COMP1730/COMP6730
Programming for Scientists

I/O and files

Outline

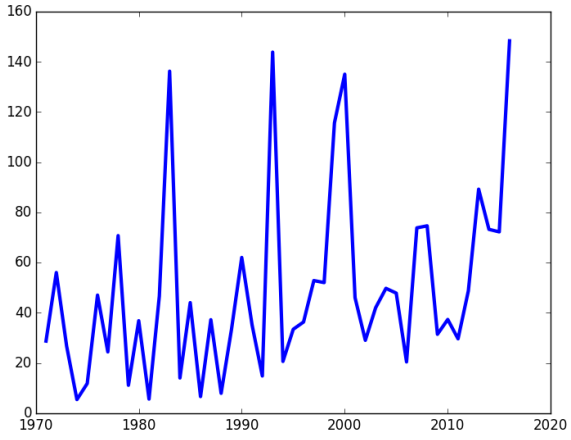
* Input and output
* Files and directories
* Reading and writing text files

Input and output

I/O: Input and Output

* A (common) way for a program to interact with the world.
  - Reading data (keyboard, files, network).
  - Writing data (screen, files, network).
* Scientific computing often means processing or generating large volumes of data.

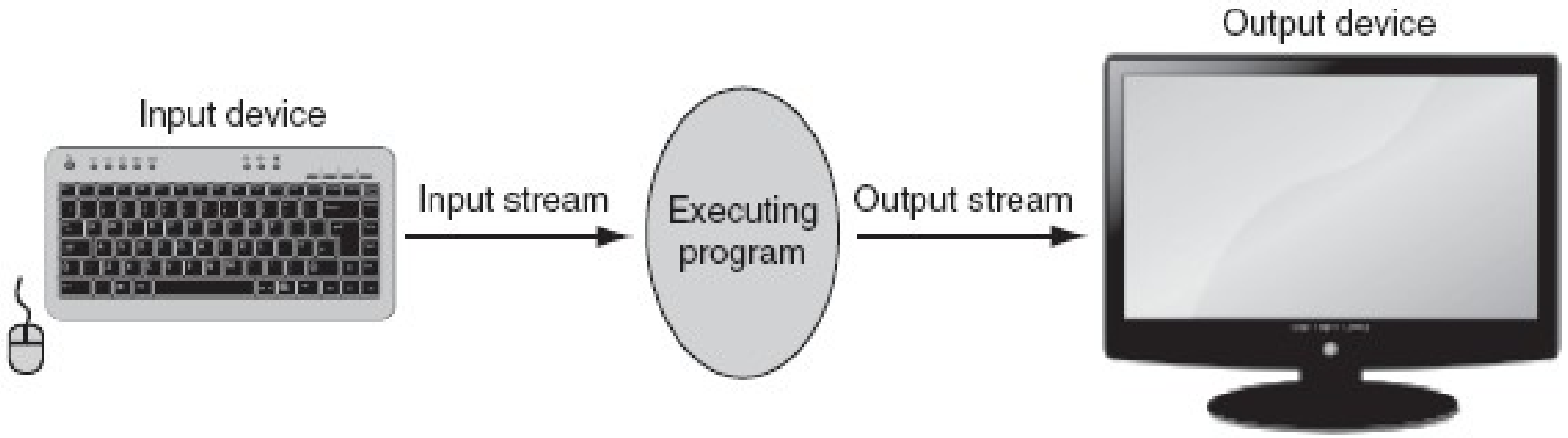
```
2016,  07,  01,   2.0,  1,  Y
2016,  07,  02,   0.0,  1,  Y
2016,  07,  03,   0.0,  1,  Y
2016,  07,  04,   0.0,   ,  Y
2016,  07,  05,   4.4,  1,  Y
2016,  07,  06,  15.4,  1,  Y
2016,  07,  07,   1.0,  1,  Y
2016,  07,  08,   0.0,  1,  Y
2016,  07,  09,   4.2,  1,  Y
2016,  07,  10,   0.0,  1,  Y
2016,  07,  11,  10.4,  1,  Y
```



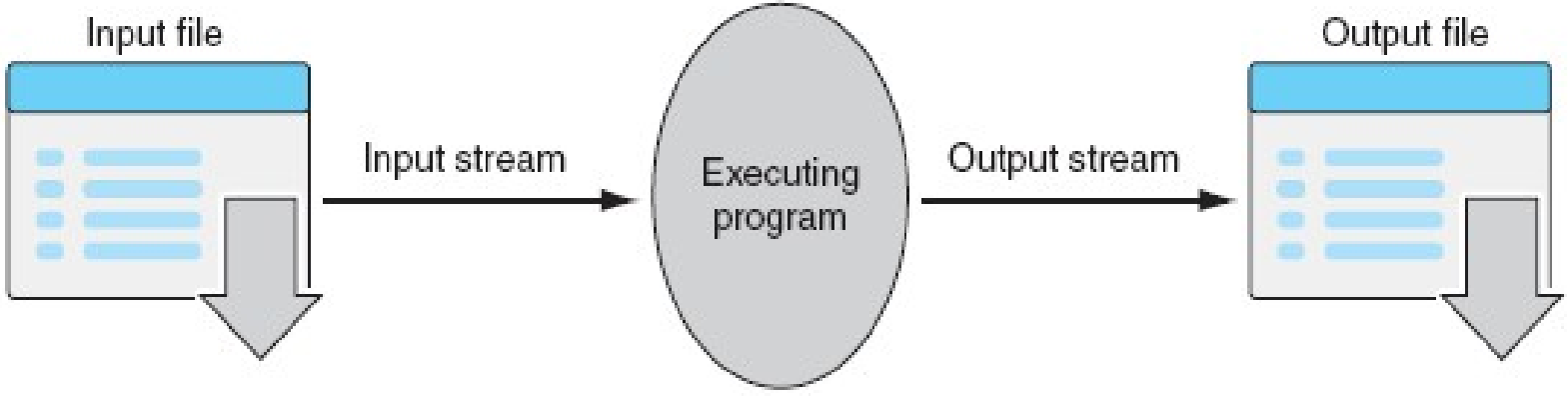
Terminal I/O

* `print(...)` generates output to the terminal (typically, screen).
* `input(...)` prints a prompt and reads input from the terminal (typically, keyboard).
  - `input` always returns a string.

```
input_str = input("Enter a number: ")
input_int = int(input_str)
```



a) Standard input and output



b) File input and output

FIGURE 5.1 Input-output streams.

Image from Punch & Enbody

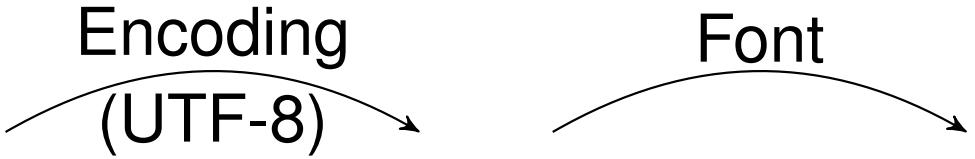
Files and directories

What is a file?

* A *file* is a collection of data on secondary storage (hard drive, USB key, network file server).
* A program can *open* a file to read/write data.
* Data in a file is a sequence of *bytes* (integer $0 \leq b \leq 255$).
  - The program reading a file must *interpret* the data (as text, image, sound, etc).
  - python & the operating system (OS) provide support for interpreting data as text.

Text encoding (recap)

* Every character has a number (an encoding): *ASCII* is a simple encoding of each character into a byte. *Unicode* is a superset of ASCII that defines numbers ("*code points*") for $>$140,000 characters (in a space for $>$1 million). Unicode can encode many languages and emojiis. The ASCII subset is commonly sufficient and used for text-based scientific data formats.

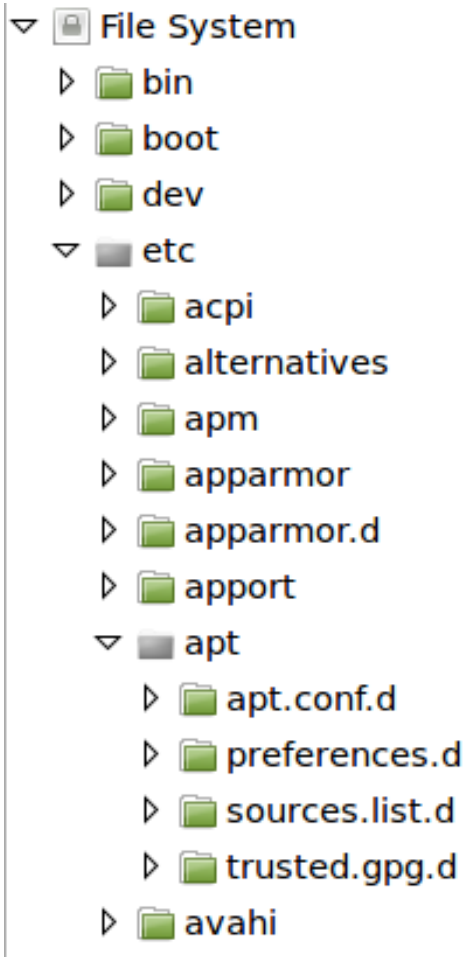


Byte(s)	Code point	Glyph
0100 0101 (69)	69	E E E

* For scientific datasets there are two major formats:
* A *text file* contains (encodings of) printable characters (including spaces, newlines, etc) and numbers are saved as decimal text, which can be examined using a text editor (e.g. csv and FASTA files in genomics).
* A *binary file* contains arbitrary data, which may not correspond to printable characters. Numeric data is saved in binary. (e.g. zip file, BAM file in genomics). Cannot be viewed in a simple text editor, but typically saves storage space and improves speed of access.

Directory structure

* Files on secondary storage are organised into *directories* (a.k.a. *folders*).
* This is an abstraction provided by the operating system.
  - It will appear differently on different operating systems.
* The directory structure is typically tree-like.



File path

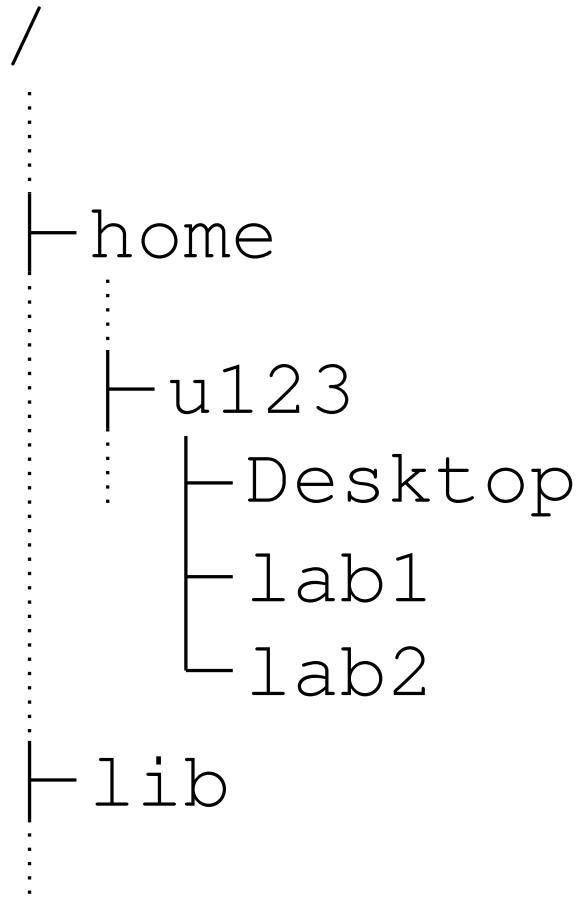
* A *path* is string that identifies the location of a file in the directory structure.
* Consists of directory names with a *separator* between each; the last name in the path is the name of the file.
* Two kinds of paths:
  - *Absolute*
  - *Relative* to the current working directory (cwd)

* When running a python file (script mode), the *current working directory* (cwd) is the directory where that file is.
* If the python interpreter was started in interactive mode (without running a file), the cwd is the directory that it was started from.
* The `os` module has functions to get (and change) the current working directory.

```
>>> import os
>>> os.getcwd()
'/home/patrik/teaching/python'
```

Example: Posix (Linux, OSX)

* Single directory tree.
  - Removable media and network file systems appear at certain places in the tree.
* The separator is `'/'`
* An absolute path starts with a `'/'`
* `'..'` means the directory above.
* File and directory names are *case sensitive*.



If the cwd is `/home/u123/lab1` then

`prob1.py` refers to `/home/u123/lab1/prob1.py`

`../lab2/prob1.py` refers to `/home/u123/lab2/prob1.py`

`../../../lib/libbz2.so` refers to `/lib/libbz2.so`

`/home/u123/Lab1/prob1.py` does not exist.

Example: Windows

* One directory tree for each “drive”; each drive is identified by a letter (`"A"` to `"Z"`)
* The separator historically was `'\'` but modern Windows OS allow `'/'` like UNIX. Note: `'\'` must be written `'\\'`
* Absolute path starts with drive letter and `':'`
* `'..'` means the directory above.
* File and directory names are *not* case sensitive.

`"C:\\Users\\patrik\\test.py"`
`"..\\lab1\\exercise1.py"` or
`"../lab1/exercise1.py"`

Reading and writing text files

File objects

* When we open a file, python creates a *file object* (or, more abstractly, “stream” object).
  - The file object is our interface to the file: all reading, writing, etc, is done through methods of this object.
  - The type of file object (and what we can do with it) depends on the *access mode* specified when the file was opened.
  - For example, *read-only*, *write-only*, *read-write* mode, etc.

Opening a file

* `open(file_path, access_mode)` opens a file and returns the file object.

```
my_file = open("notes.txt", "r")
first_line = my_file.readline()
second_line = my_file.readline()
my_file.close()
```

* Must close the file when done.
* After calling `file_obj.close()`, we can do no more read/write calls on `file_obj`.

Access modes

* *access_mode* is a string, made up of *flags*.

		if the file exists...	if it does not exist...
r	read only		Error
w	write only	Erases file content	Creates a new (empty) file
a	write only	Appends new content at end of file	Creates a new (empty) file
r+	read/write	Reads/overwrites from beginning of file	Error
w+	read/write	Erases file content	Creates a new (empty) file
a+	read/write	Reads/overwrites starting at end of file	Creates a new (empty) file

Note: under Windows, for historical reasons, you should also add “b” to these file modes (binary mode), otherwise certain end of line characters, which differ in Windows, can be modified when reading and writing data.

with statement

* As we saw in the csv example earlier in the course, the *with* statement can simplify closing files and is recommended in modern python code (in the following slides we will explicitly close files to demonstrate the close syntax).

```
import csv
with open("filename.csv") as csvfile:
    reader_iter = csv.reader(csvfile)
    next(reader_iter) # skip the header
    data = [ row for row in reader_iter ]
```

Caution

* Be careful with write modes. Erased or overwritten files cannot be recovered.
* Can we check if an existing file will be overwritten?

  Yes
  - `os.path.exists(`*`file_path`*`)` returns `True` or `False`.
  - Catching exceptions (more later in the course).

Reading text files

* *file_obj*`.readline()` reads the next line of text and returns it as a string, *including* the newline character (`'\n'`).
* *file_obj*`.read(`*size*`)` reads at most *size* characters and returns them as a string.
  - If *size* `< 0`, reads to end of file.
* If already at end-of-file, `readline` and `read` return an empty string.
* *file_obj*`.readlines()` reads all remaining lines of text returning them as a list of strings.

File position

* A file is sequence of bytes.
  - But the file object is *not* a sequence type!
* The file object keeps track of where in the file to read (or write) next.
  - The next read operation (or iteration) starts from the current position.
* When a file is opened for reading (mode `'r'`), the starting position is 0 (beginning of the file).
* File position is *not* the line number.

* Suppose `"notes.txt"` contains:

```
First line
Second line
last line
```

* Then

```
>>> fo = open("notes.txt", "r")
>>> fo.read(4)
'Firs'
>>> fo.readline()
't line\n'
>>> fo.readlines()
['Second line\n', 'last line\n']
```

Iterating through a file

* Python's text file objects are *iterable*.
* Iterating yields one line at time.

```
my_file = open("notes.txt", "r")
line_num = 1
for line in my_file:
    print(line_num, ':', line)
    line_num = line_num + 1
my_file.close()
```

Writing text files

* Access mode `'w'` (or `'a'`) opens a file for writing (text).
* *`file_obj`*`.write(`*`string`*`)` writes the string to the file.
  - Note: `write` does not add a newline to the end of the string.
* `print(..., file=`*`file_obj`*`)` prints to the specified file instead of the terminal.

Buffering

* File objects typically have an I/O buffer.
  - Writing to the file object adds data to the buffer; when full, all data in it is written to the file ("flushing" the buffer).
* Closing the file flushes the buffer.
  - If the program stops without closing an output file, the file may end up incomplete.
* *Always close the file when done!*

Programming problem

* Read a python source code file, and
  - print each line;
  - prefix each line of *code* with a line number;
  - for numbering, count only lines containing code (not empty lines, or lines with only comments).

Takehome

* File system is organised into directories and files in a tree-like structure.
* File path uses '/' (Linux, macOS) or '\' separator (Windows).
* Python file object is iterable but not a sequence.
* Good practice: Write `fileobj=open('abc')` and `fileobj.close()` immediately before adding code in-between, or (better) use the `with` statement.