

PROGRAMMING IN PYTHON I

Fast Numerical Computations in Python



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FAST NUMERICAL COMPUTATIONS IN PYTHON



Motivation

- Everything in Python is an object and code is executed line by line
 - Very convenient to use
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 - Very convenient to use
 - Slow, since optimization of the code is difficult at runtime
- We can use modules in Python that allow us to write fast code in Python
 - By providing optimized functions (e.g., NumPy, ...)
 - By providing tools for optimizing Python-like code (e.g., Numba, PyTorch, Tensorflow, ...)

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- NumPy mainly deals with (multidimensional) array data based on the `numpy.ndarray` object
- Documentation/Tutorials:
<https://numpy.org/doc/stable/index.html>

Arrays in NumPy (1)

- Elements are stored as one block with contiguous addresses in memory
- Elements are fast to access since we can quickly compute their addresses

Memory:

...	byte	byte	byte	byte	byte	byte	byte	byte	...
-----	------	------	------	------	------	------	------	------	-----

Address: ... 105 106 107 108 109 110 111 112 ...

Memory to store a 16-bit integer:

byte	byte
------	------

Storing 4 16-bit integers in memory:

...	byte	byte	byte	byte	byte	byte	byte	byte	...
-----	------	------	------	------	------	------	------	------	-----

... 105 106 107 108 109 110 111 112 ...

↑ ↑ ↑ ↑
Addresses of our integers

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 - Operations on elements can be optimized and are faster

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 - **Column-major** order: Consecutive elements of a column reside next to each other

Multidimensional Arrays: Example (1)

- We want to store a 2D array with 3 rows and 5 columns
 - 5 elements per row, 3 per column, 15 in total

0	1	2	3	4
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- Now, we want to access the element in the 4th column $c = 3$ and the 3rd row $r = 2$ (indices starting at 0 with $n_r = 5$ elements per row)

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$$n_r \cdot r + c = 5 \cdot 2 + 3 = 13$$

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- This is automatically done in the background for you, you do not have to worry about the correct index calculation

Indexing in NumPy

- Accessing NumPy arrays is similar to Python lists

- ☐ Index via integers:

`my_array[i]`

- ☐ Slicing is possible and fast (since elements are consecutively stored in memory):

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- ☐ Indexing using lists of indices, boolean index masks, ...

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- More examples in the accompanying code file

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[[1 2 3]  
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The shape of this array is (2, 3), i.e., the first axis has a length of 2 and the second axis has a length of 3

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- Many NumPy methods in the provided library require to specify the axis on which to perform some operation