error is called an **Exception** and colored red in the above output. It is given in the first line and repeated with explanation in the last line. Traceback also reports the functions involving the error, from the outermost to the innermost. Each arrow (colored green) marks the program line causing the error. The last item in the traceback is the actual position where the error occurred; the 2nd line having `return m % n == 0` in this case. The `divisible()` function containing the error line is called by the 7th line, the `count()` function, which is called by 14th line of the program. By looking at the error output, you will see the whole chain of calls that lead your program to the error state. The last one is the most important one, where Python tried to execute an operation and failed.

The reason for failure is `ZeroDivisionError` in this case. If you trace the program with input value 0, you will see that Python tried to evaluated `m % 0 == 0` for some m value. The remainder operator is division based

and dividing something by 0 is impossible mathematically. All programming languages reject this operation by a run-time error, and this is the Python style.

The following are the most common exceptions and run-time errors in Python:

Exception	Reason
KeyboardInterrupt	User presses Ctrl-C; not an error but user intervention
ZeroDivisionError	Right-hand side of / or % is 0
AttributeError	Object/class does not have a member
EOFError	input() function gets End-of-Input by user
IndexError	Container index is not valid (negative or larger than length)
KeyError	dict has no such key
FileNotFoundException	The target file of open() does not exist
TypeError	Wrong operand or parameter types, or wrong number of parameters for functions
ValueError	The given value has correct type but the operation is not supported for the given value

The following code illustrates each of these errors (except for the user-generated ones):

```
b = 0
a = a / b      # ZeroDivisionError

x = [1,2,3]
print(x.length)    # AttributeError: lists does not have a length attribute (use len(x))

print(x[4])      # IndexError: last valid index of list x is 2

person = { 'name' : 'Han', 'surname': 'Solo' }
print(person['Name'])  # KeyError: person does not have 'Name' key but 'name'

fp = open("example.txt") # FileNotFoundError: file "example.txt" does not exist

print([1,2,3] / 12)    # TypeError: Division is not defined for lists

def f(x, y):
    return x*x+y

print(f(5))      # TypeError: Only one element is supplied instead of 2.

print(int('thirtytwo')) # ValueError: string value does not represent an integer

a,b,c=[1,2,3,4]    # ValueError: too many values on the right hand side
```

7.1.4 Logical Errors

This is the worst among all errors because Python does not raise an error. It single-mindedly keeps running your program; however, your program has a mistake about what it intends to compute. In other words, it simply does not do what it is supposed to do because of an error.

Such an error can be due to a small typo, improper nesting of blocks, bad initialization of variables, and many other reasons. However, the code segment containing the error has correct syntax and hence, it does not cause a run-time error. As a result, you will not know such an error exists until you see some problems in your output.

The following are a few examples for logical errors:

```
y = x / x+1      #you meant y = x / (x+1), forgetting about precedence

lastresult = 0
def missglobal(x):
    result = x*x+1      #you intend to update the global variable
    if lastresult != result:  #but you assign a local variable instead
        lastresult = result  #you should have used "global lastresult"

def returnsnothing(x, y):
    y = x*x+y*y
    if x <= y:
        return x      #if x > y, the function returns nothing
    print(returnsnothing(0.1, 0.1))  #does not have any value. prints "None"

s = 1
while i < n:      #you forgot incrementing i as i+=1
    s += s*x/i      #loop will run forever. "infinite loop"
```

7.2 How to Work with Errors

Errors are unavoidable in programming. As you get experience, they will decrease but they will still be there. Fortunately, we have methods to have less errors but completely getting rid of them is not possible.

The following is a list of strategies for eliminating errors:

1. Program with care
2. Place controls in your code
3. Handle exceptions
4. Write verification code and raise exceptions
5. Debug your program
6. Write test cases

Those strategies can be applied by programmers with different experience levels. In the extreme case, assuring quality of programs and software testing are important professions of the software engineering discipline and handled by dedicated engineers.

7.2.1 Program with Care

The best way to write error-free programs is not to cause one in the first place. Instead of cleaning your living room every day, you may just choose not to throw garbage around. Programming is similar, the great percentage of errors are due to the careless acts of a programmer.

Programming is **not** an evolutionary process where you start from an ugly code and make it better and better as you correct errors. This way of programming is possible but not efficient. You better spend some time before starting to write code to design your solution and develop a strategy: which functions you need, which data structures you use, which algorithms you use, and which order you will write the code. It is a good practice to divide your problem into pieces (functions for example). Write one function at a time and test it before going into the next step.

This strategy will get better as you become a more experienced programmer but nothing stops you from paying more attention on your first day of coding.

7.2.2 Place Controls in Your Code

The values that a variable can have or a function may return are not known in advance. Especially, what input user may provide is completely untrustable. Also, there are other environmental issues like existence of a file.

If you have such an untrustable value, the next operation may fail as a result of it like:

```
a = [1,2,3]
age = {'Han': 30, 'Leia': 20, 'Luke': 20}

# CASE 1
n = int(input())
print(a[n])      # will fail for n > 2 or n < -2

# CASE 2
name = input()
print(age[name])  # will fail names other than 'Han', 'Leia', 'Luke'

# CASE 3
x = float(input())
y = math.sqrt(x)  # will fail for x < 0
y = 1 / x        # will fail for x == 0
```

In order to deal with such errors, you can check all values, especially user supplied ones. Checking all input values before starting a computation is called **Input Sanitization**.

```
# CASE 1 with sanitization
n = int(input())
if 0 <= n < len(a):
    print(a[n])
else:
    print("n is not valid:", n)

# CASE 2 with sanitization
name = input()
if name in age:  # membership test for dictionaries
    print(age[name])
```

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```

else:
    print("dictionary does not have member:", name)

# CASE 3 with sanitization
x = float(input())
if x >= 0:
    y = math.sqrt(x)
else:
    print("invalid for sqrt operation: ", x)

if x != 0:
    y = 1 / x
else:
    print("divisor cannot be 0")

```

Writing such conditions look like a tedious job at first, but dealing with them while your program is running is much worse for users. If you are writing a program that will be really useful, you have to do these types of input checks.

7.2.3 Handle Exceptions

This is an alternative to putting check conditions in your code. Sometimes there are too many conditions, one for each step of your computation, so that each line of code opens a new if block and nests like the branches of a tree. Instead of writing whole nested-sequence of if ... else statements, exceptions give you a chance to handle all errors in the same place. Especially, they allow you to handle the errors in the caller function rather than the original place where error occurred. Before we can see how this works, we have to learn a new syntax first:

```

try:
    .... # a block with possible errors
    .... # if there are function calls here
    .... # and error occurs in the function, we can handle error here
except exceptionname: # exceptionname is optional
    .... # this is error handling block.
    .... # when there is an error, execution jumps here

```

This try-except block has two parts: A group of code (after try:) that possibly generates run-time errors and a second or more blocks to handle the errors. When the first error occurs in the try part, the execution jumps to the except part. If except part matches the corresponding block, it is executed. Multiple except blocks are allowed for different kinds of exceptions. except :, without an exception name, matches all errors and can be used to handle all of them one block.

The following is the same example in the previous section, but errors are handled in the same place.

```

import math

a = [1,2,3]
age = {'Han': 30, 'Leia': 20, 'Luke': 20}

try:
    n = int(input())

```

(continues on next page)

```

print(a[n])      # will fail for n > 2 or n < -2

name = input()
print(age[name])  # will fail names other than 'Han', 'Leia', 'Luke'

x = float(input())
y = math.sqrt(x)  # will fail for x < 0
y = 1 / x        # will fail for x == 0

except IndexError:
    print('List index is not valid')
except KeyError:
    print('Dictionary does not have such key')
except ValueError:
    print('Invalid value for square root operation')
except ZeroDivisionError:
    print('Division by zero does not have value')
except:
    print('None of the known errors. Something happened even if nothing happened')

```

None of the known errors. Something happened even **if** nothing happened

You can try the above example with different inputs:

1. -1
2. 2 'Obi'
3. 2 'Han' -2
4. 2 'Han' 0
5. 2 'Han' 1

The first will have `a[n]` raise an `IndexError`. The second will have `age[name]` raise a `KeyError`. The third will have `sqrt(x)` raise a `ValueError`. The fourth will have `1 / x` raise a `ZeroDivisionError`. The last one will have no error and finish the try block and continue with the next instruction jumping over except blocks. You can also create exceptions with `raise` statement. `raise ValueError` will create the error.

Exceptions save you from nested if .. else statements for data validation, e.g.:

```

if cond1:
    ..1..
    if cond2:
        ..2..
        if cond3:
            ..3..
            ..4..  # success at last
    else:
        # report error
else:
    # report error
else:
    # report error

```

is harder to read compared to the following:

```

try:
    if !cond1:
        raise Error

..1..

if !cond2:
    raise Error

..2..

if !cond3:
    raise Error

..3..
..4.. # success
except :
    ... Error handling

```

which is more flat and allows you to focus on the actual code.

7.2.4 Write verification code and raise exceptions

Even if you sanitize user input and check all arguments for valid values, your program can still have logical errors and it might calculate incorrect intermediate/final values. If your program consists of multiple steps, a logical error in step one will cause step two to calculate an incorrect value and this will create a *snowball effect*, potentially causing all steps and the last to fail.

For example, you wrote a function for solving second-order equations $ax^2 + bx + c = 0$, named it `solvesecond(a,b,c)` which returns (x_1, x_2) as the roots. You are (*almost*) sure that you always send correct a,b,c values to this function. However, it won't hurt if you add a check like the following:

```

def solvesecond(a,b,c):
    det = b*b - 4*a*c
    # the following is the verification code
    if det < 0:
        print("Equation has no real roots for", a, b, c)
        raise ValueError
    ....
    ...

```

The `math.sqrt` function would have raised the exception anyway. However, you add extra error message about what caused the problem. Also, in logical errors, there is no run-time error and this error may be as serious as finding imaginary roots.

7.2.5 Debug Your Code

Finding the position and the cause of a programming error and fixing it is called **debugging**. It involves pinpointing the position of the error, reasons causing the error and updating the code so that it does not cause the error any more.

Debugging methods are explained in detail in its own section below.

7.2.6 Write Test Cases

In order to make sure your program is working properly, in other words, it contains no logical errors, you need to test it. Testing is an important yet non-trivial part of all engineering disciplines.

In order to test a program, you should create a set of inputs, run your program for each input case and collect the outputs. If there is a way of verifying the outputs, you can verify them. For example, if you solve an equation, you substitute the found variable in the equation to test if it holds:

```
(x1, x2) = findrootsecond(a,b,c)

if a*x1*x1 + b*x1 + c != 0 or a*x2*x2 + b*x2 +c != 0:
    print('test failed for', a, b, c, 'roots', x1, x2)
```

You can generate millions of such numbers and automatically verify them.

If the problem is not verifiable, you can get a set of known solutions and compare your solutions against the known solutions.

7.3 Debugging

Debugging is an act of looking for errors in a code, finding what causes the errors and correcting them. As even the modest programs can go as large as hundreds of lines of code, debugging is not an easy task. Even if a run-time error gives you the exact location of the error, the variable value causing the error can be owing to a different place in your code and you will not get the variable state of the program at the moment.

Debugging is an iterative activity. You divide your program into parts and eliminate each part one by one, ruling out the error: Narrow down all possibilities step by step to find the exact step where you made the mistake. Run-time errors help you speed-up this process.

There are several methods for debugging. A programmer may use one or more of them for debugging.

The following is a sample program with an error (you may check the Colab link and run this interactive example):

```
def startswith(srcstr, tarstr):
    "check if tarstr starts with srcstr
    like srcstr="abra" tarstr="abracadabra"
    for i in range(len(srcstr)): # check all characters of srcstr
        if srcstr[i] != tarstr[i]: # if does not match return False
            return False
    return True # if False is not returned yet, it matches
```

(continues on next page)

```
def findstr(srcstr, tarstr):
    "Find position of srcstr in tarstr"
    for i in range(len(tarstr)):
        # if srcstr is same as tarstr from i to rest
        # return i
        if startswith(srcstr, tarstr[i:]):
            return i
    return -1

print(findstr("ada", "abracadabra"))
print(findstr("aba", "abracadabra"))
```

which outputs the following when run:

```
5
-----
IndexError                                Traceback (most recent call last)
<ipython-input-3-b00405b7708c> in <module>()
    18
    19 print(findstr("ada", "abracadabra"))
--> 20 print(findstr("aba", "abracadabra"))

1 frames
<ipython-input-3-b00405b7708c> in startswith(srcstr, tarstr)
    3     like srcstr="abra" tarstr="abracadabra" "
    4     for i in range(len(srcstr)): # check all characters of srcstr
--> 5         if srcstr[i] != tarstr[i]: # if does not match return False
    6             return False
    7     return True # if False is not returned yet, it matches

IndexError: string index out of range
```

The first call returns 5, which is printed on screen, telling us that "ada" is at position 5 of "abracadabra", matches after "abrac". However, the second call should return -1 since the "aba" substring does not exist in "abracadabra" but it generates an error.

7.3.1 Debugging Using Debugging Outputs

This is one of the simplest, oldest but still an effective method for debugging a program. In this method, you add extra output lines that shed light on the behaviour of your program. This way, you can trace where your program diverted from the expected behaviour. For example (you may check the Colab link and run this interactive example):

```
def startswith(srcstr, tarstr):
    "check if tarstr starts with srcstr
    like srcstr="abra" tarstr="abracadabra" "
    for i in range(len(srcstr)): # check all characters of srcstr
        print("check if ", srcstr, '!=', tarstr, 'for i=', i)
        if srcstr[i] != tarstr[i]: # if does not match return False
            return False
    return True # if False is not returned yet, it matches
```

(continues on next page)

```

def findstr(srcstr, tarstr):
    "Find position of srcstr in tarstr"
    for i in range(len(tarstr)):
        # if scrstr is same as tarstr from i to rest
        # return i
        print("calling startswith", srcstr, tarstr[i:])
        if startswith(srcstr, tarstr[i:]):
            return i
    return -1

print(findstr("aba", "abracadabra"))

```

which outputs the following when run:

```

calling startswith aba abracadabra
check if aba != abracadabra for i= 0
check if aba != abracadabra for i= 1
check if aba != abracadabra for i= 2
calling startswith aba bracadabra
check if aba != bracadabra for i= 0
calling startswith aba racadabra
check if aba != racadabra for i= 0
calling startswith aba acadabra
check if aba != acadabra for i= 0
check if aba != acadabra for i= 1
calling startswith aba cadabra
check if aba != cadabra for i= 0
calling startswith aba adabra
check if aba != adabra for i= 0
check if aba != adabra for i= 1
calling startswith aba dabra
check if aba != dabra for i= 0
calling startswith aba abra
check if aba != abra for i= 0
check if aba != abra for i= 1
check if aba != abra for i= 2
calling startswith aba bra
check if aba != bra for i= 0
calling startswith aba ra
check if aba != ra for i= 0
calling startswith aba a
check if aba != a for i= 0
check if aba != a for i= 1
-----
```

```

IndexError                                     Traceback (most recent call last)
<ipython-input-6-b415ffe46a64> in <module>()
  19     return -1
  20
--> 21 print(findstr("aba", "abracadabra"))


```

```

1 frames
<ipython-input-6-b415ffe46a64> in findstr(srcstr, tarstr)
  15     # return i
  16     print("calling startswith", srcstr, tarstr[i:])

```

(continues on next page)

```

--> 17     if startswith(srcstr, tarstr[i]):
18         return i
19     return -1

<ipython-input-6-b415ffe46a64> in startswith(srcstr, tarstr)
    4   for i in range(len(srcstr)): # check all characters of srcstr
    5       print("check if ", srcstr, '!=', tarstr, 'for i=', i)
--> 6       if srcstr[i] != tarstr[i]: # if does not match return False
    7           return False
    8   return True # if False is not returned yet, it matches

```

IndexError: string index out of range

In the output, you can see that execution failed after output “check if aba != a for i= 1”. Therefore, we can reason that an error occurred at the next step. The following test is:

```
if srcstr[i] != tarstr[i] for "aba" and "a" for i = 1.
```

Apparently, getting tarstr[1] for tarstr == "a" fails since the length of tarstr is 1 and the only valid index is 0. There are different ways to get rid of this error. One quick solution is to test if lengths of srcstr and tarstr are compatible as len(tarstr) >= len(srcstr) should hold in startswith. The programmer should have considered this and handled this case. Now, we can correct it as a result of our debugging session.

Of course, debugging output should be added in the correct places with sufficient descriptive information. If you add too much debugging output, you may be lost in output lines. If there is not sufficient output, you may not find the error.

For generic tracing of programs with multiple functions, you can use the following Python magic called **decorator**, which reports all function calls with parameters when a function is decorated as (you may check the Colab link and run this interactive example):

```

def tracedec(f):
    def traced(*p, **kw):
        print(' ' * tracedec.level + "->", f.__name__, '(p, kw)')
        tracedec.level += 1
        val = f(*p, **kw)
        tracedec.level -= 1
        print(' ' * tracedec.level + "<-", f.__name__, 'returns', val)
        return val
    return traced
tracedec.level = 0

```

```

@tracedec
def startswith(srcstr, tarstr):
    "check if tarstr starts with srcstr
    like srcstr="abra" tarstr="abracadabra" "
    for i in range(len(srcstr)): # check all characters of srcstr
        if srcstr[i] != tarstr[i]: # if does not match, return False
            return False
    return True # if False is not returned yet, it matches

```

```

@tracedec
def findstr(srcstr, tarstr):
    "Find position of srcstr in tarstr"
    for i in range(len(tarstr)):

```

(continues on next page)

```
# if scrstr is same as tarstr from i to rest
# return i
if startswith(srcstr, tarstr[i:]):
    return i
return -1

print(findstr("aba", "abracadabra"))
```

which outputs the following when run:

```
-> findstr (('aba', 'abracadabra') {})
-> startswith (('aba', 'abracadabra') {})
<- startswith returns False
-> startswith (('aba', 'bracadabra') {})
<- startswith returns False
-> startswith (('aba', 'racadabra') {})
<- startswith returns False
-> startswith (('aba', 'cadabra') {})
<- startswith returns False
-> startswith (('aba', 'adabra') {})
<- startswith returns False
-> startswith (('aba', 'dabra') {})
<- startswith returns False
-> startswith (('aba', 'abra') {})
<- startswith returns False
-> startswith (('aba', 'bra') {})
<- startswith returns False
-> startswith (('aba', 'ra') {})
<- startswith returns False
-> startswith (('aba', 'a') {})

IndexError                                Traceback (most recent call last)
<ipython-input-2-f5cc3f720290> in <module>()
      30
      31
---> 32 print(findstr("aba", "abracadabra"))

3 frames
<ipython-input-2-f5cc3f720290> in traced(*p, **kw)
      3     print(' * tracedec.level + "->", f.__name__, '(', p, kw, ')')
      4     tracedec.level += 1
----> 5     val = f(*p, **kw)
      6     tracedec.level -= 1
      7     print(' * tracedec.level + "<-", f.__name__, 'returns ', val)

<ipython-input-2-f5cc3f720290> in findstr(srcstr, tarstr)
      25     # if scrstr is same as tarstr from i to rest
      26     # return i
---> 27     if startswith(srcstr, tarstr[i:]):
      28         return i
      29 return -1
```

(continues on next page)

```
<ipython-input-2-f5cc3f720290> in traced(*p, **kw)
  3     print(' * tracedec.level + "->", f.__name__, '(,p, kw,)')
  4     tracedec.level += 1
---> 5     val = f(*p, **kw)
  6     tracedec.level -= 1
  7     print(' * tracedec.level + "<-", f.__name__, 'returns ', val)
```

```
<ipython-input-2-f5cc3f720290> in startswith(srcstr, tarstr)
  15     like srcstr="abra" tarstr="abracadabra" ""
  16     for i in range(len(srcstr)): # check all characters of srcstr
---> 17         if srcstr[i] != tarstr[i]: # if does not match return False
  18             return False
  19     return True # if False is not returned yet, it matches
```

IndexError: string index out of range

Putting ‘@tracedec’ before function definitions will give you the entry and return states of these functions. How this decorator works and the ‘@’ syntax are far beyond the scope of this book. You may adapt and use this example if it suits you.

7.3.2 Handle the Exception to Get More Information

One problem with the run-time errors is that they do not give information about the current state of the program, basically the set of variables. They give the traceback which includes the line causing the exception and how program came to that state (which functions are active). In order to get the values of the variables, you can handle the exception and add log output to the handler as follows (you may check the Colab link and run this interactive example):

```
def startswith(srcstr, tarstr):
    "check if tarstr starts with srcstr
     like srcstr="abra" tarstr="abracadabra" "
    try:
        for i in range(len(srcstr)): # check all characters of srcstr
            if srcstr[i] != tarstr[i]: # if does not match return False
                return False
    except IndexError:
        print('Error: srcstr: ', srcstr, ', tarstr: ', tarstr, ', i:', i)
        raise IndexError      # if you like, generate an additional exception
    return True # if False is not returned yet, it matches

def findstr(srcstr, tarstr):
    "Find position of srcstr in tarstr"
    for i in range(len(tarstr)):
        # if scrstr is same as tarstr from i to rest
        # return i
        if startswith(srcstr, tarstr[i:]):
            return i
    return -1

findstr("aba", "abracadabra")
```

which outputs the following when run:

```
Error: srcstr: aba , tarstr: a , i: 1
```

```
-----  
IndexError          Traceback (most recent call last)  
<ipython-input-11-b4556283ff77> in startswith(srcstr, tarstr)  
  5     for i in range(len(srcstr)): # check all characters of srcstr  
----> 6         if srcstr[i] != tarstr[i]: # if does not match return False  
  7             return False
```

```
IndexError: string index out of range
```

During handling of the above exception, another exception occurred:

```
-----  
IndexError          Traceback (most recent call last)  
2 frames  
<ipython-input-11-b4556283ff77> in startswith(srcstr, tarstr)  
  8     except IndexError:  
  9         print('Error: srcstr: ',srcstr, ', tarstr: ', tarstr, ', i:',i)  
---> 10     raise IndexError      # if you like generate error again  
 11     return True    # if False is not returned yet, it matches  
 12
```

```
IndexError:
```

This way, we get the output:

```
Error: srcstr: aba , tarstr: a , i: 1
```

which gives us the state of the variables at the moment of the error.

7.3.3 Use Python Debugger

All programming environments come with a **debugger software** which helps a programmer to execute a program step by step, observe the current state, add break-points (stops) to inspect, and provide a controlled execution environment.

For compiled languages, debuggers are external programs getting user's program as input. For Python, it is a module called **pdb**, which stands for *Python DeBugger*. If you use an integrated development environment (IDE), a debugger is embedded in the tool so you can use it via the graphical user interface controls. Otherwise, you can use the command line interface.

In the command line, the only thing you need to do is to put:

```
import pdb
```

at the beginning of your program, and type:

```
pdb.set_trace()
```

at any place you like to stop execution and go into the **debugging mode***. When you run your program or call a function, your program will start executing and when the execution hits one of the trace points, execution will stop and a debugger prompt ((Pdb)) will be displayed:

```
> <ipython-input-14-110393975fb5>(7)startswith()
-> for i in range(len(srcstr)): # check all characters of srcstr
(Pdb) h
```

Documented commands (type help <topic>):

```
=====EOF c d h list q rv undisplay
a cl debug help ll quit s unt
alias clear disable ignore longlist r source until
args commands display interact n restart step up
b condition down j next return tbreak w
break cont enable jump p retval u whatis
bt continue exit l pp run unalias where
```

Miscellaneous help topics:

```
=====exec pdb
```

The first line tells which function and line execution have been stopped. When h or help is typed, the following help lines are displayed. Single-two letter commands are abbreviated forms of the longer ones (e.g. a for args, b for break, c for cont, cl for clear, ...).

After this point, you can use next (n) to execute the program line by line. If the current statement has a function call, you may choose to go into the function call using the step (s) command. Otherwise, next will call and return it in single step. During debugging, print (p) command can be used to print content of a variable. The following is a summary of the useful commands of the debugger:

Command	Description
next	Execute current line and stop at the next statement, jump over functions
step	Execute current line, if there is a function go into it
args	show arguments of the current function
break	Add a new breakpoint. Execution will stop at that line too
clear	Remove the breakpoint(s)
cont	Continue execution until hitting a break point
print	print current value of the variable
display	display variable value whenever it changes in current function
list	list program in current line
ll	list current function
return	continue execution until current function returns
where	show currently active functions, which function calls brought code here

The following is an example run (you may check the Colab link and run this interactive example):

```
import pdb

def startswith(srcstr, tarstr):
    """check if tarstr starts with srcstr
    like srcstr="abra" tarstr="abracadabra" """
    pdb.set_trace()
    for i in range(len(srcstr)): # check all characters of srcstr
        if srcstr[i] != tarstr[i]: # if does not match return False
            return False
```

(continues on next page)

```

return True # if False is not returned yet, it matches

def findstr(srcstr, tarstr):
    "Find position of srcstr in tarstr"
    for i in range(len(tarstr)):
        # if scrstr is same as tarstr from i to rest
        # return i
        if startswith(srcstr, tarstr[i:]):
            return i
    return -1

print(findstr("aba", "abra"))

```

which outputs the following when run:

```

><ipython-input-18-bf80973a0bf6>(7)startswith()
-> for i in range(len(srcstr)): # check all characters of srcstr
(Pdb) cont
><ipython-input-18-bf80973a0bf6>(7)startswith()
-> for i in range(len(srcstr)): # check all characters of srcstr
(Pdb) help

```

Documented commands (`type help <topic>`):

```

=====
EOF  c      d      h      list   q      rv      undisplay
a      cl     debug  help   ll     quit   s       unt
alias clear  disable ignore longlist r      source until
args   commands display interact n      restart step up
b      condition down j      next   return tbreak w
break cont   enable jump   p      retval u      whatis
bt    continue exit  l      pp     run    unalias where
bt
=====
```

Miscellaneous help topics:

```

=====
exec pdb

(Pdb) cont
><ipython-input-18-bf80973a0bf6>(7)startswith()
-> for i in range(len(srcstr)): # check all characters of srcstr
(Pdb) cont
><ipython-input-18-bf80973a0bf6>(7)startswith()
-> for i in range(len(srcstr)): # check all characters of srcstr
(Pdb) cont
=====

IndexError          Traceback (most recent call last)
<ipython-input-18-bf80973a0bf6> in <module>()
  20 return -1
  21
--> 22 print(findstr("aba", "abra"))

1 frames
<ipython-input-18-bf80973a0bf6> in findstr(srcstr, tarstr)
  16     # if scrstr is same as tarstr from i to rest
  17     # return i
=====
```

(continues on next page)

```

--> 18     if startswith(srcstr, tarstr[i:]):
19         return i
20     return -1

<ipython-input-18-bf80973a0bf6> in startswith(srestr, tarstr)
    5     like srcstr="abra" tarstr="abracadabra" ""
    6     pdb.set_trace()
----> 7     for i in range(len(srcstr)): # check all characters of srcstr
    8         if srestr[i] != tarstr[i]: # if does not match return False
    9             return False

```

IndexError: string index out of range

Debuggers are powerful tools especially when you have complex code interacting with many modules and functions. However, you need time to master and control it. The good news is if you use an integrated development interface, they are easier to control.

7.4 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- Different types of errors: Syntax, type, run-time and logical errors.
- How to deal with errors.
- Exceptions and exception handling.
- Debugging by “printing” values, exception handling and a debugger.

7.5 Further Reading

- Python’s built-in exceptions: <https://docs.python.org/3/library/exceptions.html>
- Python’s document on errors and exceptions: <https://docs.python.org/3/tutorial/errors.html>

8 | Scientific and Engineering Libraries

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In this chapter, we will cover several libraries that are very functional in scientific & engineering-related computing problems. In order to keep our focus on the practical usages of these libraries and considering that this is an introductory textbook, the coverage in this chapter is in not intended to be comprehensive.

8.1 Numerical Computing with NumPy

NumPy can be considered as a library for working with vectors and matrices. NumPy calls vectors and matrices as *arrays*.

Installation Notes

To be able to use the NumPy library, you will need to download it from numpy.org and install it on your computer. If you are using a Python package manager (e.g. pip), you can install it directly using: \$ pip install numpy. Note that if you are using Colab or another Jupyter Notebook viewer, the platform may already have numpy installed.

8.1.1 Arrays and Their Basic Properties

Let us consider a simple vector and a matrix:

$$\text{array1} = \begin{pmatrix} 1 & 2 & 3 \end{pmatrix} \quad (8.1.1)$$

and

$$\text{array2} = \begin{pmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \end{pmatrix} \quad (8.1.2)$$

Let us see how we can represent and work with these two arrays in NumPy:

```
>>> import numpy as np      # Import the NumPy library
>>> array1 = np.array([1, 2, 3])
>>> array2 = np.array([[1, 2, 3], [4, 5, 6]])
>>> type(array1)
<class 'numpy.ndarray'>
>>> type(array2)
<class 'numpy.ndarray'>
```

(continues on next page)

```
>>> array1
array([1, 2, 3])
>>> array2
array([[1, 2, 3],
       [4, 5, 6]])
>>> print(array2)
[[1 2 3]
 [4 5 6]]
```

We see from this example that we can pass lists of numbers as arguments to `np.array` function which creates a NumPy array for us. If the argument is a nested list, each element of the list is used as a row of a 2D array.

Arrays can contain any data type as elements; however, we will limit ourselves to numbers (integers and real numbers) in this chapter.

Shapes, Dimensions and Number of Elements of Arrays. The first thing we can do with a NumPy array is check its shape. For our example `array1` and `array2`, we can do so as follows:

```
>>> array1.shape
(3,)
>>> array2.shape
(2,3)
```

where we can see that `array1` is a one-dimensional array with 3 elements and `array2` is a 2×3 array (a 2D matrix).

For a 2D array, a shape value (R, C) denotes the number of rows first (R), which is sometimes also called the first dimension, and then the number of columns (C), which is the second dimension. For n D arrays with $n > 2$, the meaning of the shape values is the same except that there are n values in the shape.

In NumPy, we can easily change the shape of an array without losing content:

```
>>> array1.reshape((3,1))
array([[1],
       [2],
       [3]])
>>> array2.reshape((1,6))
array([[1, 2, 3, 4, 5, 6]])
```

For many applications, we will need to access the number of dimensions of an array. For this purpose, we can use `.ndim` value:

```
>>> array1.ndim
1
>>> array2.ndim
2
```

The number of elements in an array is another important value that we are frequently interested in. To access that, we can use the `.size` value:

```
>>> array1.size
3
>>> array2.size
6
```

Accessing elements in arrays. NumPy allows the same indexing mechanisms that you can use with Python's native container data types. For NumPy, let us look at some examples:

```
>>> array1[-1]
3
>>> array2[1][2]
6
>>> array2[-1]
array([4, 5, 6])
```

Creating arrays. We have already seen that we can create arrays using the `np.array()` function. However, there are other ways for creating arrays conforming to predefined specifications. We can for example create arrays filled with zeros or ones (note that the argument is a tuple describing the shape of the matrix):

```
>>> np.zeros((3, 4))
array([[0., 0., 0., 0.],
       [0., 0., 0., 0.],
       [0., 0., 0., 0.]])
>>> np.ones((2,6))
array([[1., 1., 1., 1., 1., 1.],
       [1., 1., 1., 1., 1., 1.]])
```

Alternatively, we can create an array filled with a range of values using `np.arange()` function:

```
>>> np.arange(1,10) # 1: starting value. 10: ending value (excluded)
array([1, 2, 3, 4, 5, 6, 7, 8, 9])
>>> np.arange(1,10,2)
array([1, 3, 5, 7, 9])
>>> np.arange(1,10).reshape((3,3))
array([[1, 2, 3],
       [4, 5, 6],
       [7, 8, 9]])
```

8.1.2 Working with Arrays

The previous section covered how we can access elements in an array and properties of an array. Now let us see how the different types of operations we can do with arrays.

Arithmetic, Relational and Membership Operations with Arrays

The arithmetic operations (`+`, `-`, `*`, `/`, `**`), the relational operations (`==`, `<`, `<=`, `>`, `>=`) and the membership operations (`in`, `not in`) that we can apply on numbers and other data types in Python can be applied on arrays with NumPy. These operations are performed elementwise. This means that the arrays that are provided as operands to a binary arithmetic operator need to have the same shape.

Let us see some examples for arithmetic operations:

```
>>> A = np.arange(4).reshape((2,2))
>>> A
array([[0, 1],
       [2, 3]])
>>> B = np.arange(4, 8).reshape((2,2))
>>> B
array([[0, 1],
       [2, 3]])
```

(continues on next page)

```

array([[4, 5],
       [6, 7]])
>>> print(B-A)
[[4 4]
 [4 4]]
>>> print(B+A)
[[ 4  6]
 [ 8 10]]
>>> A
array([[0, 1],
       [2, 3]])
>>> B
array([[4, 5],
       [6, 7]])

```

Note here that these operations create a new array whose elements are the results of applying the operation. Therefore, the original arrays are not modified. If you are interested in in-place operations that modify an existing array during the operation, you can use combined statements such as `+=`, `-=`, `*=`.

Relational and membership operations are also applied elementwise and we can easily anticipate the outcomes of such operations, e.g. as follows:

```

>>> A < B
array([[ True, True],
       [ True, True]])
>>> B > A
array([[ True, True],
       [ True, True]])
>>> A > B
array([[False, False],
       [False, False]])
>>> 4 in B
True
>>> 10 in B
False

```

Useful Functions

NumPy arrays provide several useful functions already provided. These include:

- Standard mathematical function such as exponent, sin, cos, square-root: `np.exp(<array>)`, `np.sin(<array>)`, `np.cos(<array>)`, `np.sqrt(<array>)`.
- Minimum and maximum: `<array object>.min()` and `<array object>.max()`.
- Summation, mean and standard deviation: `<array object>.sum()`, `<array object>.mean()` and `<array object>.std()`.

Note that minimum, maximum, summation, mean and standard deviation can be applied on the whole array as well as along a pre-specified dimension (specified with an `axis` parameter). Let us see some examples to clarify this important aspect:

```

>>> A
array([[0, 1],
       [2, 3]])
>>> A.sum()
6
>>> A.sum(axis=0)
array([2, 4])

```

(continues on next page)

```
>>> A.sum(axis=1)
array([1, 5])
>>> A.sum(axis=2)
Traceback (most recent call last):
File "<stdin>", line 1, in <module>
File "/usr/local/lib/python3.7/site-packages/numpy/core/_methods.py", line 47, in _sum
    return umr_sum(a, axis, dtype, out, keepdims, initial, where)
numpy.AxisError: axis 2 is out of bounds for array of dimension 2
```

where we see that axes start being numbered from zero.

Splitting and Combining Arrays

For many problems, we will need to split an array into multiple arrays or combine multiple arrays into one. For splitting arrays, we can use functions such as np.hsplit (for horizontal split), np.vsplit (for vertical split) and np.array_split (for more general split operations). Below is an example for hsplit and vsplit:

```
>>> L = np.arange(16).reshape(4,4)
>>> L
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11],
       [12, 13, 14, 15]])
>>> np.hsplit(L,2) # Divide L into 2 arrays along the horizontal axis
[array([[ 0,  1],
       [ 4,  5],
       [ 8,  9],
       [12, 13]]), array([[ 2,  3],
       [ 6,  7],
       [10, 11],
       [14, 15]])]
>>> np.vsplit(L,2)
[array([[0, 1, 2, 3],
       [4, 5, 6, 7]]), array([[ 8,  9, 10, 11],
       [12, 13, 14, 15]])]
```

Note that the resultant arrays are provided as a Python list. Note also that hsplit and vsplit functions work on even sizes (i.e. they can split into equally sized arrays) – for general split operations, you can use array_split.

For combining multiple arrays, we can use np.hstack (for horizontal stacking), np.vstack (for vertical stacking) and np.stack (for more general stacking operations). Below is an example (for the A and B arrays that we have created before):

```
>>> A
array([[0, 1],
       [2, 3]])
>>> B
array([[4, 5],
       [6, 7]])
>>> np.hstack((A, B))
array([[0, 1, 4, 5],
       [2, 3, 6, 7]])
>>> np.vstack((A, B))
array([[0, 1],
```

(continues on next page)

```
[2, 3],
[4, 5],
[6, 7]]
```

Iterations with Arrays.

NumPy library already provides for us many functionalities that we might need while working with arrays. However, in many circumstances those will not be necessary and we will need to be able to iterate over the elements of arrays and perform custom algorithmic steps.

Luckily, iteration with arrays is very similar to how we would perform iterations with other container data types in Python. Let us see some examples:

```
>>> L
array([[ 0,  1,  2,  3],
       [ 4,  5,  6,  7],
       [ 8,  9, 10, 11],
       [12, 13, 14, 15]])
>>> for r in L:
...     print("row: ", r)
...
row: [0 1 2 3]
row: [4 5 6 7]
row: [8 9 10 11]
row: [12 13 14 15]
```

where we see that iteration over a multi-dimensional array iterates over the first dimension. To iterate over each element, we have at least two options:

```
>>> for element in L.flat:
...     print(element)
...
0
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
>>> for r in L:
...     for element in r:
...         print(element)
...
0
1
```

(continues on next page)

```

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

```

Now let us implement one of the operations we have seen above in Python from scratch as an exercise:

```

import numpy as np

def horizontal_stack(A,B):
    """A function that combines two 2D arrays A and B.
    A and B need to have the same height.
    """
    # Let us get dimensions first and check whether A and B
    # are compatible for stacking.
    (H_A, W_A) = A.shape
    (H_B, W_B) = B.shape
    if H_A != H_B:
        print("Arguments A and B have incompatible heights!")
        return None
    # Let us create an empty `result` array:
    H_result = H_A #or H_B
    W_result = W_A + W_B
    result = np.zeros((H_result, W_result))

    # Now let us iterate over each position in A and B and place
    # their elements into the corresponding positions
    for i in range(H_A):
        for j in range(W_A):
            result[i][j] = A[i][j]
        for j in range(W_B):
            result[i][j+W_A] = B[i][j]

    return result

# Let us test our code:
M = np.random.randn(2,2) # Create a random 3x4 array
N = np.random.randn(2,3) # Create a random 3x6 array
print("Random array M is:\n", M)
print("Random array N is:\n", N)
print("Horizontal stacking of M and N yields:\n", horizontal_stack(M, N))

```

Random array M is:
[[0.87441013 -0.46506587]]

(continues on next page)

```
[ 0.43470365 -1.09605215]]
Random array N is:
[[-0.74886418  0.9568392 -0.19811215]
 [-0.06708416  1.68393368 -1.03013149]]
Horizontal stacking of M and N yields:
[[ 0.87441013 -0.46506587 -0.74886418  0.9568392 -0.19811215]
 [ 0.43470365 -1.09605215 -0.06708416  1.68393368 -1.03013149]]
```

8.1.3 Linear Algebra with NumPy

Now let us give a flavour of the Linear Algebra operations provided by NumPy. Note that some of these operations is provided in the module `numpy.linalg`.

Transpose.

The transpose operation flips a matrix along the diagonal. For an example matrix A ,

$$A = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \quad (8.1.3)$$

its transpose is the following:

$$A^T = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix} \quad (8.1.4)$$

In NumPy, the transpose of a matrix can be easily accessed by accessing its `.T` member variable or by calling its `.transpose()` member function:

```
>>> A
array([[1, 2],
       [3, 4]])
>>> A.T
array([[1, 3],
       [2, 4]])
>>> A
array([[1, 2],
       [3, 4]])
```

Note that `.T` is simply a member variable of the array object and is not defined as an operation. Try finding the transpose of A with `A.transpose()` and see that you obtain the expected result. Note also that the transpose operation does not change the original array.

Inverse.

The inverse of an $n \times n$ matrix A is an $n \times n$ matrix A^{-1} that yields an $n \times n$ identity matrix I when multiplied:

$$A \times A^{-1} = I. \quad (8.1.5)$$

In NumPy, we can use `np.linalg.inv(<array>)` to find the inverse of a square array. Here is an example:

```

>>> A
array([[1, 2],
       [3, 4]])
>>> A_inv = np.linalg.inv(A)
>>> A_inv
array([[-2.,  1.],
       [ 1.5, -0.5]])

```

Let us check whether the inverse was correctly calculated:

```

>>> np.matmul(A, A_inv)
array([[1.0000000e+00, 0.0000000e+00],
       [8.8817842e-16, 1.0000000e+00]])

```

which is the identity matrix (I) except for some rounding error at index (1, 0) owing to floating point approximation. However, as we have seen in Chapter 2, while writing our programs, we should compare numbers such that $8.8817842e-16$ can be considered to be equal to zero.

Determinant, norm, rank, condition number, trace

While working with matrices, we often require the following properties which can be easily calculated. For the sake of brevity and to keep the focus, we will omit their explanations:

Matrix Property	How to Calculate with NumPy
Determinant ($ A $ or $\det(A)$)	<code>np.linalg.det(A)</code>
Norm ($\ A\ $)	<code>np.linalg.norm(A)</code>
Rank ($\text{rank}(A)$)	<code>np.linalg.matrix_rank(A)</code>
Condition number ($\kappa(A)$)	<code>np.linalg.cond(A)</code>
Trace ($\text{tr}(A)$)	<code>np.trace(A)</code>

Dot Product, Inner Product, Outer Product, Matrix Multiplication

The product of two matrices can be calculated in different ways:

- `np.dot(a, b)`: For vectors (1D arrays), this is equivalent to the dot product (i.e. $\sum_i \mathbf{a}_i \times \mathbf{b}_i$ for two vectors **a** and **b**). For 2D arrays and arrays with more dimensions, the result is matrix multiplication.
- `np.inner(a,b)`: For vectors, this is dot product (like `np.dot(a,b)`). For higher-dimensional arrays, the result is a sum product over the last axes. Consider the following example for clarification on this:

```

>>> A
array([[0, 1],
       [2, 3]])
>>> B
array([[4, 5],
       [6, 7]])
>>> np.inner(A,B)
array([[ 5,  7],
       [23, 33]])

```

The last axes for both A and B are the horizontal axes. Therefore, each first-axis element of A (i.e. [0, 1] and [2,3]) is multiplied with each first-axis element of B ([4, 5] and [6, 7]).

- `np.outer(a,b)`: Outer product is defined on vectors such that $\text{result}[i,j] = a[i] * b[j]$.

- `np.matmul(a,b)`: Matrix multiplication of matrices a and b. The result is simply calculated as $\text{result}_{ij} = \sum_k \mathbf{a}_{ik} \mathbf{b}_{kj}$, as also illustrated in Fig. 8.1.1.

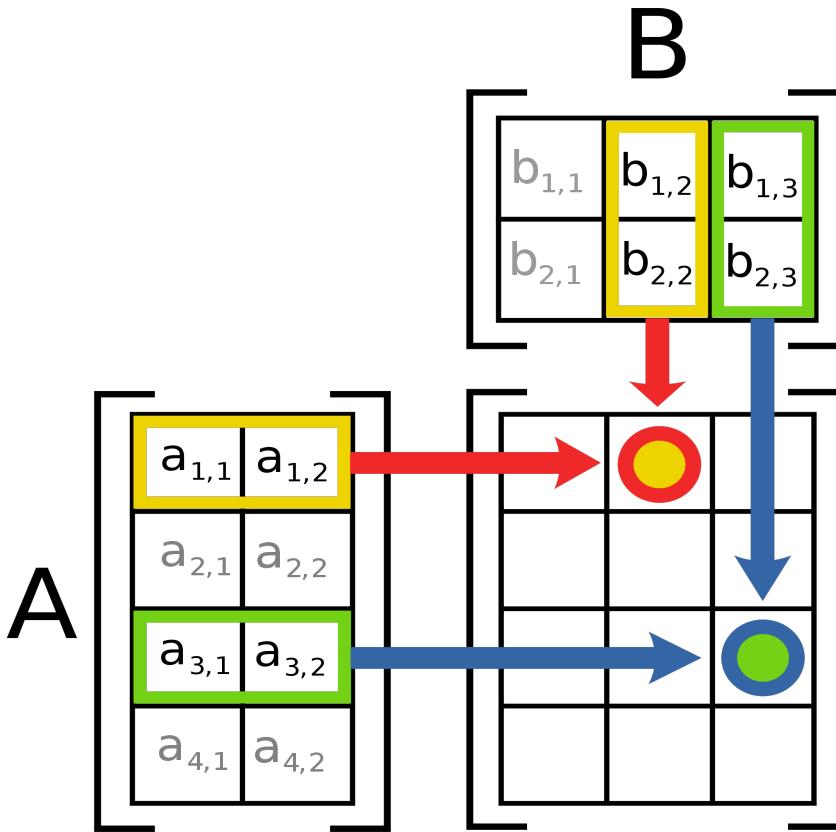


Fig. 8.1.1: Illustration of matrix multiplication of two matrices A and B. (Figure source: Wikipedia)

Eigenvectors and Eigenvalues

Explaining eigenvectors and eigenvalues is beyond the scope of the book. However, we can briefly remind that eigenvectors and eigenvalues are the variables that satisfy the following for a matrix A which can be considered as a transformation in a vector space:

$$Av = \lambda v. \quad (8.1.6)$$

In other words, v is such a vector that A just changes its scale by a factor λ .

In NumPy, eigenvectors and eigenvalues can be obtained by `np.linalg.eigh(<array>)` which returns a tuple with the following two elements:

1. Eigenvalues (λ) in decreasing order.
2. Eigenvectors (v) as a column matrix. I.e. $v[:, i]$ is the eigenvector corresponding to the eigenvalue $\lambda[i]$.

Matrix Decompositions

Numpy also provides many frequently used matrix decompositions, as listed below:

Matrix Decomposition	How to Calculate with NumPy
Cholesky decomposition	linalg.cholesky(A)
QR factorization	np.linalg.qr(A)
Singular Value Decomposition	linalg.svd(a)

Solve a linear system of equations

Given a linear system of equations as follows:

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \dots + a_{1n}x_n &= b_1, \\ a_{21}x_1 + a_{22}x_2 + \dots + a_{2n}x_n &= b_2, \\ &\dots \\ a_{n1}x_1 + a_{22}x_2 + \dots + a_{nn}x_n &= b_n, \end{aligned} \tag{8.1.7}$$

which can be represented in compact form as:

$$\mathbf{ax} = \mathbf{b}, \tag{8.1.8}$$

can be solved in NumPy using `np.linalg.solve(a, b)`.

Below is an easy example:

```
>>> A
array([[0, 1],
       [2, 3]])
>>> B
array([3, 4])
>>> np.linalg.solve(A,B)
array([-2.5,  3. ])
>>> X = np.linalg.solve(A,B)
>>> X
array([-2.5,  3. ])
```

which can be easily verified using multiplication:

```
>>> np.inner(A, X)
array([3., 4.])
```

which is equal to B.

8.1.4 Why Use NumPy? Efficiency Benefits

The previous sections have illustrated how capable the NumPy library is and how easily we can do many calculations with the pre-defined functionalities e.g. in its linear algebra module. Since we can access each element of an array using Python's indexing mechanisms, we can be tempted to implementing those functionalities ourselves, from scratch.

However, those functionalities in NumPy are *not* implemented in Python but in C, another high-level programming language where programs are directly compiled into machine executable binary code. Therefore, they would execute much faster in comparison to what we would be implementing in Python.

The following example illustrates this. When executed, you should see an order of $\sim \$1000$ difference in running time.

In other words, you are strongly advised, whenever possible, to use NumPy's existing functions and routines, and to write every operation in vector or matrix form as much as possible if you are working with matrices.

```
import numpy as np
from time import time

def matmul_2D(M, N):
    """Custom defined matrix multiplication for two 2D matrices M and N"""
    (H_M, W_M) = M.shape
    (H_N, W_N) = N.shape
    if W_M != H_N:
        print("Dimensions of M and N mismatch!")
        return None

    result = np.zeros((H_M, W_N))
    for i in range(H_M):
        for j in range(W_N):
            for k in range(W_M):
                result[i][j] += M[i][k] * N[k][j]

    return result

# First let us check that our code works as expected
M = np.random.randn(2,3)
N = np.random.randn(3,4)

print("Our matmul_2D result: \n", matmul_2D(M, N))
print("Correct result: \n", np.matmul(M, N))

# Now let us measure the running-time performances
# Create two 2D large matrices
M = np.random.randn(100, 100)
N = np.random.randn(100, 100)

# Option 1: Use NumPy's matrix multiplication
t1 = time()
result = np.matmul(M, N)
t2 = time()
print("NumPy's matmul took ", t2-t1, "ms.")

# Option 2: Use our matmul_2D function
t1 = time()
result = matmul_2D(M, N)
t2 = time()
print("Our matmul_2D function took ", t2-t1, "ms.")
```

```
Our matmul_2D result:
[[ 1.00870245  1.80029584  2.19231301  1.01315496]
 [ 1.23248392 -0.41201987  5.81237397  0.04080299]]
Correct result:
[[ 1.00870245  1.80029584  2.19231301  1.01315496]
 [ 1.23248392 -0.41201987  5.81237397  0.04080299]]
NumPy's matmul took 0.00021505355834960938 ms.
Our matmul_2D function took 1.1434831619262695 ms.
```

8.2 Scientific Computing with SciPy

SciPy is a library that includes many methods and facilities for Scientific Computing. It is closely linked with NumPy so much that NumPy needs to be imported first to be able to use SciPy.

Installation Notes

To be able to use the SciPy library, you will need to download it from scipy.org and install it on your computer. If you are using a Python package manager (e.g. pip), you can install it directly using: `$ pip install scipy`. Note that if you are using Colab or another Jupyter Notebook viewer, the platform may already have `scipy` installed.

Below is a list of some modules provided by SciPy. Even a brief coverage of these modules is not feasible in a chapter. However, we will see an example in Chapter 12 using SciPy's stats and optimize modules.

Module	Description
cluster	Clustering algorithms
constants	Physical and mathematical constants
fftpack	Fast Fourier Transform routines
integrate	Integration and ordinary differential equation solvers
interpolate	Interpolation and smoothing splines
io	Input and Output
linalg	Linear algebra
ndimage	N-dimensional image processing
odr	Orthogonal distance regression
optimize	Optimization and root-finding routines
signal	Signal processing
sparse	Sparse matrices and associated routines
spatial	Spatial data structures and algorithms
special	Special functions
stats	Statistical distributions and functions

8.3 Data handling & analysis with Pandas

Pandas is a very handy library for working with files with different formats and analyzing data in different format. To keep things simple, in this section we will just look at CSV files. Note that the facilities for other formats are very similar.

Installation Notes

To be able to use the Pandas library, you will need to download it from pandas.pydata.org and install it on your computer. If you are using a Python package manager (e.g. pip), you can install it directly using: `$ pip install pandas`. Note that if you are using Colab or another Jupyter Notebook viewer, the platform may already have `pandas` installed.

8.3.1 Supported File Formats

As we have seen before, Python already provides facilities for reading and writing files. However, if you need to work with “structured” files such as CSV, XML, XLSX, JSON, HTML, the native facilities of Python would need to be extended significantly.

That’s where Pandas comes in. It complements Python’s native facilities to be able to work with structured files for both reading data from them and creating new files. Below is a list of the different file formats that Pandas supports and the corresponding functions for reading or writing them.

Table 10.1. The file formats supported by the Pandas library. The table is adapted from and the reader is encouraged to check the following page to see a more up-to-date list: Pandas IO Reference.

Format Type	Data Description	Reader	Writer
text	CSV	read_csv	to_csv
text	Fixed-Width Text File	read_fwf	•
text	JSON	read_json	to_json
text	HTML	read_html	to_html
text	Local clipboard	read_clipboard	to_clipboard
•	MS Excel	read_excel	to_excel
binary	OpenDocument	read_excel	•
binary	HDF5 Format	read_hdf	to_hdf
binary	Feather Format	read_feather	to_feather
binary	Parquet Format	read_parquet	to_parquet
binary	ORC Format	read_orc	•
binary	Msgpack	read_msgpack	to_msgpack
binary	Stata	read_stata	to_stata
binary	SAS	read_sas	•
binary	SPSS	read_spss	•
binary	Python Pickle Format	read_pickle	to_pickle
SQL	SQL	read_sql	to_sql
SQL	Google BigQuery	read_gbq	to_gbq

8.3.2 Data Frames

Pandas library is built on top of a data type called DataFrame which is used to store all types of data while working with Pandas. In the following, we will illustrate how you can get your data into a DataFrame object:

1. Loading data from a file. If you have your data in a file that is supported by Pandas, you can use its reader for directly obtaining a DataFrame object. Let us look at an example CSV file:

```
# Download an example CSV file:  
!wget -nc https://raw.githubusercontent.com/sinankalkan/CENG240/master/figures/ch10_example.csv  
  
# Import the necessary libraries  
import pandas as pd  
  
# Read the file named 'ch10_example.csv'  
df = pd.read_csv('ch10_example.csv')  
  
# Print the CSV file's contents:  
print("The CSV file contains the following:\n", df, "\n")  
  
# Check the types of each column  
df.dtypes
```

File ‘ch10_example.csv’ already there; not retrieving.

The CSV file contains the following:

```
Name  Grade  Age  
0   Jack  40.2  20  
1  Amanda  30.0  25  
2   Mary  60.2  19  
3   John  85.0  30  
4  Susan  70.0  28  
5   Bill  58.0  28  
6   Jill  90.0  27  
7   Tom  90.0  24  
8  Jerry  72.0  26  
9  George  79.0  22  
10 Elaine  82.0  23
```

```
Name    object  
Grade  float64  
Age    int64  
dtype: object
```

Note the following critical details:

- read_csv file automatically understood that our CSV file had a header (“Name Surname”, “Grade (over 100)” and “Age”). If your file does not have a header, you can call read_csv with the header parameter set to None as follows: pd.read_csv(filename, header=None).

- read_csv read all columns in the CSV file. If you wish to load only some of the columns (e.g. ‘Name Surname’, ‘Age’ in our example), you can relay this using the names parameter as follows: pd.read_csv(filename, names=['Name Surname', 'Age']).

2. Convert Python data into a ``DataFrame``. Alternatively, you can have already a Python data object which you can provide as argument to a DataFrame constructor as illustrated with the following example:

```
lst = [('Jack', 40.2, 20), ('Amanda', 30, 25), ('Mary', 60.2, 19)]
df = pd.DataFrame(data = lst, columns=['Name', 'Grade', 'Age'])
print(df)
```

	Name	Grade	Age
0	Jack	40.2	20
1	Amanda	30.0	25
2	Mary	60.2	19

In many cases, we will require the rows to be associated with names, or sometimes called as keys. For example, instead of referring to a row as “the row at index 1”, we might require accessing a row with a non-integer value. This can be achieved as follows (note how the printed DataFrame looks different):

```
names = ['Jack', 'Amanda', 'Mary']
lst = [(40.2, 20), (30, 25), (60.2, 19)]
df = pd.DataFrame(data = lst, index=names, columns=['Grade', 'Age'])
print(df)
```

	Grade	Age
Jack	40.2	20
Amanda	30.0	25
Mary	60.2	19

Alternatively, we can obtain a DataFrame from a dictionary, which might be easier for us to create data column-wise – note that the column names are obtained from the keys of the dictionary:

```
d = {'Grade': [40.2, 30, 60.2],
      'Age': [20, 25, 19]}
names = ['Jack', 'Amanda', 'Mary']
df = pd.DataFrame(data = d, index=names)
print(df)
```

	Grade	Age
Jack	40.2	20
Amanda	30.0	25
Mary	60.2	19

8.3.3 Accessing Data with DataFrames

We can access data columnwise or row-wise.

1. Columnwise access.

For columnwise access, you can use `df['Name']`, which returns a sequence of values. To access a certain element in that sequence, you can either use an integer index (as in `df['Name'][1]`) or named index if it has been defined (as in `df['Name']['Amanda']`). The following example illustrates this for the example DataFrame we have created above:

```

>>> print(df)
   Grade Age
Jack  40.2 20
Amanda 30.0 25
Mary   60.2 19
>>> print(df['Grade'][1])
30.0
>>> print(df['Grade']['Amanda'])
30.0

```

2. Rowwise access.

To access a particular row, you can either use integer indexes with `df.iloc[<row index>]` or `df.loc[<row name>]` if a named index is defined. This is illustrated below:

```

>>> print(df)
   Grade Age
Jack  40.2 20
Amanda 30.0 25
Mary   60.2 19
>>> print(df.iloc[1])
Grade 30.0
Age   25.0
Name: Amanda, dtype: float64
>>> print(df.loc['Amanda'])
Grade 30.0
Age   25.0
Name: Amanda, dtype: float64

```

You can also provide both column index and name index in a single operation, i.e. [`<row index>, <column index>`] or [`<row name>, <column name>`] as illustrated below:

```

>>> df.loc['Amanda','Grade']
30.0
>>> df.iloc[1, 1]
25

```

While accessing a DataFrame with integer indexes, you can also use Python's slicing; i.e. [start:end:step] indexing.

8.3.4 Modifying Data with DataFrames

Although modifying data in a DataFrame is simple, you need to be careful about one crucial concept: Let us say you use column and row names to change the contents of a cell and you access first the column and then the corresponding row as follows:

```

>>> print(df)
   Grade Age
Jack  40.2 20
Amanda 30.0 25
Mary   60.2 19
>>> df['Grade']['Amanda'] = 45
/usr/local/lib/python3.6/dist-packages/ipykernel_launcher.py:6: SettingWithCopyWarning:

```

(continues on next page)

A value is trying to be set on a copy of a slice from a DataFrame

See the caveats in the documentation: https://pandas.pydata.org/pandas-docs/stable/user_guide/indexing.html
 ↵#returning-a-view-versus-a-copy

This is called *chained indexing* and Pandas will give you a warning that you are modifying a DataFrame that was *returned* while accessing columns or rows in your original DataFrame: `df['Grade']` returns a direct access for the original Grade column or a copy to it and depending on how your data is structured and stored in the memory, the end result may be different and your change might not be reflected on the original DataFrame.

Instead, you should use a single access operation as illustrated below (you may do this with `loc` and `iloc` as well):

```
>>> print(df)
   Grade Age
Jack  40.2 20
Amanda 30.0 25
Mary   60.2 19
>>> df.loc['Amanda','Grade'] = 45
>>> df.iloc[1,1] = 30
>>> print(df)
   Grade Age
Jack  40.2 20
Amanda 45.0 30
Mary   60.2 19
```

With these facilities, you can now access every item in a DataFrame and modify them.

8.3.5 Analyzing Data with DataFrames

Once we have our data in a DataFrame, we can use Pandas's built-in facilities for analyzing our data. One very simple way to analyze data is via descriptive statistics, which you can access with `df.describe()` and `df[<column>].value_counts()`:

```
print(df)
df.describe()
```

```
   Grade Age
Jack  40.2 20
Amanda 30.0 25
Mary   60.2 19
```

Apart from these descriptive functions, Pandas provides functions for sorting (using `.sort_values()` function), finding the maximum or the minimum (using `.max()` or `.min()` functions) or finding the largest or smallest n values (using `.nsmallest()` or `.nlargest()` functions):

```
print("Maximum grade is: ", df['Grade'].max())
print("\nRecords sorted according to age:\n", df.sort_values(by="Age"))
print("\n\nTop two grades are:\n", df['Grade'].nlargest(2))
```

```
Maximum grade is: 60.2
```

```
Records sorted according to age:
```

	Grade	Age
Mary	60.2	19
Jack	40.2	20
Amanda	30.0	25

```
Top two grades are:
```

```
Mary 60.2
```

```
Jack 40.2
```

```
Name: Grade, dtype: float64
```

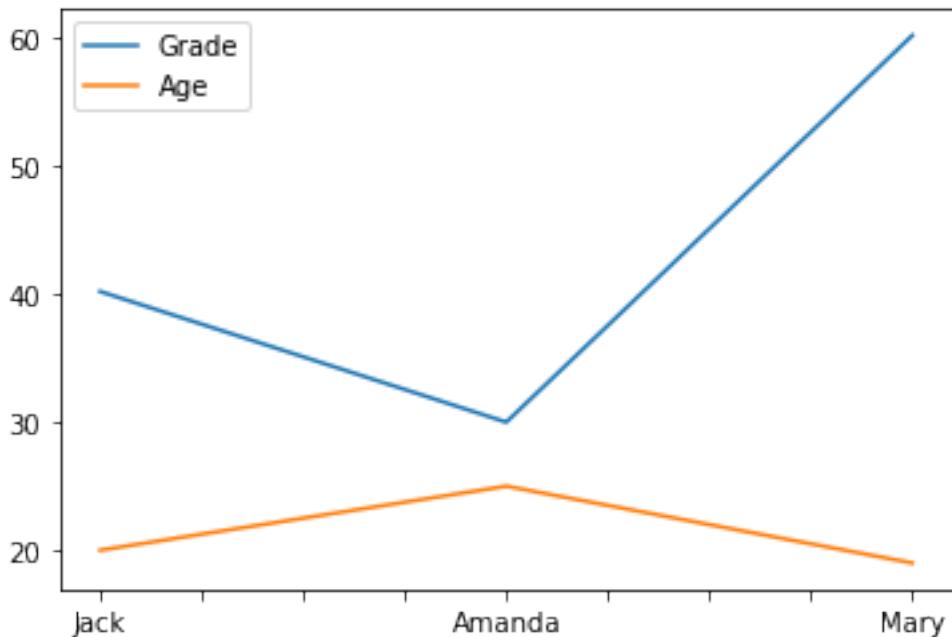
Note that, the displayed output includes the names because we selected names as the indices for accessing the rows.

8.3.6 Presenting Data in DataFrames

Pandas provides a very easy mechanism for plotting your data via `.plot()` function. Examples are provided below to illustrate how you can plot your own data. This plotting facility is provided by the Matplotlib which we will see next.

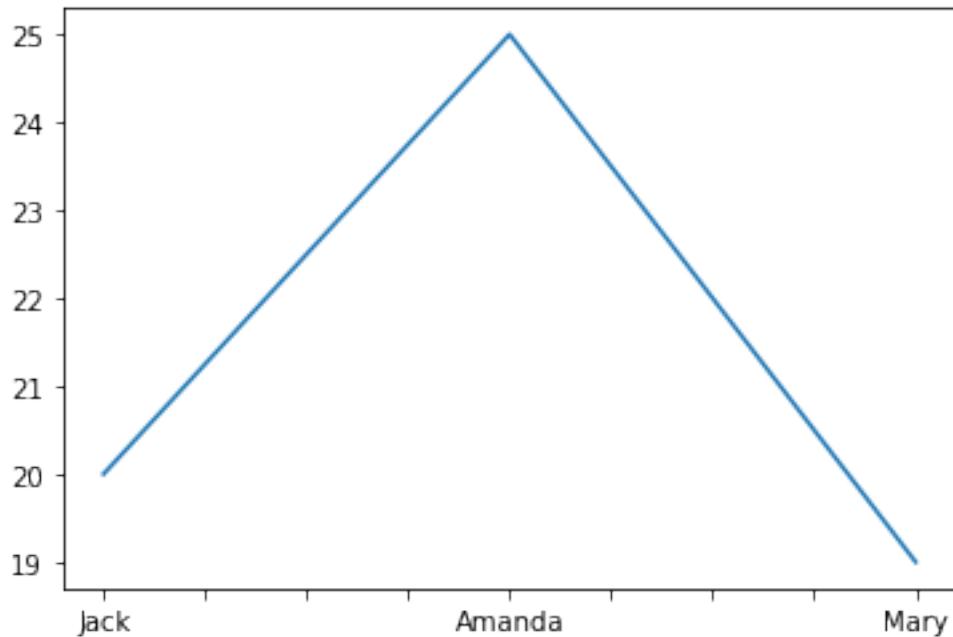
```
#Plots all columns in different colours  
df.plot()
```

```
<AxesSubplot:>
```



```
# Plots a single column  
df['Age'].plot()
```

```
<AxesSubplot:>
```



8.4 Plotting data with Matplotlib

Matplotlib is a very capable library for drawing different types of plots in Python. It is very well integrated with Numpy, Scipy and Pandas, and therefore, all these libraries are very frequently used together seamlessly.

Installation Notes

To be able to use the matplotlib library, you will need to download it from <https://matplotlib.org/> and install it on your computer. If you are using a Python package manager (e.g. pip), you can install it directly using:
\$ pip install matplotlib. Note that if you are using Colab or another Jupyter Notebook viewer, the platform may already have pandas installed.

8.4.1 Parts of a Figure

A figure consists of the following elements (see also Fig. 8.4.1): - Title of the figure. - Axes, together with their ticks, tick labels, and axis labels. - The canvas of plot, which consists of a drawing of your data in the form of a dots (scatter plot), lines (line plot), bars (bar plot), surfaces etc. - Legend, which informs the perceiver about the different plots in the canvas.

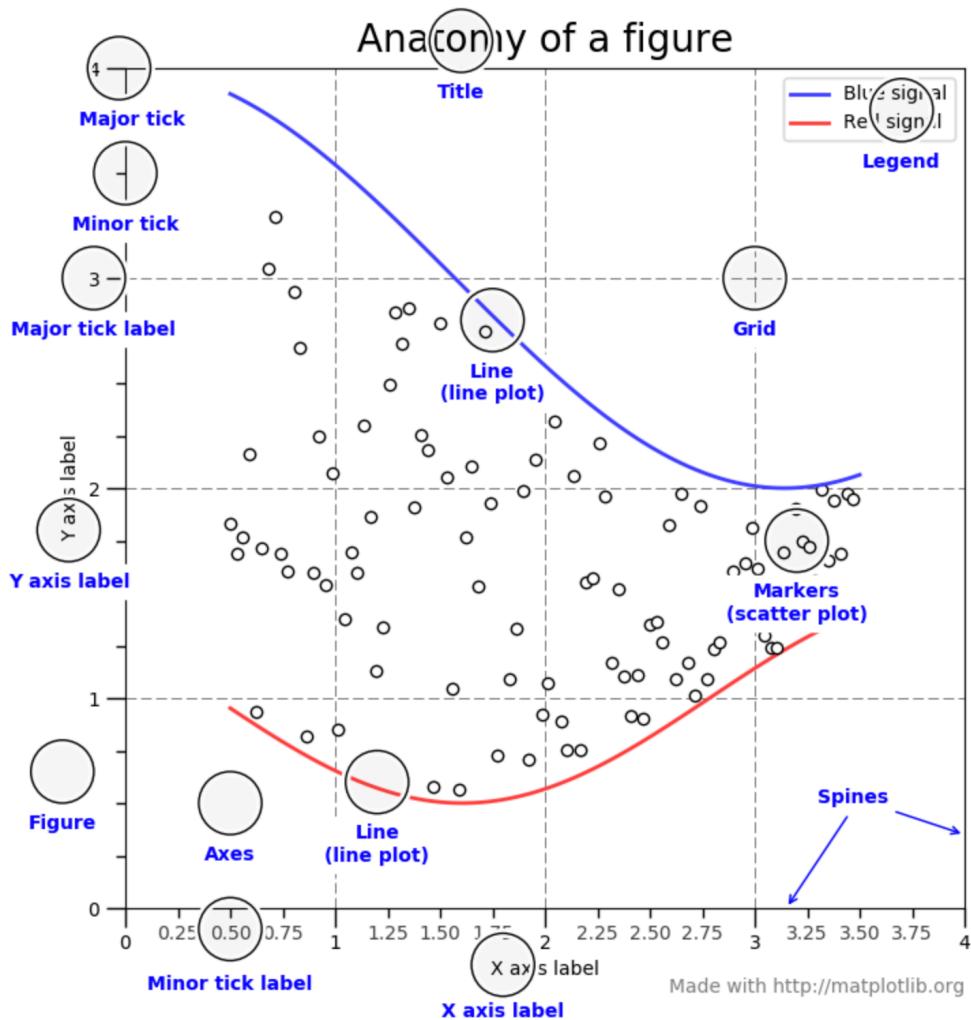


Fig. 8.4.1: A figure consists of several components all of which you can change in matplotlib easily. Figure source: Matplotlib Usage Guides.

8.4.2 Preparing your Data for Plotting

Matplotlib expects numpy arrays as input and therefore, if you have your data in a numpy array, you can directly plot it without any data type conversion. With pandas DataFrame, the behavior is not guaranteed and therefore, it is recommended that the values in a DataFrame are first converted to a numpy array, using e.g.:

```
print(df)
age_array = df['Age'].values
print("The 'Age' values in an array form are:", age_array)
print("The type of our new data is: ", type(age_array))
```

```

Grade Age
Jack 40.2 20
Amanda 30.0 25
Mary 60.2 19
The Age values in an array form are: [20 25 19]
The type of our new data is: <class 'numpy.ndarray'>

```

8.4.3 Drawing Single Plots

There are two ways to plot with matplotlib: In an object-oriented style or the so-called Pyplot style:

1. Drawing in an Object-Oriented Style.

In this style, we create a figure object and an axes object and work with those to create our plots. This is illustrated in the following example:

```

import matplotlib.pyplot as plt
import numpy as np

# Uniformly sample 50 x values between -2 and 2:
x = np.linspace(-2, 2, 50)

# Create an empty figure
fig, ax = plt.subplots()

# Plot y = x
ax.plot(x, x, label='y=x')

# Plot y = x^2
ax.plot(x, x**2, label='y=x^2')

# Plot y = x^3
ax.plot(x, x**3, label='y=x^3')

# Set the labels for x and y axes:
ax.set_xlabel('x')
ax.set_ylabel('y')

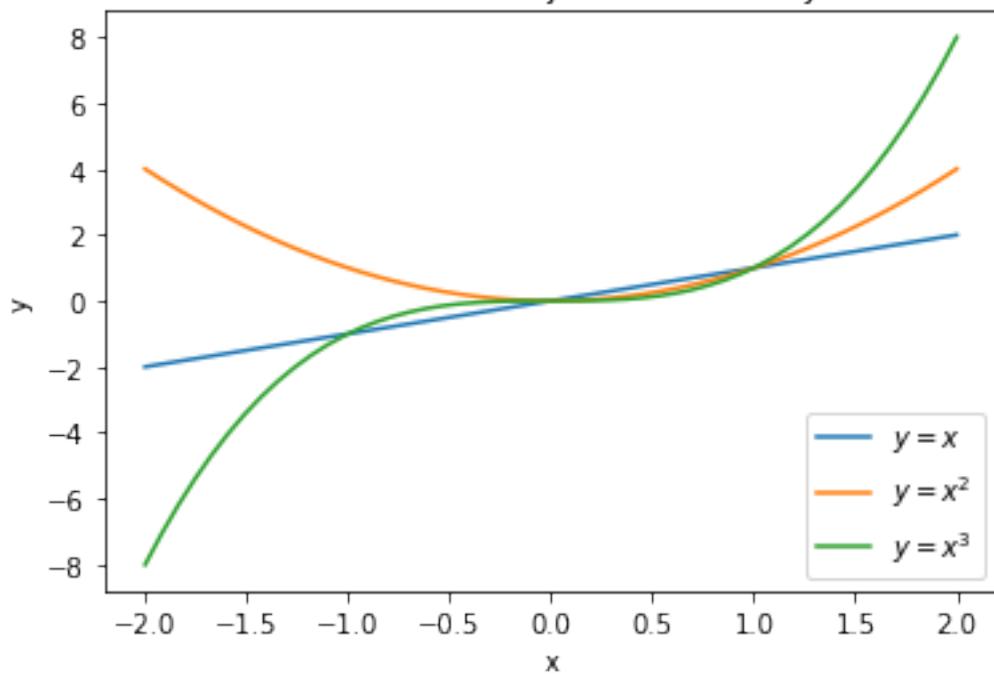
# Set the title of the figure
ax.set_title("Our First Plot -- Object-Oriented Style")

# Create a legend
ax.legend()

```

```
<matplotlib.legend.Legend at 0x11daa03a0>
```

Our First Plot -- Object-Oriented Style

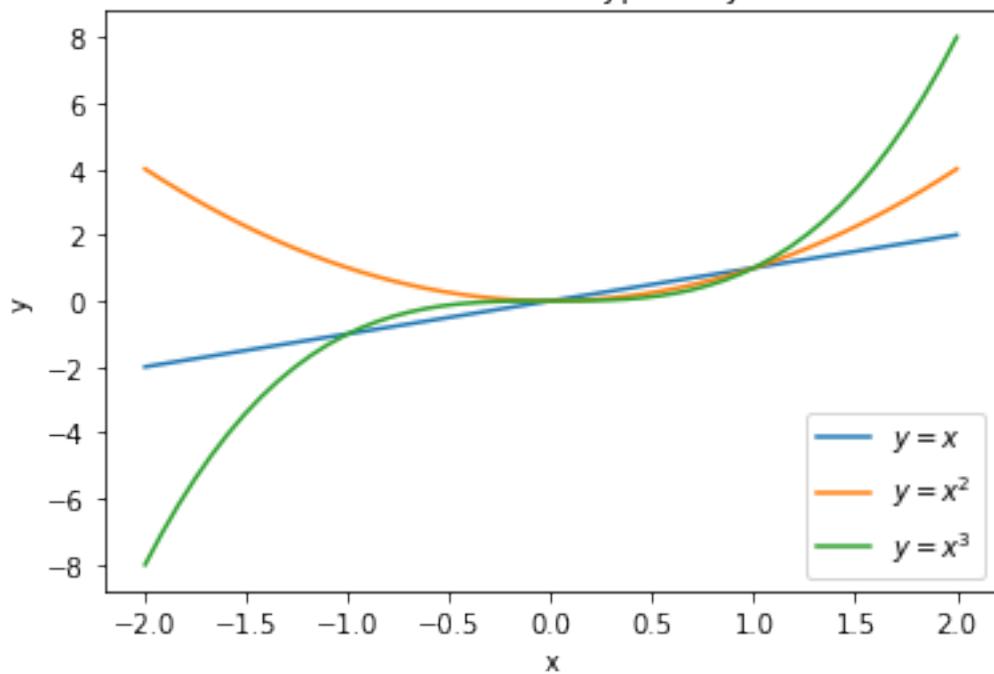


2. Drawing in a Pyplot Style. In the Pyplot style, we directly call functions in the pyplot module (matplotlib.pyplot) to create a figure and draw our plots. This style does not work with an explicit figure or axes objects. This is illustrated in the following example:

```
# Uniformly sample 50 x values between -2 and 2:  
x = np.linspace(-2, 2, 50)  
  
# Plot y = x  
plt.plot(x, x, label='y=x')  
  
# Plot y = x^2  
plt.plot(x, x**2, label='y=x^2')  
  
# Plot y = x^3  
plt.plot(x, x**3, label='y=x^3')  
  
# Set the labels for x and y axes:  
plt.xlabel('x')  
plt.ylabel('y')  
  
# Set the title of the figure  
plt.title("Our First Plot -- Pyplot Style")  
  
# Create a legend  
plt.legend()
```

```
<matplotlib.legend.Legend at 0x11dbf1a30>
```

Our First Plot -- Pyplot Style



8.4.4 Drawing Multiple Plots in a Figure

In many situations, you will need to draw multiple plots side by side in a single figure. This can be performed in the object-oriented style using the `subplots()` function to create a grid and then use the created subplots and axes to draw the plots. This is illustrated with an example below:

```
# Create a 2x2 grid of plots
fig, axes = plt.subplots(2, 2)

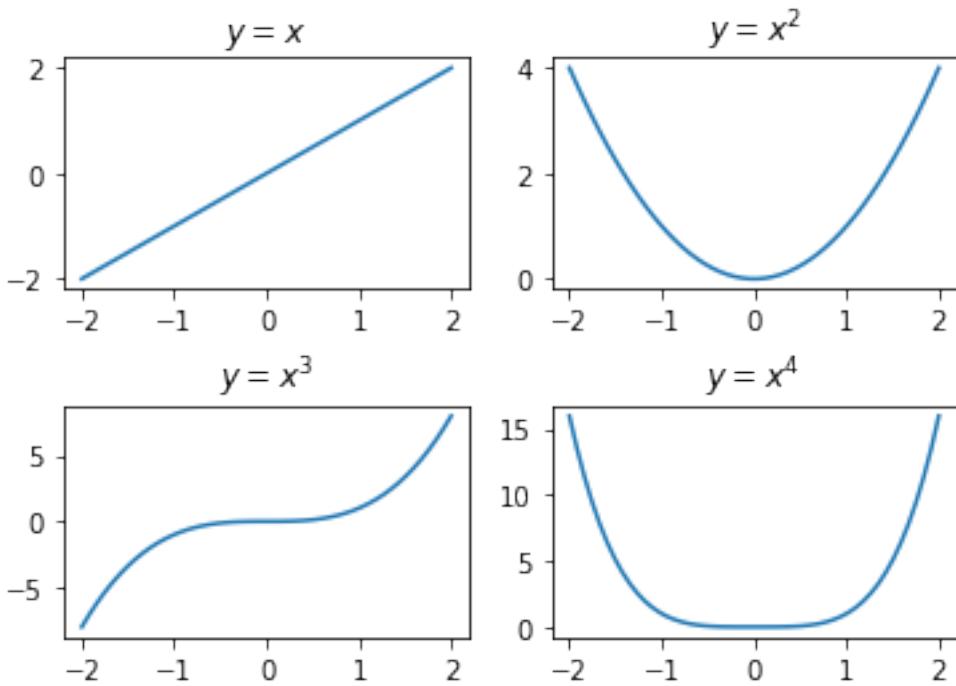
# Plot (1,1)
axes[0,0].plot(x, x)
axes[0,0].set_title("$y=x$")

# Plot (1,2)
axes[0,1].plot(x, x**2)
axes[0,1].set_title("$y=x^2$")

# Plot (2,1)
axes[1,0].plot(x, x**3)
axes[1,0].set_title("$y=x^3$")

# Plot (2,2)
axes[1,1].plot(x, x**4)
axes[1,1].set_title("$y=x^4$")

# Adjust vertical space between rows
plt.subplots_adjust(hspace=0.5)
```



It is possible to do this in the PyPlot style as well, as illustrated below:

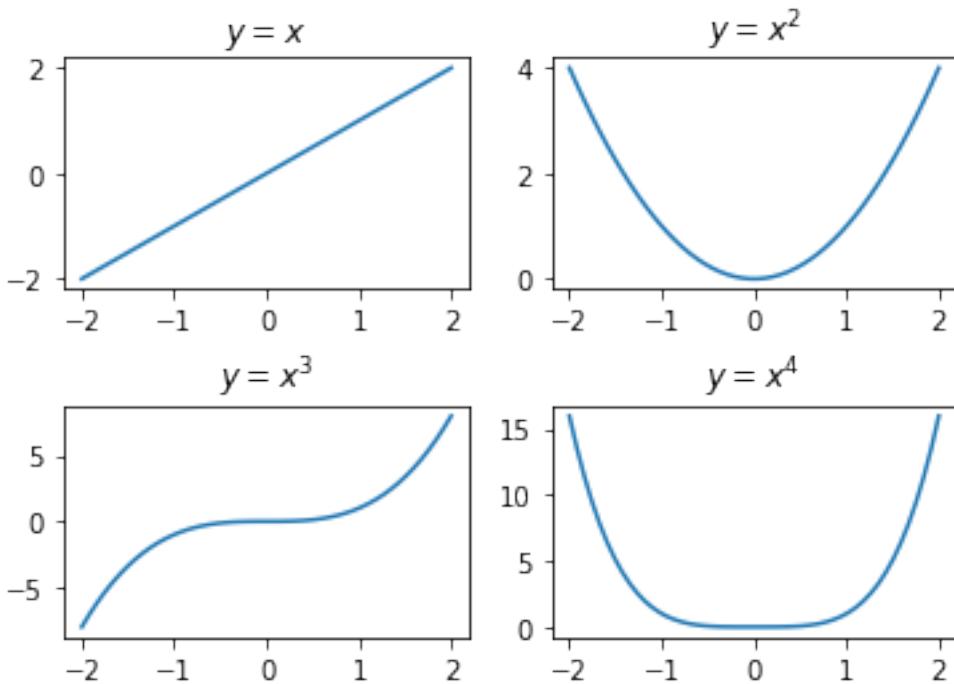
```
# Plot (1,1)
plt.subplot(2, 2, 1)
plt.plot(x, x)
plt.title('$y=x$')

# Plot (1,2)
plt.subplot(2, 2, 2)
plt.plot(x, x**2)
plt.title('$y=x^2$')

# Plot (2,1)
plt.subplot(2, 2, 3)
plt.plot(x, x**3)
plt.title('$y=x^3$')

# Plot (2,2)
plt.subplot(2, 2, 4)
plt.plot(x, x**4)
plt.title('$y=x^4$')

# Adjust vertical space between rows
plt.subplots_adjust(hspace=0.5)
```



8.4.5 Changing elements of a plot

All elements that are visualized in Figure 10.4.1 can be changed in matplotlib. We will skip these details to keep our focus in the book to the practical uses of these libraries. The interested reader can look up the extensive documentation at <https://matplotlib.org/2.1.1/contents.html> or look at the help page of a function (e.g. `help(plt.plot)`) to see how to modify all elements of a figure.

8.5 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- NumPy arrays and their properties: array shape, dimensions, sizes, elements.
- Accessing and modifying elements of a NumPy array.
- Simple algebraic functions on NumPy arrays.
- SciPy and its basic capabilities.
- Pandas, DataFrame, loading files with Pandas.
- Accessing and modifying content in DataFrames.
- Analyzing and presenting data in DataFrames.
- Matplotlib and different ways to make plots.
- Drawing single and multiple plots. Changing elements of a plot.

8.6 Further Reading

- NumPy documentation: <https://numpy.org/doc/>
- SciPy documentation: <https://docs.scipy.org/doc/scipy/reference/>
- Pandas documentation: <https://pandas.pydata.org/docs/>
- Matplotlib documentation: <https://matplotlib.org/2.1.1/contents.html>

Exercises

- Define functions that work like the sum, mean, min and max operations provided by NumPy. These functions should take a single 2D array and return the result as a number. You can assume that the operation applies to the whole array and not to a single axis.
- Create a simple CSV file using your favorite spreadsheet editor (e.g. Microsoft Excel or Google Spreadsheets) and create a file with your exams and their grades as two separate columns. Save the file, upload it to the Colab notebook and do the following:
 - Load the file using Pandas.
 - Calculate the mean of your exam grades.
 - Calculate the standard deviation of your grades.
- Using Matplotlib, generate the following plots with suitable names for the axes and the titles.
 - Draw the following four functions in separate single plots: $\sin(x)$, $\cos(x)$, $\tan(x)$, $\cot(x)$.
 - Draw these four functions in a single plot.
 - Draw a multiple 2x2 plot where each subplot is one of the four functions.

9 | An Application: Approximation and Optimization

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In this chapter, as an application for programming with Python, we will cover some mathematical methods widely used in many disciplines. We will start with Taylor Series for approximating a function. We will then see Newton's method for finding the roots of a function $f(x)$, which can also be considered as an application of Taylor series. Finally, we will cover how we can extend Newton's method for finding the minimum of a function.

9.1 Approximating Functions with Taylor Series

In some engineering or scientific problems, we have limited access to a function: We might be provided only the value of the function or its derivatives at certain input values and we might be required to make estimations (approximations) about the values of the function at other input values. Taylor's series is one method that provides us a very elegant solution for approximating a function.

The Taylor series of a function $f(\cdot)$ is essentially an infinite sum of terms that converges to the value of the function at x , i.e. $f(x)$. In more formal terms:

$$f(x) = f(a) + \frac{f'(a)}{1!}(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \frac{f'''(a)}{3!}(x - a)^3 \dots \quad (9.1.1)$$

which can be re-written in a more compact form:

$$f(x) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!}(x - a)^n. \quad (9.1.2)$$

In the limit ($n \rightarrow \infty$), $f(x)$ will be equal to its Taylor series. However, in realistic applications, it is impractical to take $n \rightarrow \infty$. In practice, we take the first m terms of the series and approximate the function with this:

$$f(x) \approx f(a) + \frac{f'(a)}{1!}(x - a) + \frac{f''(a)}{2!}(x - a)^2 + \frac{f'''(a)}{3!}(x - a)^3 \dots + \frac{f^{(m)}(a)}{m!}(x - a)^m, \quad (9.1.3)$$

ignoring the terms for $n > m$.

Note that the denominator ($n!$) gets large values quickly when n gets large. Therefore, higher-order terms in the Taylor series are likely to be very small values. For this reason, taking the first m terms in the series do provide sufficient approximations to $f(x)$ in practice.

We can provide some intuition for the Taylor Series as follows: If we know the value of function f at $x = a$, then we can calculate the value of the function at any other value of x as long as we know all (or the first m) derivatives of the function at $x = a$, i.e. $f^{(n)}(a)$ for $n = 1, \dots, \infty$ (or m). To see this, consider just the Taylor Series approximation with the first two terms: $f(x) \approx f(a) + \frac{f'(a)}{1!}(x - a)$, which is illustrated in Fig. 9.1.1.

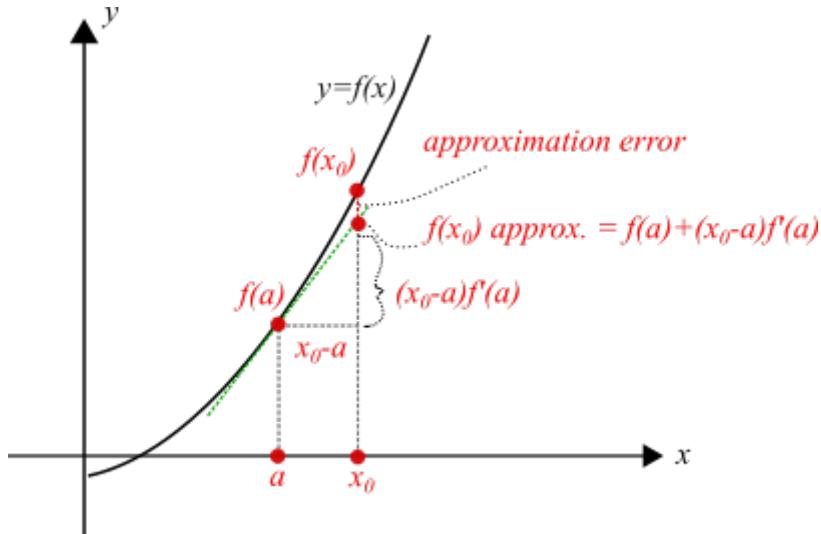


Fig. 9.1.1: Taylor Series approximates a function by using its derivatives. The drawing illustrates $f(x_0)$ being approximated (with the first term of the Taylor Series only) by the known value of the function $f(a)$ and the derivative $f'(a)$ at that point. Green line denotes the tangent line at $f(a)$ whose slope is $f'(a)$.

9.1.1 Taylor Series Example in Python

Let us take a “simple” function, namely $f(x) = x^3$, and approximate it with a few terms of the Taylor Series expansion:

```
# x^3 function
def xcube_a(a): return a*a*a

# Function for the derivatives of x^3
# Inputs: n (integer) => derivative degree
#          a (real number) => constant at which derivative is calculated
def xcube_nth_deriv_at_a(n, a):
    if n == 1: return 3*a*a # 1st derivative: 3x*x
    if n == 2: return 6*a # 2nd derivative: 6x
    if n == 3: return 6 # 3rd derivative: 6
    if n > 3: return 0 # nth derivative (n>3): 0

# Factorial function
def fact(n): return 1 if n < 1 else n*fact(n-1)

# Function approximating x^3 with m terms of the Taylor series
def xcube_approx(x, m):
    a = 1 # You can try different a values
    result = xcube_a(a)
    for n in range(1, m+1):
        result += xcube_nth_deriv_at_a(n, a)/fact(n)*pow(x-a, n)
```

(continues on next page)

```
return result
```

```
# Now let us evaluate how close our approximation is for various values of m.
import numpy as np
import matplotlib.pyplot as plt

# Let us compare the approximations for a set of x values:
x_vector=np.arange(-5, 5, 0.1)

# Find the approximations for our x values:
y_m_1=[xcube_approx(x,1) for x in x_vector]
y_m_2=[xcube_approx(x,2) for x in x_vector]
y_m_3=[xcube_approx(x,3) for x in x_vector]

# We have our ground truth (correct) values:
y_correct=[x*x*x for x in x_vector]

# Let's plot the results and the correct function ( $x^{**3}$ )
# We have a multi-plot plot, so we will use subplot() function
plt.rcParams['figure.figsize']= 15, 4 # Sets the figure size

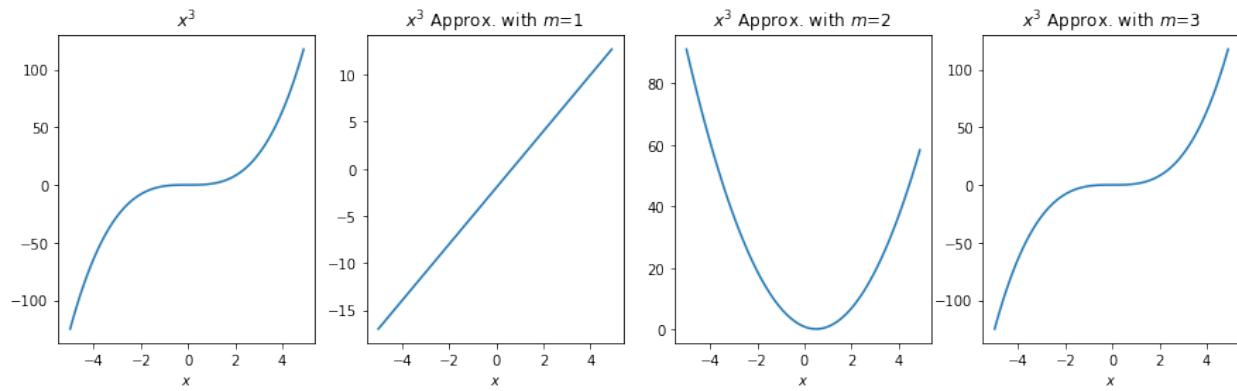
# First subplot: The correct (original) function that we are approximating
plt.subplot(1, 4, 1)
plt.plot(x_vector,y_correct, label=' $x^{**3}$ ')
plt.title('$x^3$')
plt.xlabel('$x$')

# Second subplot: Approximation with one term
plt.subplot(1, 4, 2)
plt.plot(x_vector,y_m_1)
plt.title("$x^3$ Approx. with $m=1$")
plt.xlabel('$x$')

# Third subplot: Approximation with two terms
plt.subplot(1, 4, 3)
plt.plot(x_vector,y_m_2)
plt.title("$x^3$ Approx. with $m=2$")
plt.xlabel('$x$')

# Fourth subplot: Approximation with three terms
plt.subplot(1, 4, 4)
plt.plot(x_vector,y_m_3)
plt.title("$x^3$ Approx. with $m=3$")
plt.xlabel('$x$')
```

Text(0.5, 0, '\$x\$')



9.2 Finding the Roots of a Function

Let us assume that we have a non-linear, continuous function $f(x)$ that intersects the horizontal axis as in Fig. 9.2.1. We are interested in finding r_0, \dots, r_n such that $f(r_i) = 0$. We call these intersections (r_0, r_1, r_2 in Fig. 9.2.1) the roots of function $f()$.

For many problems in Engineering and Mathematics, finding the values of these intersections is very useful. For example, many problems requiring solutions to equations like $g(x) = h(x)$ can be reformulated as a root finding problem for $g(x) - h(x) = 0$.

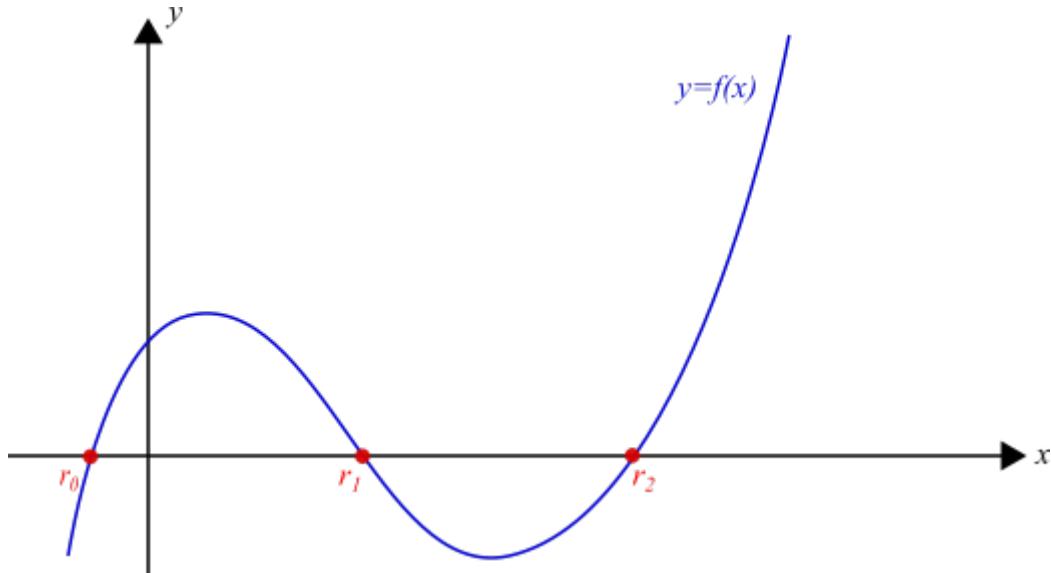


Fig. 9.2.1: Finding the roots of a function $f(x)$ means finding r_0, \dots, r_n for which the function is zero, $f(r_i) = 0$.

9.2.1 Newton's Method for Finding the Roots

Newton's method is one of the many methods for finding the roots of a function. It is a very common method that randomly starts at an x_0 value and iteratively takes one step at a time towards a root. The method can be described with the following iterative steps:

Step 1: Set an iteration variable, i , to 0. Initialize x_i randomly; however, if you have a good guess, it is always better to initialize x_i with it. For our example function $f(x)$ in Fig. 9.2.1, see the selected x_i in Fig. 9.2.2.

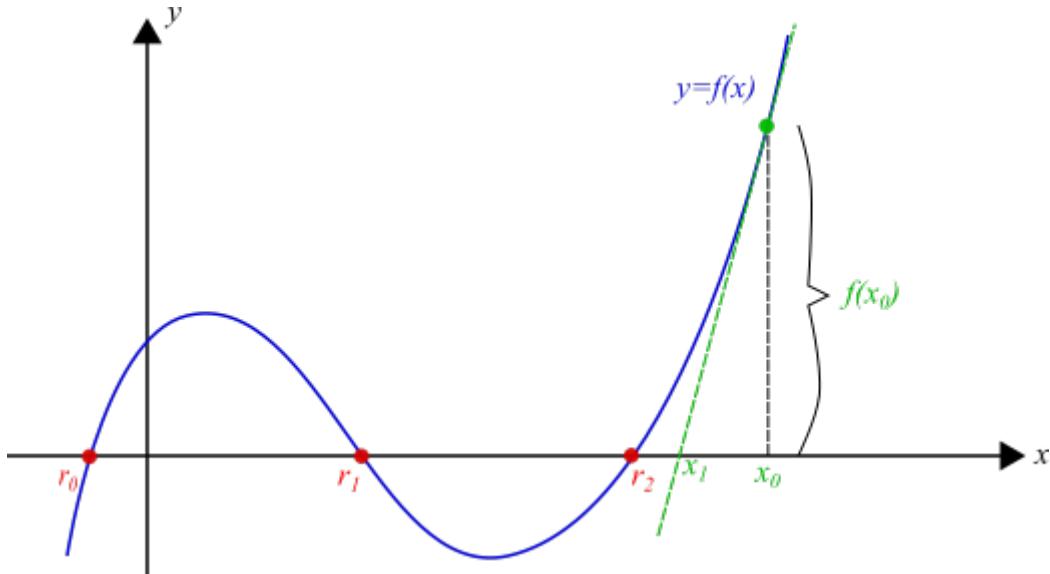


Fig. 9.2.2: One initial step of Newton's method. The tangent line at $f(x_0)$ is used to calculate the next value of x_i , getting us closer to a root.

Step 2: Find the intersection of the tangent line at x_i with the horizontal axis. The tangent line to the function at x_i is illustrated as the green dashed line in Figure 11.3. This line can be easily derived using x_i and $f'(x_i)$.

Let us use x_{i+1} to denote the intersection of the tangent line with the horizontal axis. Using the definition of the derivative and simple geometric rules, we can easily show that x_{i+1} satisfies the following:

$$\frac{x_i - x_{i+1}}{f(x_i)} = \frac{1}{f'(x_i)}, \quad (9.2.1)$$

with which we can formulate how we can find x_{i+1} as follows:

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)}. \quad (9.2.2)$$

Step 3: Repeat Step 2 by replacing $x_i \leftarrow x_{i+1}$ until “convergence”.

The intuition behind the Newton's method is simple: For a linear function such as $y = ax + b$, the root is $r = -b/a$, which can be easily derived from the slope and a known y value. For a non-linear function $y = f(x)$, we make an approximation by assuming $f()$ to be linear at point x_0 and use the slope of this linear approximation to find a new x_0 that is closer to the root.

9.2.2 Misc Details on Newton's Method for the Curious

It is not possible to cover all aspects of these elegant methods in detail. However, it would be a shame to skip the following details and hide them from a curious mind.

The Taylor Series Perspective for Newton's Method

Newton's method for finding a root of a function $f()$ works iteratively starting from an initial value x_0 by using the first-order expansion of $f()$ around x_i :

$$f(x_{i+1}) \approx f(x_i) + \frac{f'(x_i)}{1!}(x_{i+1} - x_i), \quad (9.2.3)$$

which can be simplified by rewriting $x_{i+1} = x_i + \delta$:

$$f(x_i + \delta) \approx f(x_i) + \frac{f'(x_i)}{1!}\delta. \quad (9.2.4)$$

We are interested in finding δ such that the approximation is equal to zero, in other words:

$$0 = f(x_i) + \frac{f'(x_i)}{1!}\delta, \quad (9.2.5)$$

which yields the delta value for which the approximation is zero:

$$\delta = -\frac{f(x_i)}{f'(x_i)}. \quad (9.2.6)$$

Plugging this into $x_{i+1} = x_i + \delta$, we obtain the equation for calculating the next value in the sequence towards a minimum of function $f()$:

$$x_{i+1} \leftarrow x_i - \frac{f(x_i)}{f'(x_i)}. \quad (9.2.7)$$

Notes on Convergence

A careful reader should have identified two important issues with Newton's method:

1- How can we be sure that this method converges to a solution, i.e. a root?

If function $f()$ satisfies certain conditions, then we can guarantee that Newton's method converges to a root. The details of these conditions and the proofs are beyond the scope of the book and the interested reader can check e.g. [Wikipedia²⁷](#).

To be on the safe side, we can limit the maximum number of steps that can we take and use the calculated value at the end.

2- If convergence can be guaranteed, how can we know that we have converged to a solution?

A common technique in such iterative algorithms is to check whether the difference between the consecutive values is tiny. In our case, if $|x_{i+1} - x_i| < \epsilon$, where ϵ is a very small number, then we can assume that consecutive steps do not lead to much change in x_i and therefore, we can stop our algorithm. Of course, the value of ϵ will be critical in determining how many iterations are needed to 'converge' to a result.

Notes on Multiple Roots

Newton's method converges only to a single root based on the initial value x_0 . In order to find other roots, the algorithm needs to be executed with a different value of x_0 , which will hopefully lead to a different root than the ones that we have identified before.

Since our knowledge about $f()$ or its roots is limited, running the algorithm for N times for different values of x_0 is the only option. If, on the other hand, we knew roughly the ranges of x where function $f()$ might have roots, then we could use this knowledge to choose better x_0 values.

²⁷ https://en.wikipedia.org/wiki/Newton%27s_method#Analysis

9.2.3 Newton's Method in Python

Let us implement Newton's method in Python and try to find the roots of an example function.

```
def find_root(f, f_deriv, x_0, max_steps=10, delta=0.001, verbose=True):
    """
    Use Newton's method to find a root of function f, given its derivative f_deriv.
    Inputs: f=>function
            f_deriv=> derivative of function f
            x_0=> initial x value
            max_steps=> maximum number of iterative steps (default: 10)
            delta=> if |x_{i+1} - x_i| < delta, then assume convergence
    """
    x_old = x_0
    for i in range(max_steps):
        # Step 2
        try:
            x_new = x_old - f(x_old) / f_deriv(x_old)
        except ZeroDivisionError:
            # Encountered division-by-zero, return None
            return None

        if verbose: print("Iteration ", i, ". (x_old, x_new): ", (x_old, x_new), " |x_new-x_old|: ", abs(x_new-x_old))
        if abs(x_new-x_old) < delta: break

        # Step 3
        x_old = x_new

    return x_new
```

```
# Let us pick a function and test our implementation
```

```
# Assume that our function is: f(x) = x^2 - 4
def f(x_i): return x_i**2-4

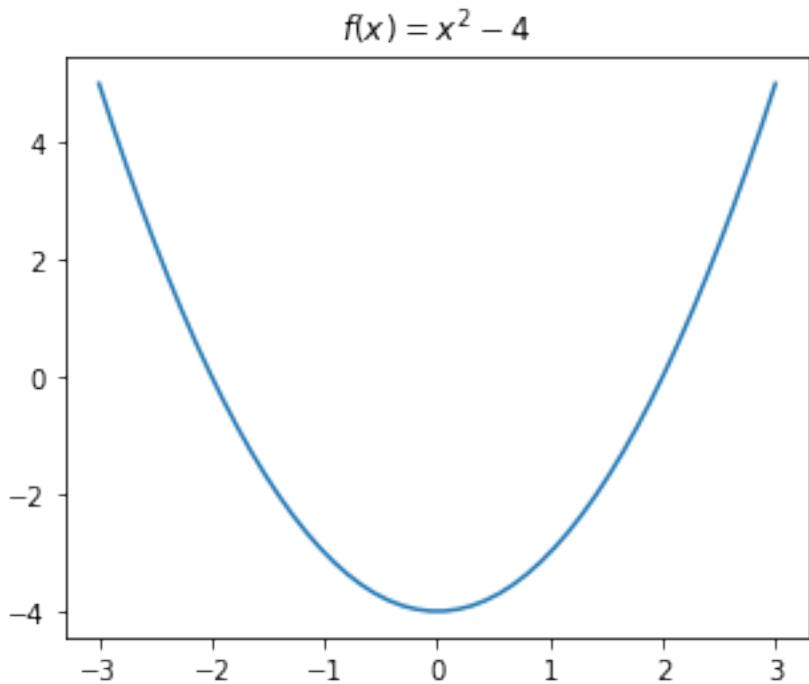
# This is the derivative, f'(x_i)
def f_deriv(x_i): return 2*x_i

# Let us draw our function first
import matplotlib.pyplot as plt
import numpy as np

def draw_f():
    # Uniformly sample 50 x values between -5 and 5:
    x = np.linspace(-3, 3, 50)

    plt.rcParams['figure.figsize'] = 5, 4
    plt.plot(x, f(x))
    plt.title('f(x)=x^2 - 4')

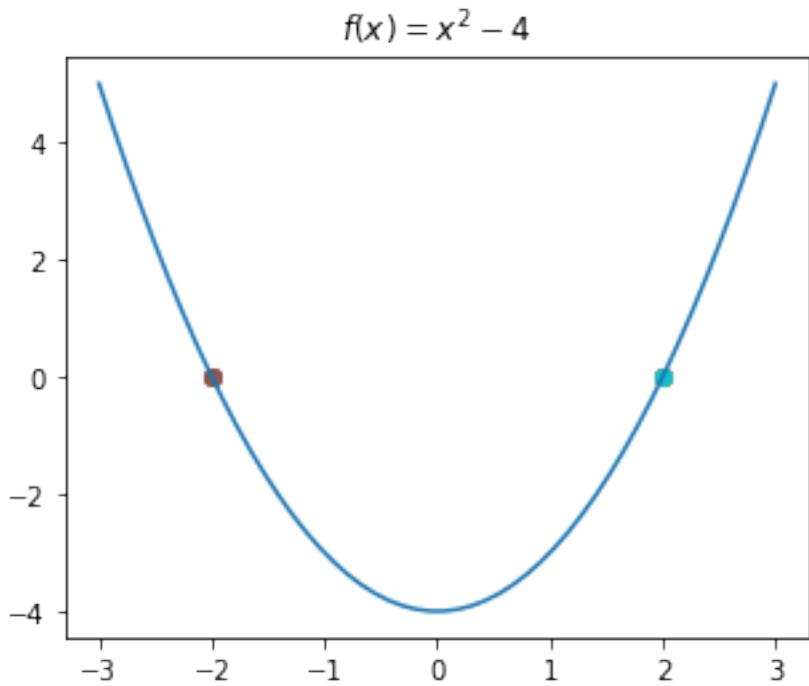
draw_f()
```



```
# Let us test our solution with 10 random initial values
import random

draw_f()
for i in range(10):
    x_0 = random.randint(-5, 5) # A random integer in [-5, 5]
    r = find_root(f, f_deriv, x_0, max_steps=50, delta=0.0001, verbose=False)
    if (not r) or (abs(f(r)) > 0.001): continue # Diverged or division-by-zero, ignore
    print("trial", i, " ended with root: ", r, " value at root, f(r): ", f(r))
    plt.scatter(r, f(r))
```

```
trial 0 ended with root: -2.000000000000002 value at root, f(r): 8.881784197001252e-15
trial 1 ended with root: 2.000000000000002 value at root, f(r): 8.881784197001252e-15
trial 2 ended with root: 2.000000000000002 value at root, f(r): 8.881784197001252e-15
trial 3 ended with root: -2.000000000006711 value at root, f(r): 2.6844304557016585e-11
trial 4 ended with root: -2.0 value at root, f(r): 0.0
trial 5 ended with root: -2.000000000006711 value at root, f(r): 2.6844304557016585e-11
trial 6 ended with root: 2.000000000000002 value at root, f(r): 8.881784197001252e-15
trial 7 ended with root: 2.0 value at root, f(r): 0.0
trial 8 ended with root: 2.000000000000002 value at root, f(r): 8.881784197001252e-15
trial 9 ended with root: 2.000000000000002 value at root, f(r): 8.881784197001252e-15
```



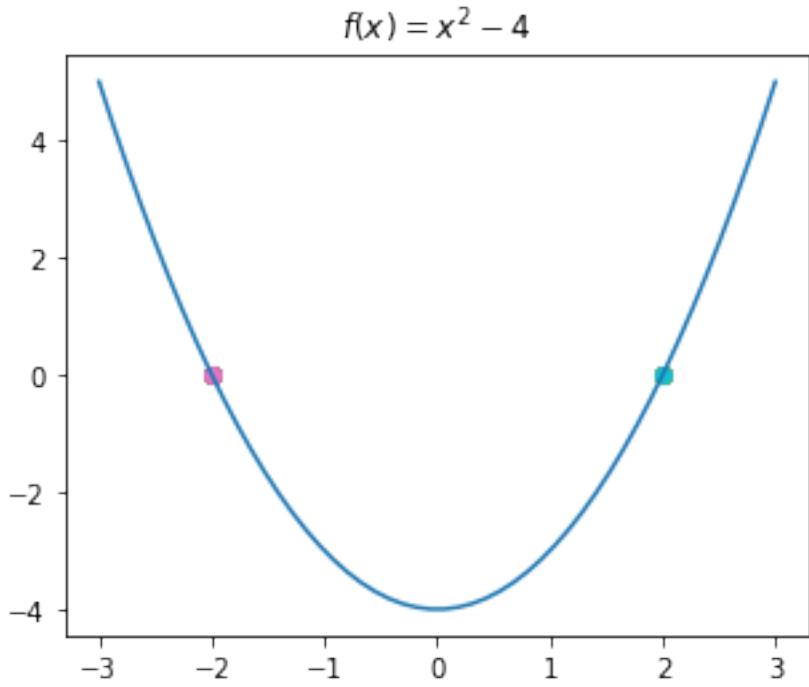
9.2.4 Newton's Method in SciPy

Let us see how we can use Newton's method from the SciPy library (from Chapter 10) to find the roots of a function. Note that we do not need to provide the derivative of the function to SciPy. It used numerical differentiation to calculate the derivative for us.

```
from scipy.optimize import newton
import random

draw_f() # Defined above
for i in range(10):
    x_0 = random.randint(-5, 5) # A random integer in [-5, 5]
    r = newton(f, x_0, fprime=None, args=(), tol=0.0001, maxiter=50)
    if (not r) or (abs(f(r)) > 0.001): continue # Diverged or division-by-zero, ignore
    print("trial", i, " ended with root: ", r, " value at root, f(r): ", f(r))
    plt.scatter(r, f(r))
```

```
trial 0 ended with root: -2.0 value at root, f(r): 0.0
trial 1 ended with root: 2.0 value at root, f(r): 0.0
trial 2 ended with root: 2.0 value at root, f(r): 0.0
trial 3 ended with root: -2.000000032851974 value at root, f(r): 1.3140789789645169e-08
trial 4 ended with root: 1.9999999996184186 value at root, f(r): -1.5263257324704682e-09
trial 5 ended with root: -2.000000075022694 value at root, f(r): 3.000907806693931e-07
trial 6 ended with root: -2.0 value at root, f(r): 0.0
trial 7 ended with root: 1.9999999996184186 value at root, f(r): -1.5263257324704682e-09
trial 8 ended with root: 1.9999999996184186 value at root, f(r): -1.5263257324704682e-09
trial 9 ended with root: 1.9999999996184186 value at root, f(r): -1.5263257324704682e-09
```



9.3 Finding a Minimum of Functions

An important problem frequently encountered in many disciplines is optimization. In such problems, as illustrated in Fig. 9.3.1, we have a function $f(x)$ and we wish to find its minimum value (f^*):

$$f^* \leftarrow \min_{x \in \mathbb{R}} f(x), \quad (9.3.1)$$

or the value (x^*) that minimizes it:

$$x^* \leftarrow \arg \min_{x \in \mathbb{R}} f(x). \quad (9.3.2)$$

In many practical settings, the functions that we work with may have multiple minima. In such a case, the minimum point, x^* , can be either (i) a *global minimum* such that there may *not* be any other point \hat{x} with $f(\hat{x}) < f(x^*)$, (ii) a *local minimum* such that x^* is the minimum of a local neighborhood.

The methods generally exploit two important cues: (i) At a minimum, the sign of the first-order derivative changes (on the sides of the minimum). (ii) At a minimum, the first derivative is zero.

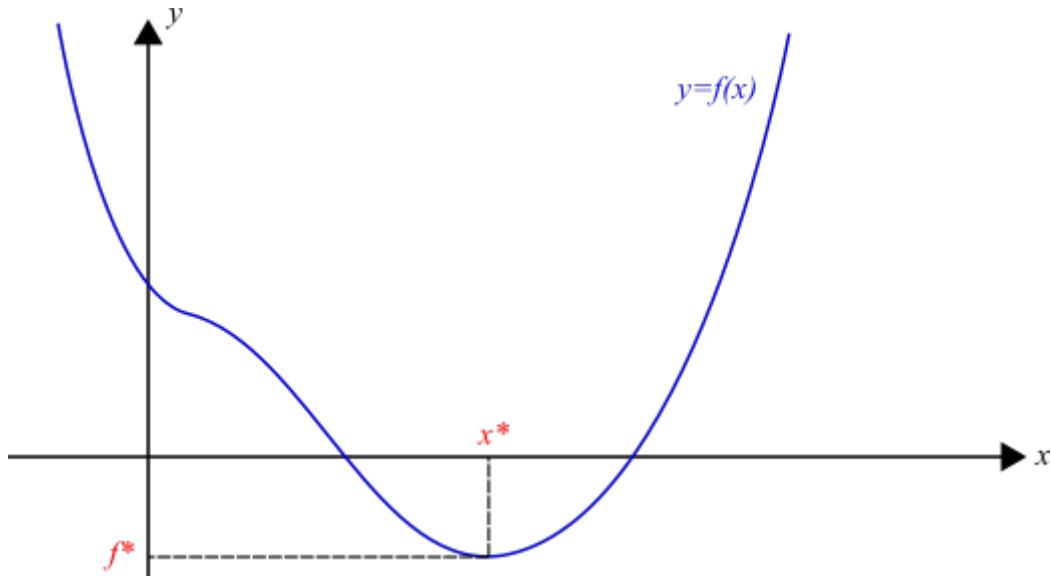


Fig. 9.3.1: Finding a minimum of a function $f(x)$ means finding x^* for which $f(x^*)$ is the lowest value (or lower than all others in a local neighborhood) that function $f()$ can take.

9.3.1 Newton's Method for Finding the Minimum of a Function

Similar to find the root of a function explained in Section 11.2, Newton's method for finding a local minimum of a function $f()$ works iteratively starting from an initial value x_0 by using the *second-order expansion* of $f()$ around x_i this time:

$$f(x_{i+1}) \approx f(x_i) + \frac{f'(x_i)}{1!}(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2, \quad (9.3.3)$$

which can be simplified by rewriting $x_{i+1} = x_i + \delta$:

$$f(x_i + \delta) \approx f(x_i) + \frac{f'(x_i)}{1!}\delta + \frac{f''(x_i)}{2!}\delta^2. \quad (9.3.4)$$

We are interested in finding δ that minimizes the approximation. This can be obtained by setting the first derivative to zero:

$$\frac{d}{d\delta} \left(f(x_i) + \frac{f'(x_i)}{1!}\delta + \frac{f''(x_i)}{2!}\delta^2 \right) = f'(x_i) + f''(x_i)\delta = 0, \quad (9.3.5)$$

which yields the delta value minimizing the approximation:

$$\delta = -\frac{f'(x_i)}{f''(x_i)}. \quad (9.3.6)$$

Plugging this into $x_{i+1} = x_i + \delta$, we obtain the equation for calculating the next value in the sequence towards a minimum of function $f()$:

$$x_{i+1} \leftarrow x_i - \frac{f'(x_i)}{f''(x_i)}. \quad (9.3.7)$$

9.3.2 Misc Details for the Curious

Notes on Convergence

Newton's method can converge to a local minimum if (i) f is a strongly convex function with Lipschitz Hessian and (ii) x_0 is close enough to $x^* \leftarrow \arg \min_{x \in \mathbb{R}} f(x)$. More formally when:

$$\|x_{i+1} - x^*\| \leq \frac{1}{2} \|x_i - x^*\|^2. \quad \forall i \geq 0. \quad (9.3.8)$$

In plain English, (i) we have a “well-shaped” local neighborhood in which we can talk about the concept of a minimum, (ii) our initial value, x_0 , is inside such a neighborhood.

Notes on Multiple Minima

Similar to the case for root finding, Newton's method converges only to a single minimum based on the initial value x_0 . In order to find other minima, the algorithm needs to be executed with a different value of x_0 , which will hopefully lead to a different minimum than the ones that we have identified before.

9.3.3 Newton's Method in Python

Now let us implement Newton's method for finding a minimum of a function from scratch, in Python.

```
def find_local_min(f_deriv, f_second_deriv, x_0, max_steps=10, delta=0.001, verbose=True):
    """
    Use Newton's method to find a local minimum of function f, given its derivative f_deriv.
    Inputs: f=>function
            f_deriv=>derivative of function f
            x_0=>initial x value
            max_steps=>maximum number of iterative steps (default: 10)
            delta=>if |x_{i+1} - x_i| < delta, then assume convergence
    """
    x_old = x_0
    for i in range(max_steps):
        try:
            x_new = x_old - f_deriv(x_old) / f_second_deriv(x_old)
        except ZeroDivisionError:
            # Encountered division-by-zero, return None
            return None

        if verbose: print("Iteration ", i, ". (x_old, x_new): ", (x_old, x_new), " |x_new-x_old|: ", abs(x_new-x_old))
        if abs(x_new-x_old) < delta: break

        # Step 4
        x_old = x_new

    return x_new

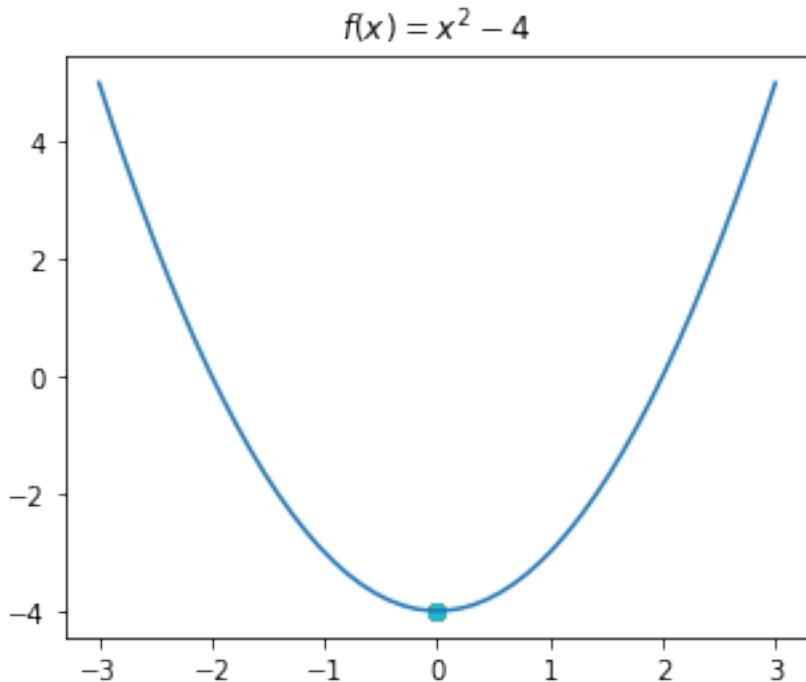
# Assume that our function is: f(x) = x^2 - 4
def f_deriv(x_i): return 2*x_i
def f_second_deriv(x_i): return 2
```

```
# Let us test our solution with 10 random initial values
import random
```

(continues on next page)

```
draw_f() # defined in Section 11.2
for i in range(10):
    x_0 = random.randint(-5, 5) # A random integer in [-5, 5]
    x_min = find_local_min(f_deriv, f_second_deriv, x_0, max_steps=50, delta=0.0001, verbose=False)
    if (x_min == None) or (abs(f_deriv(x_min)) > 0.001): continue # Diverged or division-by-zero, ignore
    print("trial", i, "led to x_min: ", x_min, ", f(x_min): ", f_deriv(x_min))
    plt.scatter(x_min, f(x_min))
```

```
trial 0 led to x_min: 0.0 , f(x_min): 0.0
trial 1 led to x_min: 0.0 , f(x_min): 0.0
trial 2 led to x_min: 0.0 , f(x_min): 0.0
trial 3 led to x_min: 0.0 , f(x_min): 0.0
trial 4 led to x_min: 0.0 , f(x_min): 0.0
trial 5 led to x_min: 0.0 , f(x_min): 0.0
trial 6 led to x_min: 0.0 , f(x_min): 0.0
trial 7 led to x_min: 0.0 , f(x_min): 0.0
trial 8 led to x_min: 0.0 , f(x_min): 0.0
trial 9 led to x_min: 0.0 , f(x_min): 0.0
```



9.3.4 Newton's Method for Finding Minima in SciPy

Unfortunately, Newton's method as explained in Section 11.3.1 does not exist in SciPy. However, there are many alternatives and we will just illustrate only one of them here.

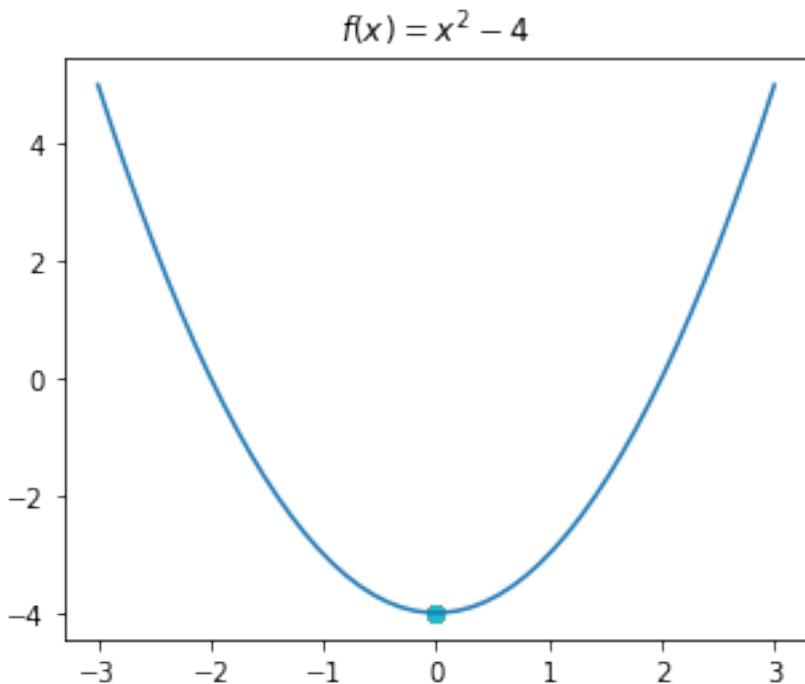
```
from scipy.optimize import minimize_scalar
import random

draw_f()
for i in range(10):
```

(continues on next page)

```
x_0 = random.randint(-5, 5) # A random integer in [-5, 5]
result = minimize_scalar(f, method='golden', tol=0.001, options={'maxiter': 50})
x_min = result['x']
print("trial", i, "led to x_min: ", x_min, ", f(x_min): ", f(x_min))
plt.scatter(x_min, f(x_min))
```

trial 0 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 1 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 2 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 3 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 4 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 5 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 6 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 7 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 8 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08
 trial 9 led to x_min: 1.4872654968309704e-08 , f(x_min): 2.974530993661941e-08



9.4 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- Taylor Series for function approximation.
- Newton's method for finding the roots and the minima of functions.
- Local minimum vs. global minimum.

9.5 Further Reading

- Taylor Series: <https://openstax.org/books/calculus-volume-2/pages/6-3-taylor-and-maclaurin-series>
- Newton's Method:
 - <https://openstax.org/books/calculus-volume-1/pages/4-9-newtons-method>
 - http://www.opentextbookstore.com/calc/2_7.pdf

Exercises

- For the Taylor series approximation of x^3 in Section 11.1.1:
 1. Discuss how and why the approximation is changing when we add more terms.
 2. Discuss why having 3 terms in the approximation yields a function that is very close to the original function.
 3. Write a Python code that checks whether an approximation is exactly the same as the function being approximated. Use this code to check whether using 3 terms in Taylor series expansion was sufficient for approximating x^3 .
- Approximate the sin function using Taylor Series:
 1. Approximate the sin function with the Taylor Series expansion by taking $a = 0$. You will need the n th derivative of sin, which turns out to be simply $\frac{d^n}{dx^n} \sin(x) = \sin(x + n\pi/2)$.
 2. Plot the approximation for different number of terms (m): 1, 2, 3 and 4. Observe what happens when more terms are added to the approximation.
 3. Compare your approximation results to those we obtained for x^3 . Discuss the reasons for similarities and differences.
- Find the roots of the following functions using Newton's Method:
 1. $f(x) = x^2 - 4$ for $x \in [-5, 5]$.
 2. $f(x) = \sin(x)$ for $x \in [0, \pi]$.
 3. $f(x) = \log(x)$ for $x \in [0.5, 2.5]$.
- Consider a second-order function, e.g. $f(x) = x^2 - 4$, which has a minimum at $x = 0$.
 1. Plot $f()$ and its derivative $f'()$ using matplotlib.
 2. Do you see a link between the root of $f'()$ and the minimum of $f()$?
 3. Using `scipy.optimize.newton()` function, which is for finding the roots of a function, find the *minimum* of function $f()$. Hint: A minimum is a root of the first order derivative.

10 | An Application: Solving a Simple Regression Problem

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In this chapter, we will cover an important problem in many disciplines: that of fitting (regressing) a function to a set of data, i.e. the regression problem. We will look at two versions, namely, linear regression and non-linear regression, using SciPy. While doing so, we will use Pandas, NumPy and Matplotlib as well, which were covered in Chapter 10.

10.1 Introduction

Let us first formulate the problem and clearly outline the notation. In a regression problem, we have a set of x, y values: $\{(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)\}$, where x_i and y_i can be multi-dimensional variables (i.e. vectors) but for the sake of simplicity, in this chapter we will work with one-dimensional x_i and y_i values. In a regression problem, we are interested in finding the function $f()$ that goes through those (x_i, y_i) values. In other words, we wish to find $f()$ that satisfies the following:

$$y_i = f(x_i). \quad (10.1.1)$$

At first, this might look difficult since we are trying to estimate a function from its input-output values and there can be infinitely many functions that can go through a finite set of (x_i, y_i) values. However, by restructuring the problem a little bit and making some assumptions on the general form of $f()$, we can solve such complicated regression problems very well.

Let us briefly describe how we can do so: We first re-write $f()$ as a parametric function and try to formulate the regression problem as the problem of finding the parameters of $f()$:

$$y = f(x) = f(x; \theta) = \sum_{i=1}^m g_i(x; \theta_i), \quad (10.1.2)$$

where $\theta = (\theta_1, \dots, \theta_n)$ is the set of parameters that we need to find to solve the regression problem; and $g_1(), \dots, g_m()$ are our “simpler” functions (compared to $f()$) whose parameters can be identified more easily compared to $f()$.

With this parameterized definition of $f()$, we can formally define regression as an optimization (minimization) problem (see also Chapter 11):

$$\theta^* \leftarrow \arg \min_{\theta \in \mathbb{R}^d} \sum_i (y_i - f(x_i; \theta))^2, \quad (10.1.3)$$

where the summation runs over the $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$ values that we are trying to regress; $(y_i - f(x_i; \theta))^2$ is the error between the estimated (regressed) value (i.e. $f(x_i; \theta)$) and the correct y_i value with θ as the parameters.

We can describe this optimization formulation in words as: Find parameters θ that minimize the error between y_i and what the function is predicting given x_i as input.

This is a minimization problem and in Chapter 11, we have seen a simple solution and how SciPy can be used for such problems. In this chapter, we will spend more time on this with sample regression problems and solutions. Namely,

- Linear regression, where $f()$ is assumed to be a line, $y = ax + b$, and θ is (a, b) .
- Non-linear regression, where $f()$ has a non-linear nature, e.g. a quadratic, exponential or logarithmic form.

10.1.1 Why is regression important?

In many disciplines, we observe an environment, an event, or an entity through sensors or some data collected in a different manner, and obtain some information about what we are observing in the form of a variable x . Each x generally has an associated outcome variable y . Or x can represent an action that we are exerting in an environment and we are interested in finding how x affects the environment by observing a variable y .

Here are some examples for x and y for which finding a function $f()$ can be really useful:

- x : The current that we are providing to a motor. y : The speed of the motor.
- x : The day of a year. y : The average rain fall on a year.
- x : The changes in stock value of a bond in the last day. y : The value of a bond in one hour.
- x : The number of COVID cases in a day. y : The number of deaths owing to COVID.

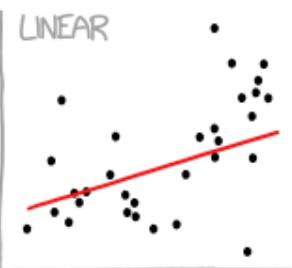
10.1.2 The form of the function

As discussed before, solving the regression problem without making any assumption about the underlying function is very challenging. We can simplify the problem by making an assumption about the function. However, an incorrect assumption can yield inaccurate regression model.

This is illustrated very well in a famous cartoon in Fig. 10.1.1. As illustrated, if the form of the function is too simple (e.g. linear), the fitted function will not be able to capture the true nature of the data. However, if the assumed function form is too complex (e.g. a higher-order polynomial), the fitted function will try to go through every data point, which may not be ideal since the data can be noisy.

Choosing the right form of the function is therefore tricky and it requires some prior idea about the function or the problem. If the relationship between x and y is known to be linear, then a linear function form should be chosen. If the relation between x and y is known to be non-linear but the exact form is unknown, x and y can be plotted first to get a feeling for the underlying form. This can give an idea for what kinds of function forms can be suitable.

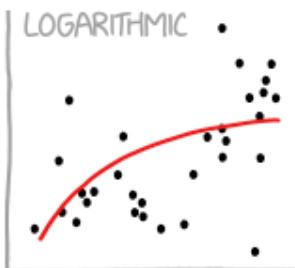
CURVE-FITTING METHODS AND THE MESSAGES THEY SEND



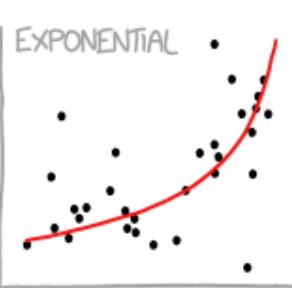
"HEY, I DID A
REGRESSION."



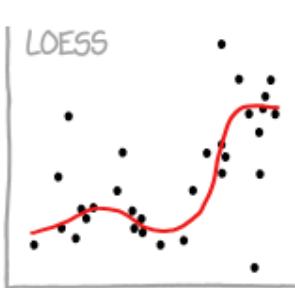
"I WANTED A CURVED
LINE, SO I MADE ONE
WITH MATH."



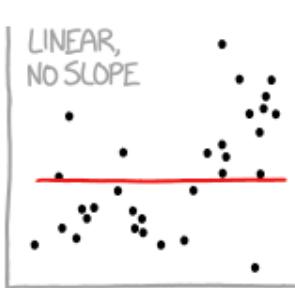
"LOOK, IT'S
TAPERING OFF!"



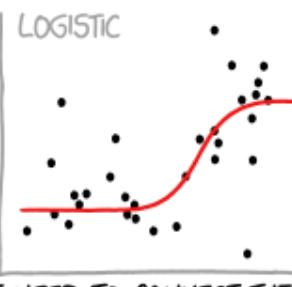
"LOOK, IT'S GROWING
UNCONTROLLABLY!"



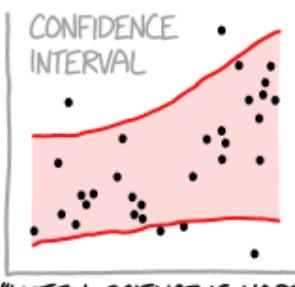
"I'M SOPHISTICATED, NOT
LIKE THOSE BUMBLING
POLYNOMIAL PEOPLE."



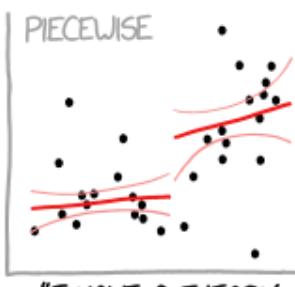
"I'M MAKING A
SCATTER PLOT BUT
I DON'T WANT TO."



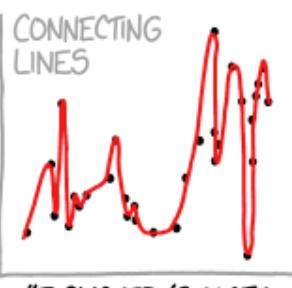
"I NEED TO CONNECT THESE
TWO LINES, BUT MY FIRST IDEA
DIDN'T HAVE ENOUGH MATH."



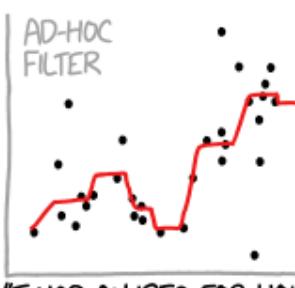
"LISTEN, SCIENCE IS HARD.
BUT I'M A SERIOUS
PERSON DOING MY BEST."



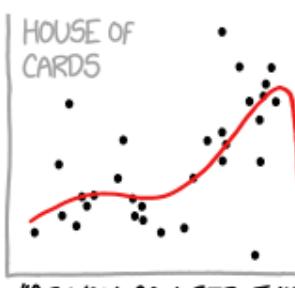
"I HAVE A THEORY,
AND THIS IS THE ONLY
DATA I COULD FIND."



"I CLICKED 'SMOOTH
LINES' IN EXCEL."



"I HAD AN IDEA FOR HOW
TO CLEAN UP THE DATA.
WHAT DO YOU THINK?"



"AS YOU CAN SEE, THIS
MODEL SMOOTHLY FITS
THE— WAIT NO NO DON'T
EXTEND IT AAAAAAA!!"

Fig. 10.11: The challenging regression problem can be simplified by making an assumption about the underlying function; as illustrated in the drawings, the function can be assumed to be linear, quadratic, logarithmic etc. However, an incorrect assumption can yield inaccurate regression. (Figure source: <https://xkcd.com/2048/>)

10.2 Least-Squares Regression

A commonly-used method for regression is called Least-Squares Regression (LSE). In LSE, the minimization problem in Section 12.1 is solved by setting the gradient of the objective to zero:

$$\frac{\partial}{\partial \theta_j} \sum_i (y_i - f(x_i; \theta))^2 = 0, \quad \text{for each } j. \quad (10.2.1)$$

Linear Least-Squares Regression. If our function is linear, i.e. $f(x_i; \theta) = \theta_1 x_i + \theta_2$, setting the gradient to zero provides us one set of equations for each θ_j . If the number of data points (x_i, y_i) is bigger than the number of variables, these equations can be easily solved to obtain θ that minimizes the objective in Section 12.1. Those interested in the derivation of the solution and its exact form can look up e.g. [Wikipedia²⁸](#).

Non-linear Least-Squares Regression. If our function is not linear, a solution can be obtained iteratively by making a linear approximation/step at each iteration using the so-called [Gauss-Newton method²⁹](#).

10.3 Linear Regression with SciPy

SciPy has a function called `scipy.stats.linregress(x, y)` which we can use to regress a line passing through a set of points. Let us go through an example to see how we can do that. Moreover, we will use our regressed line to analyze some properties of our data.

10.3.1 Create Artificial Data

To keep things simple, let us generate some artificial data in Python and save it in a file called `ch12_linear_data.csv`. We have already run this code and saved this CSV file on web – in the following steps, we will continue with this file on the web. However, you can change the following code to generate data in different forms and with different noise levels and observe how the different regression methods perform.

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

def plot_func(f, params, xs, legend):
    ys = f(xs, *params) # This is called parameter unpacking -- Google and learn this
    plt.plot(xs, ys, label=legend)

def line_func(x, a, b):
    """Line function."""
    #(a,b) = params
    return a*x + b

xs = np.linspace(-10, 10, 100)
ys = line_func(xs, 3, 0.5) + np.random.normal(0, 4, xs.size) # add random noise

df = pd.DataFrame({'x': xs, 'y': ys})
df.to_csv("ch12_linear_data.csv")
```

(continues on next page)

²⁸ https://en.wikipedia.org/wiki/Linear_least_squares

²⁹ https://en.wikipedia.org/wiki/Gauss%20%80%93Newton_algorithm

```
print("Created {0} many data points and saved them into CSV file.".format(xs.size))
```

Created 100 many data points **and** saved them into CSV file.

10.3.2 Download and Visualize Data

Let us download the ch12_linear_data.csv file from web so that we can provide you the experience of a full data analysis pipeline.

```
# Let us download our data
!wget -nc https://raw.githubusercontent.com/sinankalkan/CENG240/master/figures/ch12_linear_data.csv

# Import the necessary libraries
import pandas as pd

# Read the file named 'ch12_linear_data.csv'
df = pd.read_csv('ch12_linear_data.csv')

# Print the CSV file's contents:
print("The CSV file contains the following:\n", df, "\n")

# Check the types of each column
df.dtypes
```

File ‘ch12_linear_data.csv’ already there; not retrieving.

The CSV file contains the following:

	Unnamed: 0	x	y
0	0	-10.000000	-25.541643
1	1	-9.797980	-21.879656
2	2	-9.595960	-30.961630
3	3	-9.393939	-22.314965
4	4	-9.191919	-28.890941
..
95	95	9.191919	23.674962
96	96	9.393939	30.717558
97	97	9.595960	32.536789
98	98	9.797980	29.463917
99	99	10.000000	21.630870

[100 rows x 3 columns]

	Unnamed: 0	int64
x		float64
y		float64
dtype: object		

```
# Let us visualize the data
import matplotlib.pyplot as plt
```

(continues on next page)

```

xs = df['x'][:].values
ys = df['y'][:].values

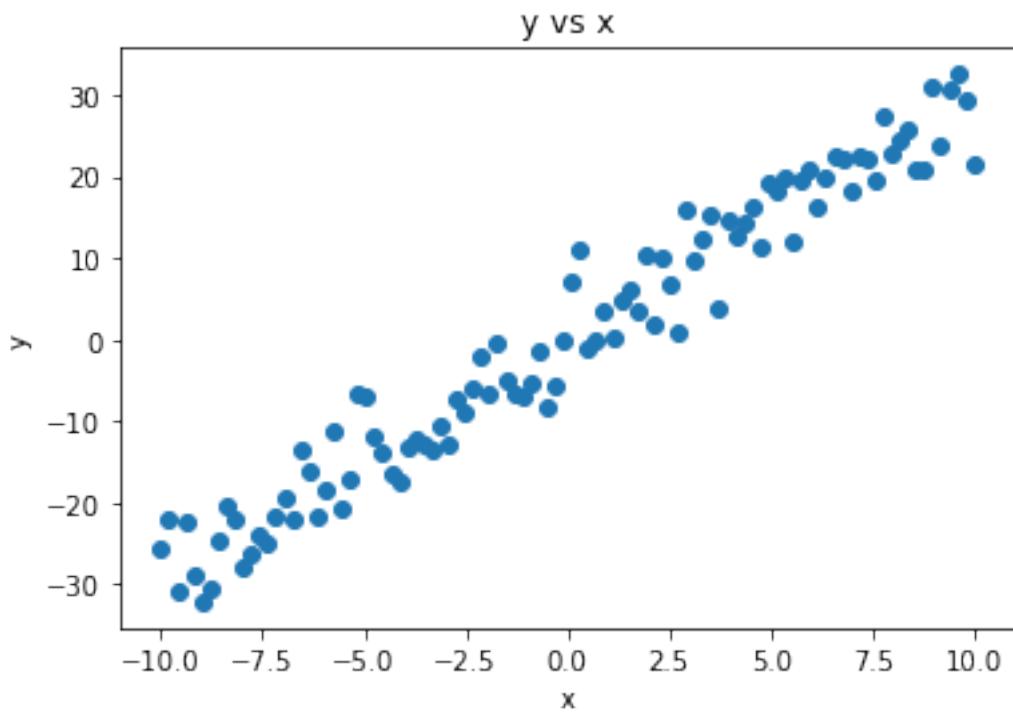
# Plot y vs. x
plt.scatter(xs, ys)

# Set the labels for x and y axes:
plt.xlabel('x')
plt.ylabel('y')

# Set the title of the figure
plt.title("y vs x")

```

```
Text(0.5, 1.0, 'y vs x')
```



We see that our data is rather noisy, though it more or less follows a linear function. Let us see whether we can capture that.

10.3.3 Fit a Linear Function with SciPy

Now, let us fit a line (linear function) to our data using `scipy.stats.linregress`. The specific method being used by this function is Least-Squares Regression which we briefly explained in Section 12.2.

```
# Import stats module
from scipy import stats

# Fit a linear model:
solution = stats.linregress(xs, ys)

# Get the slope (a) and the intercept (b) in y = ax + b
a_estimated = solution.slope
b_estimated = solution.intercept

print("The estimated solution is: y = %4f x + %4f" % (a_estimated, b_estimated))
```

The estimated solution is: $y = 2.962724 x + 0.109122$

10.3.4 Analyze the Solution

We have obtained a solution. Now, let us analyze how good the solution is. We can do that qualitatively (by visual inspection) or quantitatively (by looking at some numerical measures of how good the fit is).

1- Qualitative Analysis. For regression, a qualitative analysis can be performed by plotting the data, the obtained solution and the correct solution. If the obtained solution goes through the data well and is close to the original solution in the graph, then we can visually confirm whether the solution looks acceptable.

Let us do this for our example:

```
# Plot y vs. x
plt.scatter(xs, ys)

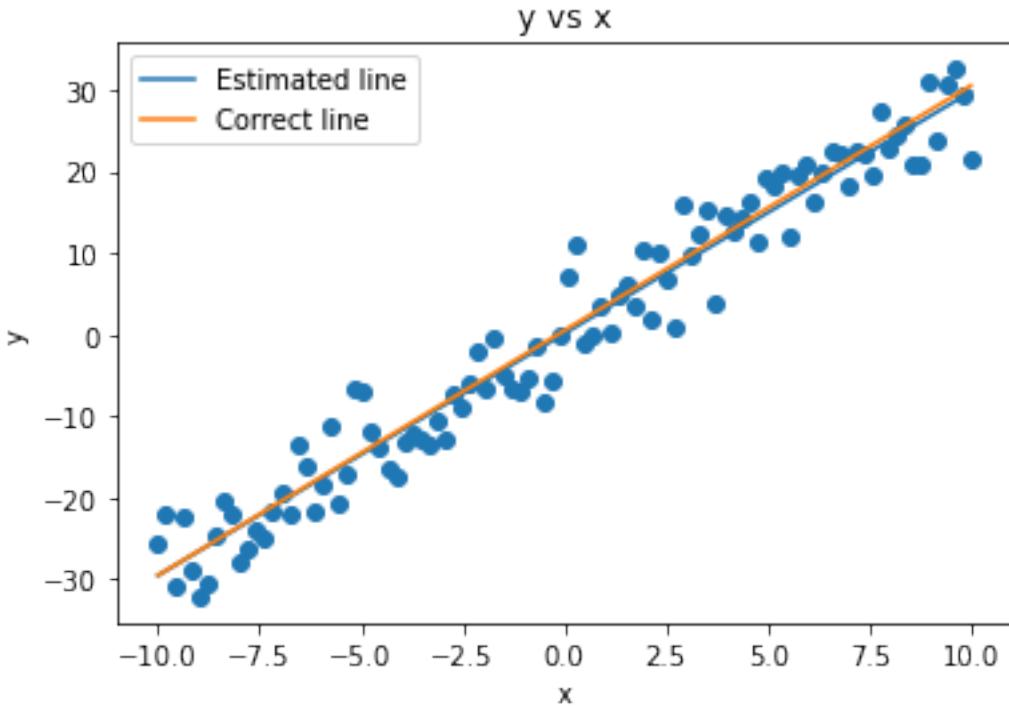
# Plot the estimated line
plot_func(line_func, (a_estimated, b_estimated), xs, "Estimated line")

# Plot the correct line
# The data was generated from y = 3x + 0.5
a_correct = 3
b_correct = 0.5
plot_func(line_func, (a_correct, b_correct), xs, "Correct line")

# Set the labels for x and y axes:
plt.xlabel('x')
plt.ylabel('y')

# Set the title of the figure
plt.title("y vs x")

# Legend
plt.legend()
```



We can confirm that the obtained solution (blue line) goes through the original data points well and it is almost identical to the correct line, i.e. the line from which we generated the original (x, y) pairs. So, our regression solution appears to be accurate visually.

2- Quantitative Analysis. Qualitative analysis can be difficult sometimes and its judgment is subjective; i.e. different observers might draw different conclusions especially in cases where the solution is different from the correct solution. Therefore, in addition to the qualitative analysis like we did above, it is very common to measure the goodness of our solution with a number.

Depending on the problem, different measures can be used. For regression, we frequently use the following three:

1. *Mean Squared Error (MSE)*. For N data points, assuming \hat{y}_i is the predicted value for x_i , MSE can be defined as follows:

$$MSE = \frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2, \quad (10.3.1)$$

which essentially accumulates the squared errors for each data point.

2. *Root Mean Squared Error (RMSE)*. RMSE is simply the square-root of MSE:

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^N (y_i - \hat{y}_i)^2}. \quad (10.3.2)$$

3. *:math: R^2` Error* (also called the coefficient of determination). R^2 is a normalized measure which considers the error of the “correct” solution as well. Since data can be noisy, this can be a better way to understand how good/bad our error value (MSE or RMSE) was. R^2 Error is defined as:

$$R^2 = 1 - \frac{\text{MSE of estimates}}{\text{MSE wrt. the mean of } y} = 1 - \frac{1/N \sum_{i=1}^N (y_i - \hat{y}_i)^2}{1/N \sum_{i=1}^N (y_i - \bar{y})^2} = 1 - \frac{\sum_{i=1}^N (y_i - \hat{y}_i)^2}{\sum_{i=1}^N (y_i - \bar{y})^2}, \quad (10.3.3)$$

where $\bar{y} = 1/N \sum_i y_i$ is the mean of y values. If $R^2 = 1$, that means MSE of the estimates is zero; i.e. we have obtained perfect regression. If $R^2 = 0$, all $y_i = \bar{y}$; in other words, all estimates are the mean of the y values, therefore the regression method did not find a good solution. If, on the other hand, $R^2 < 0$, that means the obtained solution is even worse than the mean y_i values.

Now let us analyze our solution using these three metrics.

```
def MSE(estimated_y, correct_y):
    """
    Mean Squared Error between the estimated_y and correct_y values.
    Inputs are both numpy arrays.
    """
    result = 0
    N = estimated_y.size
    for i in range(N):
        result += (estimated_y[i] - correct_y[i]) ** 2
    return result / N

def RMSE(estimated_y, correct_y):
    """
    Root Mean Squared Error between the estimated_y and correct_y values.
    Inputs are both numpy arrays.
    """
    return MSE(estimated_y, correct_y) ** 0.5

def R_squared(estimated_y, correct_y):
    """
    R^2 error between the estimated_y and correct_y values.
    Inputs are both numpy arrays.
    """
    MSE_of_estimates = MSE(estimated_y, correct_y)
    mean_y = correct_y.mean()
    mean_y_array = np.full(correct_y.size, mean_y)
    MSE_wrt_mean_of_y = MSE(estimated_y, mean_y_array) # an array filled with mean-y
    result = 1 - MSE_of_estimates / MSE_wrt_mean_of_y

    return result

estimated_y = xs * a_estimated + b_estimated
correct_y = ys

print("MSE Error: ", MSE(estimated_y, correct_y))
print("RMSE Error: ", RMSE(estimated_y, correct_y))
print("R-squared Error: ", R_squared(estimated_y, correct_y))
```

```
MSE Error: 14.421275615638306
RMSE Error: 3.7975354660145446
R-squared Error: 0.9516878523484535
```

We see that we have obtained very low errors. Especially the R^2 value is very close to one, which suggests good approximation of the regressed line to the underlying solution. Note that since our data was noisy, it was not possible to obtain $R^2 = 1$.

10.4 Non-linear Regression with SciPy

Let us now see how we can perform non-linear regression.

10.4.1 Create Artificial Data

To keep things simple, let us generate some artificial data in Python and save it in a file called ch12_nonlinear_data.csv. We have already run this code and saved this CSV file on web – in the following steps, we will continue with this file on the web. However, you can change the following code to generate data in different forms and with different noise levels and observe how the different regression methods perform.

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

def nonlinear_f(xs, params):
    (a,b) = params
    return a*np.sin(xs)+b

xs = np.linspace(-10, 10, 100)
ys = nonlinear_f(xs, params=(3, 0.5)) + np.random.normal(0, 0.7, xs.size) # add random noise

df = pd.DataFrame({'x': xs, 'y': ys})
df.to_csv("ch12_nonlinear_data.csv")

print("Created {} many data points and saved them into CSV file.".format(xs.size))
```

Created 100 many data points **and** saved them into CSV file.

10.4.2 Download and Visualize Data

Let us download the ch12_linear_data.csv file from web so that we can provide you the experience of a full data analysis pipeline.

```
# Let us download our data
!wget -nc https://raw.githubusercontent.com/sinankalkan/CENG240/master/figures/ch12_nonlinear_data.csv

# Import the necessary libraries
import pandas as pd

# Read the file named 'ch12_nonlinear_data.csv'
df = pd.read_csv('ch12_nonlinear_data.csv')

# Print the CSV file's contents:
print("The CSV file contains the following:\n", df, "\n")

# Check the types of each column
df.dtypes
```

```
File 'ch12_nonlinear_data.csv' already there; not retrieving.
```

The CSV file contains the following:

```
Unnamed: 0      x      y
0      0 -10.000000 1.721089
1      1 -9.797980 0.708420
2      2 -9.595960 0.347027
3      3 -9.393939 0.287755
4      4 -9.191919 0.594612
..    ...
95     95  9.191919 1.280956
96     96  9.393939 -0.629524
97     97  9.595960 -0.004467
98     98  9.797980 0.233133
99     99 10.000000 -0.838783
```

[100 rows x 3 columns]

```
Unnamed: 0      int64
x            float64
y            float64
dtype: object
```

```
# Let us visualize the data
import matplotlib.pyplot as plt

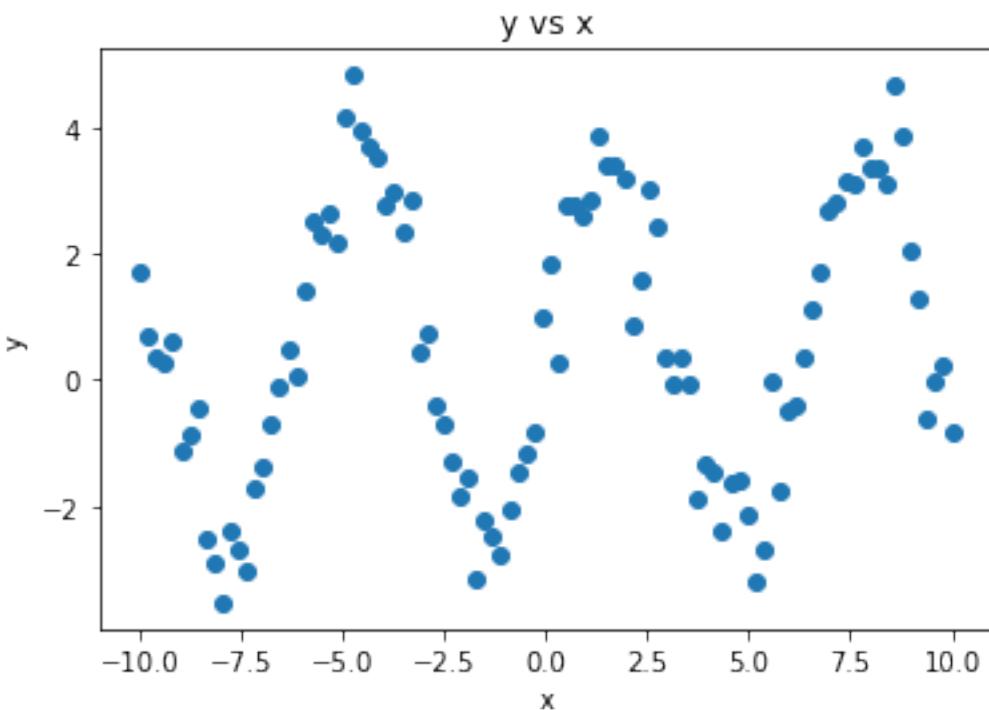
xs = df['x'][:].values
ys = df['y'][:].values

# Plot y vs. x
plt.scatter(xs, ys)

# Set the labels for x and y axes:
plt.xlabel('x')
plt.ylabel('y')

# Set the title of the figure
plt.title("y vs x")
```

```
Text(0.5, 1.0, 'y vs x')
```



10.4.3 Fitting a Non-linear Function with SciPy

For non-linear regression, we will use `scipy.optimize.curve_fit` which internally performs Non-linear Least-squares Regression.

```
# Import optimize module
from scipy import optimize

def nonlinear_f(x, a, b):
    return a * np.sin(x) + b

# Fit a linear model:
solution, _ = optimize.curve_fit(nonlinear_f, xs, ys, method='lm')

print("The estimated solution is: ", solution)
```

The estimated solution is: [3.03810507 0.56551062]

10.4.4 Analyzing the Solution

Similar to our analysis in Section 12.3.4, let us analyze our solution qualitatively and quantitatively.

1- Qualitative Analysis. Let us first analyze the found solution qualitatively.

```
# Plot y vs. x
plt.scatter(xs, ys)

# Plot the estimated line
```

(continues on next page)

```

plot_func(nonlinear_f, solution, xs, "Estimated curve")

# Plot the correct curve
plot_func(nonlinear_f, (3, 0.5), xs, "Correct curve")

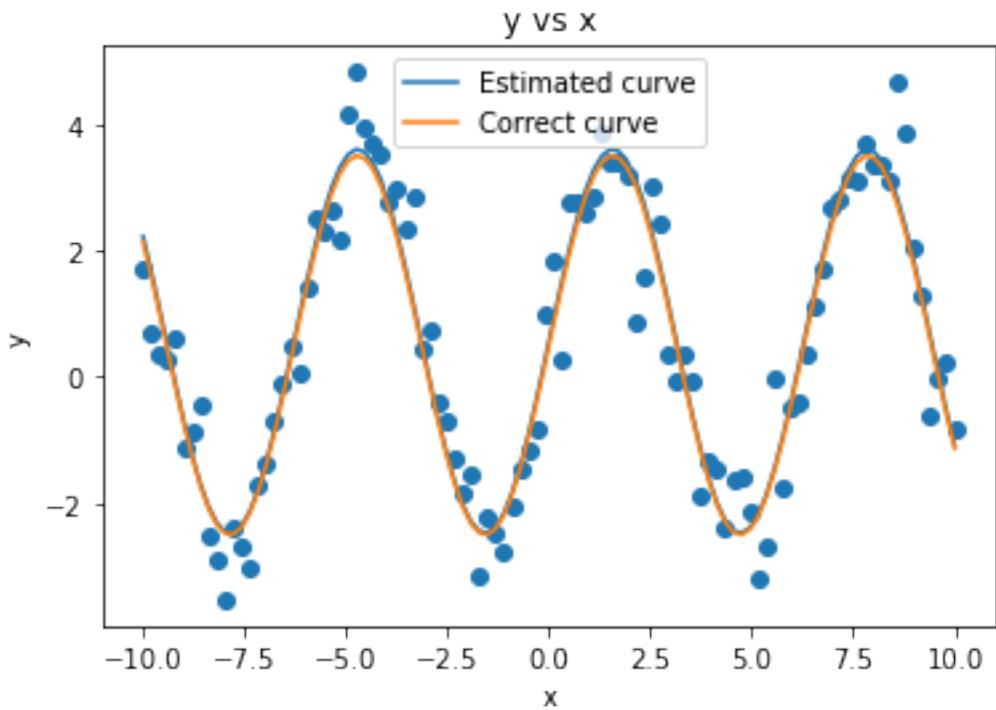
# Set the labels for x and y axes:
plt.xlabel('x')
plt.ylabel('y')

# Set the title of the figure
plt.title("y vs x")

# Legend
plt.legend()

```

<matplotlib.legend.Legend at 0x132d74d00>



Visually, it appears that our estimated solution is a very good fit for the data and it overlaps nicely with the correct function with which we had generated the data.

2- Quantitative Analysis. Now, let us look at some the metrics we have defined in Section 12.3 to get a better feeling for how good our fit was:

```

estimated_y = nonlinear_f(xs, *solution)
correct_y = ys

print("MSE Error: ", MSE(estimated_y, correct_y))
print("RMSE Error: ", RMSE(estimated_y, correct_y))
print("R-squared Error: ", R_squared(estimated_y, correct_y))

```

MSE Error: 0.4719959515976198
RMSE Error: 0.6870196151476461
R-squared Error: 0.892495976237392

We see again that we have obtained low error values, despite the noise. However, we couldn't obtain perfect regression ($R^2 = 1$) since our data was very noisy.

10.5 Important Concepts

We would like our readers to have grasped the following crucial concepts and keywords from this chapter:

- Regression problem and its uses.
- Least-squares regression.
- Linear vs. non-linear regression.
- Linear and non-linear regression with SciPy.
- Qualitatively and quantitatively analyzing a regression solution.

10.6 Further Reading

- The Elements of Statistical Learning, a free book that provides a good coverage of linear and non-linear regression: <https://web.stanford.edu/~hastie/ElemStatLearn/>
- Practical Regression and Anova using R, another free book that provides a practical coverage: <https://cran.r-project.org/doc/contrib/Faraway-PRA.pdf>

Exercises

1. For clarity, we implemented the error metrics in Section 12.3 using for loops. Re-implement them using NumPy functions without using explicit for or while loops.
2. Generate 100 random (x, y) values from a non-linear function, e.g. $y = x^2$, for $x \in [-10, 10]$ and use the linear regression steps in Section 12.3 to regress a linear solution. Qualitatively and quantitatively analyze the obtained solution.
3. Choose your favorite city and download its temperature readings for two consecutive days from [meteoblue³⁰](#). Download the readings as CSV files and load them using Pandas. Plot the data using Matplotlib and see the general shape of the function. Choose a suitable non-linear function and follow the steps in Section 12.4 to regress a function to the temperature data. Measure also how good the function represents the temperature readings of the second day.

³⁰ <https://content.meteoblue.com/en/content/view/full/2879>