Introduction to python 3

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Outline

1. The basics
2. SciPy
3. The numpy package
4. The scipy package
5. Plotting with python
6. Symbolic computing with Sympy

The basics

Python references

- Good python book *Python 3 (2017 edition)* by Johannes Ernesti and Peter Kaiser
- online documentation: `https://docs.python.org/3.6/`

Historical facts

- developed in the nineties by Guido van Rossum in Amsterdam at Centrum voor Wiskunde en Informatica
- the name "python" comes from the comedy "*Monty Python*"
- python **version 3.0** was released in December 2008
- one of the most popular programming languages
- designed for *functional* and *object oriented* programming
- programs that partially use python:
  - Google Mail
  - Google Maps
  - YouTube
  - Dropbox
  - reddit
  - Battlefield 2
  - BitTorrent

Why python?

What does python offer?

- Interactive
- Interpreted
- Modular
- Object-oriented
- Portable
- High level
- Extensible in C++ & C

Why is python good for scientifc computing?

- open source / free
- many libraries, e.g.,
- scientific computing: numpy, scipy
- symbolic math: sympy
- plotting: matplotlib
- excellent PDE solver software: ngsolve, FEniCs, Firedrake, ...

How to start python?

- Python can either be used **interactively**: simply type "python3" or "ipython3" (to start IPython) into the shell
- we can also **execute python code** written in a file "file.py" by typing "python3 file.py" into the shell

Let's start with a hello world example:

Listing 1: hello_world.py

```python
""" This is our first program """

print("Hello world!")
```

Float

declaration of floats

```
>>> x = 987.27
>>> x
987.27
```

division

```
>>> y = 2.27
>>> x/y
434.92070484581495
```

floor division

```
>>> x//y
434.0
```

multiplication

```
>>> x*y
2241.1029
>>> x*-y
-2241.1029
```

addition and subtraction

```
>>> x = 987.27
>>> y = 2.0
>>> x+y
989.27
>>> x-y
985.27
```

powers

```
>>> x**2
974702.0529
>>> x**3
962294095.766583
>>> x**0.5 # square root
31.4208529483208
```

Integers

calculator

```
>>> 1+3
4
>>> 3-10
-7
>>> 30*3
90
```

declaration of integer

```
>>> x = 987
>>> x
987
>>> int(10.0)
10

>>> y = 2
>>> x/y
493.5
>>> 5/3
1.6666666666666667
```

floor division

```
>>> x//y
493
```

conversion of float to integer

```
>>> x = 1.4
>>> y = int(x)
>>> y
1
>>> x + 3
4.4
```

- remember: float + int = float

Complex number

- imaginary unit in python is j
- recall $(a+ib)*(c+id) := ac-db+i(bc+ad)$

```
>>> z = 1.0 + 5j  # complex number with real 1 and imag 5
>>> z.conjugate()  # conjugate complex number
(1-5j)

>>> z = complex(1,5) # equivalent to 1+5j

>>> z.imag # return imaginary part
5.0
>>> z.real # return real part
1.0
```

Complex number (continued)

multiplication of complex numbers

```
>>> z1 = 1 + 4j
>>> z2 = 2 - 4j

>>> z1*z2  # multiply z1 and z2
(18+4j)

>>> # Let us verify this is correct

>>> a, b, c, d  = z1.real, z1.imag, z2.real, z2.imag

>>> a*c - b*d
18.0
>>> b*c + a*d
4.0
```

Strings

declaration of strings

```
>>> a = "hello" # assign hello
>>> a
'hello'
```

addition of strings

```
>>> a+a
'hellohello'
>>> a+" cool"
'hello cool'
```

referencing letters

```
>>> fourth =   a[3]  # 4th letter
>>> fourth
'l'
>>> last = a[-1]  # last letter
>>> last
'o'
```

conversion of float and integer to string

```
>>> x = 987.27
>>> s1 = str(x)
>>> s1
'987.27'
>>> n = 10
>>> s2 = str(n)
>>> s2
'10'
```

Strings (continued)

lower and upper case

```
>>> a = "hello" # assign hello
>>> a.upper()
'HELLO'

>>> a = "HELLO"
>>> a.lower()
'hello'
>>> a
'HELLO'

>>> a = "Hello"
>>> a.swapcase()
'hELLO'
>>> a
'Hello'
```

accessing letters

```
>>> s = "This is a long sentence!"
>>> s[::3] # every third letter
'Tss nstc'
>>> s = "z"
>>> 10*s
'zzzzzzzzzz'
```

Splitting and concatenation

```
>>> name = "This is a long sentence."
>>> name.split()
['This', 'is', 'a', 'long', 'sentence.']
>>> name
'This is a long sentence.'
```

inserting strings

```
>>> 'Insert here: {}'.format('Inserted string')
'Insert here: Inserted string'
```

Lists

declaration of list

```
>>> l = []   # empty list
>>> l
[]
>>> l = [1, 2, 3] # integers list
>>> l
[1, 2, 3]
>>> l = [1.0, 3.0, 3,0] # float list
```

lists can contain anything

```
>>> l1 = [1,2,3]
>>> l2 = ["hello", [], "new"]
>>> l = [l1, l2]
>>> l
[[1, 2, 3], ['hello', [], 'new']]
```

other ways to generate lists

```
>>> l1 = [1]*5
>>> l1
[1, 1, 1, 1, 1]
>>> l2 = [k for k in range(5)]
>>> l2
[0, 1, 2, 3, 4]
```

The last command is similar to the mathematical definition $\{k : \ k = 0, 1, 2, 3, 4\}$.

addition of lists

```
>>> l1 = [1,2,3]
>>> l2 = [4,5,6]
>>> l1+l2
[1, 2, 3, 4, 5, 6]
```

multiplication of lists is not supported!!

More on lists

The *list* class has the following methods:

- append
- clear
- copy
- count
- extend
- index
- insert
- pop
- remove
- reverse
- sort

```
>>> l = [1, 2, 3, 4, 4]
>>> l
[1, 2, 3, 4, 4]

>>> l.reverse()
>>> l
[4, 4, 3, 2, 1]

>>> l.pop(3)
2
>>> l
[4, 4, 3, 1]

>>> # print every 2nd element
>>> # start with index 1
>>> # go until end of list -1
>>> # the : operation is called slicing
>>> l[1:-1:2]
[4]
```

Tuple

- tuple are essentially uneditable lists. We use round parenthesis.
- referencing possible, but no assignment
- to be used when list should not be modified

declaration of list

```
>>> l = ()  # empty tuple
>>> l
()
>>> l = (1, 2, 3) # tuple of integers
>>> l
(1, 2, 3)
>>> l = tuple([1.0, 3.0, 3,0]) # conversion of list to tuple
>>> l
(1.0, 3.0, 3, 0)
```

adding tuples

```
>>> l+l
(1.0, 3.0, 3, 0, 1.0, 3.0, 3, 0)
>>> 4*l
(1.0, 3.0, 3, 0, 1.0, 3.0, 3, 0, 1.0, 3.0, 3, 0, 1.0, 3.0, 3, 0)
```

Bool and logical operators

bool True or False

```
>>> t = True
>>> t
True
>>> f = False
>>> f
False
>>> f == t
False
```

"and", "or", and "not

```
>>> t and f
False
>>> t or f
True
>>> not f == t
True
```

Possibilities for "or":

x	y	x or y
True	True	True
True	False	True
False	True	True
False	False	False

Possibilities for "and":

x	y	x and y
True	True	True
True	False	False
False	True	False
False	False	False

If-else

simple if-else statement

Listing 2: if_else.py

```
if condition:
    command
else:
    another command
```

When we have more than one condition we use *elif*:

Listing 3: if_else2.py

```
if condition1:
    first command
elif condition2:
    second command
else:
    third command
```

If-else example

Listing 4: if_else_ex.py

```
if x == 1:
    print("x has value 1")
elif x == 2:
    print("x has value 2")
```

Listing 5: if_else_ex2.py

```
if x == 1:
    print("x has value 1")
else:
    print("x has another value")
```

for loop

Listing 6: for_loop.py

```
for n in range(10):
    print(n)
```

- Here *n* ranges from 0 to 9 and is printed after each loop.
- general syntax is *range(start, stop, steps)*
- *start* and *steps* are optional

Listing 7: for_loop2.py

```
l = [0, 1, 'hello', True, False]

for n in l:
    print(n)
```

for loop (continued)

- use *enumerate* to count the element in the loop

Listing 8: for_loop_en.py

```
l = ['one', 'two', 'three', 'four', 'five']

for n, s in enumerate(l):
    print('Item number ', n, ' item itself ', s)
```

While loop

The syntax of a python while loop is as follows.

```
while statement:
    do stuff
```

- "do stuff" is executed as long as statement is true.
- notice again the indention!
- use `break` to leave a while loop
- use `continue` to go to the next loop

Listing 9: while_loop.py

```
counter = 10

while counter > 0:
    print("counter is", counter)
    counter -= 1
```

Functions

Let's have a look at an example function.

Listing 10: func.py

```
def my_func(x):
    x = x + 1.0
    return x
```

- indention in python replaces brackets!!!
- a function always starts with *def*
- a *return* is not mandatory
- without *return* the function returns None.

Functions (continued)

- anonymous functions can be defined using *lambda* keyword

```
>>> f = lambda x: x**2 # define lambda function f
>>> f(2)
4
```

a more complicated example

```
>>> f = lambda x: x**2 if x < 0 else x**3
>>> f(2)
8
```

Listing 11: lambda_func.py

```
def f(x):
    if x < 0:
        return x**2
    else:
        return x**3
```

Functions (optional arguments)

- It is possible to give functions optional arguments.

Listing 12: func_opt.py

```
def f(x, y=None):

    if y == None:
        return x**2
    else:
        return x**2 + y**2
print(f(1))
print(f(1,2))
```

Dictionaries

- make a dictionary with {} and : to signify a *key* and a *value*

```
>>> value1 = 1.0
>>> value2 = 2.0
>>> my_dict = {'key1':value1,'key2':value2}

>>> print(my_dict)
{'key1': 1.0, 'key2': 2.0}

>>> my_dict['key1'] # access value1
1.0

>>> 'key2' in my_dict
True
```

Dictionaries (continued)

Accessing the values and the keys

```
>>> # Make a dictionary with {} and : to signify a key and a value
>>> value1 = 1.0
>>> value2 = 2.0
>>> my_dict = {'key1':value1,'key2':value2}


>>> print(my_dict.values())  # return values of dictionary
dict_values([1.0, 2.0])

>>> print(my_dict.items()) # return items
dict_items([('key1', 1.0), ('key2', 2.0)])

>>> print(my_dict.keys()) # return keys
dict_keys(['key1', 'key2'])
```

Sets

- sets are unordered lists

declaration of sets

```
>>> S = set([1,2,3,4])  # def. a set S
>>> S
{1, 2, 3, 4}

>>> S = {1,2,3,4} # equiv. definition
>>> S
{1, 2, 3, 4}
```

union $\cup$ and subtraction $\setminus$ of sets

```
>>> S1 = {1,2,3}
>>> S2 = {2,3,4}

>>> S1 - S2   # subtract S1 from S2
{1}
>>> S2 - S1   # subtract S2 from S1
{4}

>>> S1 | S2   # union of S1 and  S2
{1, 2, 3, 4}

>>> S1^S2   # symmetric difference
{1, 4}
```

Sets (continued)

alternative definition

```
>>> S1 = {2,3,4,5}
>>> S2 = {1,2,3,4}

>>> S1.intersection(S2)
{2, 3, 4}

>>> S2.union(S1)
{1, 2, 3, 4, 5}

>>> S1.difference(S2)
{5}
```

union ∪ and subtraction \ of sets

```
>>> S1 = set([1,2,3])
>>> S2 = set([2,3,4])

>>> S1 - S2   # S1/S2
{1}
>>> S2 - S1   # S2/S1
{4}

>>> S1 | S2 # union of S1 and S2
{1, 2, 3, 4}
```

adding and deleting elements

```
>>> S1.add(10) # add 10 to list
>>> S1
{10, 1, 2, 3}

>>> S1.discard(10) # remove element 10
>>> S1
{1, 2, 3}
```

Python key words

- We already know a few python key words.
- The *keywords* are part of the python programming language.
- you cannot use these names for variables or functions

and	def	finally	in	or	while
as	del	for	is	pass	with
assert	elif	from	lambda	raise	yield
break	else	global	None	return	
class	except	if	nonlocal	True	
continue	False	import	not	try	

Figure: List of python keywords

Importing modules

- import a module with command `import module_name`
- a function **func** in **module_name** can be accessed by `module_name.func`
- including with different name use `import module_name as mn`
- import specific function: `from module_name import func`
- import everything with `from module_name import *`

Math modul

Let us consider as an example the *math* package.

```
>>> import math  # import math module and use name "math"
>>> math.pi
3.141592653589793
>>> del(math) # remove math package

>>> import math as m # import math module with name "m"
>>> m.pi
3.141592653589793
>>> del(m)

>>> from math import pi # import constant pi from math
>>> pi
3.141592653589793

>>> from math import pi as pipi # import constant pi from math with name "pipi"
>>> pipi
3.141592653589793
```

Immutable vs mutable datatypes

- Python distinguishes two datatypes: mutable and immutable.
- immutable: float, int, string, tuple
- mutable: set, list, dict

The build-in function `id(variable)` shows the unique identity of a python object.

```
>>> s1 = "CompMath"
>>> s2 = "CompMath"

>>> id(s1)
140199884781872
>>> id(s2)
140199884781872

>>> s1 is s2  # check if s1 is s2
True
>>> s1 == s2  # check if s1 has same values as s2
True
```

Immutable vs mutable datatypes (continued)

Let us now check lists.

```
>>> l1 = [0.1, "CompMath"]
>>> l2 = [0.1, "CompMath"]

>>> id(l1)
140199887587912
>>> id(l2)
140199887930568

>>> l1 is l2  # check if l1 is l2
False
>>> l1 == l2  # check if l1 has same values as l2
True
```

So both lists are different, but have exactly the same values.

Immutable vs mutable datatypes (continued)

```
>>> l1 = [0.1, "CompMath"]
>>> l2 = l1

>>> l1 is l2  # check if s1 is s2
True
>>> l1 == l2  # check if s1 has same values as s2
True

>>> id(l1)
140199887587400
>>> id(l2)
140199887587400

>>> l1[0] = 0.0
>>> l1
[0.0, 'CompMath']
>>> l2
[0.0, 'CompMath']
```

- So l1 and l2 share the same reference. Changing l1 also changes l2.

Immutable vs mutable datatypes (continued)

So how can we copy a list?

```
>>> l1 = [0.1, "CompMath"]
>>> l2 = l1[:]  # this generates a copy of l1

>>> l1 is l2  # check if s1 is s2
False
>>> l1 == l2  # check if s1 has same values as s2
True

>>> id(l1)
140199887587912
>>> id(l2)
140199887930568
```

Immutable vs mutable datatypes (continued)

- if list elements are mutable itself the previous copying does not work as one might expect

```
>>> change = [0, 0, 0]
>>> l1 = [1, 2, change]
>>> l2 = l1[:]  # change is not copied here
```

In this case one can use deepcopy of the module copy.

```
>>> change = [0, 0, 0]
>>> l1 = [1, 2, change]
>>> import copy
>>> l2 = copy.deepcopy(l1)
```

a is b vs a==b

- The way python 3 is implemented the integer numbers [-5, 256] are cached. For integers in this range python only returns a reference to the same element.

```
>>> a = 1
>>> b = 1
>>> id(a)
94069709345536
>>> id(b)
94069709345536
>>> a is b ## a and b same
True
>>> a == b
True
```

```
>>> c = 1000
>>> d = 1000
>>> id(c)
140199884624432
>>> id(d)
140199884624528
>>> c is d  ## two different references
False
>>> c == d
True
```

Local vs global variables

How to figure our which variables are defined so far?

- `dir()` - list defined variables in scope
- `globals()` - dict of global variables
- `locals()` - dict of local variables in scope (including values)

Local vs global variables - example

Listing 13: dirs.py

```
b = 0.

def f(x):
    a = 0.0

    print("local variables in f", locals())
    print("local variables f", dir())

    return x

print("local variables in current scope", locals())

print(f(0.1))
```

Classes

Listing 14: class_ex.py

```
class simple:
    pass
```

- keyword `class` defines a class with name simple
- keyword `pass` means that the class simple does nothing

Classes

Listing 15: class_ex2.py

```
class simple_two:
    a = 0.1
    s = "hello"

t = simple_two() # define class instance

print(t.a) # print variable a
```

- keyword `class` defines a class with name simple
- keyword `pass` means that the class simple does nothing

Classes - constructor

Listing 16: class_construct.py

```python
class test:

    def __init__(self, a = 0.0):  # constructor
        self.a = a

C1 = test(0.1)  # create instance C1 with value a = 0.1
C2 = test()  # create instance C2 with default value

print(C1.a) # print value of variable a
```

- a class constructor is defined by `__init__`, which is called upon initialisation of the class
- the class test has an optimal argument *a*, which is by default 0.0

Classes - methods

Listing 17: class_method.py

```python
class test:

    def __init__(self):
        print("This is the constructor.")

    def func(self):
        print("This is the func.")

C = test() # create instance C
C.func()   # call func()
```

- the first argument of a method (here func(self)) must be self
- function is accessed via `C.func()`

Classes - methods

Listing 18: class_method2.py

```
class test:

    def __init__(self):
        print("This is the constructor.")

    def func2(self, b):
        print("This is func2 with b = {}".format(b))

C = test()
C.func2(0.3) # call func2(0.3)
```

- the first argument of a method (here func(self)) must be self (see next slide)

What is self?

- self is basically a reference to the class instance
- the name does not have to be "self", but it is recommended
- the first argument of a method in a class is always self

Listing 19: self.py

```
class test:

    def __init__(self):
        print("This is the constructor.")

    def we_call_self(self):
        print("This is self", self)

C = test()
C.we_call_self()
print("This is C", C)
```

Inheriting classes

As in C++ we can inherit classes. The basic syntax is as follows:

```
class Derived_ClassName(Base_ClassName):
    statement-1
    .
    .
    .
    statement-N
```

Inheriting classes: example

Listing 20: inherit.py

```
class Base_Class:

    def f(self, x):
        return x

class Derived_Class(Base_Class):

    def g(self, x, y):
        return x + y
```

- `Base_Class()` contains the functions `f(x)`
- `Derived_Class` extends `Base_Class()` by `g(x, y)`

Reading files

- we can read a file with `open("filename", 'r')`

We now want to read the file

Listing 21: readme.txt

```
This is CompMath.

We want to read this file.
```

```
>>> file = open("code/code_lec2/readme.txt", 'r')
>>> print(file.readlines())
['This is CompMath.\n', '\n', 'We want to read this file.\n']
>>> file.close()
```

Writing to files

- we can write to a file with `open("filename", 'w')`
- if "filename" is not there it will be created

```
file = open("code/code_lec2/writeme.txt", 'w+')
file.write("We write this into writeme.txt")
file.close()
```

Further options of `open()`

The function open has the following options. (Taken from `help(open)`).

'r'	open for reading (default)
'w'	open for writing, truncating the file first
'x'	create a new file and open it for writing
'a'	open for writing, appending to the end of the file if it exists
'b'	binary mode
't'	text mode (default)
'+'	open a disk file for updating (reading and writing)
'U'	universal newline mode (deprecated)

Reading and writing lines

Now suppose we want to add text to the beginning of the file *prepend.txt*

```
file = open("prepend.txt", 'a+')  # open file prepend.txt
file.seek(0)  # start at beginning of file
s = ["This text should go at the beginning."]
file.writelines(s)
file.close()
```

Doc-Strings

What is a doc string?

- doc-string is convenient way do describe document modules, functions, classes, and methods.

How do we define a doc string?

- a doc-string has the syntax `""" documentation here """`

How do we use a doc string?

- The doc string can be accessed with `.__doc__`.

Doc-String: example

Listing 22: doc_string.py

```
""" This is a doc string. """

def f(x, y = 0.0):
    """
    This function adds numbers x and y.
    The variable y is optional. Default is y = 0.0
    """
    return x + y

#print("call doc string with f.__doc__:", f.__doc__)
print("alternatively use help(f):", help(f))
```

Decorators

The basic decorator code structure is as follows:

```
def decor(func):
    def inner():
        func()
    return inner
```

Usage:

```
dec = decor(func)
```

- decor is a wrapper function - essentially a function that returns a function
- the decorator gets as argument a function (`func()`) and returns another function (`inner()`)
- the "actual" coding happens inside the `inner` function

Decorators - Example 1

Listing 23: decorator_.py

```
from math import exp

def f(x, y):
    return exp(x*y) + y

def deco(func):
    y = 0.0 # define value for y
    def f1(x):
        return func(x, y)
    return f1
```

Decorators - Example 2

Listing 24: decorator2_.py

```
from math import exp

def f(x, y):
    return exp(x*y) + y

def deco(func, y):   # decorator has y as argument
    def f1(x):
        return func(x, y)
    return f1

de = deco(f, 5)

print(de(0.1))
```

Decorators - Example 3

Listing 25: decorator3_.py

```
from math import sin, cos

def func_comp(fun1, fun2):
    def f1(x):
        return fun1(fun2(x))
    return f1

de = func_comp(cos, sin)

print(de(0.1))
```

Recursion without loops

Suppose we want to implement the factorial `n!`. A loop approach would be as follows:

Listing 26: factorial_loop.py

```
def fac(n):
    val = 1
    for k in range(1, n+1):
        val = val*k

    return val

print(fac(10))
```

Recursion without loops

As second approach without loops is

Listing 27: factorial_loop_free.py

```
def fac(n):
    if n == 1:
        return 1
    else:
        return n*fac(n-1) ## function fac called with n-1

print(fac(10))
```

Recursion without loops

- using second approach avoid calling function multiple times!! Consider

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{1}{x_n}\right).$$

Listing 28: babylon_bad.py

```
def babylon(n):
    x0 = 10
    if n == 1:
        return x0
    else :
        return (1/2)*(babylon(n-1) + 2/babylon(n-1))
```

problem: if a_n is number of function calls, then $a_n = 2a_{n-1}$and hence $a_n = 2^n$ function calls are need. In total to compute recursion at stage n we need $\sum_{\ell=0}^{n} a_\ell = 2^{n+1} - 1$.

Recursion without loops

- using second approach avoid calling function multiple times!! Consider

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{1}{x_n}\right).$$

Listing 29: babylon_good.py

```
def babylon(n):
    x0 = 10
    if n == 1:
        return x0
    else:
        xn = babylon(n-1)
        return (1/2)*(xn + 2/xn)
```

better: here we have $a_n = a_{n-1}$, so $a_n = a_0 = 1$ and hence in total $\sum_{\ell=0}^{n} a_\ell = n+1$.

$*args$ and $**kwargs$

- sometimes the number of arguments a function gets is unknown. Then we can use `*arg` and `**kwargs`.
- `kwargs` - keyword arguments; `args` - normal arguments
- The actual names args and kwargs are irrelevant, we could also use $*va$, only the star $*$ matters; same for kwargs.

Basic syntax is as follows:

```
def f(farg, *args, **kwargs):
    # do something with args, farg and kwargs
```

- inside the function `f` `args` will be a tuple and `kwargs` a dictionary.
- the order of `farg`, `args` and `kwargs` matters: positional argument follows keyword argument

∗*args*- example 1

Listing 30: args_ex1.py

```
def f(*args):
    print(type(args))
    print(args)

f(1,2,3)
f([1,],3,4,'hello')
```

$*$*args*- example 2

- To illustrate $*$*args*, we want implement the polynomial $p(x) = a_n x^n + \cdots + a_1 x + a_0$.
- The number n of coefficients $a_0, \dots, a_n \in \mathbf{R}$ is variable; hence we can define a python function `polynom(x,*args)`.

*args- example 2

Listing 31: args_ex2.py

```
def polynom(x, *args):

    n = len(args)
    val = 0.0

    print(type(args))
    for k in range(n):
        val += args[k]*x**k

    return val

a = (1, 2, 3, 4)
print(polynom(0.1, *a))
print(polynom(0.1, 1, 2, 3, 4))
```

*kwargs - example 1

With kwargs we can give a function an arbitrary number of optional keyword arguments.

Listing 32: kwargs_ex1.py

```
def f(**kwargs):
    print(type(kwargs))
    print(kwargs)

f(a=1, b=2, c=3)
d = {'a':1, 'b':1, 'c':1}
f(**d)
```

Measuring time - in ipython shell

- in the ipython shell one can use `time` to measure the time a function call takes
- usage: `%time sin(1)` to find the time it took to eval sin at 1.
- to get more accurate average use %timeit which runs 1000000 loops

Measuring time

- to measure time of code segments we can use the time module

Listing 33: measuring_time.py

```
import time   # time module

def tic():  # start  measuring time
    global  start
    start  = time.time()

def toc():  # end measuring time
    if  'start'  in  globals():
        print("time:  {}.".format(str(time.time()-start)))
    else:
        print("toc():  start  time not  set")
```

Measuring time (continued)

Let us now use the functions `tic` and `toc` to measure for instance the time to evaluate `sin` and `cos`.

Listing 34: measuring_time.py

```
from measure_time import tic, toc
from math import sin, cos

tic()
sin(1.0)
cos(1.0)
toc()
```

What is time.time()

- The function `time.time()` return time since epoch in second.
- For Unix system, January 1, 1970, 00:00:00 at UTC is epoch.

We test this:

```
>>> import time
>>> time.time()  # epoch time in second
1558355501.1507561
>>> time.time()/(60*60*24*365.25) # convert in years
49.381305965942126

>>> T = time.time()/(60*60*24*365.25)
>>> 2019 - T
1969.6186940340551
```

Measuring time of function evals

- we can now combine our knowledge of decorators, `*args` and `**kwargs` and the time measurement to write a function which measures the execution time of a function.
- rather than putting `tic` and `toc` before and after a function in the code, we want to have a function `calculate_time(func)` which measures the execution of `func`.

Measuring time of function evals - example 1

Listing 35: measuring_time.py

```
import time

def calculate_time(func):

    def inner1(*args, **kwargs):

        begin = time.time()
        func(*args, **kwargs)
        end = time.time()

        print("Total time taken in : ", func.__name__, end - begin)

    return inner1
```

Measuring time of function evals - example 1

Listing 36: measuring_time2.py

```
from measure_time_func import calculate_time
import math

# test how long it takes to eval sin
SIN = calculate_time(math.sin)
SIN(10)
```

Call by reference vs. call by value

- function calls in python are call by reference **if** the object that is passed is mutable
- for immutable objects (e.g., `float`, `tuple`, `int`) only a copy is passed

Call by value

Listing 37: func_call_by_ref.py

```python
l = [1,2]
print('id', id(l)) # print identity of l
print('l', l, '\n') # print list l

def add(l_):
    l_ += [1]

add(l) # call add()

print('id', id(l))
print('l', l)
```

Call by reference

Listing 38: func_call_by_val.py

```python
a = 1
print('id', id(a))
print('a', a)

def add(a):
    a += 1

print('id', id(a))
print('a', a)
```

Evaluating functions at multiple values

- How to evaluate a function `f(x)` for a list of values, say, `l = [1, 2, 3, 4, 4, 4]`?
- solution: use `map(f, l)`

```
>>> f = lambda x: x**4
>>> l = [1, 2, 3, 4, 4, 4]
>>> map(f, l)
<map object at 0x7f82d453dd30>
>>> print(list(map(f,l)))
[1, 16, 81, 256, 256, 256]
```

a+=1 vs. a = a+1

- for mutable objects `a += b` returns the same reference of a
- for mutable objects `a = a + b` return a new object a

```
>>> a = 1
>>> id(a)
94069709345536
>>> a += 1
>>> id(a)
94069709345568

>>> a = 1
>>> a = a + 1
>>> id(a)
94069709345568
```

```
>>> a = [1,2,3]
>>> id(a)
140199887588104
>>> a = a + [1]
>>> id(a)
140199888211336

>>> a = [1,2,3]
>>> id(a)
140199884749256
>>> a += [1]
>>> id(a)
140199884749256
```

SciPy

Online resources

- SciPy is collection of open source software for scientific computing in Python:
  - numpy
  - scipy
  - matplotlib
  - pandas
  - sympy
  - IPython
  - and more ...

Online documentation: `https://scipy.org/doc.html`

The numpy package

The numpy package

The numpy module offers the following functionalities:

- a powerful N-dimensional array object
- sophisticated (broadcasting) functions
- basic linear algebra functions
- basic Fourier transforms
- sophisticated random number capabilities
- tools for integrating Fortran and C/C++ code

The numpy package is usually imported as follows:

```
import numpy as np
```

Numpy arrays

- arrays are defined by `a = np.array([], dtype = datatype)`
- *dtype* is optional
- each entry of an array has to hold same data type (unlike python arrays)
- example: `a = np.array([1,2], dtype = float)` or shorter `a = np.array([1.,2.])`

- online lectures: `https://scipy-lectures.org/intro/numpy/operations.html`
- official docu: `https://docs.scipy.org/doc/numpy/reference/`

Accessing arrays

```
>>> # let's define an array
>>> a = np.array([1,2,3])
>>> a
array([1, 2, 3])
>>> type(a)
<class 'numpy.ndarray'>
```

```
>>> # accessing arrays
>>> A = np.array([[1,2,3], [2,2,2]])
>>> A
array([[1, 2, 3],
       [2, 2, 2]])
>>> A[0,1] # element (0,1)
2
>>> A[0][1] # element (0,1)
2
>>> A[0]  # first row
array([1, 2, 3])
>>> A[0][:] # same
array([1, 2, 3])
>>> A[:, 0] # first column
array([1, 2])
```

Accessing arrays (continued)

```
>>> # let's define an array
>>> a = np.array([[1,2,3], [0,-1,2]])

>>> ind = [0, 1]

>>> a[:,ind]
array([[ 1,  2],
       [ 0, -1]])
```

```
>>> # accessing arrays
>>> A = np.array([[1,2,3], [2,2,2]])
>>> A
array([[1, 2, 3],
       [2, 2, 2]])
>>> A[0,1] # element (0,1)
2
>>> A[0][1] # element (0,1)
2
>>> A[0]  # first row
array([1, 2, 3])
>>> A[0][:] # same
array([1, 2, 3])
>>> A[:, 0] # first column
array([1, 2])
```

Array multiplication

- Matrix multiplication between arrays via `np.dot(A,B)` or `A@B`
- `A*B` multiplies A and B elementwise!!!

```
>>> A = np.array([[1,2], [2,3]])
>>> B = np.array([[0,1], [1,1]])

>>> A@B  # matrix prod of A and B
array([[2, 3],
       [3, 5]])
>>> np.dot(A,B) # same
array([[2, 3],
       [3, 5]])
```

```
>>> A*B
array([[0, 2],
       [2, 3]])
```

More standard operations on array

- tensor product of array a and b via `np.outer(a,b)` or `a[:,np.newaxis]*b[np.newaxis,:]`
- sum all elements of array A via `A.sum()`; sum only first axis `A.sum(axis=1)`

```
>>> A = np.array([[1,2], [2,3]])
>>> B = np.array([[0,1], [1,1]])

>>> A@B
array([[2, 3],
       [3, 5]])
>>> np.dot(A,B)
array([[2, 3],
       [3, 5]])

>>> A
array([[1, 2],
       [2, 3]])
```

```
>>> a = np.array([1,2,3])
>>> b = np.array([3,4,5])
>>> np.outer(a,b) # tensor product
array([[ 3,  4,  5],
       [ 6,  8, 10],
       [ 9, 12, 15]])
>>> a[np.newaxis].T*b[np.newaxis] # same --
array([[ 3,  4,  5],
       [ 6,  8, 10],
       [ 9, 12, 15]])

>>> np.cross(a,b) # vector product of a and
array([-2,  4, -2])
```

Standard matrices

- numpy implements standard matrices such as the identity

```
>>> I = np.identity(4)
>>> I
array([[1., 0., 0., 0.],
       [0., 1., 0., 0.],
       [0., 0., 1., 0.],
       [0., 0., 0., 1.]])

>>> I_c = np.identity(4, dtype=complex)
>>> I_c
array([[1.+0.j, 0.+0.j, 0.+0.j, 0.+0.j],
       [0.+0.j, 1.+0.j, 0.+0.j, 0.+0.j],
       [0.+0.j, 0.+0.j, 1.+0.j, 0.+0.j],
       [0.+0.j, 0.+0.j, 0.+0.j, 1.+0.j]])
```

```
>>> F = np.eye(3)
>>> F
array([[1., 0., 0.],
       [0., 1., 0.],
       [0., 0., 1.]])

>>> F = np.eye(4,2)
>>> F
array([[1., 0.],
       [0., 1.],
       [0., 0.],
       [0., 0.]])
```

Standard matrices (continued)

```
>>> F = np.eye(4,k=2)
>>> F
array([[0., 0., 1., 0.],
       [0., 0., 0., 1.],
       [0., 0., 0., 0.],
       [0., 0., 0., 0.]])

>>> F = np.eye(4,k=-2)
>>> F
array([[0., 0., 0., 0.],
       [0., 0., 0., 0.],
       [1., 0., 0., 0.],
       [0., 1., 0., 0.]])
```

```
>>> E = np.ones(3)
>>> E
array([1., 1., 1.])

>>> E = np.ones((2,3))
>>> E
array([[1., 1., 1.],
       [1., 1., 1.]])

>>> F = np.full((3,2),1/3)
>>> F
array([[0.33333333, 0.33333333],
       [0.33333333, 0.33333333],
       [0.33333333, 0.33333333]])
```

Concatenating matrices

- We can "glue" matrices together with np.concatentate.

```
>>> A = np.array([[1,2,3],[2,2,2]])
>>> A
array([[1, 2, 3],
       [2, 2, 2]])
>>> B = np.ones((3,2))
>>> B
array([[1., 1.],
       [1., 1.],
       [1., 1.]])

>>> AB = np.concatenate((A,B.T), axis=1)
>>> AB
array([[1., 2., 3., 1., 1., 1.],
       [2., 2., 2., 1., 1., 1.]])
```

Arrays and functions

- functions can be evaluated at arrays (similarly to map with list)
- return value is of the shape of input array
- this avoids loops and is fast

```
>>> def f(x):
...     return x**2
...
>>> a = np.array([[1,2,3], [2,3,4]])
>>> print(f(a))
[[ 1  4  9]
 [ 4  9 16]]
```

Arrays and functions (continued)

```
>>> def f(x):
...     return x**2
...
>>> a = np.array([[1,2,3], [2,3,4]])
>>> print(f(a))
[[ 1  4  9]
 [ 4  9 16]]
```

This code corresponds to

$$f(a) = \begin{pmatrix} f(a_{00}) & f(a_{01}) & f(a_{02}) \\ f(a_{10}) & f(a_{11}) & f(a_{12}) \end{pmatrix}.$$

Arrays and functions (continued)

```
>>> def f(x, y):
...     return x**2 + y**2
...
>>> a = np.array([[1,2,3], [2,3,4]])
>>> b = np.array([[0,5,6], [0,2,4]])
>>> print(f(a,b))
[[ 1 29 45]
 [ 4 13 32]]
```

This code corresponds to

$$f(a,b) = \begin{pmatrix} f(a_{00}, b_{00}) & f(a_{01}, b_{01}) & f(a_{02}, b_{02}) \\ f(a_{00}, b_{00}) & f(a_{01}, b_{01}) & f(a_{02}, b_{02}) \end{pmatrix}.$$

Arrays and functions (continued)

```
>>> def f(x, y):
...     return x[0]**2 + x[1]**2*y[0] + y[1]**2
...
>>> a = np.array([[1,2,3], [2,3,4]])
>>> b = np.array([[0,5,6], [0,2,4]])
>>> f(a,b)
array([  1,  53, 121])
```

This code corresponds to

$$f(a,b) = \left(f\left(\begin{pmatrix} a_{00} \\ a_{10} \end{pmatrix}, \begin{pmatrix} b_{00} \\ b_{10} \end{pmatrix} \right) \quad f\left(\begin{pmatrix} a_{01} \\ a_{11} \end{pmatrix}, \begin{pmatrix} b_{01} \\ b_{11} \end{pmatrix} \right) \quad f\left(\begin{pmatrix} a_{02} \\ a_{12} \end{pmatrix}, \begin{pmatrix} b_{02} \\ b_{12} \end{pmatrix} \right) \right).$$

```
>>> [f(a[:,0],b[:,0]), f(a[:,1],b[:,1]), f(a[:,2],b[:,2])]
[1, 53, 121]
```

Arrays and functions (continued)

- What is the advantage of arrays over python lists? Answer: speed
- Reason: numpy arrays are saved into contiguous blocks in the memory, while python lists are scattered over the memory. (Note: this is not true for `dtype = object`)

```
>>> r = np.random.rand(10000)  # Random array of length 10000
>>> from time import time

>>> def f(x):
...     return x**2 + np.sin(x**3)
...
>>> a = time()
>>> arr1 = f(r)
>>> print(time() - a)
0.0014252662658691406

>>> a = time()
>>> arr2 = np.array(list(map(f,r)))
>>> print(time() - a)
```

Arrays and functions (continued)

- some functions need to be rewritten to support evaluation on arrays

For instance the function:

$$\Theta(x) := \begin{cases} 1 & x > 0 \\ 0 & x \leq 0 \end{cases}.$$

In this case `np.where(cond, val1, val2)` is helpful, which returns `val1` if `cond` is `True` and `val2` if `cond` is `False`.

```
>>> a = np.array([1,2,-3])
>>> def theta1(x):
...     if x>0:
...         return 1
...     else:
...         return 0
...
>>> #theta1(a)   gives error
```

```
>>> a = np.array([1,2,3])
>>> def theta2(x):
...     return np.where(x>0,1,0)
...
>>> theta2(a)
array([1, 1, 1])
```

Broadcasting arrays

- typically only arrays of the same dimension are added; however it is also possible to add arrays of different dimension
- in this case a new array is created and the dimension missing is "filled up"

What happens is for instance the following:

$$\begin{pmatrix} a_1 & a_2 & a_2 \end{pmatrix} + \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} = \begin{pmatrix} a_1 & a_2 & a_3 \\ a_1 & a_2 & a_3 \\ a_1 & a_2 & a_3 \end{pmatrix} + \begin{pmatrix} b_1 & b_1 & b_1 \\ b_2 & b_2 & b_2 \\ b_3 & b_3 & b_3 \end{pmatrix}$$

```
>>> a = np.array([[1,2,4]])
>>> b = np.array([[0],[0],[0]])
>>> a+b
array([[1, 2, 4],
       [1, 2, 4],
       [1, 2, 4]])
```

Broadcasting arrays

Now why is this useful? For instance:

```
>>> a = np.array([1,2,3,1])
>>> a = a + 1 # new array is created with each element +1
>>> a
array([2, 3, 4, 2])

>>> a += 1  # each element of a is increased by 1

>>> a
array([3, 4, 5, 3])
```

The same broadcasting works for - and *. For instnace

```
>>> a = np.array([[1,2,3]])
>>> b = np.array([[1,1,1]]).T

>>> a*b
array([[1, 2, 3],
       [1, 2, 3],
       [1, 2, 3]])
```

More element wise operations

We can compare matrices element wise.

```
>>> A = np.array([[1,2,3],[2,3,4]])
>>> B = A+1
>>> B[0,0] -= 2

>>> A>B
array([[ True, False, False],
       [False, False, False]])

>>> A<B
array([[False,  True,  True],
       [ True,  True,  True]])

>>> np.any(A<B)
True
>>> np.all(A<B)
False
```

Diagonal matrices

- create diagonal matrices with `np.diag(a)`
- extract diagonal of matrix with `np.diag(A)`

```
>>> a = np.array([(-k)**k for k in range(4)])
>>> a
array([  1,  -1,   4, -27])

>>> diag(a)
array([[  1,   0,   0,   0],
       [  0,  -1,   0,   0],
       [  0,   0,   4,   0],
       [  0,   0,   0, -27]])
```

Tridiagonal matrices

Example of a tridiagonal matrix

$$T_N = \begin{pmatrix} 2 & -1 & & 0 \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ 0 & & -1 & 2 \end{pmatrix}.$$

```
>>> a = 2*ones(4)
>>> b = -ones(3)

>>> T = diag(a,0)+diag(b,-1)+diag(b,1)
>>> T
array([[ 2., -1.,  0.,  0.],
       [-1.,  2., -1.,  0.],
       [ 0., -1.,  2., -1.],
       [ 0.,  0., -1.,  2.]])
```

Block matrices

Example

- Let A, B, C, D be matrices. Then in numpy with `block` we can define the new matrix $\begin{pmatrix} A & B \\ C & D \end{pmatrix}$.
- If we only want $\begin{pmatrix} A & B \end{pmatrix}$ or $\begin{pmatrix} A \\ C \end{pmatrix}$, we can also use `vstack` or `hstack`.

```
>>> B = ones((2,2))
>>> C = B.copy()
>>> A = array([[1,2],[1,2]])
>>> D = A.copy()

>>> block([[A,B],[C,D]])
array([[1., 2., 1., 1.],
       [1., 2., 1., 1.],
       [1., 1., 1., 2.],
       [1., 1., 1., 2.]])
```

```
>>> B = 4*eye(2)
>>> hstack([B,B])
array([[4., 0., 4., 0.],
       [0., 4., 0., 4.]])

>>> vstack([B,B])
array([[4., 0.],
       [0., 4.],
       [4., 0.],
       [0., 4.]])
```

Reshaping arrays

- shape of an array a can be displayed by a.shape or np.shape(a).
- for reshape an array use a.reshape(shape), where shape is a tuple

```
>>> a = np.array([[1,2,3],[0,0,5]])
>>> a.shape # print shape
(2, 3)
>>> a.T # transpose array
array([[1, 0],
       [2, 0],
       [3, 5]])
>>> a.T.shape  # shape of transposed
(3, 2)
```

```
>>> a = np.array([[1,2,3],[0,0,5]])
>>> a.reshape((1,6))
array([[1, 2, 3, 0, 0, 5]])

>>> a.reshape((6,1))
array([[1],
       [2],
       [3],
       [0],
       [0],
       [5]])
>>> a.reshape((6,1)).reshape((3,2))
array([[1, 2],
       [3, 0],
       [0, 5]])
```

More functions of array

```
>>> A = np.array([1,1])
>>> dir_A = [s for s in dir(A) if s[0] != '_']

>>> for s in range(0,len(dir_A),7):
...         print(dir_A[s:s+7])
...
['T', 'all', 'any', 'argmax', 'argmin', 'argpartition', 'argsort']
['astype', 'base', 'byteswap', 'choose', 'clip', 'compress', 'conj']
['conjugate', 'copy', 'ctypes', 'cumprod', 'cumsum', 'data', 'diagonal']
['dot', 'dtype', 'dump', 'dumps', 'fill', 'flags', 'flat']
['flatten', 'getfield', 'imag', 'item', 'itemset', 'itemsize', 'max']
['mean', 'min', 'nbytes', 'ndim', 'newbyteorder', 'nonzero', 'partition']
['prod', 'ptp', 'put', 'ravel', 'real', 'repeat', 'reshape']
['resize', 'round', 'searchsorted', 'setfield', 'setflags', 'shape', 'size']
['sort', 'squeeze', 'std', 'strides', 'sum', 'swapaxes', 'take']
['tobytes', 'tofile', 'tolist', 'tostring', 'trace', 'transpose', 'var']
['view']
```

More functions of the numpy module

A list of all functions in the numpy package can be obtained by typing `dir(numpy)` in the ipython shell.

For instance the names of (for space reasons here) of all functions starting with 's':

```
>>> import numpy
>>> dir_s = [s for s in dir(numpy) if s[0] == 's']
>>> for k in range(0,len(dir_s),5):
...       print(dir_s[k:k+5])
...
['s_', 'safe_eval', 'save', 'savetxt', 'savez']
['savez_compressed', 'sctype2char', 'sctypeDict', 'sctypeNA', 'sctypes']
['searchsorted', 'select', 'set_numeric_ops', 'set_printoptions', 'set_string_f
['setbufsize', 'setdiff1d', 'seterr', 'seterrcall', 'seterrobj']
['setxor1d', 'shape', 'shares_memory', 'short', 'show_config']
['sign', 'signbit', 'signedinteger', 'sin', 'sinc']
['single', 'singlecomplex', 'sinh', 'size', 'sometrue']
['sort', 'sort_complex', 'source', 'spacing', 'split']
['sqrt', 'square', 'squeeze', 'stack', 'std']
['str', 'str0', 'str_', 'string_', 'subtract']
['sum', 'swapaxes', 'sys']
```

linalg module

- `linalg` is a submodule of `numpy`, which provides basic linear algebra tools
- it is recommended to rather use the linear algebra package of `scipy`

Typing `help(numpy.linalg)` shows:

- norm	Vector or matrix norm
- inv	Inverse of a square matrix
- solve	Solve a linear system of equations
- det	Determinant of a square matrix
- lstsq	Solve linear least-squares problem
- pinv	Pseudo-inverse (Moore-Penrose) calculated using a singular value decomposition
- matrix_power	Integer power of a square matrix

The scipy package

Online resources

- full documentation of latest scipy version (2511 pages)
  `https://docs.scipy.org/doc/scipy-1.2.1/scipy-ref-1.2.1.pdf`
- online lectures: `https://scipy-lectures.org`

Basic module structure of library scipy

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

Getting help via `help(scipy)` in ipython shell.

Scipy vs. Numpy?

- Numpy <u>should do</u>: indexing, sorting, reshaping, basic elementwise functions
- Scipy <u>should do</u>: numerical algorithms
- Problem: Numpy is backward compatible with previous versions; hence it also contains numerical algorithms
- But: Scipy has usually more fully fledged algorithms

SciPy imports all the functions from the NumPy namespace.

scipy.linalg - solving linear systems

Most important functions:

- inv - Find the inverse of a square matrix
- solve - Solve a linear system of equations
- det - Find the determinant of a square matrix
- norm - Matrix and vector norm
- lstsq - Solve a linear least-squares problem
- pinv - Pseudo-inverse (Moore-Penrose) using lstsq
- pinv2 - Pseudo-inverse using svd
- kron - Kronecker product of two arrays

Solving linear equation

Let $A \in \mathbf{R}^{d\times d}$ and $b \in \mathbf{R}^d$. Then we can solve $Ax = b$ with scipy as follows:

```
>>> from scipy.linalg import solve

>>> A = array([[0,2,3],[2,2,2],[2,3,4]])
>>> b = array([1,1,1])

>>> x = solve(A,b)
>>> print(x)
[-0.5  2.  -1. ]

>>> # test if correct

>>> norm(A@x-b)
0.0
```

Solve options

- Question: What method does `linagl.solve` call to solve the system?
- Answer: it depends on the structure of `A`.
- You can tell `linalg.solve` what type of matrix it is via `assume_a`.

`linalg.solve(A,b, assume_a = 'opt')`

generic matrix	'gen'
symmetric	'sym'
hermitian	'her'
positive definite	'pos'

- 'gen' $\rightarrow$ LU factorisation
- 'pos' $\rightarrow$ $LL^\top$ (or Cholesky) factorisation
- 'sym' $\rightarrow$ $LDL^\top$ factorisation
- 'her' $\rightarrow$ LDL^H facorisation

Solve option - LAPACK

- The function `linalg.solve` calls the LAPACK functions ?GESV, ?SYSV, ?HESV, and ?POSV.
- LAPACK is a package written in Fortran 90 provides routines for
  - solving systems of simultaneous linear equations
  - least-squares solutions of linear systems of equations
  - eigenvalue problems
  - singular value problems.

scipy.linalg - decompositions

These functions allow different decompositions $A = CD$ of a matrix $A \in \mathbf{R}^{d\times d}$ into to matrices $C \in \mathbf{R}^{d\times d}$ and $D \in \mathbf{R}^{d\times d}$.

lu	- LU decomposition of a matrix
lu_solve	- Solve Ax=b using back substitution with output of lu_factor
svd	- Singular value decomposition of a matrix
svdvals	- Singular values of a matrix
null_space	- Construct orthonormal basis for the null space of A using svd
ldl	- LDL.T decomposition of a Hermitian or a symmetric matrix
cholesky	- Cholesky decomposition of a matrix
qr	- QR decomposition of a matrix
schur	- Schur decomposition of a matrix
hessenberg	- Hessenberg form of a matrix

scipy.linalg - eigenvalue problems

Given $A \in \mathbf{R}^{d\times d}$(or $\in \mathbf{C}^{d\times d}$) we want solve the eigenvalue problem: find $(\lambda, v) \in \mathbf{C} \times \mathbf{C}^d$, such that $Av = \lambda v$.

- eig - Find the eigenvalues and eigenvectors of a square matrix
- eigvals - Find just the eigenvalues of a square matrix
- eigh - Find the e-vals and e-vectors of a Hermitian or symmetric matrix
- eigvalsh - Find just the eigenvalues of a Hermitian or symmetric matrix
- eig_banded - Find the eigenvalues and eigenvectors of a banded matrix
- eigvals_banded - Find just the eigenvalues of a banded matrix

scipy.linalg - eigenvalue problems

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

>>> [D, V] = linalg.eig(A)
>>> D
array([-1.10977223,  8.10977223,  0.        ])
>>> V
array([[-0.85872789,  0.44526277,  0.40824829],
       [ 0.36234405,  0.63314337, -0.81649658],
       [ 0.36234405,  0.63314337,  0.40824829]])

>>> A = array([[0, -1],[0,1]])

>>> linalg.eig(A)
(array([0., 1.]), array([[ 1.        , -0.70710678],
       [ 0.        ,  0.70710678]]))
```

Solving singular linear system

If A is not regular A^{-1} does not exist. However one can always solve

$$\min_{x\in\mathbf{R}^d} \|Ax-b\|_2^2,$$

which is called *least square problem*/(Problem der kleinsten Quadrate). In scipy this can be solved with `linalg.lstsq(A,b)`.

```
>>> A = array([[1,2,3],[3,3,3],[3,3,3]])
>>> b = np.array([1,2,1])

>>> x = linalg.lstsq(A,b)[0]
>>> x
array([0.16666667, 0.16666667, 0.16666667])
```

Solving singular linear system: pseudo inverse

Let $b \in \mathbf{R}^m$. The pseudo inverse of a matrix $A \in \mathbf{R}^{m\times n}$ is denote by A^+ and defined by its action $A^+b := x$, where $x \in \mathbf{R}^n$ is the solution to

$$\min_{x\in\mathbf{R}^n} \|Ax - b\|_2^2,$$

with minimal norm $\|x\|_2$.

- In scipy the pseudo inverse is defined by `scipy.linalg.pinv` or `scipy.linalg.pinv2`.
- The first method uses `scipy.linalg.lstsq` and second computes uses the singular value decomposition of A.

Example 1

For example let $\hat{A} \in \mathbf{R}^{d\times d}$ be invertible and define

$$A := \begin{pmatrix} \hat{A} & 0 \\ 0 & 0 \end{pmatrix} \in \mathbf{R}^{(d+\ell)\times(d+\ell)}.$$

Then

$$A^+ = \begin{pmatrix} \hat{A}^{-1} & 0 \\ 0 & 0 \end{pmatrix}$$

Example 2

(a) If the matrix $A \in \mathbf{R}^{m\times n}$ is injective, then $A^\top A$ is injective and thus invertible.
(b) If A is injective, then the pseudo inverse is $A^+ = (A^\top A)^{-1}A^\top : \mathbf{R}^m \to \mathbf{R}^n$.

Proof.

ad (a): Let $x \in \mathbf{R}^d$ be such that $A^\top Ax = 0$. Then $0 = A^\top Ax \cdot x = Ax \cdot Ax = \|Ax\|_2^2 = 0$ and hence $Ax = 0$. It follows $x = 0$ since A is injective. This shows that $A^\top A$ is injective and therefore also surjective (and hence bijective)
ad (b): In numerics lectures. $\square$

Example 2

Consider for instance

$$A = \begin{pmatrix} 1 & 0 \\ 2 & 0 \\ 1 & 1 \end{pmatrix}, \; A^\top = \begin{pmatrix} 1 & 2 & 1 \\ 0 & 0 & 1 \end{pmatrix} \quad \Rightarrow \quad A^\top A = \begin{pmatrix} 6 & 1 \\ 1 & 1 \end{pmatrix}.$$

Hence using (b) from the previous slide:

$$(A^\top A)^{-1} = \frac{1}{5}\begin{pmatrix} 1 & -1 \\ -1 & 6 \end{pmatrix} \quad \Rightarrow \quad A^+ = \frac{1}{5}\begin{pmatrix} 1 & 2 & 0 \\ -1 & -2 & 5 \end{pmatrix}.$$

```
>>> A = array([[1, 0],[2,0],[1,1]])
>>> 5 * pinv(A)
array([[ 1.00000000e+00,  2.00000000e+00,  2.45275636e-16],
       [-1.00000000e+00, -2.00000000e+00,  5.00000000e+00]])
```

Solving singular linear system: pseudo inverse

In scipy the pseudo inverse can be computed via `scipy.linalg.pinv`.

```
>>> A = np.zeros((3,3))
>>> A_ = np.array([[1,2],[2,1]])

>>> A[0:2,0:2] = A_

>>> pinv(A)
array([[-0.33333333,  0.66666667,  0.        ],
       [ 0.66666667, -0.33333333,  0.        ],
       [ 0.        ,  0.        ,  0.        ]])

>>> inv(A_)
array([[-0.33333333,  0.66666667],
       [ 0.66666667, -0.33333333]])
```

Solving singular linear system: pseudo inverse

```
>>> A = np.zeros((3,3))
>>> A_ = np.array([[1,2],[2,1]])

>>> A[0:2,0:2] = A_

>>> b = np.array([1,2,1])

>>> pinv(A)@b
array([ 1.00000000e+00, -2.22044605e-16,  0.00000000e+00])

>>> lstsq(A,b)[0]
array([ 1.00000000e+00, -1.16957102e-16,  0.00000000e+00])
```

Plotting with python

Plotting in python

Plotting tools in python

There are many tools to plot in python:

- matplotlib (mostly 2d plotting) https://matplotlib.org
- mayavi (3d plotting) https://docs.enthought.com/mayavi/mayavi/
- bokeh (for plotting in web browser) https://bokeh.pydata.org
- seaborn (plotting of statistical data) https://seaborn.pydata.org
- ...

matplotlib

matplotlib and pyplot

- matplotlib is a python library for mostly 2D plotting
- pyplot is a submodule of matplotlib and allows matlab-like plotting
- you can use matplotlib interactively in `ipython` shell by typing `%matplotlib` in ipython shell
- after you can import as follows `import matplotlib.pyplot as plt`

pylab

matplotlib docu says: Since heavily importing into the global namespace may result in unexpected behavior, the use of pylab is strongly discouraged. Use matplotlib.pyplot instead.

np.linspace

np.linspace

- `numpy.linspace(start, stop, num=50, endpoint=True, retstep=False,...)`
- divides the interval (start,stop) into num parts and if endpoint=True the point stop belongs to output

```
>>> x = np.linspace(0,1,4)
>>> x
array([0.        , 0.33333333, 0.66666667, 1.        ])

>>> x, y = np.linspace((0,1), (3,4), 5).T
>>> x
array([0.  , 0.75, 1.5 , 2.25, 3.  ])
>>> y
array([1.  , 1.75, 2.5 , 3.25, 4.  ])
```

Simple line plot - matplotlib.pyplot.plot

```
plot(*args, scalex=True, scaley=True, data=None, **kwargs)[source]
```

Listing 39: line_plot.py

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

x = np.linspace(0,10,100) # divide [0,10] into 100 parts
y = x**2 # y[i] = x[i]**2

plt.plot(x, y)          # plot x and y using default line style and color
plt.show()
```

Simple line plot - more options

`help(plot)` for a full set of options

Listing 40: line_plot2.py

```python
import matplotlib.pylab as plt
import numpy as np

x = np.linspace(0,10,100) # divide [0,10] into 100 parts
y = x**2 # y[i] = x[i]**2

plt.plot(x, y, color = 'r', marker = 'x', linestyle = '--',
     linewidth = 2, markersize = 4)
# use color red, style x, and linestyle "dashed"

plt.show()
```

Simple line plot - labels and legend

Listing 41: line_plot3.py

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

x = np.linspace(0,2*np.pi,100)  # x values
y = np.sin(x)**2  # y values

plt.plot(x,y)
plt.xlabel('x')  # x label
plt.ylabel('$sin^2(x)$') # y label
plt.legend(('sin(x)',))
#plt.xlim(0,1)  ## restrict x to (0,1)
#plt.ylim(0,0.5) ## restrict y to (0,0.5)
plt.show()
```

Scatter point

Listing 42: scatter_2d.py

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

# gives always the same random output
np.random.seed(19680801)

N = 50
x = np.random.rand(N)
y = np.random.rand(N)
colors = np.random.rand(N)
area = (30 * np.random.rand(N))**2 # 0 to 15 point radii

plt.scatter(x, y, s=area, c=colors, alpha=0.5)
plt.show()
```

Multiple plots

Listing 43: mult_plots.py

```python
import matplotlib.pyplot as plt
plt.figure(1)                # figure number 1
plt.subplot(121)             # 121 = 1 number rows
                             #       2 number columns
                             #       1 plot first
plt.plot([1, 2, 3])          # plot into 121
plt.subplot(122)             # the second subplot in the first figure
plt.plot([4, 5, 6])          # plot into 122

plt.figure(2)                # figure number 2
plt.plot([4, 5, 6], 'o')     # creates a subplot(111) by default
plt.show()
```

Subplots - more control

Listing 44: subplots.py

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

fig, (ax1,ax2) = plt.subplots(2,1, sharex = True)
# create figure with 2 subplots
# they share the x axis
# other options: sharex, sharey : bool or {'none', 'all', 'row', 'col'}
x = np.linspace(0,1)

ax1.plot(x,x**2)
ax2.plot(x,x**4)
plt.show()
```

Axes and figure

Axes and figures

- matplotlib distinguishes the figure and axis.
- the figure is the window where the plotting happens; generate figure with `plt.figure(num)`, if `num` is not specified it is by default 1
- axes contain the x and y axes and the plot; add axes to figure via `fig.add_axes([left, bottom, width, height])`.

Commands add axes:

- `Figure.add_axes`
- `pyplot.subplot`
- `Figure.add_subplot`
- `Figure.subplots`
- `pyplot.subplots`

Axes and figure - example

Listing 45: axes_figure.py

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

fig = plt.figure()  # generate figure

ax1 = fig.add_axes([0.1, 0.1, 0.4, 0.4]) # add axes at (0.1,0.1)
                                         # size 0.4 x 0.4
ax2 = fig.add_axes([0.5, 0.5, 0.4, 0.4]) # another one

x = np.linspace(0,1)
ax1.plot(x,x**2) # plot into ax1
ax2.plot(x,x**3) # plot into ax2
plt.show()
```

3D plotting with `mplot3d`

- matplotlib allows simple 3D plotting using the library `mpl_toolkits.mplot3d`
- online docu of mplot3d:
  `https://matplotlib.org/mpl_toolkits/mplot3d/tutorial.html`
- for fancier plots use, e.g., paraview, mayavi (see below)

Available plotting functions

- `Axes3D.scatter(xs, ys, zs=0, *args, **kwargs)`
- `Axes3D.plot_wireframe(X, Y, Z, *args, **kwargs)`
- `Axes3D.plot_surface(X, Y, Z, *args, **kwargs)`
- `Axes3D.quiver(*args, **kwargs)`
- `Axes3D.text(x, y, z, s, zdir=None, **kwargs)`

plot_surface

Listing 46: plot_3d_surf.py

```python
from mpl_toolkits.mplot3d import Axes3D # only needed for projection below
import numpy as np
import matplotlib.pyplot as plt

fig = plt.figure()
ax = fig.add_subplot(111, projection='3d')

theta = np.linspace(0, np.pi, 100) # divide [-4pi, 4pi] into 100
phi = np.linspace(0, 2*np.pi, 100) # same

theta, phi = np.meshgrid(theta,phi)

x = np.sin(theta)*np.cos(phi) # compute sin(theta[i]) * cos(phi[i])
y = np.sin(theta)*np.sin(phi) # compute sin(theta[i]) * sin(phi[i])
z = np.cos(theta) # compute cos(theta[i])

ax.plot_surface(x, y, z, label='surface plot', rstride = 5, cstride = 5) # plot into figure
#ax.plot_wireframe(x, y, z, label='wireframe surface plot', rstride = 10, cstride = 10) # plot into figure
#ax.legend() # put legend

plt.show() # show plot
```

plot_curve

Listing 47: plot_3d_curve.py

```
from mpl_toolkits.mplot3d import Axes3D # only needed for projection below

import numpy as np
import matplotlib.pyplot as plt

plt.rcParams['legend.fontsize'] = 10

fig = plt.figure()
ax = fig.gca(projection='3d')

theta = np.linspace(-4 * np.pi, 4 * np.pi, 100) # divide [-4pi, 4pi] into 100

z = np.linspace(-2, 2, 100) # divide [-2,2] into 100
r = z**2 + 1 # compute r[i] = z[i]**2 + 1

x = r * np.sin(theta) # compute r[i]* sin(theta[i])
y = r * np.cos(theta) # compute r[i]* cost(theta[i])

ax.plot(x, y, z, label='parametric curve') # plot into figure
ax.legend() # put legend

plt.show() # show plot
```

Plotting with mayavi

- Mayavi has better rendering and is more suitable for large data.
- You need to install it, e.g. on ubuntu `pip install --user mayavi`
- it is free: BSD license
- online documentation: `http://docs.enthought.com/mayavi/mayavi/`
- mayavi also ships with gui

In python we mayavi via

```
from mayavi import mlab
```

Simple surface plot with `surf`

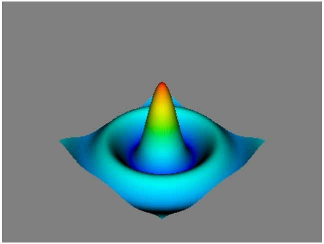
Here is how you can plot the surface $\varphi : \mathbf{R}^2 \to \mathbf{R}^3$, $\varphi(u,v) := \left(u, v, \frac{\sin(r(u,v))}{r(u,v)}\right)$ with $r(u,v) = \sqrt{u^2+v^2}$.

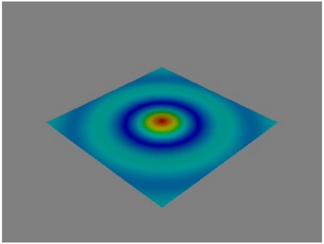
Listing 48: may_3d_surf.py

```
import numpy as np
from mayavi import mlab

x, y = np.mgrid[-10:10:100j, -10:10:100j]
r = np.sqrt(x**2 + y**2)
z = np.sin(r)/r

mlab.surf(z, warp_scale='auto')
#mlab.surf(x,y,z)  # plot flat

#mlab.outline()
#mlab.axes()  # put axes
mlab.show()  # show plot
#mlab.gcf()
#mlab.options.offscreen = True
#mlab.savefig("surf_flat.jpg")
#mlab.close()
```

Surface plot - example

Here is the result





mgrid

- `mgrid` generates a mesh grid, that is two 2D arrays which hold the x and y values over which a function is plotted
- for instance `mgrid[0:1:10j,0:2:10j]` generates a mesh grid where the xrange goes from 0 to 1 and is divided into 10 parts. Similarly the yrange goes from 0 to 2 and is also divided into 10 parts
- note that the 10j is indeed a complex number

mgrid - example

```
>>> X, Y = np.mgrid[0:1:5j,0:2:5j]
>>> X
array([[0.  , 0.  , 0.  , 0.  , 0.  ],
       [0.25, 0.25, 0.25, 0.25, 0.25],
       [0.5 , 0.5 , 0.5 , 0.5 , 0.5 ],
       [0.75, 0.75, 0.75, 0.75, 0.75],
       [1.  , 1.  , 1.  , 1.  , 1.  ]])
>>> Y
array([[0. , 0.5, 1. , 1.5, 2. ],
       [0. , 0.5, 1. , 1.5, 2. ],
       [0. , 0.5, 1. , 1.5, 2. ],
       [0. , 0.5, 1. , 1.5, 2. ],
       [0. , 0.5, 1. , 1.5, 2. ]])
```

```
>>> x = np.linspace(0,1,5)
>>> y = np.linspace(0,2,5)
>>> X, Y = np.meshgrid(x,y)
>>> X
array([[0.  , 0.25, 0.5 , 0.75, 1.  ],
       [0.  , 0.25, 0.5 , 0.75, 1.  ],
       [0.  , 0.25, 0.5 , 0.75, 1.  ],
       [0.  , 0.25, 0.5 , 0.75, 1.  ],
       [0.  , 0.25, 0.5 , 0.75, 1.  ]])
>>> Y
array([[0. , 0. , 0. , 0. , 0. ],
       [0.5, 0.5, 0.5, 0.5, 0.5],
       [1. , 1. , 1. , 1. , 1. ],
       [1.5, 1.5, 1.5, 1.5, 1.5],
       [2. , 2. , 2. , 2. , 2. ]])
```

mgrid - example (continued)

```
>>> X = np.linspace(0,1,4)*np.ones((5,1))
>>> Y = np.linspace(2,3,5)*np.ones((4,1))
>>> X
array([[0.        , 0.33333333, 0.66666667, 1.        ],
       [0.        , 0.33333333, 0.66666667, 1.        ],
       [0.        , 0.33333333, 0.66666667, 1.        ],
       [0.        , 0.33333333, 0.66666667, 1.        ],
       [0.        , 0.33333333, 0.66666667, 1.        ]])
>>> Y
array([[2.  , 2.25, 2.5 , 2.75, 3.  ],
       [2.  , 2.25, 2.5 , 2.75, 3.  ],
       [2.  , 2.25, 2.5 , 2.75, 3.  ],
       [2.  , 2.25, 2.5 , 2.75, 3.  ]])
```

Listing 49: may_3d.py

```
from numpy import pi, sin , cos, mgrid
from mayavi import mlab

dphi, dtheta = pi/250.0, pi/250.0
[phi,theta] = mgrid[0:pi+dphi*1.5:dphi,0:2*pi+dtheta*1.5:dtheta]
m0 = 4; m1 = 3; m2 = 2; m3 = 3; m4 = 6; m5 = 2; m6 = 6; m7 = 4;
r = sin(m0*phi)**m1 + cos(m2*phi)**m3 + sin(m4*theta)**m5 + cos(m6*theta)**m7
#r = 1
x = r*sin(phi)*cos(theta)
y = r*cos(phi)
z = r*sin(phi)*sin(theta)

# View it.
s = mlab.mesh(x, y, z)
mlab.show()
```

Symbolic computing with Sympy

Online resources

Online

- home: `https://www.sympy.org/en/index.html`
- git repository: `https://github.com/sympy/sympy`

According to sympy webpage here are reasons why to use it:

- **Free**: Licensed under BSD, SymPy is free both as in speech and as in beer.
- **Python-based**: SymPy is written entirely in Python and uses Python for its language.
- **Lightweight**: SymPy only depends on mpmath, a pure Python library for arbitrary floating point arithmetic, making it easy to use.
- **A library**: Beyond use as an interactive tool, SymPy can be embedded in other applications and extended with custom functions.

After installing sympy (it is not part of the standard library) you import it with

```
from sympy import *
```

Variables in sympy

variables in sympy are defined via `x = Symbol('x')` or for several at once `x,y,z = symbols('x y z')`.

```
>>> from sympy import *
>>> x,y,z = symbols('x y z')

>>> x+x
2*x

>>> x+y
x + y

>>> x**y
x**y
```

Evaluation, simplification and differentiation

- function is defined by `f = x**2 - 2*x +1 + y**2 -2*y + 1`
- differentiation w.r.t x, `diff(f,'x')`
- simplification `simplify(f)`
- expand expression `expand`

```
>>> from sympy import *
>>> x, y = symbols('x y')
>>> f = x**2 - 2*x +1 + y**2 -2*y + 1

>>> diff(f, x)
2*x - 2
>>> diff(f, y)
2*y - 2

>>> simplify(f)
x**2 - 2*x + y**2 - 2*y + 2
```

Expanding and factorisation

- factorisation `factor(f)`
- expand expression `expand(f)`

```
>>> from sympy import *
>>> x, y = symbols('x y')
>>> f = (x-1)**4 + y**2 -2*y + 1

>>> expand(f)
x**4 - 4*x**3 + 6*x**2 - 4*x + y**2 - 2*y + 2

>>> factor(f)
x**4 - 4*x**3 + 6*x**2 - 4*x + y**2 - 2*y + 2

>>> factorint(64)
{2: 6}
```

lambdify sympy expressions

We can transform a sympy expression into a lambda function via `lambdify`. This is useful since we can then use matplotlib or mayavi to plot the function.

```
>>> from sympy import *
>>> x = symbols('x')
>>> f = (x-1)**4 +  1 + sin(x)
>>> df = diff(f)

>>> f_ = lambdify(x, f, 'numpy') # lambda function f_
>>> df_ = lambdify(x, df, 'numpy') # lambda function df_
```

Taylow series expansion

We can also do a Taylor expansion of for instance

$$e^x = \sum_{\ell=0}^{\infty} \frac{x^\ell}{\ell!}.$$

```
>>> from sympy import *
>>> init_printing(use_unicode=False) # make it look nice

>>> x = symbols('x')
>>> exp(x).series(x, 0, 6)
         2    3    4     5
        x    x    x     x      / 6\
1 + x + -- + -- + -- + --- + O\x /
        2    6    24   120
>>> (1/cos(x)).series(x, 0, 10)
     2      4       6        8
    x    5*x    61*x    277*x      / 10\
1 + -- + ---- + ----- + ------ + O\x   /
    2     24     720     8064
```

lambdify sympy expressions: example 1

Listing 50: lamfy.py

```
from sympy import *
import numpy as np
import matplotlib.pylab as plt

x = symbols('x')
f = (x-1)**4 + 1 + sin(x)
df = diff(f)

f_ = lambdify(x, f, 'numpy') # lambda function f_
df_ = lambdify(x, df, 'numpy') # lambda function df_

x = np.linspace(-10,10,100)

plt.plot(x,f_(x),'b', label = 'f_(x)')
plt.plot(x,df_(x),'r', label = 'df_(x)')
plt.legend()
plt.show()
```

Plotting of sympy expressions

Sympy supports the following plotting methods of symbolic expressions:

- `plot`: 2D line plots
- `plot_parametric`: 2D parametric plots
- `plot_implicit`: 2D implicit and region plots
- `plot3d`: 3D plots of functions in two variables
- `plot3d_parametric_line`: 3D line plots, defined by a parameter
- `plot3d_parametric_surface`: 3D parametric surface plots

Implicit plots in 2d

plot_implicit in sympy only works in 2d

```
from sympy import *
var('x y') # or x,y = symbols('x y')
f = x**2 + y**2 - 1
plotting.plot_implicit(f, (x,0,1), (y,0,1))
# or alternatively
plotting.plot_implicit(Eq(x**2+y**2,1), (x,0,1),(y,0,1))
```

Curve in 3d

`plot3d_parametric_surface` in sympy only works in 2d

```
from sympy import *
var('s') # or s = Symbol('s')
ux = sin(s)
uy = cos(s)
uz = s
plotting.plot3d_parametric_line(ux, uy, uz, (s, 0, 5*pi))
```