

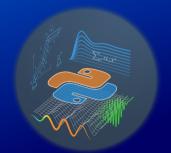


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# Python for Engineers Pythonkurs für Ingenieur:innen

Performance Optimization Performanzoptimierung Dresden (Online), 2023-12-05

https://tu-dresden.de/pythonkurs
https://python-fuer-ingenieure.de



#### **Outline**

- Introduction
- Timing
- General Tips
- Compiled Code





#### Introduction

#### What is performance?

- runtime
- memory requirements (RAM, hard disk)
- power consumption
- → In this lecture: only **execution time** considered (most important in most cases, easy to measure, correlated with power consumption)

#### **Facts**

- Python: slower than compiled languages (interpreters)
- in many applications: difference not even perceptible (0.1s vs. 0.01s)
- runtime optimization of code itself often very time consuming
- → conflict of goals: execution vs. development time

#### Introduction

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#### Facts

- Python: slower than compiled languages (interpreters)
- in many applications: difference not even perceptible (0.1s vs. 0.01s)
- · runtime optimization of code itself often very time consuming
- → conflict of goals: execution vs. development time
- ⇒ general tips to follow from the start
- ⇒ specific optimization of runtime for **critical algorithm parts**

### Time Measurement (I)

- module time
- time.time() returns "epoch-time" (also called "UNIX-timestamp") time  $\hat{=}$  seconds since 01/01/1970 00:00:00.00
- advantage: very simple
- disadvantage: additional ("boilerplate") code distributed in the program

```
import time

s = 0
start = time.time()

for i in range(1000000):
    s += i**(0.5)

print("Duration [s]:", time.time() - start)
```





#### **Time Measurement (II)**

- module timeit, see docs
- runtime measurement of a statement (mostly function call)
- good for comparison of code snippets for special problem
- statement must be passed as string or callable
- advantages: non-invasive, averaging of multiple runs





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```
Listing: example-code/time-example.py

import math; from timeit import timeit

def root1(x=2): return x**0.5

def root2(): return math.sqrt(2)

N = int(1e6)
print("2**0.5: ", timeit("2**0.5", number=N), "sqrt(2):", timeit("math.sqrt(2)", setup="import math", number=N))

# func calls without argument
print("root1(): ", timeit(root1, number=N), "root2():", timeit(root2, number=N))

# func calls with argument (timeit(root2(x=2), number=N))) would "see" only the return value
# Thus, wee need to pass the function call as string. Then the 'globals'- keyword argument is also needed.
print("root1(x=2):", timeit("root1(x=2)", number=N, globals=globals()))
```





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• See also: "magic macros" for both IPython and Jupyter: %time and %timeit





# **Professional Timing: Profiling (I)**

- module cProfile: detailed runtime analysis of a (possibly very large) program →
  Find bottleneck.
- · profiling creates overhead, i. e. program runs slightly slower than without it
- results as print output or to file for use in analysis tools
- argument is passed as string

```
Listing: example-code/profile-example.py
import cProfile
import math

def main():
    s = 0
    for i in range(100000):
        s += math.sqrt(i)

cProfile.run("main()")
```

#### alternative (command line call):

```
python -m cProfile -s cumtime test.py > test.txt
```

- sorted by cumulative time
- ... > test.txt redirects output to file: test.txt
- with option -o test.prfl will redirect results in binary format to file test.prfl (can then be evaluated with pstats, see docs).

### **Profiling (II)**

#### Output of the example

```
100004 function calls in 0 021 seconds
Ordered by: standard name
ncalls tottime percall
                          cumtime percall filename: lineno (function)
          0.000
                   0.000
                            0.021
                                     0.021 <string>:1(<module>)
                                     0.021 profile-example.pv:4(main)
          0.014
                  0.014
          0.000
                  0.000
                            0.021
                                     0.021 (built-in method builtins.exec)
         0.006
                  0.000
                            0.006
                                     0.000 {built-in method math.sgrt}
                                     0.000 (method 'disable' of 'lsprof.Profiler' objects)
          0.000
                  0.000
                            0.00
```

- shows which function was called how often and how much time it needed
- → find starting points for optimization
- interesting here: only  $\approx \frac{1}{3}$  of the runtime for sqrt needed
- rest: overhead (function call, loop)





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- rest: overhead (function call, loop)
- Further analysis: pstats, see docs





### **General Tips (I)**

- optimize code only when there is an actual need ("Premature optimisation is the root of all evil.")
- $\rightarrow$  use profiling and identify only the worthwhile jobs.
- · optimize only correct code
- use unit tests to ensure correctness of the code during/after rework
  - order: "Make it run. Make it right. Make it fast."
- use appropriate libraries for respective problem
- e.g. numpy for numerics
  - is written in C/Fortran  $\rightarrow$  much faster than pure Python
- Python scripts usually faster than Jupyter Notebooks (rendering overhead)





### **General Tips (II)**

use appropriate data types: tuple or dict instead of list.
 example: "element Lookup"

```
res = 3 in {1: True, 2: True, 3: True} # effort: O(1) (= const)
res = 3 in [1, 2, 3] # effort O(n)
```

- in (nested) loops: move functionality "from inside to outside".
  - initializations of variables
  - calculations → intermediate results save/cache
  - ightarrow execute statements only as often as necessary, but as rarely as possible
  - "loops in functions" are faster than "functions in loops" (every function-call costs time)
- create auxiliary **local variables** to avoid "points" (e. g. from object orientation):
  - each point ( obj.attr ) means attributes/member lookup,
  - local caching is worthwhile especially in loops

```
root = math.sqrt
# ...
root(2) # inside a loop avoid name-lookup
```





#### **Outdated Tips (III)**

Often recommended but not so effective (anymore) w.r.t speedup

- use iterators (e.g. range (4) instead of [0, 1, 2, 3])
  - background: iterators generate function to calculate next element,
  - more memory-efficient than generating whole sequence in advance
- use list comprehension instead of for -loops

```
r = [ str(k) for k in [1, 2, 3] ]
# instead of
r = []
for k in [1, 2, 3]:
    r.append(str(k))
```

• vectorize functions for array operations ( numpy.vectorize ), see docs

```
def f(x):
    if x > 2: return x*100
    else:    return x

xx = np.arange(5)
# f(xx) # -> ValueError
f_vect = np.vectorize(f)
f_vect(xx) # -> array([ 0,  1,  2, 300, 400])
```

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#### Possible combinations (embedding compiled code in Python):

- "Just in Time" compilation of certain code sections (e.g. module numba)
- compile Python code into cython
  - very similar to Python but statically typed and compiled  $\rightarrow$  fast
- ctypes
  - Can load external libraries into Python (e.g. \*.dll on Windows, \*.so on Unix)
  - → very powerful and flexible
  - Not considered here; if necessary see python-c-code-example (github)
  - mostly useful if C-library already exists (or is needed anyway, e.g. for target hardware)

#### Just-in-time-Compilation with numba

- Significant acceleration potential for mathematical operations.
- Necessary: pip install numba
- Example: "Mandelbrot set"
  - (simple math, high numerical effort, visual result).

```
Listing: example-code/numba1.py (14-29)

# Decorator for just-in-time comp. (-> 30x speedup)

@jit

def mandel(x, y, max_iters):
    """
    Given a complex number x + y*j, determine
    if it is part of the Mandelbrot set given
    a fixed number of iterations.
    """

i = 0

c = complex(x, y)

z = 0.0j

for i in range(max_iters):
    z = z*z + c

    if (z.real*z.real + z.imag*z.imag) >= le3:
        return i
```





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```
Listing: example-code/numba1.py (14-29)
# Decorator for just-in-time comp. (-> 30x speedup)
                                                                           0.75
@jit
                                                                           0.50
def mandel(x, v, max iters):
                                                                           0.25
                                                                          -0.25
                                                                          -0.50
                                                                          -0.75
    i = 0
    c = complex(x, v)
    z = 0.01
    for i in range(max_iters):
         7 = 7*7 + C
        if (z.real*z.real + z.imag*z.imag) >= 1e3:
             return i
```





#### Cython (I)

- Cython is a separate programming language, installation: pip install cython
- Very close to Python but with explicit **static type** information
- ightarrow can be compiled to C automatically ightarrow compilable ightarrow faster
- details: see docs

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- details: see docs
- procedure:
  - Develop algorithm in pure Python ("Make it run" + "Make it right")
  - Translate Python to Cython manually
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#### Typically 3 files, e. g.

- mandel-cython.pyx: cython source code
- mandel-cython-setup.py : for compiling
- mandel-cython-main.py : to import and call compiled code

#### Listing: example-code/mandel-cython.pyx

```
# Cython source code
cimport numby as no # for the special numby stuff
cdef inline int mandel (double real, double imag, int max iterations=20):
    Mandelbrot set given a fixed number of iterations. """
    cdef double z real = 0.. z imag = 0.
    cdef int i
    for i in range(0, max_iterations):
        z real, z imag = ( z real*z real - z imag*z imag + real,
                           2*z real*z imag + imag )
        if (z real*z real + z imag*z imag) >= 1000:
            return i
    # return -7
    return 255
def create fractal (double min x, double max x, double min y, int nb iterations,
                            np.ndarray[np.uint8_t, ndim=2, mode="c"] image not None):
    cdef int width, height, x, y, start_y, end_y
   cdef double real, imag, pixel_size
    width = image.shape[0]
    height = image.shape[1]
    pixel_size = (max_x - min_x) / width
    for x in range(width):
        real = min x + x*pixel size
        for y in range (height):
            imag = min v + v*pixel size
            image[x, y] = mandel(real, imag, nb iterations)
```

# Cython (III)

script for conversion Cython → C:

```
Listing: example-code/mandel-cython-setup.py

"script for conversion of cython-code to c-code"

from distutils.core import setup
from distutils.extension import Extension
from Cython.Distutils import build_ext
import numpy # to get includes

setup(
    cmdclass = {'build_ext': build_ext},
    ext_modules = [Extension("mandelcy", ["mandel-cython.pyx"], )],
    include_dirs = [numpy.get_include(),],
}
```

- Command: python mandel-cython-setup.py build\_ext --inplace
- → C code is compiled and an importable library is created





### Cython (IV)

• Calling the compiled code and visualization of Mandelbrot set:

Listing: example-code/mandel-cython-main.py

```
import numpy as np
import matplotlib.pyplot as plt
import mandelcy # our Cython module (for the real work)
import time
# define section of the Gaussian number plane
min x = -1.5
max x = 0.15
min v = -1.5
\max v = \min v + \max x - \min x
# to have same section like numba script
\# min_x = -2; max_x = 1; min_y = -1.5
nb iterations = 255
t1 = time.time()
dataarray = np.zeros((500, 500), dtype=np.uint8)
t2 = time.time()
print("Time needed", t2 - t1)
# execution of the compiled code
mandelcy.create_fractal(min_x, max_x, min_y, nb_iterations, dataarray)
dataarray = dataarray.T[::-1, :] # Transpose and reverse order along first axis
plt.imshow(dataarray, extent=(min x, max x, min v, max x), cmap=plt.cm.plasma)
plt.savefig("mandel-cython.png")
plt.show()
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                                                                                            -0.4
min v = -1.5
\max v = \min v + \max x - \min x
                                                                                            -0.6
                                                                                            -0.8
# to have same section like numba script
                                                                                            -1.0
\# min_x = -2; max_x = 1; min_y = -1.5
                                                                                            -1.2
nb iterations = 255
                                                                                             -1.50 -1.25 -1.00 -0.75 -0.50 -0.25 0.00
t1 = time.time()
dataarray = np.zeros((500, 500), dtype=np.uint8)
                                                                                     (\rightarrow 500x \text{ speedup (Py vs Cy))}
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### **Summary**

- ∃ many ways to tweak Python code to make it faster
- If that is not enough:
  - identify bottle necks using profiling
- replace critical program parts with compiled code
  - just-in-time compilation numba (effort: low)
  - manual port to cython (effort: moderate)
  - custom C code using ctypes (effort might be considerable)





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  - just-in-time compilation numba (effort: low)
  - manual port to cython (effort: moderate)
  - custom C code using ctypes (effort might be considerable)
  - (∃ more possibilities, e.g. PyPy )
- not covered here:
  - threading/multiprocessing, parallelization via asyncio
  - pyjion ("drop-in JIT Compiler for Python 3.10")



