

Fakultät Elektrotechnik und Informationstechnik Institut für Regelungs- und Steuerungstheorie

INTRODUCTION TO SCIENTIFIC PROGRAMMING WITH PYTHON

Carsten Knoll



Outline

Introduction

Symbolic Computation (sympy)

Interactive Documents with Jupyter Notebook

Numeric Computation (numpy and scipy)

2d Visualization (matplotlib)

Final remarks

About

About me

- Post-doc at Institute of Control Theory
- Co-Founder of University Group for Free Software and Free Knowledge
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- Truncated, compressed and translated version of a one-semester-course
- Formerly organized by Sebastian Voigt, Christoph Statz, Dr.-Ing. Ines Gubsch, Ingo Keller, Peter Seifert and others
- Modules
 - 1. Introduction to Python
 - 2. Symbolic computation
 - 3. Numeric computation
 - 4. 2d visualization

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- A Contains didactic simplifications

Why Python? (1)

Python as Programming Language

- Clean readable syntax (few overhead)
- Allowed paradigms object oriented, procedural, functional
- Useful and powerful standard data types (list, tuple, dict, set, ...)
- Extensive and powerful standard library (batteries included)
- Simple modularization (import this)
- Good error handling (Exceptions)
- Simple integration of external code (C, C++, Fortran)

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\Rightarrow

- Easy to learn
- Problem oriented (powerful and flexible)

Additionally: platform independent / free and open source / big and active Community

Why Python? (2)

Python as a tool for scientists

- Symbolic computation (basic algebra, differentiation, solving equations, ...)
- Numeric computation Rechnen (lin. algebra, solving ODEs, optimization, ...)
- Visualization (2D, 3D, in publication quality)
- Grafical user interface (GUI)
- Communication with external (lab) devices (RS232, GPIB, ...)
- Parallelization

Installation: instal-script.txt

- Different methods available (depending on operating system)
- Recommendation: https://repo.continuum.io/miniconda/

```
# paste these commands in your terminal line by line
# use CTRL-SHIFT-V

# download the installer
wget https://repo.continuum.io/miniconda/Miniconda3-latest-Linux-x86_64.sh -0
    miniconda.sh

bash ./miniconda.sh -b # execute it in batch mode

# add miniconda3 to system path
echo "export PATH=\"$HOME/miniconda3/bin:\$PATH\"" >> "/.bashrc

# install important packages via conda
conda install --yes ipython jupyter sympy numpy scipy matplotlib
# install IDE (spyder) and personal debug-helper
pip install spyder ipydex
```

- Background information:
 - We use Python 3.6 (most recent version available with miniconda)
 - Python 3.x is not 100% backward compatible, ∃ still much 2.7-code

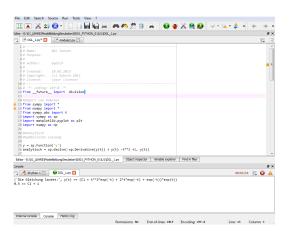
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- Jupyter Notebook (with Python Kernel)
 - Command: \$ jupyter notebook
 - Backend: (local) webserver; frontend: interactive document in browser
 - Notebooks combine source code, program-output and documentation (incl. LATEX-formulas)

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- Integrated Development Environment (we use spyder)
 - Command: \$ spyder3
 - Adapted text editor
 - Much more features (we wont use today)

Integrated Development Environment (IDE)



- Start from command line:
 - \$ spyder
- Other text editors also possible
 - Important: Indention: 4 spaces
- Avoid Tab-characters

Code-Example

```
Listing: hello-world.py
import math
print("Hello World")
a = 10
b = 20.5
c = a + b + 3**2
print(math.sqrt(c))
while True: # start infinite loop
    x = input("Your name? ") # returns a str-object
    if x == "q":
       break # finish loop
    print("Hello ", x)
```

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        break # finish loop
    print("Hello ", x)
```

- Indention have syntactical meaning
- de facto standard: 4 spaces (in IDE: block wise with <Tab>(→) and <Shift+Tab> (←))
- 01_appendix-syntax-and-types.pdf

Exercise: Embedded IPython

```
Listing: ipython1.py
import math
# import embedded shell
from ipydex import IPS
a = 10
b = 20.5
c = a + b + 3**2
d = math.sqrt(c)
# run embedded shell
IPS()
# try: math.sqrt?, math.s<TAB>, history (up, down), %magic
# exit with CTRI.-D
```

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sympy Overview

```
Listing: sympy1.py 1:18
import sympy as sp
x = sp.Symbol("x")
a, b, c, z = sp.symbols("a b c z") # create several symbols at once
some_formula = a*b*x*b + b**2*a*x - c*b*(2*a/c*x*b-1/(b*2))
print(some_formula) # -> -b*c*(-1/(2*b) + 2*a*b*x/c) + 2*a*x*b**2
print(some_formula.expand()) # -> c/2
# some calculus
y = sp.sin(x)*sp.exp(3*x)*sp.sqrt(a)
print(y) \# -> a**(1/2)*exp(x)*sin(x)
# derive
y.diff(x) # -> 3*sqrt(a)*exp(3*x)*sin(x) + sqrt(a)*exp(3*x)*cos(x)
# trigonometric simplification
print(sp.trigsimp(sp.sin(x)**2+sp.cos(x)**2)) # \rightarrow 1
```

Substitute: <expr>.subs(...)

- Comparable with <str>.replace(old, new)
- Useful for: coordinate transformation manual simplification, (partial) function evaluation
- · Returns new expression, original unchanged

```
Listing: sympy1.py 21:28
```

```
# 2 arguments:
# substitute x with z-1
y2 = y.subs(x, z-1)
# 1 argument (list of 2-tuples):
# substitute x with z-1 and a with 25 (in this order)
y3 = y.subs([(x, z-1), (a, 25)])
```

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```

• Exercise: Use IPS() to explore the content of the variables

Numerical Formula Evaluation (lambdify)

```
Listing: sympy2.py
import sympy as sp
from ipydex import IPS
a, b, c, x = sp.symbols("a b c x") # create symbols
# define expression
f = a*sp.sin(b*x)
# create python-function
f_xa_fnc = sp.lambdify((a, b, x), f, modules="numpy")
# evaluate function
print(f_xa_fnc(1.2, 0.5, 3.14))
IPS()
# use magic commands to investigate speedup
# %time f_xa_fnc(1, 1, 1)
# %time f.subs([(a, 1), (b, 1), (x, 1)]).evalf()
```

More Important Methods / Functions / Types

- sp.Matrix([[x, a+b], [c*x, sp.sin(x)]]): Matrices
- <mtrx>.jacobian(xx): Jacobian of a vector
- sp.solve(x**2 + x a, x): solve equations and systems of equations
- <expr>.atoms(), <expr>.atoms(sp.sin): get "'atoms" (all or specific ones)
- <expr>.args: arguments of the respective class (terms of the sum, factors)
- sp.sympify(...): adapt data types
- sp.integrate(<expr>, <var>): integration
- sp.series(...): series expansion
- sp.limit(<var>, <value>): limit
- <expr>.as_num_denom(): get numerator and denominator
- sp.Polynomial(x**7+a*x**3+b*x+c, x, domain='EX'): polynomials
- sp.Piecewise(...): piecewise defined functions

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Jupyter



- Web application for interactive data science and scientific computing
- Start with:
 - \$ cd notebooks
 - \$ jupyter notebook ./
- Important keyboard shortcuts:

Command Mode (press Esc to enable)

- Shift-Return execute cell, activate next
- h show keyboard shortcuts
- m change cell type to markdown
- y change cell type to code
- a new cell above

Edit Mode (press Return to enable)

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- Shift-Tab tooltip
- Ctrl-Z undo

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- → Now play around with example-notebook1.ipynb and sympy-notebook1.ipynb

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Numpy

- Basic numeric algorithms around a special data type:
- numpy.ndarray
- No (slow) python loops \rightarrow almost as fast as C or Fortran
- Explained with material from datacamp.com



Lists Recap

- Powerful
- Collection of values
- Hold different types
- Change, add, remove
- Need for Data Science
 - Mathematical operations over collections
 - Speed



Illustration

```
In [1]: height = [1.73, 1.68, 1.71, 1.89, 1.79]
In [2]: height
Out[2]: [1.73, 1.68, 1.71, 1.89, 1.79]
In [3]: weight = [65.4, 59.2, 63.6, 88.4, 68.7]
In [4]: weight
Out[4]: [65.4, 59.2, 63.6, 88.4, 68.7]
In [5]: weight / height ** 2
TypeError: unsupported operand type(s) for **: 'list' and 'int'
```



Solution: NumPy

- Numeric Python
- Alternative to Python List: NumPy Array
- Calculations over entire arrays
- Easy and Fast
- Installation
 - In the terminal: pip3 install numpy



NumPy

```
In [6]: import numpy as np
In [7]: np_height = np.array(height)
In [8]: np_height
Out[8]: array([ 1.73,  1.68,  1.71,  1.89,  1.79])
In [9]: np_weight = np.array(weight)
In [10]: np_weight
Out[10]: array([ 65.4,  59.2,  63.6,  88.4,  68.7])
In [11]: bmi = np_weight / np_height ** 2
In [12]: bmi
Out[12]: array([ 21.852,  20.975,  21.75 ,  24.747,  21.441])
```

NumPy

```
Element-wise calculations
In [8]: np_height
Out[8]: array([ 1.73, 1.68, 1.71, 1.89, 1.79])
In [10]: np weight
Out[10]: array([ 65.4, 59.2, 63.6, 88.4, 68.7])
In [12]: bmi
Out[12]: array([ 21.852, 20.975,
                                  21.75 ,
                                            24.747.
                                                    21.4417)
                = 65.5/1.73 ** 2
```



Comparison

```
In [13]: height = [1.73, 1.68, 1.71, 1.89, 1.79]
In [14]: weight = [65.4, 59.2, 63.6, 88.4, 68.7]
In [15]: weight / height ** 2
TypeError: unsupported operand type(s) for **: 'list' and 'int'

In [16]: np_height = np.array(height)
In [17]: np_weight = np.array(weight)
In [18]: np_weight / np_height ** 2
Out[18]: array([ 21.852, 20.975, 21.75 , 24.747, 21.441])
```

NumPy: remarks



NumPy Subsetting

```
In [24]: bmi
Out[24]: array([ 21.852, 20.975, 21.75 , 24.747, 21.441])
In [25]: bmi[1]
Out[25]: 20.975
In [26]: bmi > 23
Out[26]: array([False, False, False, True, False], dtype=bool)
In [27]: bmi[bmi > 23]
Out[27]: array([ 24.747])
```





INTRO TO PYTHON FOR DATA SCIENCE

2D NumPy Arrays

Type of NumPy Arrays

```
In [1]: import numpy as np
In [2]: np_height = np.array([1.73, 1.68, 1.71, 1.89, 1.79])
In [3]: np_weight = np.array([65.4, 59.2, 63.6, 88.4, 68.7])
In [4]: type(np_height)
Out[4]: numpy.ndarray
In [5]: type(np_weight)
Out[5]: numpy.ndarray
```



2D NumPy Arrays

```
In [6]: np_2d = np.array([[1.73, 1.68, 1.71, 1.89, 1.79],
                          [65.4, 59.2, 63.6, 88.4, 68.7]])
In [7]: np_2d
Out[7]:
array([[ 1.73, 1.68, 1.71, 1.89, 1.79],
       [65.4, 59.2, 63.6, 88.4, 68.7]])
In [8]: np 2d.shape
                        2 rows, 5 columns
Out[8]: (2, 5)
In [9]: np.array([[1.73, 1.68, 1.71, 1.89, 1.79],
                  [65.4, 59.2, 63.6, 88.4, "68.7"]])
Out[9]:
                                                    Single type!
array([['1.73', '1.68', '1.71', '1.89', '1.79'],
       ['65.4', '59.2', '63.6', '88.4', '68.7']],
     dtvpe='<U32')
```

DataCamp

Subsetting

```
o 1 2 3 4
array([[ 1.73,  1.68,  1.71,  1.89,  1.79], o
[ 65.4,  59.2,  63.6,  88.4,  68.7]]) 1
```

```
In [10]: np_2d[0]
Out[10]: array([ 1.73,  1.68,  1.71,  1.89,  1.79])

In [11]: np_2d[0][2]
Out[11]: 1.71

In [12]: np_2d[0,2]
Out[12]: 1.71
```

DataCamp

Subsetting



Subsetting

```
array([[ 1.73, 1.68, 1.71, 1.89, 1.79], 0
  [ 65.4, 59.2, 63.6, 88.4, 68.7]]) 1
```

- How numpy manages different shapes in element-wise calculations
- Trivial example: 2d-array + scalar → scalar is "blown up"
- 2d-array + 1d-array ?

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General Rule

Length along the last axis of both operands must match or one of both equals 1.

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Length along the last axis of both operands must match or one of both equals 1.

•	Example:	RGB-Image Scale	(3d array): (1d array):	256	256	3
		Result	(3d array):	256	256	3

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	•	Result	(3d array):	256	256	3

- Powerful but not intuitive → possible confusion
 ValueError: shape mismatch: objects cannot be broadcast to a single shape
- → Recommendation interactive trial and error

List of imortant numpy-functions

- arange, linspace (create arrays)
- min, max, argmin, argmax, sum (array → scalars)
- sin, cos, exp, abs, real, imag (array → array)
- Change shape: <arr>. T (transpose), reshape, flatten, vstack, hstack

Linear Algebra

- Matrix multiplication: dot(a,b)
- Submodule: numpy.linalg:
 - det, inv, solve (lin. eq. system), eig (Eigenvalues and vectors),
 - pinv (pseudoinverse), svd (singular value decomposition), ...

Package scipy

- Based on numpy
- Offers functionality for
 - Physical constants
 - More linear algebra
 - Signal processing (FFT, Filter, ...)
 - Statistics
 - Optimization
 - Interpolation
 - Numerical integration ("simulation")

scipy.optimize.fsolve and fmin

- fsolve: find (one) root of a (nonlinear) function $\mathbf{f}: \mathbb{R}^n \to \mathbb{R}^n$
- Important: initial guess
- Example (with n = 12): approximate solution of equation $x + 2.3 \cdot \cos(x) = 1$
- $f(x) = x + 2.3 \cdot \cos(x) 1 \stackrel{!}{=} 0$

```
Listing: scipy1.py
import numpy as np
from scipy import optimize

def fnc1(x):
    return x + 2.3*np.cos(x) -1

sol = optimize.fsolve(fnc1, 0) # -> array([-0.723632])
# proof:
sol + 2.3*np.cos(sol) # -> array([ 1.])
```

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# proof:
sol + 2.3*np.cos(sol) # -> array([ 1.])
```

- fmin: find minimum of $f: \mathbb{R}^n \to \mathbb{R}$
- Exercise: reproduce the the above result using fmin

Theory: Numerical solution of ODEs ("Simulation")

- State space representation
 - System of first order ODEs $\dot{\mathbf{z}} = \mathbf{f}(\mathbf{z}, t)$
 - Solution (flow) $t \mapsto \mathbf{z}(t)$ (depends on initial condition $\mathbf{z}(0)$)

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 - Solution (flow) $t \mapsto \mathbf{z}(t)$ (depends on initial condition $\mathbf{z}(0)$)
- Example harmonic oscillator: $\ddot{y} + 2\delta \dot{y} + \omega^2 y = 0$
- Preparation: ODE of 2nd order → two ODEs 1st order: state: z = (z₁, z₂)^T with z₁ := y, z₂ := y

$$\dot{z}_1 = z_2
\dot{z}_2 = -2\delta z_2 - \omega^2 z_1 \quad (= \ddot{y})$$

• ∃ several integration algorithms (Euler, Runge-Kutta, ...)

Practice: Numerical solution of ODEs ("Simulation")

```
Listing: scipy2.py

from scipy.integrate import odeint
import numpy as np
delta, omega = .1, 1

def rhs(z,t):
    """ rhs = right hand side [function] """
    z1, z2 = z # unpacking state
    z1_dot = z2
    z2_dot = -2*delta*z2 - omega**2*z1
    return [z1_dot, z2_dot]

tt = np.arange(0, 100,.01) # 100s dt = 0.1
z0 = [3, 0] # initial state for [z1, z2]
zz = odeint(rhs, z0, tt) # call integration algorithm
```

• Notice: rhs is an "ordinary" object (type: function)

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- Notice: rhs is an "ordinary" object (type: function)
- Exercises:
 - a) Print the shape of the array zz
 - b) Plot the function $t \mapsto y(t)$

Practice: Numerical solution of ODEs ("Simulation")

```
Listing: scipy2.py

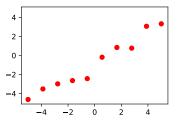
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import numpy as np
delta, omega = .1, 1

def rhs(z,t):
    """ rhs = right hand side [function] """
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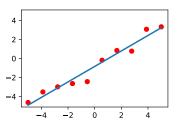
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- Exercises:
 - a) Print the shape of the array zz
 - b) Plot the function $t \mapsto y(t)$
 - c) Simulate the Van der Pol oscillator and plot the phase portrait

Regression (scipy.polyfit):



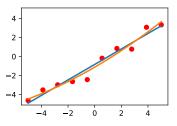
Regression (scipy.polyfit):

Linear regression



Regression (scipy.polyfit):

- Linear regression
- · Also: higher order



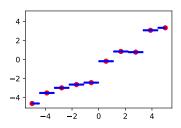
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- Linear regression
- · Also: higher order

Interpolation

(scipy.interpolation):

- Piecewise polynomial (→ Spline)
- Arbitrary order (here: order = 0)

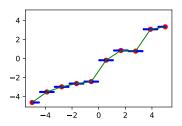


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- · Also: higher order

Interpolation (scipy.interpolation):

- Piecewise polynomial (→ Spline)
- Arbitrary order (here: order = 1)



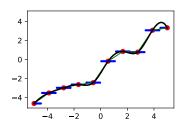
Regression (scipy.polyfit):

- Linear regression
- · Also: higher order

Interpolation

(scipy.interpolation):

- Piecewise polynomial (→ Spline)
- Arbitrary order (here: order = 2)



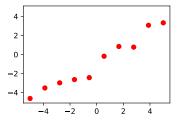
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Hybrid (also scipy.interpolation):

"smoothened spline" (smoothness coefficient)

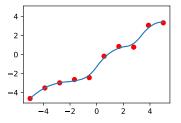
Regression (scipy.polyfit):

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(scipy.interpolation):

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Hybrid (also scipy.interpolation):

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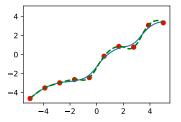
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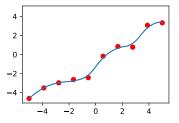
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Hybrid (also scipy.interpolation):

"smoothened spline" (smoothness coefficient)

See scipy-interpolation.py

Outline

Introduction

Symbolic Computation (sympy)

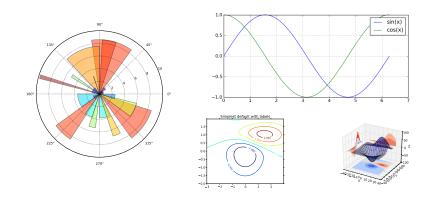
Interactive Documents with Jupyter Notebook

Numeric Computation (numpy and scipy)

2d Visualization (matplotlib)

Final remarks

matplotlib Overview (1)



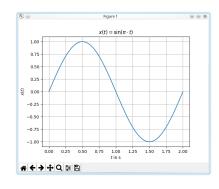
Much more examples (including code): https://matplotlib.org/gallery.html

matplotlib Overview (2)

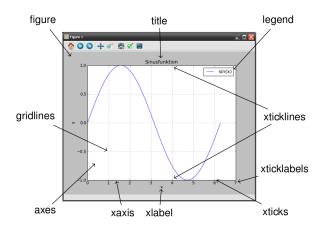
- Defacto standard for 2d-plots with python
- (also some limited 3d-features)
- Supports many kinds of plots (see gallery)
- Two types of results
 - Interaktive (with zooming, panning)
 - Publication ready vector graphics
- Support for LATEX-formulas (axis-label, title, ...)
- Animations possible
- Drawback: Performance

Simple Plot

```
Listing: matplotlib1.pv
from matplotlib import pyplot as plt
import numpy as np
tt = np.linspace(0, 2, 100)
xx = np.sin(np.pi*tt)
plt.plot(tt, xx)
# add some candy
plt.grid()
plt.xlabel("$t$ in s")
plt.vlabel("$x(t)$")
plt.title(r"$x(t)=\sin(\pi \cdot t)$")
# note the usage of a raw-string
# (beginning with r")
# -> no special meaning of
# backslash-character (\)
plt.show()
```



Terminology



Cheatsheet: Line Styles

Three possibilities:

1. very short as format string:

2. short with abbreviated keyword arguments :

3. long with full keyword arguments:

short form	long form	Output
'' oder '' '' '' ''	None 'solid' (default) 'dashed' 'dashdot' 'dotted'	

Cheatsheet: Line Styles

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1. very short as format string:

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short form	long form	Output
", oder ",	None 'solid' (default)	
,,	'dashed'	
) = ,)	'dashdot'	
* ; *	'dotted'	

Exercise: Draw three fancy curves with different linestyles (and widths and colors).

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Important but not covered topics

- Exception handling and usage of assert
- lambda-functions and list comprehension
- Scoping, Decorators (Functions of Functions)
- Test driven development (Link) / unittests
 - Software that tests software
 - No new feature without a test
 - Python: import unittest
- Documentation
 - Without docs your software is unklikely to be used (even by you).
 - Minimum: """Write docstrings!"""
 - Better: use Sphinx
- Be aware of PEP8 (style guide / best practices)
- Use a separate virtualenv for each project
- Revision control: Use git!

Links

Official docs

- http://docs.sympy.org/latest/modules/
- https://docs.scipy.org/doc/numpy-1.13.0/reference/
- https://docs.scipy.org/doc/scipy/reference/
- https://matplotlib.org/contents.html

Use also: google, stackoverflow, ...