TECHNISCHE UNIVERSITÄT DRESDEN

Fakultät Elektrotechnik und Informationstechnik Institut für Regelungs- und Steuerungstheorie

INTRODUCTION TO SCIENTIFIC PROGRAMMING WITH PYTHON

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Outline

Introduction

Symbolic Computation (`sympy`)

Interactive Documents with Jupyter Notebook

Numeric Computation (`numpy` and `scipy`)

2d Visualization (`matplotlib`)

Final remarks

About

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- Post-doc at Institute of Control Theory
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About this course

- 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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  4. 2d visualization
- ⚠ Contains didactic simplifications

Why Python? (1)

Python as Programming Language

- Clean readable syntax (few)
- 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)
- Motivation $\nearrow$, frustration $\searrow$

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 -O
     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

Possibilities to Invoke Python

- Default interactive interpreter
  - Command: `$ python` or `$ python3`
  - Can execute every Python-command
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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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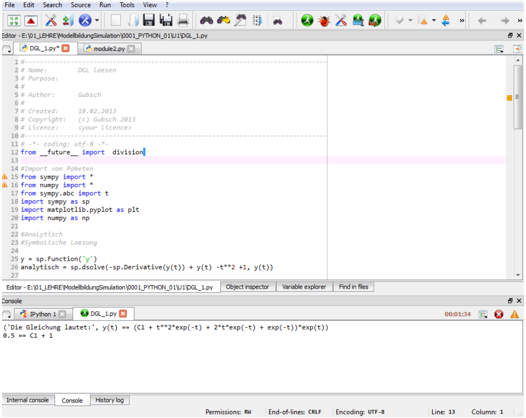
  - Notebooks combine source code, program-output and documentation (incl. LaTeX-formulas)
- Integrated Development Environment (we use spyder)
  - Command: `$ spyder`
  - Adapted text editor
  - Much more features (we wont use today)

Integrated Development Environment (IDE)



- Start from command line:
  `$ spyder`
- Other text editors also possible
- **Important:** Indention: 4 space
- Avoid TABs

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
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- 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 CTRL-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)) # -> 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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→ Now play around with `example-notebook1.ipynb` and `sympy-notebook1.ipynb`

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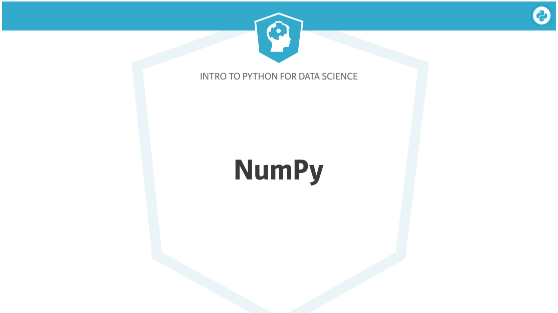
Numpy

- Basic numeric algorithms around a special data type:
- `numpy.ndarray`
- No (slow) python loops → 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

Source: github.com/datacamp

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 [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)

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Out[10]: array([ 65.4,  59.2,  63.6,  88.4,  68.7])

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Out[12]: array([ 21.852,  20.975,  21.75 ,  24.747,  21.441])
```

```
= 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])
```

Source: github.com/datacamp

NumPy: remarks

```
In [19]: np.array([1.0, "is", True])
Out[19]:
array(['1.0', 'is', 'True'],
      dtype='<U32')

In [20]: python_list = [1, 2, 3]

In [21]: numpy_array = np.array([1, 2, 3])

In [22]: python_list + python_list
Out[22]: [1, 2, 3, 1, 2, 3]

In [23]: numpy_array + numpy_array
Out[23]: array([2, 4, 6])
```

NumPy arrays: contain only one type

Different types: different behavior!

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])
```

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
```

ndarray = N-dimensional array

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
Out[8]: (2, 5)
```

2 rows, 5 columns

```
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]:
array([['1.73', '1.68', '1.71', '1.89', '1.79'],
       ['65.4', '59.2', '63.6', '88.4', '68.7']],
      dtype='<U32')
```

Single type!

Source: github.com/datacamp

Subsetting

```
            0       1       2       3       4
array([[ 1.73,  1.68,  1.71,  1.89,  1.79],    0
       [ 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
```

Source: github.com/datacamp

Subsetting

	0	1	2	3	4	
array([[	1.73,	1.68,	1.71,	1.89,	1.79],	0
[	65.4,	59.2,	63.6,	88.4,	68.7]])	1

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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

In [13]: np_2d[:,1:3]
Out[13]:
array([[  1.68,   1.71],
       [ 59.2 ,  63.6 ]])
```

Subsetting

	0	1	2	3	4	
array([[	1.73,	1.68,	1.71,	1.89,	1.79],	0
[	65.4,	59.2,	63.6,	88.4,	68.7]])	1

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In [10]: np_2d[0]
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Out[12]: 1.71

In [13]: np_2d[:,1:3]
Out[13]:
array([[  1.68,   1.71],
       [ 59.2 ,  63.6 ]])

In [14]: np_2d[1,:]
Out[14]: array([ 65.4,  59.2,  63.6,  88.4,  68.7])
```

Broadcasting

- How numpy manages different shapes in element-wise calculations
- Trivial example: 2d-array + scalar $\rightarrow$ scalar is “blown up”
- 2d-array + 1d-array ?

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

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- Example:

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

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RGB-Image	(3d array):	256	256	3
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- 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 $\rightarrow$ scalars)
- `sin`, `cos`, `exp`, `abs`, `real`, `imag` (array $\rightarrow$ 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 $\mathbf{f} : \mathbb{R}^n \rightarrow \mathbb{R}^n$
- Important: initial guess
- Example (with $n = 12$): approximate solution of equation $x + 2.3 \cdot \cos(x) = 1$
- $f(x) = x + 2.3 \cdot \cos(x) - 1 \overset{!}{=} 0$

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.])
```

scipy.optimize.fsolve and fmin

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- **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 $\rightarrow$ two ODEs 1st order:
  state: $\mathbf{z} = (z_1, z_2)^T$ with $z_1 := y$, $z_2 := \dot{y}$

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

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]

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    a) Print the shape of the array zz
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- Exercises:
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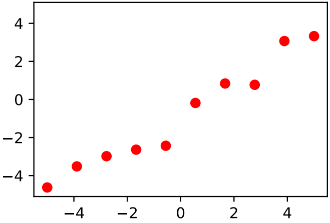
  c) Simulate the Van der Pol oscillator and plot the phase portrait

Regression, Interpolation

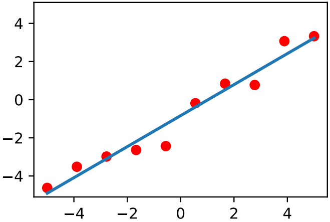
Regression (`scipy.polyfit`):



Regression, Interpolation

Regression (`scipy.polyfit`):

- Linear regression



Regression, Interpolation

Regression (`scipy.polyfit`):

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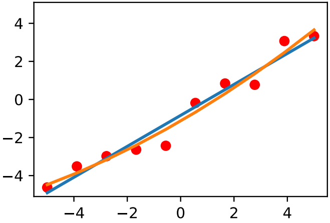
- Also: higher order



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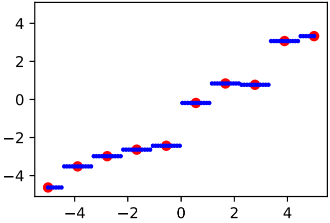
Interpolation (`scipy.interpolation`) :

- Piecewise polynomial ($\rightarrow$ Spline)
- Arbitrary order (here: order = 0)



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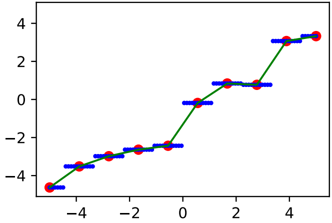

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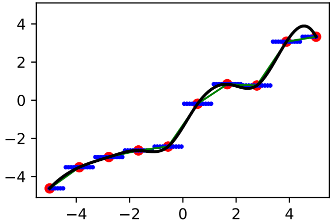

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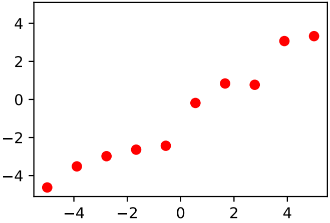

Hybrid (also `scipy.interpolation`):

- ”smoothened spline“ (smoothness coefficient)

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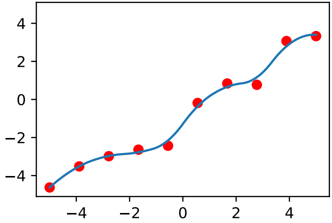

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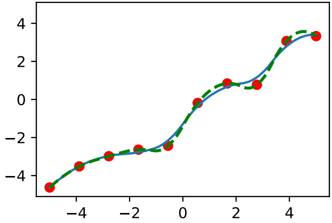

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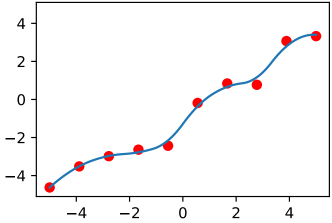

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see `scipy-interpolation.py`

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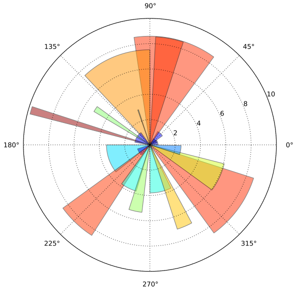
Interactive Documents with Jupyter Notebook

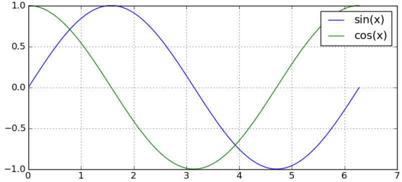
Numeric Computation (`numpy` and `scipy`)

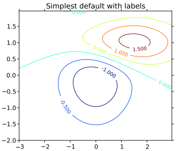
2d Visualization (`matplotlib`)

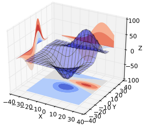
Final remarks

`matplotlib` Overview (1)









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

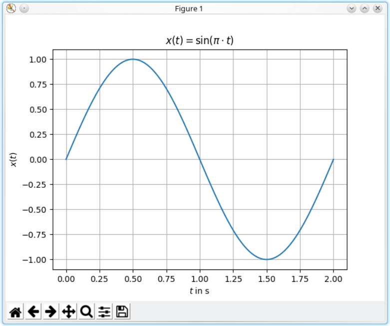
Overview (2)

- 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

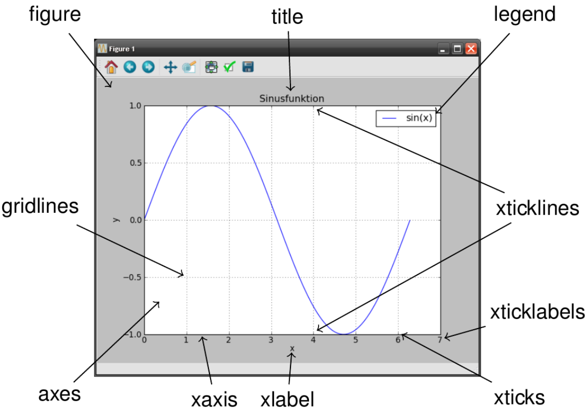
Simple Plot

Listing: matplotlib1.py

```
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.ylabel("$x(t)$")

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:
   `plot(x, y, '--')`
2. short with abbreviated keyword arguments :
   `plot(x, y, ls='--')`
3. long with full keyword arguments:
   `plot(x, y, linestyle='dashed')`

short form	long form	Output
`''` oder `' '`	`None`	
`'-'`	`'solid'` (*default*)	
`'--'`	`'dashed'`	
`'-.'`	`'dashdot'`	
`':'`	`'dotted'`	

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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, ...