PYTHON
Introduction to the Basics

October 2022 | S. Linner, M. Lischewski, M. Richerzhagen | Forschungszentrum Jülich

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Table of Contents

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

What is Python?

Python: Dynamic programming language which supports several different programing paradigms:

- Procedural programming
- Object oriented programming
- Functional programming

Standard: Python byte code is executed in the Python interpreter (similar to Java)
$\rightarrow$ **platform independent code**

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Why Python?

- Extremely versatile language
  - Website development, data analysis, server maintenance, numerical analysis, ...
- Syntax is clear, easy to read and learn (almost pseudo code)
- Common language
- Intuitive object oriented programming
- Full modularity, hierarchical packages
- Comprehensive standard library for many tasks
- Big community
- Simply extendable via C/C++, wrapping of C/C++ libraries
- **Focus: Programming speed**

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

History

- Start implementation in December 1989 by Guido van Rossum (CWI)
- 16.10.2000: Python 2.0
  - Unicode support
  - Garbage collector
  - Development process more community oriented
- 3.12.2008: Python 3.0
  - Not 100% backwards compatible
- most popular programming language (TIOBE Index)
- Recommendation for scientific programming (Nature News, NPG, 2015)
- Current version: Python 3.10.8
- Python2 is out of support since 2020![1]

---

[1] https://python3statement.org/

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Zen of Python

- 20 software principles that influence the design of Python:
  1. Beautiful is better than ugly.
  2. Explicit is better than implicit.
  3. Simple is better than complex.
  4. Complex is better than complicated.
  5. Flat is better than nested.
  6. Sparse is better than dense.
  7. Readability counts.
  8. Special cases aren't special enough to break the rules.
  9. Although practicality beats purity.
  10. Errors should never pass silently.
  11. Unless explicitly silenced.
  12. ...

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Is Python fast enough?

- For user programs: Python is fast enough!
- Most parts of Python are written in C
- For compute intensive algorithms: Fortran, C, C++ might be better
- Performance-critical parts can be re-implemented in C/C++ if necessary
- First analyse, then optimise!

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Hello World!

```python
#!/usr/bin/env python3

# This is a commentary
print("Hello world!")
```
hello_world.py

```
$ python3 hello_world.py
Hello world!
$
```

```
$ chmod 755 hello_world.py
$ ./hello_world.py
Hello world!
$
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Hello User

```python
#!/usr/bin/env python3

name = input("What's your name? ")
print("Hello", name)
```

hello_user.py

```
$ ./hello_user.py
What's your name? Rebecca
Hello Rebecca
$
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Strong and Dynamic Typing

Strong Typing:

- Object is of exactly one type! A string is always a string, an integer always an integer
- Counterexamples: PHP, JavaScript, C: `char` can be interpreted as `short`, `void *` can be everything

Dynamic Typing:

- No variable declaration
- Variable names can be assigned to different data types in the course of a program
- An object's attributes are checked only at run time
- Duck typing (an object is defined by its methods and attributes)
  When I see a bird that walks like a duck and swims like a duck and quacks like a duck, I call that bird a duck.[2]

---
[2]James Whitcomb Riley

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Example: Strong and Dynamic Typing

types.py

```python
#!/usr/bin/env python3
number = 3
print(number, type(number))
print(number + 42)
number = "3"
print(number, type(number))
print(number + 42)
```

```
3 <class 'int'>
45
3 <class 'str'>
Traceback (most recent call last):
  File "types.py", line 7, in <module>
    print(number + 42)
TypeError: can only concatenate str (not "int") to str
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE
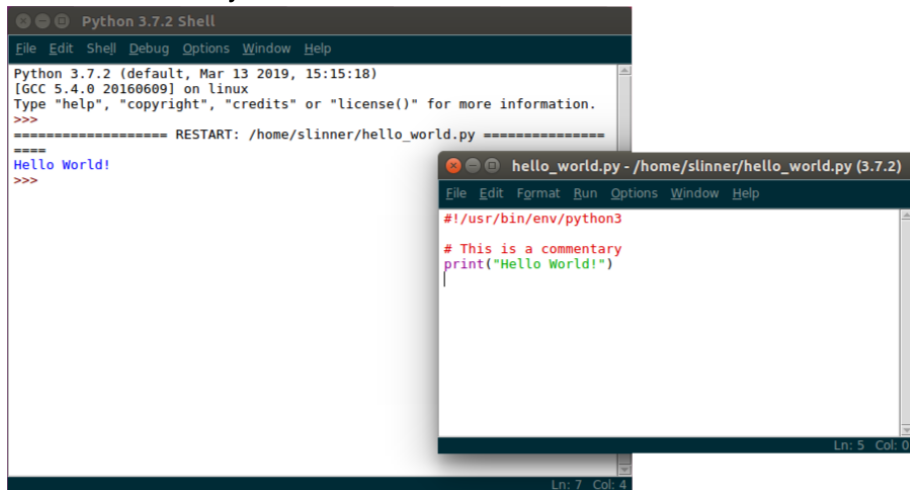
Interactive Mode

The interpreter can be started in interactive mode:

```
$ python3
Python 3.7.2 (default, Mar 13 2019, 15:15:18)
[GCC 5.4.0 20160609] on linux
Type "help", "copyright", "credits" or "license" for
more information.
>>> print("hello world")
hello world
>>> a = 3 + 4
>>> print(a)
7
>>> 3 + 4
7
>>>
```

IDLE

- **I**ntegrated **D**eve**L**opment **E**nvironment
- Part of the Python installation

Documentation

Online help in the interpreter:

- **help()**: general Python help
- **help(obj)**: help regarding an object, e.g. a function or a module
- **dir ()**: all used names
- **dir (obj)**: all attributes of an object

Official documentation: http://docs.python.org/

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Documentation

```
>>> help(dir)
Help on built-in function dir:
...
>>> a = 3
>>> dir()
['__builtins__', '__doc__', '__file__', '__name__', 'a']
>>> help(a)
Help on int object:
...
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Differences Python 2 – Python 3 (incomplete)

	Python 2	**Python 3**
shebang[1]	`#!/usr/bin/python`	`#!/usr/bin/python3`
IDLE cmd[1]	idle	idle3
print cmd (syntax)	`print`	`print()`
input cmd (syntax)	`raw_input()`	`input()`
unicode	`u"..."`	all strings
integer type	`int/long`	`int` (infinite)
...	hints in each chapter	

$\Rightarrow$ `http://docs.python.org/3/whatsnew/3.0.html`

---

[1] linux specific

JÜLICH Forschungszentrum — JÜLICH SUPERCOMPUTING CENTRE

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Numerical Data Types

- `int` : integer numbers (infinite)
- `float` : corresponds to `double` in C
- `complex` : complex numbers (`j` is the imaginary unit)

```
a = 1

c = 1.0
c = 1e0

d = 1 + 0j
```

Operators on Numbers

- **Basic arithmetics**: `+` , `-` , `*` , `/`
  <u>hint:</u> *Python 2* $\Rightarrow$ $1/2 = 0$
  Python 3 $\Rightarrow$ $1/2 = 0.5$

- **Div and modulo operator**: `//` , `%` , `divmod(x, y)`

- **Absolute value**: `abs(x)`

- **Rounding**: `round(x)`

- **Conversion**: `int(x)` , `float(x)` , `complex(re [, im=0])`

- **Conjugate of a complex number**: `x.conjugate()`

- **Power**: `x ** y` , `pow(x, y)`

Result of a composition of different data types is of the "bigger" data type.

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Bitwise Operation on Integers

Operations:

- **AND**: `x & y`

- **OR**: `x | y`

- **exclusive OR (XOR)** :
  `x ^ y`

- **invert**: `~x`

- **shift right n bits**: `x >> n`

- **shift left n bits**: `x << n`

Use `bin(x)` to get binary
representation string of `x` .

```
>>> print(bin(6),bin(3))
0b110 0b11
>>> 6 & 3
2
>>> 6 | 3
7
>>> 6 ^ 3
5
>>> ~0
-1
>>> 1 << 3
8
>>> pow(2,3)
8
>>> 9 >> 1
4
>>> print(bin(9),bin(9>>1))
0b1001 0b100
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Strings

Data type: `str`

- `s = 'spam'`, `s = "spam"`
- Multiline strings: `s = """spam"""`
- No interpretation of escape sequences: `s = r"sp\nam"`
- Generate strings from other data types: `str(1.0)`

```
>>> s = """hello
... world"""
>>> print(s)
hello
world
>>> print("sp\nam")
sp
am
>>> print(r"sp\nam")   # or: print("sp\\nam")
sp\nam
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

String Methods

- Count appearance of substrings: `s.count(sub [, start[, end]])`
- Begins/ends with a substring? `s.startswith(sub [, start[, end]])`, `s.endswith(sub[, start[, end]])`
- All capital/lowercase letters: `s.upper()`, `s.lower()`
- Remove whitespace: `s.strip([chars])`
- Split at substring: `s.split([sub [,maxsplit]])`
- Find position of substring: `s.index(sub[, start[, end]])`
- Replace a substring: `s.replace(old, new[, count])`

More methods: `help(str)`, `dir(str)`

Lists

Data type: `list`

- `s = [1, "spam", 9.0, 42]` , `s = []`
- **Append an element**: `s.append(x)`
- Extend with a second list: `s.extend(s2)`
- Count appearance of an element: `s.count(x)`
- Position of an element: `s.index(x[, min[, max]])`
- Insert element at position: `s.insert(i, x)`
- Remove and return element at position: `s.pop([i])`
- **Delete element**: `s.remove(x)`
- Reverse list: `s.reverse()`
- **Sort**: `s.sort([cmp[, key[, reverse]]])`
- Sum of the elements: `sum(s)`

Tuple

Data type: `tuple`

- `s = 1, "spam", 9.0, 42`

  `s = (1, "spam", 9.0, 42)`
- Constant list
- Count appearance of an element: `s.count(x)`
- Position of an element: `s.index(x[, min[, max]])`
- Sum of the elements: `sum(s)`

Tuple

Data type: `tuple`

- `s = 1, "spam", 9.0, 42`

  `s = (1, "spam", 9.0, 42)`
- Constant list
- Count appearance of an element: `s.count(x)`
- Position of an element: `s.index(x[, min[, max]])`
- Sum of the elements: `sum(s)`

Multidimensional tuples and lists

- List and tuple can be nested (mixed):

```
>>> A=([1,2,3],(1,2,3))
>>> A
([1, 2, 3], (1, 2, 3))
>>> A[0][2]=99
>>> A
([1, 2, 99], (1, 2, 3))
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Lists, Strings and Tuples

- Lists are **mutable**
- Strings and tuples are **immutable**
  - No assignment `s[i] = ...`
  - No appending and removing of elements
  - Functions like `x.upper()` return a new string!

```
>>> s1 = "spam"
>>> s2 = s1.upper()
>>> s1
'spam'
>>> s2
'SPAM'
```

Operations on Sequences

Strings, lists and tuples have much in common: They are **sequences**.

- Does/doesn't s contain an element?
  `x in s`, `x not in s`
- **Concatenate sequences**: `s + t`
- Multiply sequences: `n * s`, `s * n`
- **i-th element**: `s[i]`, i-th to last element: `s[-i]`
- Subsequence (slice): `s[i:j]`, with step size k: `s[i:j:k]`
- Subsequence (slice) from beginning/to end: `s[:-i]`, `s[i:]`, `s[:]`
- **Length** (number of elements): `len(s)`
- **Smallest/largest element**: `min(s)`, `max(s)`
- Assignments: `(a, b, c) = s`
  $\rightarrow$ `a = s[0]`, `b = s[1]`, `c = s[2]`

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Indexing in Python

positive index	0	1	2	3	4	5	6	7	8	9	10
element	P	y	t	h	o	n		K	u	r	s
negative index	-11	-10	-9	-8	-7	-6	-5	-4	-3	-2	-1

```
>>> kurs = "Python Kurs"
>>> kurs[2:2]

>>> kurs[2:3]
t
>>> kurs[2]
t
>>> kurs[-4:-1]
Kur
>>> kurs[-4:]
Kurs
>>> kurs[-6:-8:-1]
no
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Boolean Values

Data type **bool**: `True`, `False`
Values that are evaluated to `False`:

- `None` (data type `NoneType`)
- `False`
- `0` (in every numerical data type)
- Empty strings, lists and tuples: `''`, `[]`, `()`
- Empty dictionaries: `{}`
- Empty sets `set()`

All other objects of built-in data types are evaluated to `True`!

```
>>> bool([1, 2, 3])
True
>>> bool("")
False
```

References

- Every object name is a reference to this object!
- An assignment to a new name creates an additional reference to this object.
  Hint: copy a list with `s2 = s1[:]` or `s2 = list(s1)`
- Operator `is` compares two references (identity),
  operator `==` compares the contents of two objects
- Assignment: different behavior depending on object type
    - Strings, numbers (simple data types): create a new object with new value
    - Lists, dictionaries, ...: the original object will be changed

Reference - Example

```
>>> x=1
>>> y=x
>>> x is y
True
>>> y=2
>>> x is y
False
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Reference - Example

```
>>> x=1
>>> y=x
>>> x is y
True
>>> y=2
>>> x is y
False
```

Reference - Example

```
>>> x=1
>>> y=x
>>> x is y
True
>>> y=2
>>> x is y
False
```

Reference - Example

```
>>> x=1
>>> y=x
>>> x is y
True
>>> y=2
>>> x is y
False
```



```
>>> s1 = [1, 2, 3, 4]
>>> s2 = s1
>>> s2[1] = 17
>>> s1
[1, 17, 3, 4]
>>> s2
[1, 17, 3, 4]
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Reference - Example


```
>>> x=1
>>> y=x
>>> x is y
True
>>> y=2
>>> x is y
False
```



```
>>> s1 = [1, 2, 3, 4]
>>> s2 = s1
>>> s2[1] = 17
>>> s1
[1, 17, 3, 4]
>>> s2
[1, 17, 3, 4]
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE
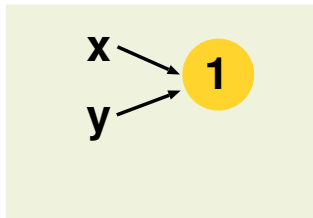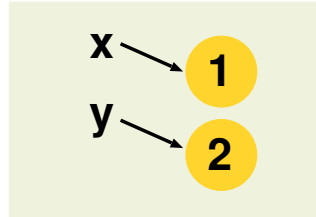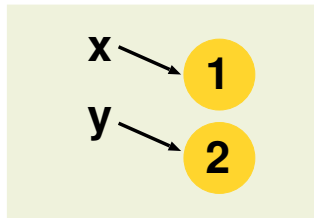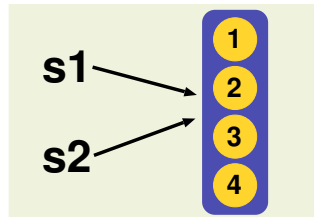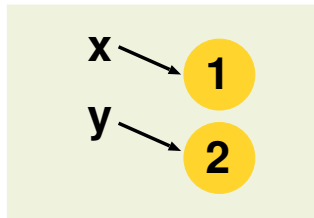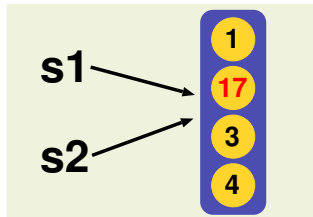
Groups

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

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

The If Statement

```python
if a == 3:
    print("Aha!")
```

- Blocks are defined by indentation! ⇒ *Style Guide for Python*
- Standard: Indentation with four spaces

```python
if a == 3:
    print("spam")
elif a == 10:
    print("eggs")
elif a == -3:
    print("bacon")
else:
    print("something else")
```

Relational Operators

- Comparison of content: `==` , `<` , `>` , `<=` , `>=` , `!=`
- Comparison of object identity: `a is b` , `a is not b`
- And/or operator: `a and b` , `a or b`
- Chained comparison: `a <= x < b` , `a == b == c` , . . .
- Negation: `not a`

```
if not (a==b) and (c<3):
    pass
```

Hint: `pass` is a No Operation (NOOP) function

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

For Loops

```python
for i in range(10):
    print(i)   # 0, 1, 2, 3, ..., 9

for i in range(3, 10):
    print(i)   # 3, 4, 5, ..., 9

for i in range(0, 10, 2):
    print(i)   # 0, 2, 4, 6, 8
else:
    print("Loop completed.")
```

- End loop prematurely: `break`
- Next iteration: `continue`
- `else` is executed when loop didn't end prematurely

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

For Loops (continued)

Iterating directly over sequences (without using an index):

```
for item in ["spam", "eggs", "bacon"]:
    print(item)
```

The `range` function can be used to create a list:

```
>>> list(range(0, 10, 2))
[0, 2, 4, 6, 8]
```

If indexes are necessary:

```
for (i, char) in enumerate("hello world"):
    print(i, char)
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

While Loops

```python
i = 0
while i < 10:
    i += 1
```

`break` and `continue` work for while loops, too.

Substitute for do-while loop:

```python
while True:
    # important code
    if condition:
        break
```

Enjoy

python™

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Functions

```python
def add(a, b):
    """Returns the sum of a and b."""

    mysum = a + b
    return mysum
```

```
>>> result = add(3, 5)
>>> print(result)
8
>>> help(add)
Help on function add in module __main__:

add(a, b)
    Returns the sum of a and b.
```

Return Values and Parameters

- Functions accept arbitrary objects as parameters and return values
- Types of parameters and return values are unspecified
- Functions without explicit return value return `None`

my_program.py

```python
def hello_world():
    print("Hello World!")


a = hello_world()
print(a)
```

```
$ python3 my_program.py
Hello World!
None
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Multiple Return Values

Multiple return values are realised using tuples or lists:

```
def foo():
    a = 17
    b = 42
    return (a, b)

ret = foo()
(x, y) = foo()
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Optional Parameters – Default Values

Parameters can be defined with default values.
Hint: It is not allowed to define non-default parameters after default parameters

plot_lines.py

```python
def fline(x, m=1, b=0): # f(x) = m*x + b
    return m*x + b

for i in range(5):
    print(fline(i),end=" ")
#force newline
print()
for i in range(5):
    print(fline(i,-1,1),end=" ")
```

```
$ python3 plot_lines.py
0 1 2 3 4
1 0 -1 -2 -3
```

Hint: `end` in `print` defines the last character, default is linebreak

Positional Parameters

Parameters can be passed to a function in a different order than specified:

```python
def printContact(name, age, location):
    print("Person:  ", name)
    print("Age:     ", age, "years")
    print("Address: ", location)

printContact(name="Peter Pan", location="Neverland", age=10)
```

displayPerson.py

```
$ python3 displayPerson.py
Person:  Peter Pan
Age:     10 years
Address: Neverland
```

Functions are Objects

Functions are objects and as such can be assigned and passed on:

```
>>> a = float
>>> a(22)
22.0
```

```
>>> def foo(fkt):
...         print(fkt(33))
...
>>> foo(float)
33.0
>>> foo(str)
33
>>> foo(complex)
(33+0j)
```

Online Help: Docstrings

- Can be used in function, modul, class and method definitions
- Is defined by a **string** as the first statement in the definition
- `help(...)` on python object returns the docstring
- Two types of docstrings: one-liners and multi-liners

```python
def complex(real=0.0, imag=0.0):
    """Form a complex number.

    Keyword arguments:
    real -- the real part (default 0.0)
    imag -- the imaginary part (default 0.0)

    """
    ...
```

Functions & Modules

- Functions thematically belonging together can be stored in a separate Python file.
  (Same for objects and classes)
- This file is called **module** and can be loaded in any Python script.
- Multiple modules available in the Python Standard Library
  (part of the Python installation)
- Command for loading a module: `import <filename>`
  (filename without ending .py)

```
import math
s = math.sin(math.pi)
```

More information for standard modules and how to create your own module see chapter
Modules and Packages on slide 91

Enjoy

python™

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

String Formatting

- Format string + class method `x.format()`
- "replacement fields": curly braces around optional arg_name (default: 0,1,2,...)

```
print("The answer is {0:4d}".format(42))
'The answer is   42'
s = "{0}: {1:08.3f}".format("spam", 3.14)
'spam: 0003.140'
```

format	purpose
	default: string
m.n**f**	floating point: **m** filed size, **n** digits after the decimal point (6)
m.n**e**	floating point (exponential): **m** filed size, 1 digit before and **n** digits behind the decimal point (default: 6)
m.n**%**	percentage: similar to format **f**, *value* $* 100$ with finalizing '%'
m**d**	Integer number: **m** field size (**0m** $\Rightarrow$ leading "0") format **d** can be replaced by **b** (binary), **o** (octal) or **x** (hexadecimal)

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Literal String Interpolation (f-strings)

- Provides a way to embed expressions inside string literals, using a minimal syntax
- Is a literal string, prefixed with 'f', which contains expressions inside braces
- Expressions are evaluated at runtime and replaced with their values.

```
>>> name = "Martin"
>>> age = 50
>>> f"My name is {name} and my age next year is {age+1}"
'My name is Martin and my age next year is 51'
>>> value = 12.345
>>> f"value={value:5.2f}"
'value=12.35'
```

Hint: Since Python 3.6!

String Formatting (deprecated, Python 2 only)

String formatting similar to C:

```python
print "The answer is %4i." % 42
s = "%s: %08.3f" % ("spam", 3.14)
```

- **Integer decimal**: d, i
- **Integer octal**: o
- **Integer hexadecimal**: x, X
- **Float**: f, F
- **Float in exponential form**: e, E, g, G
- **Single character**: c
- **String**: s
- Use %% to output a single % character.

Command Line Input

User input in Python 3:

```
user_input = input("Type something: ")
```

User input in Python 2:

```
user_input = raw_input("Type something: ")
```

Hint: In Python 2 is `input("...")` $\iff$ `eval(raw_input("..."))`

Command line parameters:

params.py

```
import sys
print(sys.argv)
```

```
$ python3 params.py spam
['params.py', 'spam']
```

Files

```
file1 = open("spam.txt", "r")
file2 = open("/tmp/eggs.json", "wb")
```

- **Read mode**: `r`
- **Write mode (new file)**: `w`
- **Write mode, appending to the end**: `a`
- **Handling binary files**: e.g. `rb`
- **Read and write (update)**: `r+`

```
for line in file1:
    print(line)
```

Operations on Files

- **Read**: `f.read([size])`

- **Read a line**: `f.readline()`

- **Read multiple lines**: `f.readlines([sizehint])`

- **Write**: `f.write(str)`

- **Write multiple lines**: `f.writelines(sequence)`

- **Close file**: `f.close()`

```python
file1 = open("test.txt", "w")
lines = ["spam\n", "eggs\n", "ham\n"]
file1.writelines(lines)
file1.close()
```

Python automatically converts `\n` into the correct line ending!

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

The `with` **statement**

File handling (open/close) can be done by the context manager `with`.
(⇒section Errors and Exceptions on slide 65).

```python
with open("test.txt") as f:
    for line in f:
        print(line)
```

After finishing the `with` block the file object is closed, even if an exception occurred inside the block.

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Syntax Errors, Indentation Errors

Parsing errors: **Program will not be executed**.

- Mismatched or missing parenthesis
- Missing or misplaced semicolons, colons, commas
- Indentation errors

add.py

```python
print("I'm running...")
def add(a, b)
    return a + b
```

```
$ python3 add.py
  File "add.py", line 2
    def add(a, b)
                 ^
SyntaxError: invalid syntax
```

Exceptions

Exceptions occur at **runtime**:

error.py

```python
import math
print("I'm running...")
math.foo()
print("I'm still running...")
```

```
$ python3 error.py
I'm running...
Traceback (most recent call last):
  File "error.py", line 3, in <module>
    math.foo()
AttributeError: module 'math' has no attribute 'foo'
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Handling Exceptions (1)

```python
try:
    s = input("Enter a number: ")
    number = float(s)
except ValueError:
    print("That's not a number!")
```

- `except` block is executed when the code in the `try` block throws an according exception
- Afterwards, the program continues normally
- Unhandled exceptions force the program to exit.

Handling different kinds of exceptions:

```python
except (ValueError, TypeError, NameError):
```

Built-in exceptions: http://docs.python.org/library/exceptions.html

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Handling Exceptions (2)

```python
try:
    s = input("Enter a number: ")
    number = 1/float(s)
except ValueError:
    print("That's not a number!")
except ZeroDivisionError:
    print("You can't divide by zero!")
except:
    print("Oops, what's happened?")
```

- Several `except` statements for different exceptions
- Last `except` can be used without specifying the kind of exception: Catches all remaining exceptions
    - Careful: Can mask unintended programming errors!

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Handling Exceptions (3)

- `else` is executed if no exception occurred
- `finally` is executed **in any** case

```python
try:
    f = open("spam")
except IOError:
    print("Cannot open file")
else:
    print(f.read())
    f.close()
finally:
    print("End of try.")
```

Exception Objects

Access to exception objects:

- `EnvironmentError` (`IOError` , `OSError`):
  Exception object has 3 attributes (`int` , `str` , `str`)
- Otherwise: Exception object is a string

spam_open.py

```python
try:
    f = open("spam")
except IOError as e:
    print(e.errno, e.filename, e.strerror)
    print(e)
```

```
$ python3 spam_open.py
2 spam No such file or directory
[Errno 2] No such file or directory: 'spam'
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Exceptions in Function Calls

draw() ← rectangle() ← line() Exception!
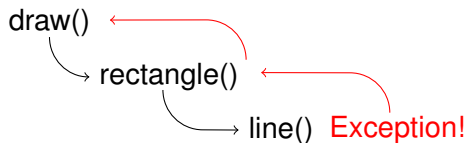
- Function calls another function.
- That function raises an exception.
- Is exception handled?
- No: Pass exception to calling function.

Raising Exceptions

Passing exceptions on:

```python
try:
    f = open("spam")
except IOError:
    print("Problem while opening file!")
    raise
```

Raising exceptions:

```python
def gauss_solver(matrix):
    # Important code
    raise ValueError("Singular matrix")
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Exceptions vs. Checking Values Beforehand

Exceptions are preferable!

```python
def square(x):
    if type(x) == int or type(x) == float:
        return x ** 2
    else:
        return None
```

- What about other numerical data types (complex numbers, own data types)? Better: Try to compute the power and catch possible exceptions! → **Duck-Typing**
- Caller of a function might forget to check return values for validity. Better: Raise an exception!

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Exceptions vs. Checking Values Beforehand

Exceptions are preferable!

```python
def square(x):
    if type(x) == int or type(x) == float:
        return x ** 2
    else:
        return None
```

```python
def square(x):
    return x ** 2
...
try:
    result = square(value)
except TypeError:
    print("'{0}': Invalid type".format(value))
```

The `with` Statement

Some objects offer context management [3] , which provides a more convenient way to write `try ... finally` blocks:

```python
with open("test.txt") as f:
    for line in f:
        print(line)
```

After the `with` block the file object is guaranteed to be closed properly, no matter what exceptions occurred within the block.

---

[3]Class method `__enter__(self)` will be executed at the beginning and class method `__exit__(...)` at the end of the context

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Sets

Set: unordered, no duplicated elements

- `s = {"a", "b", "c"}`
  alternative `s = set(`*[sequence]*`)` , required for empty sets.
- **Constant set**: `s = frozenset(`*[sequence]*`)`
  e.g. empty set: `empty = frozenset()`
- **Subset**: `s.issubset(t)` , `s <= t` , strict subset: `s < t`
- **Superset**: `s.issuperset(t)` , `s >= t` , strict superset: `s > t`
- **Union**: `s.union(t)` , `s | t`
- **Intersection**: `s.intersection(t)` , `s & t`
- **Difference**: `s.difference(t)` , `s - t`
- **Symmetric Difference**: `s.symmetric_difference(t)` , `s ^ t`
- **Copy**: `s.copy()`

As with sequences, the following works:

`x in s` , `len(s)` , `for x in s` , `s.add(x)` , `s.remove(x)`

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Dictionaries

- Other names: Hash, Map, Associative Array
- Mapping of key $\rightarrow$ value
- Keys are unordered

```
>>> store = { "spam": 1, "eggs": 17}
>>> store["eggs"]
 17
>>> store["bacon"] = 42
>>> store
{'eggs': 17, 'bacon': 42, 'spam': 1}
```

- Iterating over dictionaries:

```
for key in store:
    print(key, store[key])
```

- Compare two dictionaries: `store == pool`
  Not allowed: `>`, `>=`, `<`, `<=`

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Operations on Dictionaries

- **Delete an entry**: `del(store[key])`
- **Delete all entries**: `store.clear()`
- **Copy**: `store.copy()`
- **Does it contain a key**? `key in store`
- **Get an entry**: `store.get(key[, default])`
- **Remove and return entry**: `store.pop(key[, default])`
- **Remove and return arbitrary entry**: `store.popitem()`

Operations on Dictionaries

- **Delete an entry**: `del(store[key])`
- **Delete all entries**: `store.clear()`
- **Copy**: `store.copy()`
- **Does it contain a key**? `key in store`
- **Get an entry**: `store.get(key[, default])`
- **Remove and return entry**: `store.pop(key[, default])`
- **Remove and return arbitrary entry**: `store.popitem()`

Views on Dictionaries

- **Create a view**: `items()` , `keys()` and `values()`
  - **List of all (key, value) tuples**: `store.items()`
  - **List of all keys**: `store.keys()`
  - **List all values**: `store.values()`
- Caution: Dynamical since Python 3

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Views Behavior: Python 2.X versus Python 3.X

Python 2 (static)

```
>>> mdict={"a":2, "d":5}
>>> mdict
{'a': 2, 'd': 5}
>>> s=mdict.items()
>>> for i in s:
        print(i)
('a', 2)
('d', 5)
>>> mdict['a']=-1
>>> mdict
{'a': -1, 'd': 5}
>>> for i in s:
        print(i)
('a', 2)
('d', 5)
```

Python 3 (dynamic)

```
>>> mdict={"a":2, "d":5}
>>> mdict
{'a': 2, 'd': 5}
>>> s=mdict.items()
>>> for i in s:
        print(i)
('a', 2)
('d', 5)
>>> mdict['a']=-1
>>> mdict
{'a': -1, 'd': 5}
>>> for i in s:
        print(i)
('a', -1)
('d', 5)
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Object Oriented Programming (OOP)

- So far: **procedural programming**
  - Data (values, variables, parameters, . . .)
  - Functions taking data as parameters and returning results
- Alternative: Group data and functions belonging together to form **custom data types**
- $\rightarrow$ Extensions of structures in C/Fortran

Using Simple Classes as Structs

my_point.py

```python
class Point:
    pass

p = Point()
p.x = 2.0
p.y = 3.3
```

- **Class**: Custom date type (here: `Point`)
- **Object**: Instance of a class (here: `p`)
- Attributes (here `x`, `y`) can be added dynamically

Hint: `pass` is a No Operation (NOOP) function

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Classes - Constructor

my_point.py

```python
class Point:
    def __init__(self, x, y):
        self.x = x
        self.y = y

p = Point(2.0, 3.0)
print(p.x, p.y)
p.x = 2.5
p.z = 42
```

- `__init__` : Is called automatically after creating an object

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Methods on Objects

```python
import math

class Point:
    def __init__(self, x, y):
        self.x = x
        self.y = y

    def norm(self):
        n = math.sqrt(self.x ** 2 + self.y ** 2)
        return n

p = Point(2.0, 3.0)
print(p.x, p.y, p.norm())
```

my_point.py

- Method call: automatically sets the object as first parameter
- → traditionally called `self`
- Careful: Overloading of methods not possible!

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Converting Objects to Strings

Default return value of `str(...)` for objects of custom classes:

```
>>> p = Point(2.0, 3.0)
>>> print(p)  # --> print(str(p))
<__main__.Point object at 0x402d7a8c>
```

Converting Objects to Strings

Default return value of `str(...)` for objects of custom classes:

```
>>> p = Point(2.0, 3.0)
>>> print(p)  # --> print(str(p))
<__main__.Point object at 0x402d7a8c>
```

This behaviour can be overwritten:

my_point.py

```
class Point:
    [...]
    def __str__(self):
        return f"({self.x}, {self.y})"
```

```
>>> print(p)
(2.0, 3.0)
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Comparing Objects

Default: `==` checks for object identity of custom objects.

```
>>> p1 = Point(2.0, 3.0)
>>> p2 = Point(2.0, 3.0)
>>> p1 == p2
False
```

Comparing Objects

Default: `==` checks for object identity of custom objects.

```
>>> p1 = Point(2.0, 3.0)
>>> p2 = Point(2.0, 3.0)
>>> p1 == p2
False
```

This behaviour can be overwritten:

my_point.py

```
class Point:
    [...]
    def __eq__(self, other):
        return (self.x == other.x) and (self.y == other.y)
```

```
>>> p1 == p2 # Check the content
True
>>> p1 is p2 # Check the identity
False
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Operator overloading

More relational operators:

- `<` : `__lt__(self, other)`
- `<=` : `__le__(self, other)`
- `!=` : `__ne__(self, other)`
- `>` : `__gt__(self, other)`
- `>=` : `__ge__(self, other)`

Numeric operators:

- `+` : `__add__(self, other)`
- `-` : `__sub__(self, other)`
- `*` : `__mul__(self, other)`
- ...

Emulating Existing Data Types

Classes can emulate built-in data types:

- Numbers: arithmetics, `int(myobj)`, `float(myobj)`, …
- Functions: `myobj(...)`
- Sequences: `len(myobj)`, `myobj[...]`, `x in myobj`, …
- Iteratores: `for i in myobj`

See documentation: `http://docs.python.org/3/reference/datamodel.html`

Class Variables

Have the same value for all instances of a class:

my_point.py

```python
class Point:
    count = 0  # Count all point objects
    def __init__(self, x, y):
        Point.count += 1  # self.__class__.count += 1
        [...]
```

```python
>>> p1 = Point(2, 3); p2 = Point(3, 4)
>>> p1.count
2
>>> p2.count
2
>>> Point.count
2
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Class Methods and Static Methods

```python
class Spam:
    spam = "I don't like spam."

    @classmethod
    def class_method(cls):
        print(cls.spam)

    @staticmethod
    def static_method():
        print("Blah blah.")
```

```python
Spam.class_method()
Spam.static_method()
s = Spam()
s.class_method()
s.static_method()
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Inheritance (1)

There are often classes that are very similar to each other.
Inheritance allows for:

- Hierarchical class structure (is-a-relationship)
- Reusing of similar code

Example: Different types of phones

- Phone
- Mobile phone (is a phone with additional functionality)
- Smart phone (is a mobile phone with additional functionality)

Inheritance (2)

```python
class Phone:
    def call(self):
        pass

class MobilePhone(Phone):
    def send_text(self):
        pass
```

MobilePhone now inherits methods and attributes from Phone.

```python
h = MobilePhone()
h.call()  # inherited from Phone
h.send_text()  # own method
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Overwriting Methods

Methods of the parent class can be overwritten in the child class:

```python
class MobilePhone(Phone):
    def call(self):
        self.find_signal()
        super().call() # or Phone.call(self)
```

Multiple Inheritance

Classes can inherit from multiple parent classes. Example:

- SmartPhone is a mobile phone
- SmartPhone is a camera

```python
class SmartPhone(MobilePhone, Camera):
    pass

h = SmartPhone()
h.call()       # inherited from MobilePhone
h.take_photo() # inherited from Camera
```

Attributes are searched for in the following order:
`SmartPhone`, `MobilePhone`, `Camera`, parent classes of `MobilePhone`, parent classes of `Camera`, ...
see: https://en.wikipedia.org/wiki/C3_linearization

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Private Attributes / Private Class Variables

- There are no private variables or private methods in Python.
- **Convention:** Mark attributes that shouldn't be accessed from outside with an underscore: `_foo`.
- To avoid name conflicts during inheritance: Names of the form `__foo` are replaced with `_classname__foo`:

```python
class Spam:
    __eggs = 3
    _bacon = 1
    beans = 5
```

```python
>>> dir(Spam)
>>> ['_Spam__eggs', ... , '_bacon', 'beans']
```

Classic (old Style) Classes

- The only class type until Python 2.1
- In Python 2 default class

New Style Classes

- Unified class model (user-defined and build-in)
- Descriptores (getter, setter)
- The only class type in Python 3
- Available as basic class in Python 2: **object**

Properties (1)

If certain actions (checks, conversions) are to be executed while accessing attributes, use
getter and **setter**:

```python
class Spam:
    def __init__(self):
        self._value = 0

    def get_value(self):
        return self._value

    def set_value(self, value):
        if value < 0:
            raise ValueError(f'Value must be positive: {value=}')
        else:
            self._value = value

    value = property(get_value, set_value)
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Properties (2)

Properties can be accessed like any other attributes:

```
>>> s = Spam()
>>> s.value = 6       # set_value(6)
>>> s.value           # get_value()
6
>>> s.value = -6      # set_value(-6)
[...]
ValueError: Value must be positive: value=-6
>>> s.value           # get_value()
6
>>> s._value = -6     # no setter called
>>> s.value           # get_value()
-6
```

- Getter and setter can be added later without changing the API
- Access to `_value` still possible

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Importing Modules

Reminder: Functions, classes and object thematically belonging together are grouped in modules.

```python
import math
s = math.sin(math.pi)
```

```python
import math as m
s = m.sin(m.pi)
```

```python
from math import pi as PI, sin
s = sin(PI)
```

```python
from math import *
s = sin(pi)
```

Online help: `dir(math)`, `help(math)`

Creating a Module (1)

Every Python script can be imported as a module.

my_module.py

```python
"""My first module: my_module.py"""

def add(a, b):
    """Add a and b."""
    return a + b

print(add(2, 3))
```

```python
>>> import my_module
5
>>> my_module.add(17, 42)
59
```

Top level instructions are executed during import!

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Creating a Module (2)

If instructions should only be executed when running as a script, not importing it:

```
my_module.py

def add(a, b):
    return a + b

def main():
    print(add(2, 3))

if __name__ == "__main__":
    main()
```

Useful e.g. for testing parts of the module.

Creating a Package

Modules can be grouped into hierarchically structured packages.

```
– numeric
    ├ __init__.py
    ├ linalg
    │   ├ __init__.py
    │   ├ decomp.py
    │   ├ eig.py
    │   └ solve.py
    └ fft
        ├ __init__.py
        └ ...
```

- Packages are subdirectories
- In each package directory:
  `__init__.py` (may be empty)

```python
import numeric
numeric.foo() # from __init__.py
numeric.linalg.eig.foo()
```

```python
from numeric.linalg import eig
eig.foo()
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Modules Search Path

Modules are searched for in (see `sys.path`):

- The directory of the running script
- Directories in the environment variable `PYTHONPATH`
- Installation-dependent directories

```
>>> import sys
>>> sys.path
['', '/usr/lib/python37.zip',
'/usr/lib64/python3.7',
'/usr/lib64/python3.7/plat-linux', ...]
```

Python's Standard Library

„**Batteries included**": comprehensive standard library for various tasks

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE
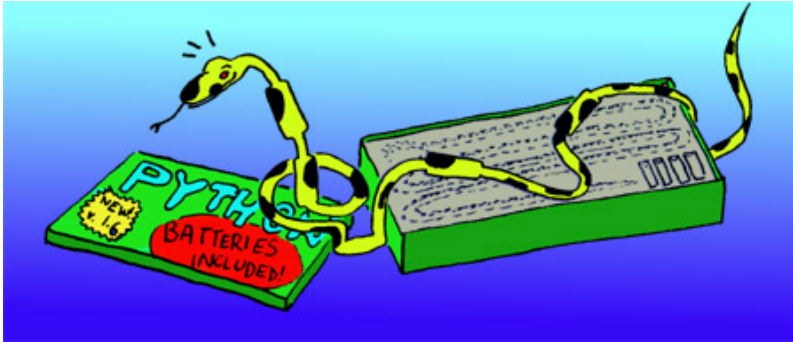
Mathematics: `math`

- Constants: `e` , `pi`
- Round up/down: `floor(x)` , `ceil(x)`
- Exponential function: `exp(x)`
- Logarithm: `log(x[, base])` , `log10(x)`
- Power and square root: `pow(x, y)` , `sqrt(x)`
- Trigonometric functions: `sin(x)` , `cos(x)` , `tan(x)`
- Conversion degree ↔ radiant: `degrees(x)` , `radians(x)`

```
>>> import math
>>> math.sin(math.pi)
1.2246063538223773e-16
>>> math.cos(math.radians(30))
0.86602540378443871
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Random Numbers: `random`

- Random integers:
  `randint(a, b)` , `randrange([start,] stop[, step])`
- Random floats (uniform distr.): `random()` , `uniform(a, b)`
- Other distibutions: `expovariate(lambd)` , `gammavariate(alpha, beta)` ,
  `gauss(mu, sigma)` , . . .
- Random element of a sequence: `choice(seq)`
- Several unique, random elements of a sequence: `sample(population, k)`
- Shuffled sequence: `shuffle(seq[, random])`

```
>>> import random
>>> s = [1, 2, 3, 4, 5]
>>> random.shuffle(s)
>>> s
[2, 5, 4, 3, 1]
>>> random.choice("Hello world!")
'e'
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Time Access and Conversion: `time`

- Classical `time()` functionality
- Time class type is a 9-tuple of `int` values (`struct_time`)
- Time starts at epoch (for UNIX: 1.1.1970, 00:00:00)
- Popular functions:
  - Seconds since epoch (as a float): `time.time()`
  - Convert time in seconds (float) to `struct_time` : `time.localtime(`*`[seconds]`*`)`
    If seconds is `None` the actual time is returned.
  - Convert `struct_time` in seconds (float): `time.mktime(t)`
  - Convert `struct_time` in formatted string: `time.strftime(format[, t])`
  - Suspend execution of current thread for secs seconds: `time.sleep(secs)`

Date and Time: `datetime`

Date and time objects:

```
d1 = datetime.date(2008, 3, 21)
d2 = datetime.date(2008, 6, 22)
dt = datetime.datetime(2011, 8, 26, 12, 30)
t = datetime.time(12, 30)
```

Calculating with date and time:

```
print(d1 < d2)
delta = d2 - d1
print(delta.days)
print(d2 + datetime.timedelta(days=44))
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Operations on Path Names: `os.path`

- Paths: `abspath(path)` , `basename(path)` , `normpath(path)` , `realpath(path)`
- Construct paths: `join(path1[, path2[, ...]])`
- Split paths: `split(path)` , `splitext(path)`
- File information: `isfile(path)` , `isdir(path)` , `islink(path)` , `getsize(path)` , …
- Expand home directory: `expanduser(path)`
- Expand environment variables: `expandvars(path)`

```
>>> os.path.join("spam", "eggs", "ham.txt")
'spam/eggs/ham.txt'
>>> os.path.splitext("spam/eggs.py")
('spam/eggs', '.py')
>>> os.path.expanduser("~/spam")
'/home/rbreu/spam'
>>> os.path.expandvars("/mydir/$TEST")
'/mydir/test.py'
```

Files and Directories: `os`

- Working directory: `getcwd()`, `chdir(path)`
- Changing file permissions: `chmod(path, mode)`
- Changing owner: `chown(path, uid, gid)`
- Creating directories: `mkdir(path[, mode])`, `makedirs(path[, mode])`
- Removing files: `remove(path)`, `removedirs(path)`
- Renaming files: `rename(src, dst)`, `renames(old, new)`
- List of files in a directory: `listdir(path)`

```python
for myfile in os.listdir("mydir"):
    os.chmod(os.path.join("mydir", myfile),
             os.path.stat.S_IRGRP)
```

Files and Directories: `shutil`

Higher level operations on files and directories. Mighty wrapper functions for `os` module.

- Copying files: `copyfile(src, dst)` , `copy(src, dst)`
- Recursive copy: `copytree(src, dst[, symlinks])`
- Recursive removal:
  `rmtree(path[, ignore_errors[, onerror]])`
- Recursive move: `move(src, dst)`

```
shutil.copytree("spam/eggs", "../beans",
                symlinks=True)
```

Directory Listing: `glob`

List of files in a directory with Unix-like extension of wildcards: `glob(path)`

```
>>> glob.glob("python/[a-c]*.py")
['python/confitest.py',
 'python/basics.py',
 'python/curses_test2.py',
 'python/curses_keys.py',
 'python/cmp.py',
 'python/button_test.py',
 'python/argument.py',
 'python/curses_test.py']
```

Run Processes: `subprocess`

Simple execution of a program:

```python
p = subprocess.Popen(["ls", "-l", "mydir"])
returncode = p.wait()  # wait for p to end
```

Access to the program's output:

```python
p = Popen(["ls"], stdout=PIPE, stderr=STDOUT)
p.wait()
output = p.stdout.read()
```

Pipes between processes (`ls -l | grep txt`)

```python
p1 = Popen(["ls", "-l"], stdout=PIPE)
p2 = Popen(["grep", "txt"], stdin=p1.stdout)
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Access to Command Line Parameters: `argparse` (1)

Python program with standard command line option handling:

```
$  ./argumentParser.py -h
usage: argumentParse.py [-h] -f FILENAME [-v]

Example how to use argparse

optional arguments:
 -h, --help                  show this help message and exit
 -f FILENAME, --file FILENAME    output file
 -v, --verbosity             increase output verbosity
```

```
$  python3 argumentParse.py -f newfile.txt -v
newfile.txt
True
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Access to Command Line Parameters: `argparse` (2)

- Simple list of parameters: → `sys.argv`
- More convenient for handling several options: `argparse`
- Deprecated module `optparse` (since Python 2.7/3.2)

argumentParse.py

```python
parser = argparse.ArgumentParser(
        description='Example how to use argparse')
parser.add_argument("-f", "--file",
                    dest="filename",
                    default="out.txt",
                    help="output file")
parser.add_argument("-v","--verbosity",
                    action="store_true",
                    help="increase output verbosity")

args = parser.parse_args()
print(args.filename)
print(args.verbosity)
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

CSV Files: `csv` (1)

CSV: Comma Seperated Values

- Data tables in ASCII format
- Import/Export by MS Excel ®
- Columns are delimited by a predefined character (most often comma)

```python
f = open("test.csv", "r")
reader = csv.reader(f)
for row in reader:
    for item in row:
        print(item)
f.close()
```

```python
f = open(outfile, "w")
writer = csv.writer(f)
writer.writerow([1, 2, 3, 4])
```

CSV Files: `csv` (2)

Handling different kinds of formats (dialects):

```python
csv.reader(csvfile, dialect='excel') # Default
csv.writer(csvfile, dialect='excel_tab')
```

Specifying individual format parameters:

```python
csv.reader(csvfile, delimiter=";")
```

Further format parameters: `lineterminator` , `quotechar` , `skipinitialspace` , . . .

Lightweight Database: `sqlite3` (1)

Database in a file or in memory; in Python's stdlib since 2.5.

```
conn = sqlite3.connect("bla.db")
c = conn.cursor()

c.execute("""CREATE TABLE Friends
             (firstname TEXT, lastname TEXT)""")
c.execute("""INSERT INTO Friends
             VALUES("Jane", "Doe")""")
conn.commit()
```

```
c.execute("""SELECT * FROM Friends""")
for row in c:
    print(row)

c.close();
conn.close()
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Lightweight Database: `sqlite3` (2)

String formatting is insecure since it allows injection of arbitrary SQL code!

```python
# Never do this!
symbol = "Jane"
c.execute("... WHERE firstname='{0}'".format(symbol))
```
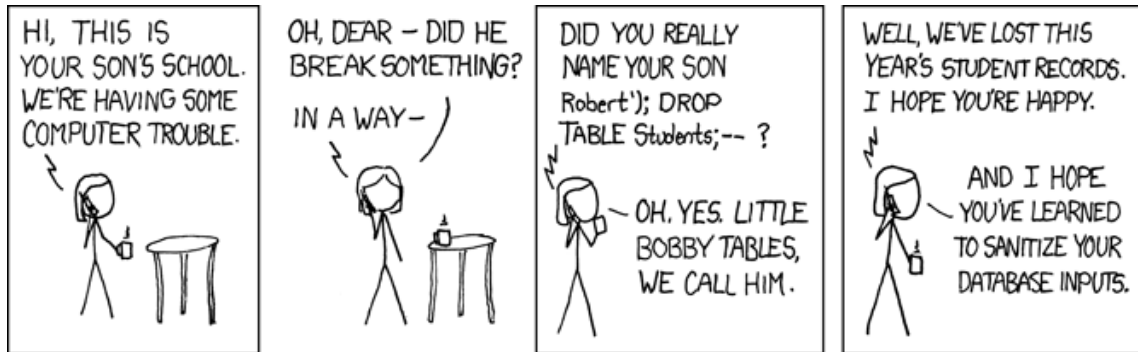
Lightweight Database: `sqlite3` **(3)**

Instead: Use the placeholder the database API provides:

```
c.execute("... WHERE name = ?", symbol)
```

```
friends = (("Janis", "Joplin"), ("Bob", "Dylan"))
for item in friends:
    c.execute("""INSERT INTO Friends
                 VALUES (?,?)""", item)
```

⇒ Python module `cx_Oracle` to access Oracle database
   Web page: http://cx-oracle.sourceforge.net/

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

XML based Client-Server Communication: `xmlrpc` (1)

- XML-RPC: **Remote Procedure Call** uses XML via HTTP
- Independent of platform and programming language
- For the client use `xmlrpc.client`

```python
import xmlrpc.client

s = xmlrpc.client.Server("http://localhost:8000")
# print list of available methods
print(s.system.listMethods())
# use methods
print(s.add(2,3))
print(s.sub(5,2))
```

Automatic type conversion for the standard data types: boolean, integer, floats, strings, tuple, list, dictionarys (strings as keys), . . .

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

XML based Client-Server Communication: `xmlrpc` (2)

- For the server use `xmlrpc.server`

```python
from xmlrpc.server import SimpleXMLRPCServer

# methods which are to be offered by the server:
class MyFuncs:
    def add(self, x, y):
        return x + y
    def sub(self, x, y):
        return x - y

# create and start the server:
server = SimpleXMLRPCServer(("localhost", 8000))
server.register_instance(MyFuncs())
server.serve_forever()
```

More Modules

- `readline` : Functionality for command line history and auto-completion
- `tempfile` : Generate temporary files and directories
- `numpy` : **Num**eric **Py**thon package
  - N-dimensional arrays
  - Supports linear algebra, Fourier transform and random number capabilities
  - Part of the SciPy stack
- `mathplotlib` : 2D plotting library, part of the SciPy stack
- ...

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Conditional Expressions

A conditional assignment as

```python
if value < 0:
    s = "negative"
else:
    s = "positive"
```

can be realized in abbreviated form

```python
s = "negative" if value < 0 else "positive"
```

List Comprehension

Allows sequences to be build by sequences. Instead of using `for`:

```python
a = []
for i in range(10):
    a.append(i**2)
```

List comprehension can be used:

```python
a = [i**2 for i in range(10)]
```

Conditional values in list comprehension:

```python
a = [i**2 for i in range(10) if i != 4]
```

Since Python 2.7: set and dictionary comprehension

```python
s = {i*2 for i in range(3)}
d = {i: i*2 for i in range(3)}
```

Dynamic Attributes

Remember: Attributes can be added to python objects at runtime:

```python
class Empty:
    pass

a = Empty()
a.spam = 42
a.eggs = 17
```

Also the attributes can be deleted at runtime:

```python
del(a.spam)
```

getattr, setattr, hasattr

Attributes of an object can be accessed by name (string):

```python
import math
f = getattr(math, "sin")
print(f(x)) # sin(x)
```

```python
a = Empty()
setattr(a, "spam", 42)
print(a.spam)
```

Useful if depending on user or data input.

Check if attribute is defined:

```python
if not hasattr(a,"spam"):
    setattr(a, "spam", 42)
print(a.spam)
```

Anonymous Function Lambda

Also known as lambda expression and lambda form

```
>>> f = lambda x, y: x + y
>>> f(2, 3)
5
>>> (lambda x: x**2)(3)
9
```

Useful if only a simple function is required as an parameter in a function call:

```
>>> friends = ["alice", "Bob"]
>>> friends.sort()
>>> friends
['Bob', 'alice']
>>> friends.sort(key = lambda a: a.upper())
>>> friends
['alice', 'Bob']
```

Functions Parameters from Lists and Dictionaries

```python
def spam(a, b, c, d):
    print(a, b, c, d)
```

Positional parameters can be created by lists:

```python
>>> args = [3, 6, 2, 3]
>>> spam(*args)
3 6 2 3
```

Keyword parameters can be created by dictionaries:

```python
>>> kwargs = {"c": 5, "a": 2, "b": 4, "d":1}
>>> spam(**kwargs)
2 4 5 1
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Variable Number of Parameters in Functions

```python
def spam(*args, **kwargs):
    for i in args:
        print(i)
    for i in kwargs:
        print(i, kwargs[i])
```

```python
>>> spam(1, 2, c=3, d=4)
1
2
c 3
d 4
```

Global and Static Variables in Functions

- `global` links the given name to a global variabile
- Static variable can be defined as an attribute of the function

```python
def myfunc():
    global max_size
    if not hasattr(myfunc, "_counter"):
        myfunc._counter = 0   # it doesn't exist yet,
                              # so initialize it
    myfunc._counter += 1
    print("{0:d}. call".format(myfunc._counter))
    print("max size is {0:d}".format(max_size))
...
```

```python
>>> max_size = 222
>>> myfunc()
1. call
max size is 222
```

Map

Apply specific function on each list element:

```
>>> li = [1, 4, 81, 9]
>>> mapli = map(math.sqrt, li)
>>> mapli
<map object at 0x7f5748240b90>
>>> list(mapli)
[1.0, 2.0, 9.0, 3.0]
>>> list(map(lambda x: x * 2, li))
[2, 8, 162, 18]
```

Functions with more than one parameter requires an additional list per parameter:

```
>>> list(map(math.pow, li, [1, 2, 3, 4]))
[1.0, 16.0, 531441.0, 6561.0]
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Filter

Similar to `map`, but the result is a `filter` object, which contains only list elements, where the function returns `True`.

filter_example.py

```python
li = [1, 2, 3, 4, 5, 6, 7, 8, 9]
liOdd = filter(lambda x: x % 2, li)
print("li =", li)
print("liOdd =", liOdd)
print("list(liOdd) =", list(liOdd))
```

```
$ python3 filter_example.py
li = [1, 2, 3, 4, 5, 6, 7, 8, 9]
liOdd = <filter object at 0x7fe4ccdcb7c0>
list(liOdd) = [1, 3, 5, 7, 9]
$
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Zip

- Join multiple sequences to one list of tuples:
  Useful when iterating on multiple sequences in parallel

```
>>> list(zip("ABC", "123"))
[('A', '1'), ('B', '2'), ('C', '3')]
>>> list(zip([1, 2, 3], "ABC", "XYZ"))
[(1, 'A', 'X'), (2, 'B', 'Y'), (3, 'C', 'Z')]
```

- Example: How to create a dictionary by two sequences

```
>>> dict(zip(("apple", "peach"), (2,0)))
{'apple': 2, 'peach': 0}
```

Iterators (1)

What happens, if `for` is applied on an object?

```
for i in obj:
    pass
```

- The `__iter__` method for `obj` is called, return an **iterator**.
- On each loop cycle the `iterator.__next__()` method will be called.
- The exception `StopIteration` is raised when there are no more elements.
- Advantage: Memory efficient (access time)

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Iterators (2)

```python
class Reverse:
    def __init__(self, data):
        self.data = data
        self.index = len(data)
    def __iter__(self):
        return self
    def __next__(self):
        if self.index == 0:
            self.index = len(self.data)
            raise StopIteration
        self.index = self.index - 1
        return self.data[self.index]
```

```python
>>> for char in Reverse("spam"):
...     print(char, end=" ")
...
m a p s
```

Generators

Simple way to create iterators:

- Methods uses the `yield` statement
  $\Rightarrow$ breaks at this point, returns element and continues there on the next
  `iterator.__next__()` call.

```python
def reverse(data):
    for element in data[::-1]:
        yield element
```

```python
>>> for char in reverse("spam"):
...     print(char, end=" ")
...
m a p s
```

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Generator Expressions

Similar to the list comprehension an iterator can be created using a generator expression:

```
>>> data = "spam"
>>> for c in (elem for elem in data[::-1]):
...     print(c, end=" ")
...
m a p s
```

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

IPython (I)

- Enhanced interactive Python shell
- Numbered input/output prompts
- Object introspection

```
In [1]: len?
Type:        builtin_function_or_method
String Form:<built-in function len>
Namespace:   Python builtin
Docstring:
len(object)

Return the number of items of a sequence or collection.
```

- System shell access

```
In [1]: a = !ls

In [2]: print(a)
['example01.py', 'example02.py', 'example03.py']
```

IPython (II)

- Tab-completion
- Command history retrieval across session
- User-extensible 'magic' commands
    - `%timeit` ⇒ Time execution of a Python statement or expression using the timeit module
    - `%cd` ⇒ Change the current working directory
    - `%edit` ⇒ Bring up an editor and execute the resulting code
    - `%run` ⇒ Run the named file inside IPython as a program
    - ⇒ *more 'magic' commands*
- ⇒ *IPython documentation*

PIP Installs Python/Packages (I)

- Command `pip`
- A tool for installing Python packages
- Python 2.7.9 and later (on the python2 series), and Python 3.4 and later include `pip` by default
- Installing Packages

```
$  pip3  install  SomePackage
$  pip3  install  --user  SomePackage       #user  install
```

- Uninstall Packages

```
$  pip3  uninstall  SomePackage
```

PIP Installs Python/Packages (II)

- Listing Packages

```
$ pip3 list
docutils (0.9.1)
Jinja2 (2.10)
Pygments (2.3.1)
Sphinx (1.1.2)
$ pip3 list --outdated
docutils (Current: 0.9.1 Latest: 0.14)
Sphinx (Current: 1.1.2 Latest: 2.10)
```

- Searching for Packages

```
$ pip3 search "query"
```

- ⇒*pip documentation*

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

pyenv - Simple Python Version Management (I)

- Easily switch between multiple versions of Python
- Doesn't depend on Python itself
- Inserts directory of *shims*[4] at the front of your `PATH`
- Easy Installation:

```
$ git clone https://github.com/yyuu/pyenv.git ~/.pyenv
$ echo 'export PYENV_ROOT="$HOME/.pyenv"' >> ~/.bashrc
$ echo 'export PATH="$PYENV_ROOT/bin:$PATH"' >> ~/.bashrc
$ echo 'eval "$(pyenv init -)"' >> ~/.bashrc
```

- ⇒*pyenv repository*

---

[4]kind of infrastructure to redirect system/function calls
metaphor: A *shim* is a piece of wood or metal to make two things fit together

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

pyenv - Simple Python Version Management (II)

- Install Python versions into `$PYENV_ROOT/versions`

```
$ pyenv install --list    # available Python versions
$ pyenv install 3.7.4     # install Python 3.7.4
```

- Change the Python version

```
$ pyenv global 3.7.4      # global Python
$ pyenv local 3.7.4       # per-project Python
$ pyenv shell 3.7.4       # shell-specific Python
```

- List all installed Python versions (asterisk shows the active)

```
$ pyenv versions
  system
  2.7.16
* 3.7.4 (set by PYENV_VERSION environment variable)
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Virtual Environments

- Allow Python packages to be installed in an isolated location
- Use cases
  - Two applications need different versions of a library
  - Install an application and leave it be
  - Can't install packages into the global site-packages directory
- Virtual environments have their own installation directories
- Virtual environments don't share libraries with other virtual environments
- Available implementations:
  - `virtualenv` (Python 2 and Python 3)
  - `venv` (Python 3.3 and later)

venv

- Create virtual environment

```
$ python3 -m venv /path/to/env
```

- Activate

```
$ source /path/to/env/bin/activate
```

- Deactivate

```
$ deactivate
```

- ⇒ *venv documentation*

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Pylint (I)

- `pylint` is the `lint` implementation for python code
- Checks for errors in Python code
- Tries to enforce a coding standard
- Looks for bad code smells
- Displays classified messages under various categories such as errors and warnings
- Displays statistics about the number of warnings and errors found in different files

Pylint (II)

- The code is given an overall mark

```
$ python3 -m pylint example.py

...

Global evaluation
-----------------
Your code has been rated at 10.00/10
          (previous run: 9.47/10, +0.53)
```

- ⇒*Pylint documentation*

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Software testing

- Part of quality management
- Point out the defects and errors that were made during the development phases
- It always ensures the users or customers satisfaction and reliability of the application
- The cost of fixing the bug is larger if testing is not done $\Rightarrow$ testing saves time
- Python testing tools
  - pytest
  - unittest
  - . . .

pytest

- Easy to get started
- `test_` prefixed test functions or methods are test items
- Asserting with the `assert` statement
- pytest will run all files in the current directory and its subdirectories of the form `test_*.py` or `*_test.py`
- Usage:

```
$ python3 -m pytest
...
$ python3 -m pytest example.py
...
```

- ⇒*pytest documentation*

JÜLICH Forschungszentrum · JÜLICH SUPERCOMPUTING CENTRE

pytest Example: Check Function Return Value

example1_test.py

```python
def incr(x):
    return x + 11

def test_incr():
    assert incr(3) == 4
```

```
$ python3 -m pytest -v example1_test.py
...
_____ test_incr _____
    def test_incr():
>       assert incr(3) == 4
E       assert 14 == 4
E        +  where 14 = incr(3)

example1_test.py:5: AssertionError
============= 1 failed in 0.00 seconds =============
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

pytest Example: Check for expected Exception

```python
import pytest

def f():
    raise SystemExit(1)

def test_error():
    with pytest.raises(SystemExit): #passes
        f()
```

pytest Example: Check for expected Exception

```python
import pytest

def f():
    raise SystemExit(1)

def test_error():
    with pytest.raises(SystemExit): #passes
        f()
```

pytest Example: Comparing Two Data Object

```python
def test_list_comparison():
    list1 = [1,3,0,8]
    list2 = [1,3,3,8]
    assert list1 == list2            #fails
```

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

pytest Example: Parameterize Test Function

```python
def incr(x):
    return x + 1

@pytest.mark.parametrize("test_input,expected", [
    (1, 2),
    (2, 3),
    (3, 4),
])
def test_incr(test_input, expected):
    assert incr(test_input) == expected
```

Enjoy

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Regular Expressions – Introduction

- Regular expression (RegExp):
  Formal language for pattern matching in strings
- Motivation: Analyze various text files:
  - Log files
  - Data files (e.g. experimental data, system configuration, . . .)
  - Command output
  - . . .
- Python module: `import re`

```
>>> re.findall(r"a.c", "abc aac aa abb a c")
['abc', 'aac', 'a c']
```

Remember:

    `r"..."` $\Rightarrow$ raw string (escape sequences are not interpreted)

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Regular Expressions – Character Classes

- Class/set of possible characters: `[!?:.,;a-z]`
- `^` at the beginning negates the class.
  e.g.: `[^aeiou]` ⇒ all characters besides the vocals
- Character class in pattern tests for **one** character
- The `.` represents **any** (one) character
- Predefined character classes:

name	character	Acr.	negated
whitespace	`[ \t\n\r\f]`	\s	\S
word character	`[a-zA-Z_0-9]`	\w	\W
digit	`[0-9]`	\d	\D

```
>>> re.findall(r"\s\d\s", "1 22 4 22 1 a b c")
[' 4 ', ' 1 ']
>>> re.findall(r"[^aeiou]", "Python Kurs")
['P', 'y', 't', 'h', 'n', ' ', 'K', 'r', 's']
```

Regular Expressions – Quantifiers

- Quantifier can be defined in ranges (min, max):
  `\d{5,7}` matches sequences of 5-7 digits
- Acronym:

{1}	one−time occurrence	Default
{0,}	none to multiple occurrences	*
{0,1}	none or one−time occurrence	?
{1,}	at least one−time occurrence	+

```
>>> re.findall(r"[ab]{1,2}", "a aa ab ba bb b")
['a', 'aa', 'ab', 'ba', 'bb', 'b']
>>> re.findall(r"\d+", "1. Python Kurs 2012")
['1', '2012']
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Regular Expressions – Anchors

- Anchors define special restrictions to the pattern matching:

```
\b      word boundary, switch between \w and \W
\B      negate \b
^       start of the string
$       end of the string
```

```
>>> re.findall(r"^\d+", "1. Python Course 2015")
['1']
```

- Look-around anchors (context):
  - Lookahead

    ```
    ab(?=c)   matches "ab" if it's part of "abc"
    ab(?!c)   matches "ab" if not followed by a "c"
    ```

  - Lookbehind

    ```
    (?<=c)ab   matches "ab" if it's part of "cab"
    (?<!c)ab   matches "ab" if not behind a "c"
    ```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Regular Expression – Rules for Pattern Matching

- Pattern analysis will start at the beginning of the string.
- If pattern matches, analysis will continue as long as the pattern is still matching (greedy).
- Pattern matching behavior can be changed to non-greedy by using the "?" behind the quantifier.
  ⇒ the pattern analysis stops at the first (minimal) matching

```
>>> re.findall(r"Py.*on", "Python ... Python")
['Python ... Python']
>>> re.findall(r"Py.*?on", "Python ... Python")
['Python', 'Python']
```

Regular Expressions – Groups

- `()` brackets in a pattern create a group
- Group name is numbered serially (starting with 1)
- The first 99 groups (`\1` - `\99`) can be referenced in the same pattern
- Patterns can be combined with logical **or** (`|`) inside a group

```
>>> re.findall(r"(\w+) \1", "Py Py abc Test Test")
['Py', 'Test']
>>>
>>> re.findall(r"([A-Za-z]+|\d+)", "uid=2765(zdv124)")
['uid', '2765', 'zdv', '124']
>>>
>>> re.findall(r"(\[.*?\]|<.*?>)", "[hi]s<b>sd<hal>")
['[hi]', '<b>', '<hal>']
```

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Regular Expressions – Group Usage

- Some `re.*` methods return a `re.MatchObject`
  ⇒ contain captured groups

re_groups.py

```python
text="adm06:x:706:1000:St.Graf:/home/adm06:/bin/bash"
grp=re.match(r"^([a-z0-9]+):x:[0-9]+:[0-9]+:(.+):.+:.+$", text)
if (grp):
    print("found:", grp.groups())
    print(" user ID=",grp.group(1))
    print(" name=",grp.group(2))
```

```
$ python3 re_groups.py
found: ('adm06', 'St.Graf')
user ID= adm06
name= St.Graf
```

JÜLICH
Forschungszentrum
JÜLICH
SUPERCOMPUTING
CENTRE

Regular Expressions – Matching Flags

- Special flags can change behavior of the pattern matching
    - `re.I` : Case insensitive pattern matching
    - `re.M` : `^` or. `$` will match at beginning/end of each line
      (not only at the beginning/end of string)
    - `re.S` : `.` also matches newline (`\n`)

```
>>> re.findall("^abc", "Abc\nabc")
[]
>>> re.findall("^abc", "Abc\nabc", re.I)
['Abc']
>>> re.findall("^abc", "Abc\nabc", re.I | re.M)
['Abc', 'abc']
>>> re.findall("^Abc.", "Abc\nabc")
[]
>>> re.findall("^Abc.", "Abc\nabc", re.S)
['Abc\n']
```

Regular Expressions – Methods (I)

findall: Simple pattern matching
$\Rightarrow$ list of strings (hits)

```
>>> re.findall(r"\[.*?\]", "a[bc]g[hal]def")
['[bc]', '[hal]']
```

sub: Query replace $\Rightarrow$ new (replaced) string

```
>>> re.sub(r"\[.*?\]", "!", "a[bc]g[hal]def")
'a!g!def'
```

search: Find first match of the pattern
$\Rightarrow$ returns `re.MatchObject` or `None`

```
if re.search(r"\[.*?\]", "a[bc]g[hal]def"):
    print("pattern matched!")
```

Regular Expressions – Methods (II)

match: Starts pattern matching at beginning of the string
⇒ returns `re.MatchObject` or `None`

```
text="adm06:x:706:1000:St.Graf:/home/adm06:/bin/bash"
grp=re.match("([a-z0-9]+):x:[0-9]+:[0-9]+:(.+):.+:.+$", text)
```

compile: Regular expressions can be pre-compiled
⇒ gain performance on reusing these RegExp multiple times
(e.g. in loops)

```
>>> pattern = re.compile(r"\[.*?\]")
>>> pattern.findall("a[bc]g[hal]def")
['[bc]', '[hal]']
```

Table of Contents

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Summary

We have learned:

- Multiple **data types** (e.g. „high level")
- Common **statements**
- Declaration and usage of **functions**
- **Modules** and packages
- Errors and **Exceptions**, exception handling
- **Object oriented programming**
- Some of the often used standard modules
- Popular tools for Python developers

Not covered yet

- Closures, decorators (function wrappers)
- Meta classes
- More standard modules: mail, WWW, XML, …
  → https://docs.python.org/3/library
- Profiling, debugging, unit-testing
- Extending and embedding: Python & C/C++ → https://docs.python.org/3/extending
- Third Party-Modules: Graphic, web programming, data bases,
  … → http://pypi.python.org/pypi

JÜLICH Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

Web Programming

- CGI scripts: Module `cgi` (standard lib)
- Web frameworks: Django, Flask, Pylons, ...
- Template systems: Cheetah, Genshi, Jinja, ...
- Content Management Systems (CMS): Zope, Plone, Skeletonz, ...
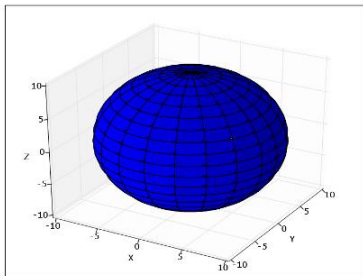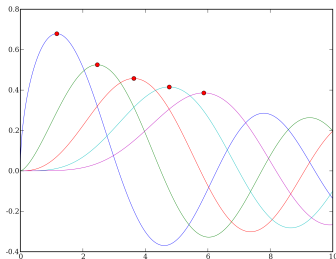- Wikis: MoinMoin, ...

NumPy + SciPy + Matplotlib = Pylab

Alternative to MatLab:
Matrix algebra, numeric functions, plotting, ...

And more ...

- **jupyter** Notebook (interactive computational environment)
- Python IDEs
  - PyCharm
  - Eclipse (PyDev)
  - ...
- Python and other languages:
  - Jython: Python code in Java VM
  - Ctypes: Access C-libraries in Python (since 2.5 in standard lib)
  - SWIG: Access C- and C++ -libraries in Python
- **PIL**: Python Imaging Library for image manipulation
- **SQLAlchemy**: ORM-Framework
  - Abstraction: Object oriented access to database

JÜLICH
Forschungszentrum
JÜLICH SUPERCOMPUTING CENTRE

Interactive High-Performance Computing with Jupyter

PRACE-Trainingskurs, online (05.04, - 07.04.2022)

- Introduction to Jupyter
- Parallel computing using Jupyter
- Coupling and control of simulations
- Interactive and in-situ visualization
- Simulation dashboards
- `https://www.fz-juelich.de/SharedDocs/Termine/IAS/JSC/DE/Kurse/2022/` `ptc-interactive-hpc-2022.html`

JÜLICH
Forschungszentrum

JÜLICH
SUPERCOMPUTING
CENTRE

Data Analysis and Plotting in Python with Pandas

Trainingskurs, online (12.05.2022)

- Introduction to Pandas
- Simple examples
- Hands-on exercises
- `https://www.fz-juelich.de/SharedDocs/Termine/IAS/JSC/DE/Kurse/2022/pandas-2022.html`

JÜLICH
Forschungszentrum | JÜLICH SUPERCOMPUTING CENTRE

High-performance computing with Python

PRACE-Trainingskurs, online tba

- Introduces Matlab programmers to the usage of Python
    1. Interactive parallel programming with IPython
    2. Profiling and optimization
    3. High-performance NumPy
    4. Just-in-time compilation with numba
    5. Distributed-memory parallel programming with Python and MPI
    6. Bindings to other programming languages and HPC libraries
    7. Interfaces to GPUs
    8. `https://www.fz-juelich.de/SharedDocs/Termine/IAS/JSC/DE/Kurse/2021/ptc-hpc-python-2021.html?nn=717802`

PyCologne

PyCologne: Python User Group Köln

- Meets on the 2nd Wednesday each month at Chaos-Computer-Club Cologne
- URL: http://pycologne.de

Enjoy