PROGRAMMING IN PYTHON I

Fast Numerical Computations in Python

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Motivation

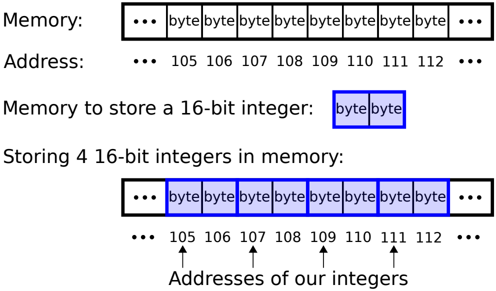
- Everything in Python is an object and code is executed line by line
  - Very convenient to use
  - Slow, since optimization of the code is difficult at runtime
- We can use modules in Python that allow us to write fast code in Python
  - By providing optimized functions (e.g., `NumPy`, ...)
  - By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

NumPy

- **NumPy** is the go-to module for numerical computations in Python
- Provides a large range of functionalities for performing scientific computations and handling array data
  - These functions are typically highly optimized and implemented in C
  - Access is still done via Python (you do not need to know C)
- 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



Arrays in NumPy (2)

- In Python, an element in a list is simply a reference to the corresponding Python object
  - Data types of objects are flexible
  - → Operations on elements are slower/clumsy (need to determine type of object before usage)
- In NumPy, an element in an array is (usually) a bit pattern that directly represents the stored value (and not a reference)
  - The array holds the information about the data type (encoding/decoding scheme for bits) used in array
  - Data type of elements in array is fixed (but we can create new arrays with a different data type)
  - **All elements** in an array have the **same data type**
  - → Operations on elements can be optimized and are faster

Multidimensional Arrays

- In Python, we already saw the concept of nested lists
  - Can be used to create 2D or nD arrays
  - Slow, since we have to access the sublists to access our elements
- In NumPy, we can store nD arrays as fast 1D arrays
  - Done by NumPy in the background
  - Store nD array in a **flat** manner
  - **Row-major** order: Consecutive elements of a row reside next to each other (NumPy default)
  - **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
5	6	7	8	9
10	11	12	13	14

- We can create a 1D array with 15 elements

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14

- We can say that
  - the first 5 (column) elements belong to the first row
  - the next 5 (column) elements belong to the second row
  - the last 5 (column) elements belong to the third row

  $\rightarrow$ row-major order

Multidimensional Arrays: Example (2)

- We agreed on row-major order
- 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)

0	1	2	3	4
5	6	7	8	9
10	11	12	13	14

- We can compute the index in the 1D array via $n_r \cdot r + c = 5 \cdot 2 + 3 = 13$

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14

- 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):
    `my_array[:i]`
- NumPy offers many more **fancy indexing** options
  - Indexing multi-dimensional arrays directly:
    `my_array[row, col]`
    `my_array[2, 4, 8, 5]`
  - Indexing using lists of indices, boolean index masks, ...
- More examples in the accompanying code file

Shapes and Axes in NumPy

- The **shape** defines the (multi-)dimensionality of an array
- Each dimension can be accessed using the corresponding **axis** (i.e., dimensions = axes)
- Example of a 2D array, i.e., an array with 2 axes

  ```
  [[1 2 3]
   [4 5 6]]
  ```

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