Data in scientific programming

Guillermo Aguilar & Pietro Berkes &

Zbigniew Jędrzejewski-Szmek & Victoria Shevchenko

Fork and clone repository
https://git.aspp.school/
ASPP/2025-plovdiv-data.git

Things one thinks about when thinking about data

Processing	Storage	Reproducibility and collaboration
• Efficient processing (no for-loops!) • Organizing data so that analyses are easy	• Size • Access ease • Access time	• Versioning • Lineage tracing (which script / other data was used to generate this?) • Ease of sharing

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Hands-on

What data structure would you use to represent…

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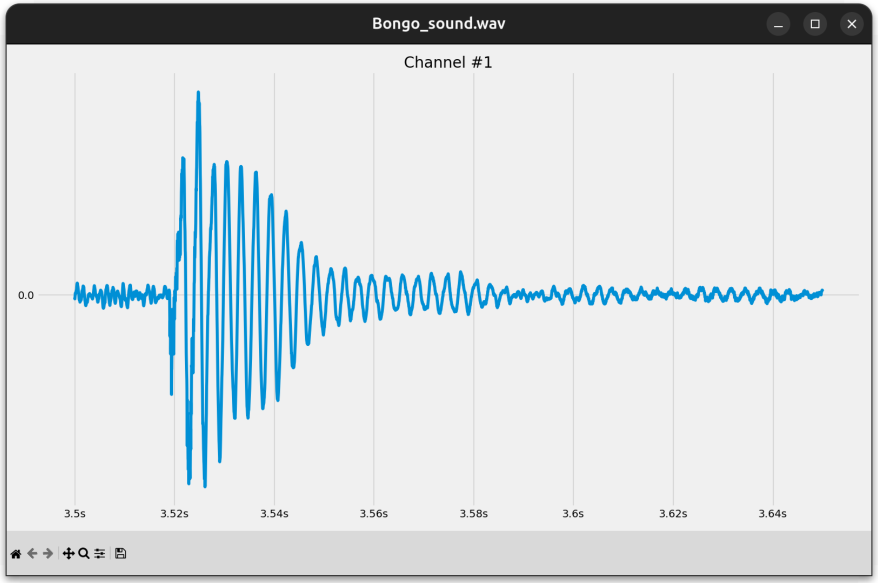
A sound wave?



Hands-on

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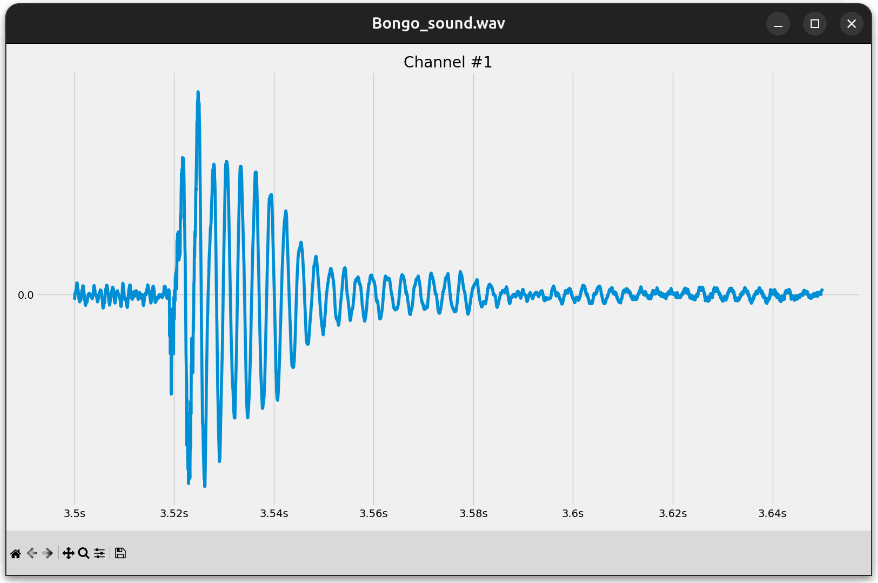
NumPy array




```
In [6]: sound_data
Out[6]: array([0.66709183, 0.55973494, 0.95416669, 0.60810949, 0.05188879,
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Hands-on

What data structure would you use to represent…

A map between color names and RGB values?

Hands-on

What data structure would you use to represent…

A map between color names and RGB values?

Dictionary

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colors_hex = {
    "tawny orange": "#CD5700",
    "very peri": "#6667AB",
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    "pink flambé": "#DC4C8B”,
    # …
}
```

Hands-on

What data structure would you use to represent…

Phone book entries?

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Pandas DataFrame

first_name	last_name	phone_nr	address	ZIP	city
John	Doe	555-1234	123 Maple St	12345	Springfield
Jane	Smith	555-5678	456 Oak St	67890	Rivertown
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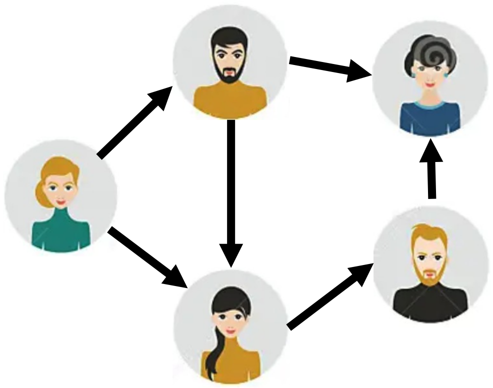
Friendship relations?



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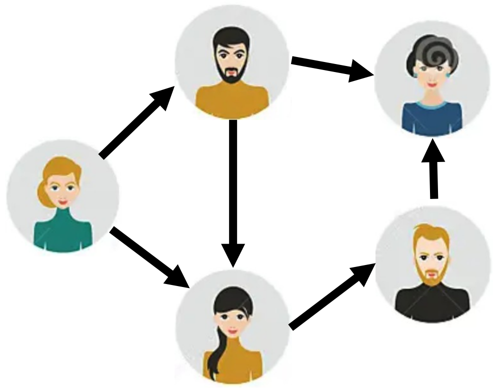
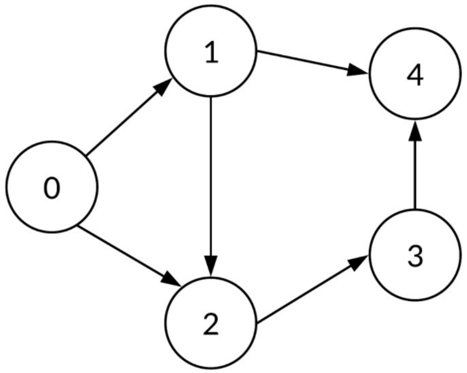


Graph



Implemented as

	0	1	2	3	4
0	0	1	1	0	0
1	0	0	1	0	1
2	0	0	0	1	0
3	0	0	0	0	1
4	0	0	0	0	0

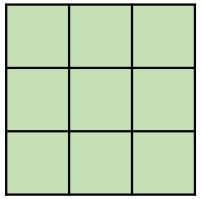
Adjacency matrix (array)

```
A_dict = {
    '0':[1,2],
    '1':[2],
    '2':[3],
    '3':[4],
    '4':[]
}
```

Dictionary

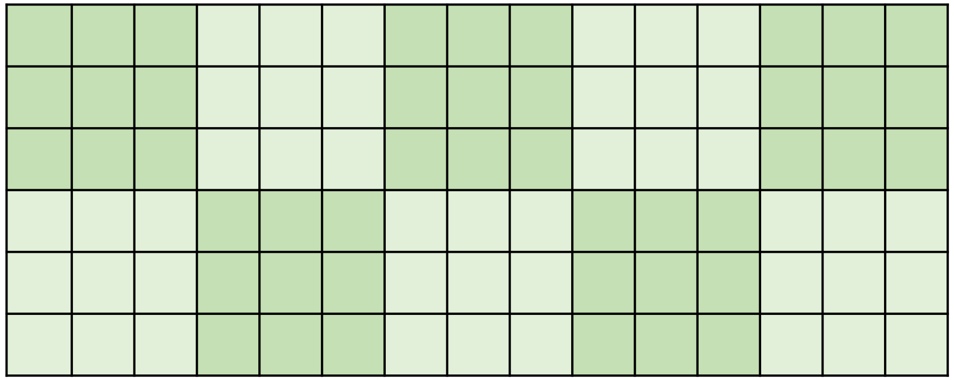
You develop your code on a small data set, how is it going to scale to the complete data set?

Development data



N data points,
Processing time T

Real data

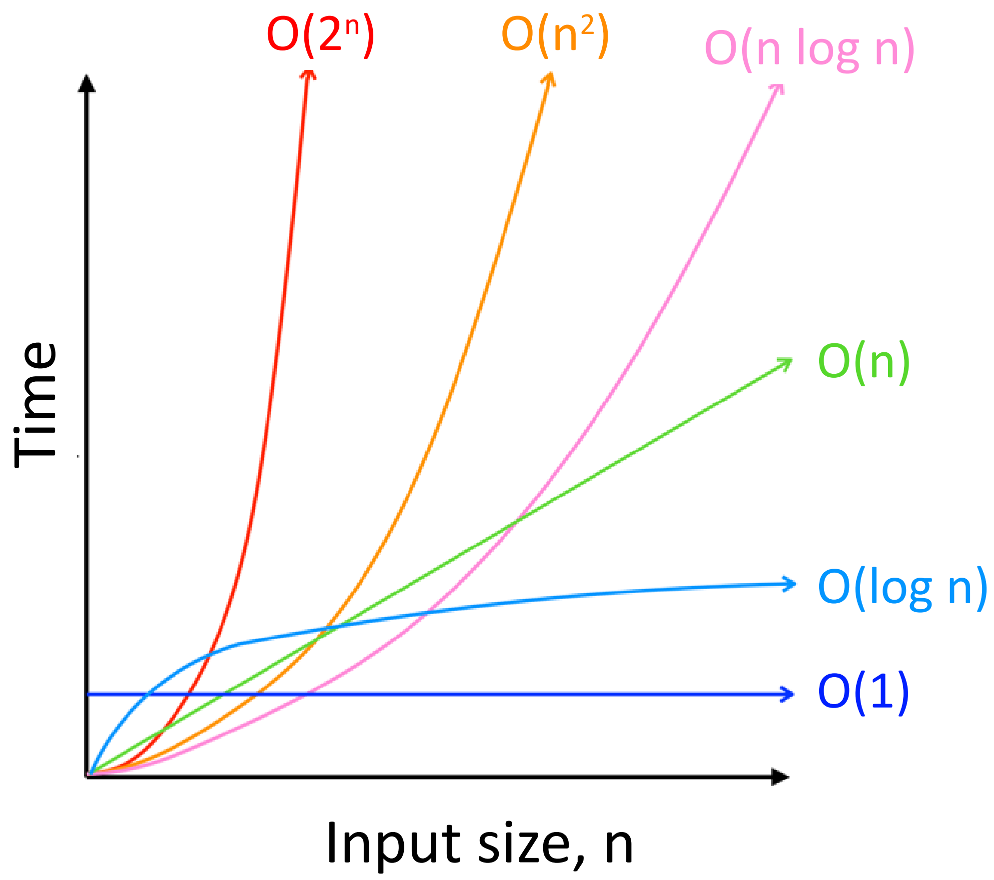


10x N data points
Processing time -> ?

We’re interested in orders of magnitude

How performance scales: big-O

Big-O class	What we call it	Time increase, when data increases 10x
O(1)	constant	1x time
O(n)	linear	10x time
O(n^2)	quadratic	100x time
O(n * log n)	linearithmic	~10-20x time
O(log n)	logarithmic	~1-2x time



Hands-on: Operations on lists

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Big-O class	Operation on lists that scales this way
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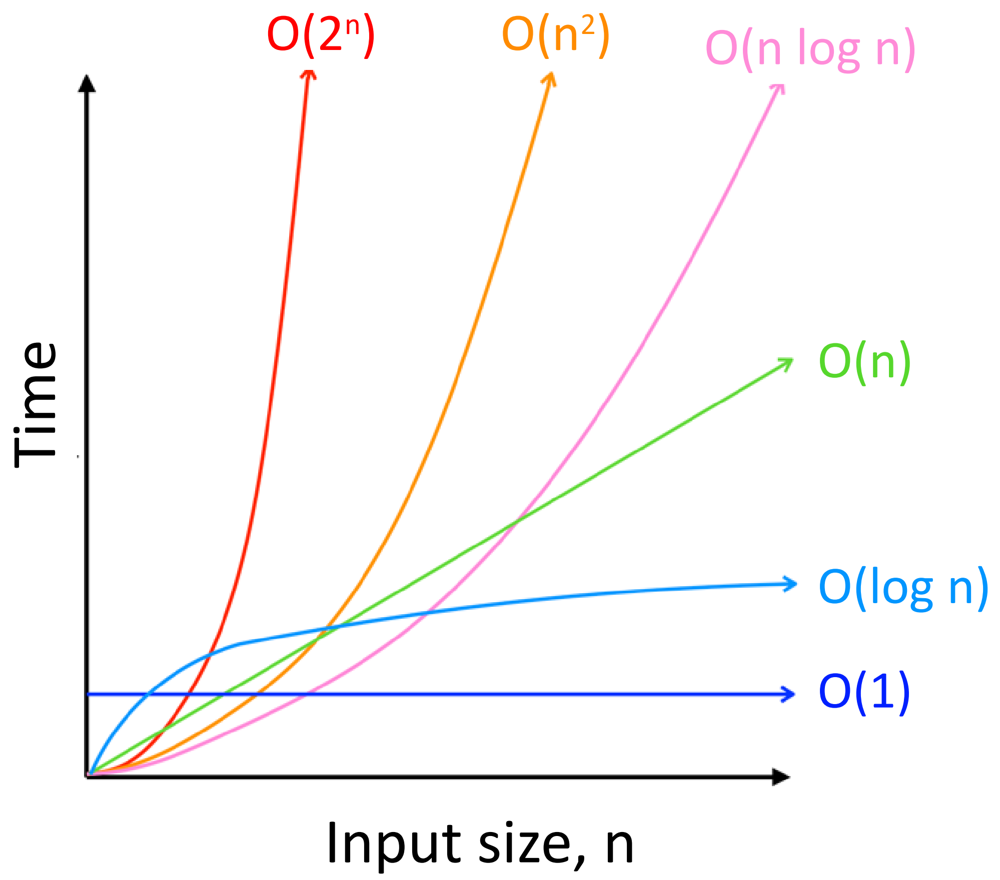

Hands-on: Operations on lists

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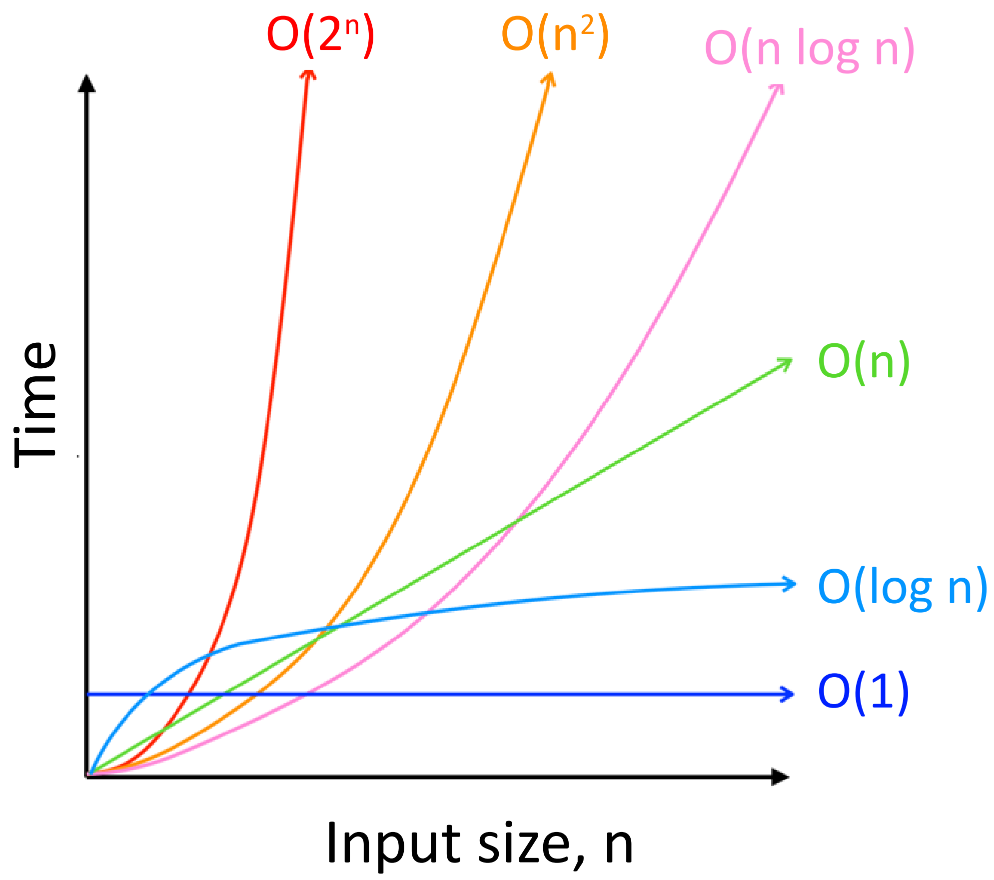
$O(n * \log n)$	linearithmic	~10-20x time
$O(\log n)$	logarithmic	~1-2x time

Big-O class	Operation on lists that scales this way
$O(1)$	Getting an element by its index
$O(n)$	Summing elements in list
$O(n^2)$	Computing distance between all pairs of elements in the list
$O(n * \log n)$	Sorting the list
$O(\log n)$	Searching an element in a sorted list



Example: Find common words

Given two lists of words, extract all the words that are in common

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']
```

Expected result: `['apple', 'orange', 'banana']`

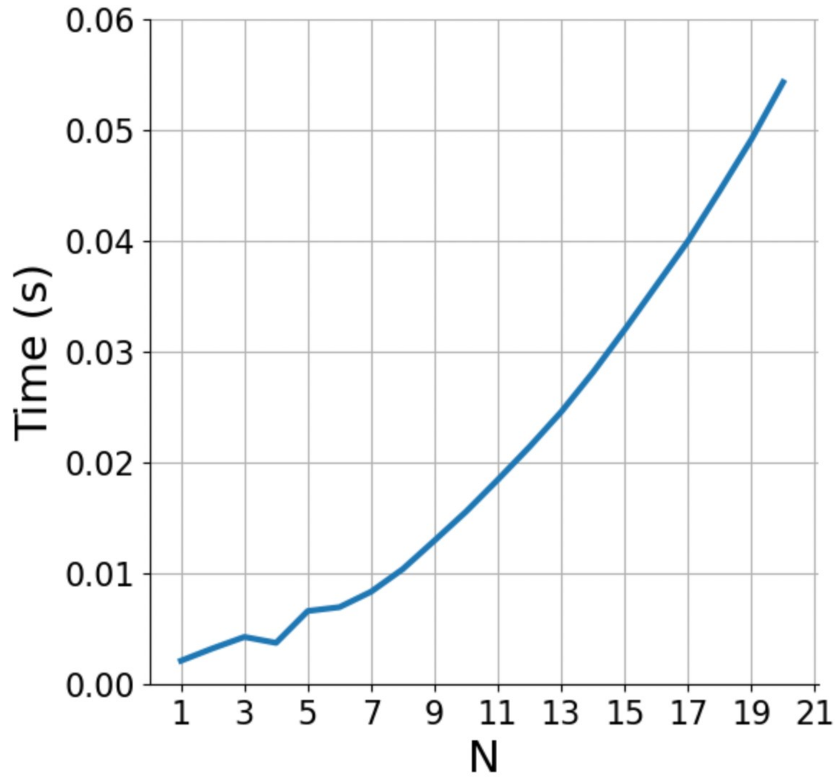
Implementation with two for-loops

```python
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

common = []
for w in words1:
    if w in words2:
        common.append(w)
```

What is the big-O complexity of this implementation?

Implementation with two for-loops

```python
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

common = []
for w in words1:          # O(N)
    if w in words2:         # O(N)
        common.append(w)  # O(1)
```



What is the big-O complexity of this implementation?

N * N ~ **$O(N^2)$**

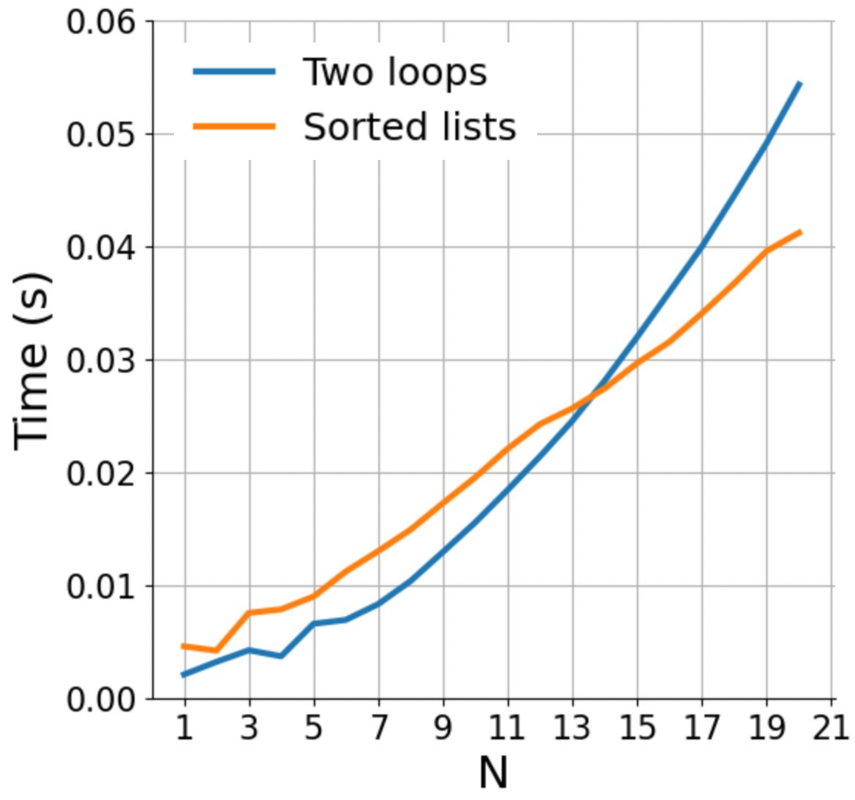
Implementation with sorted lists

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

words1 = sorted(words1)  # ['apple', 'banana', 'melon', 'orange', 'peach']
words2 = sorted(words2)  # ['apple', 'avocado', 'banana', 'kiwi', 'orange']

common = []
idx2 = 0
for w in words1:
    while idx2 < len(words2) and words2[idx2] < w:
        idx2 += 1

    if idx2 >= len(words2):
        break

    if words2[idx2] == w:
        common.append(w)
```

What is the big-O complexity of this implementation?

Implementation with sorted lists

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

words1 = sorted(words1)      # O(N * log(N))
words2 = sorted(words2)      # O(N * log(N))

common = []
idx2 = 0
for w in words1:                                        # O(N)
    while idx2 < len(words2) and words2[idx2] < w:      # O(N) in total
        idx2 += 1

    if idx2 >= len(words2): # O(1)
        break

    if words2[idx2] == w:   # O(1)
        common.append(w)
```



What is the big-O complexity of this implementation?

2 * (N * log(N)) + 2 * N ~ **O(N log N)**

Implementation with sets

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

words2 = set(words2)

common = []
for w in words1:
    if w in words2:
        common.append(w)
```

What is the big-O complexity of this implementation?

Implementation with sets

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words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
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words2 = set(words2)       # O(N)

common = []
for w in words1:           # O(N)
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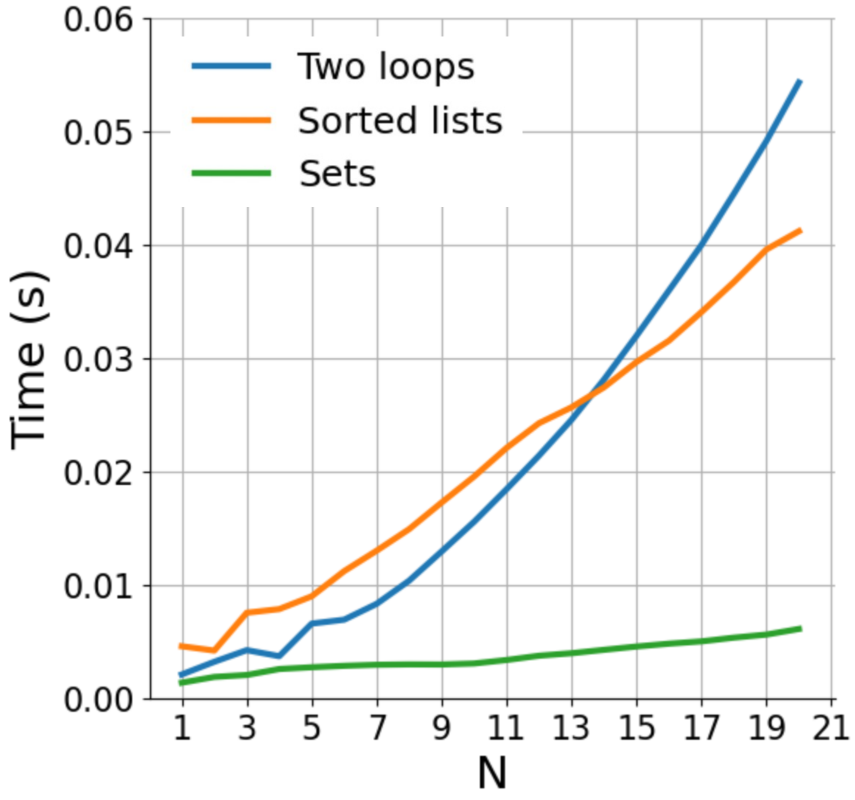
        common.append(w)       # O(1)
```



What is the big-O complexity of this implementation?

N + N ~ **O(N)**

Basic reference sheet about Python data structures

Lists: collection of ordered, arbitrary data

Getting an element by index	O(1)
Appending	O(1)
Inserting an element at index	O(n)
Sorting	O(n log n)
Finding an element by value (e.g., “if element in my_list: …”, list.index, etc.)	O(n)
Copy a list	O(n)

Dictionaries (“hashmaps”)

Inserting	O(1)
Finding a value by key (e.g., “if element in my_dict: …”)	O(1)
Create dictionary from lists	O(n)

Sets: it’s dictionaries without values

Inserting	O(1)
Finding a value by key (e.g., “if element in my_set: …”)	O(1)
Create set from list	O(n)

See also: https://wiki.python.org/moin/TimeComplexity

Hands-on

Exercise

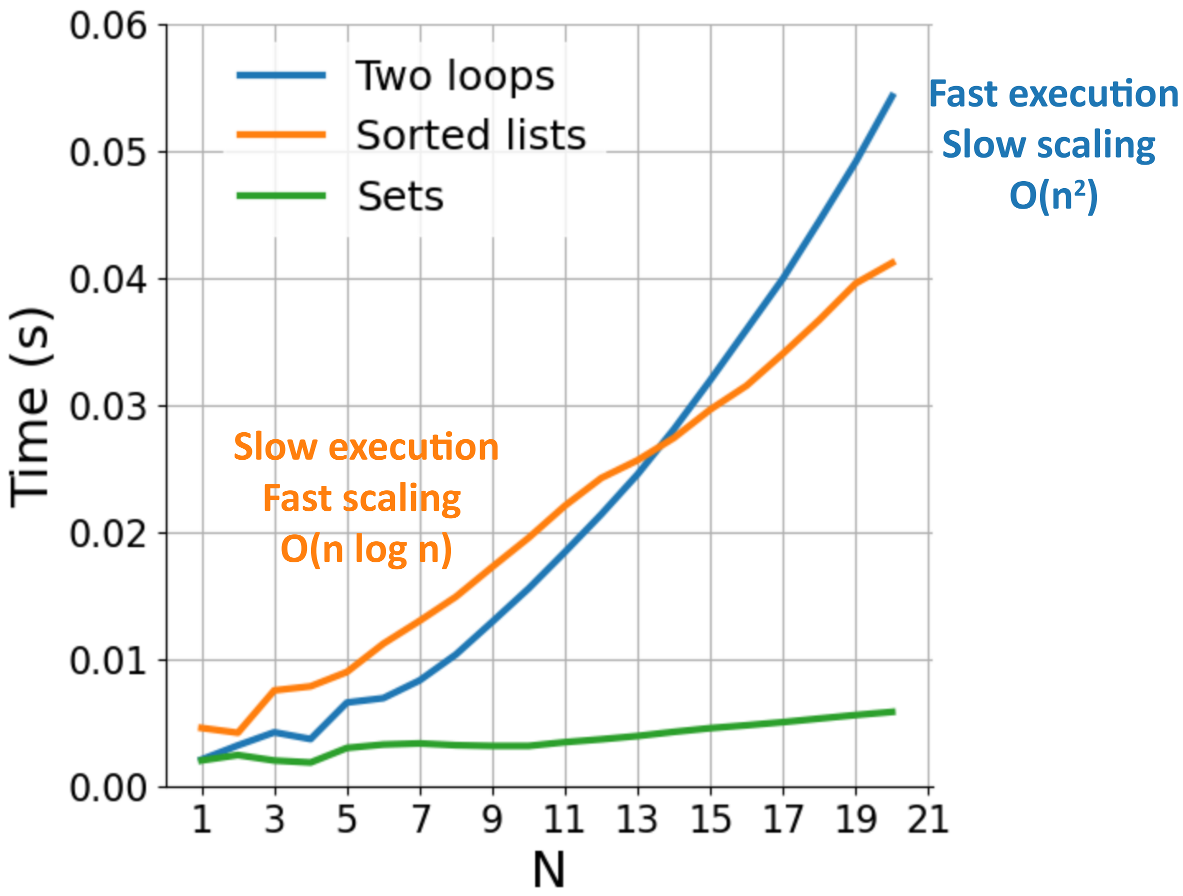
exercises/match_tarots

- Open the notebook `match_tarots`, and follow the instructions!

- Submit a PR for Issue #1 on
  `git.aspp.school/ASPP/2025-plovdiv-data`

How does rewriting in C change the performance?

(rewriting in C, parallelization; same algorithm)



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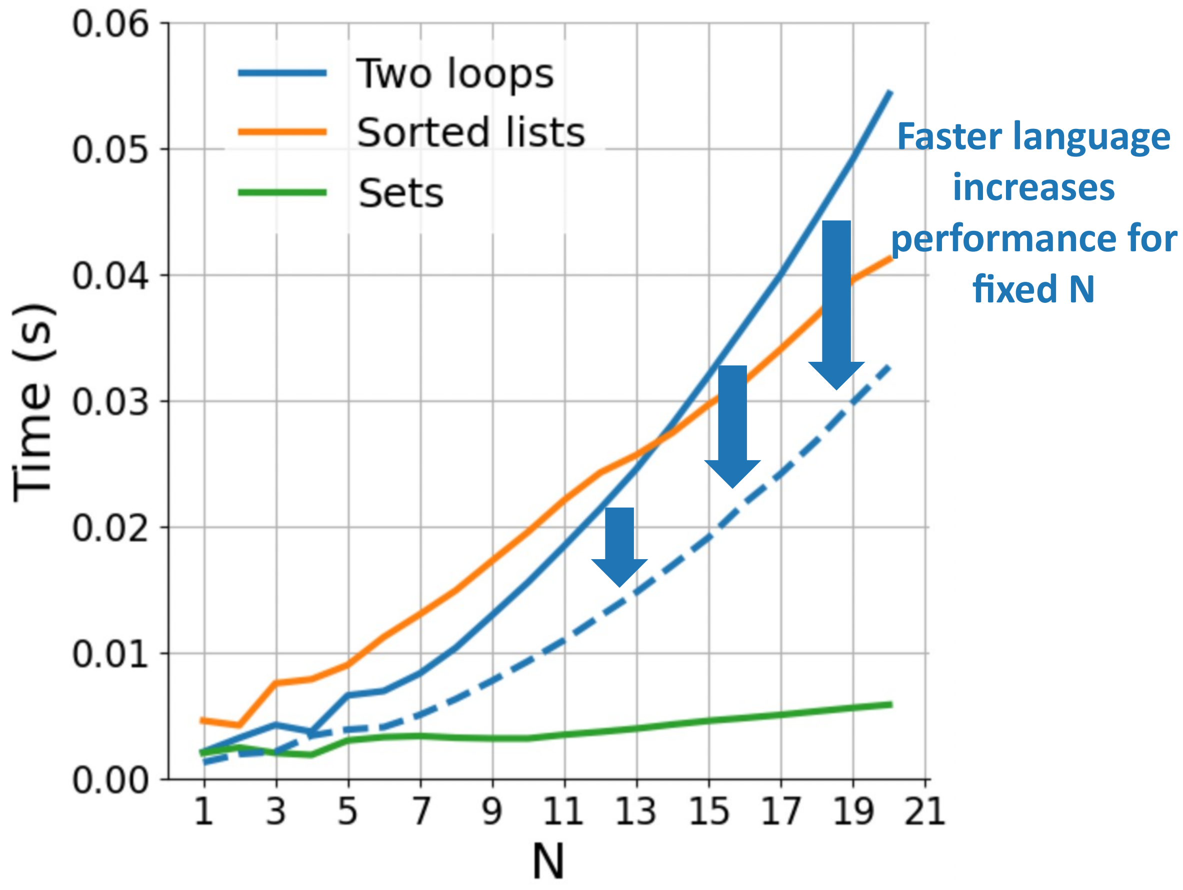

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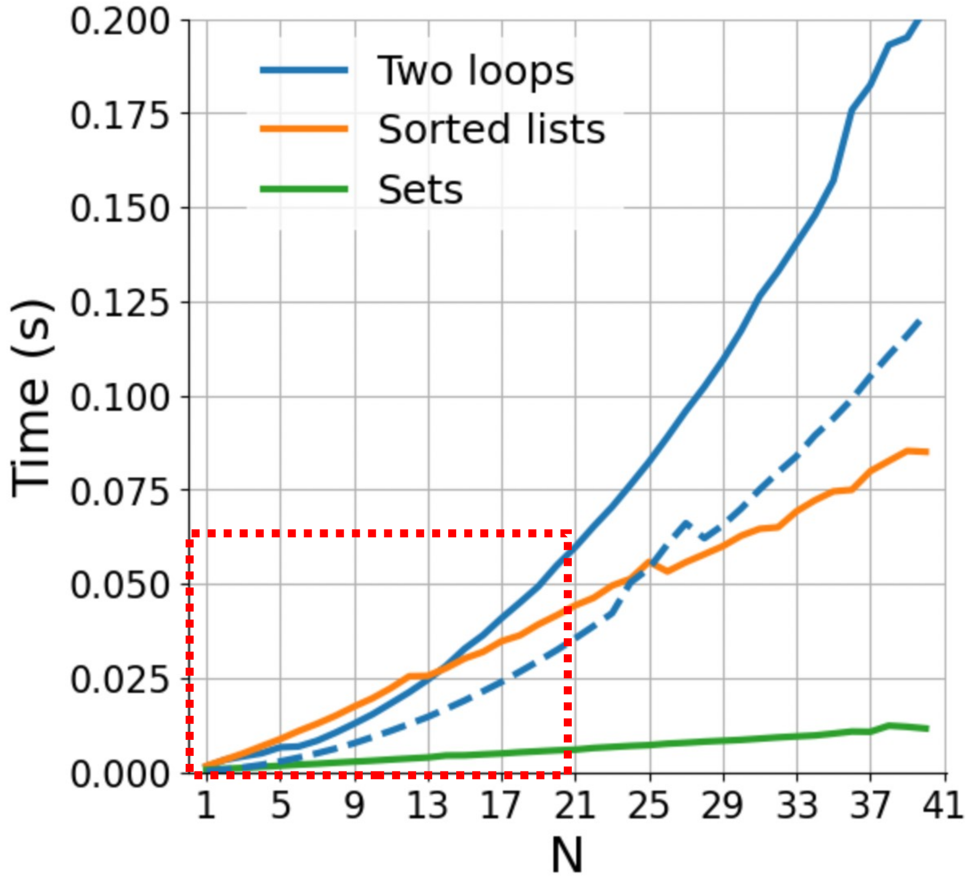

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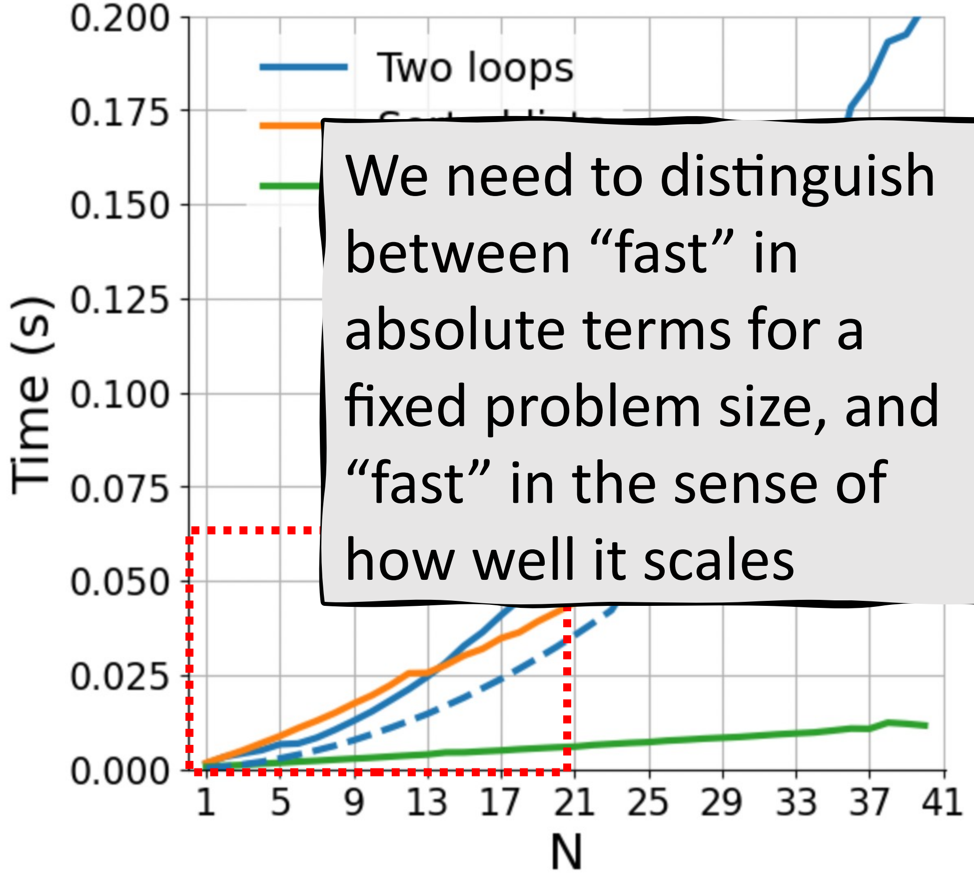

We need to distinguish between “fast” in absolute terms for a fixed problem size, and “fast” in the sense of how well it scales

COMING UP NEXT:
NumPy and the array data structure

Some data structures

- list: ordered, heterogeneous storage, stack/queue, fast access by index, slow search
- set: unordered
- dictionary
- arrays: e.g. numpy, HDF5
- tables: e.g. pandas, dask, spark, SQL
- graph: social network structure
- tree: to rapidly search a dataset
- heap
- stack
- queue
- priority queue

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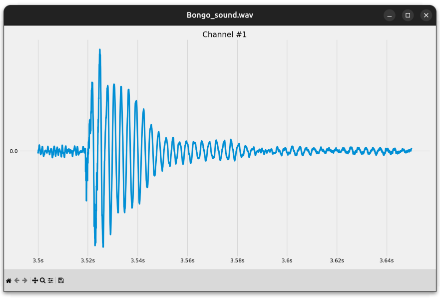

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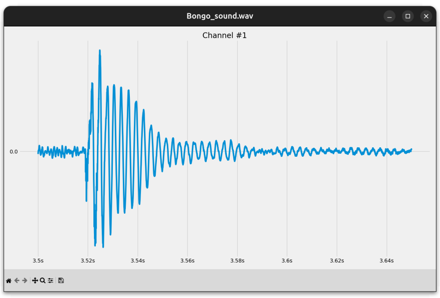

NumPy array

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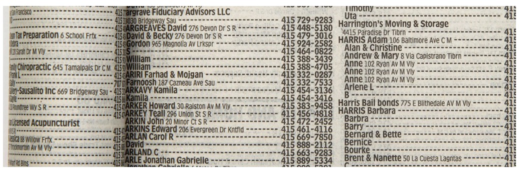
Phone book entries?



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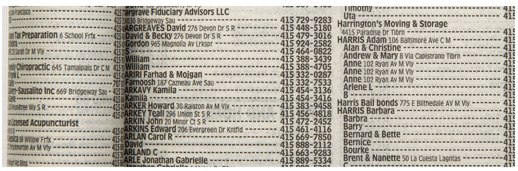

Pandas DataFrame

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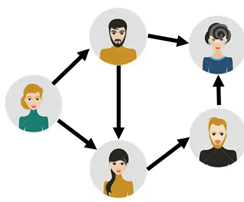

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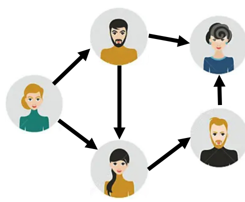
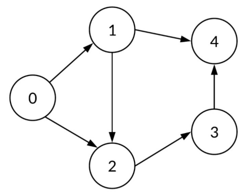


Graph



Implemented as

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Adjacency matrix (array)

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A_dict = {
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```
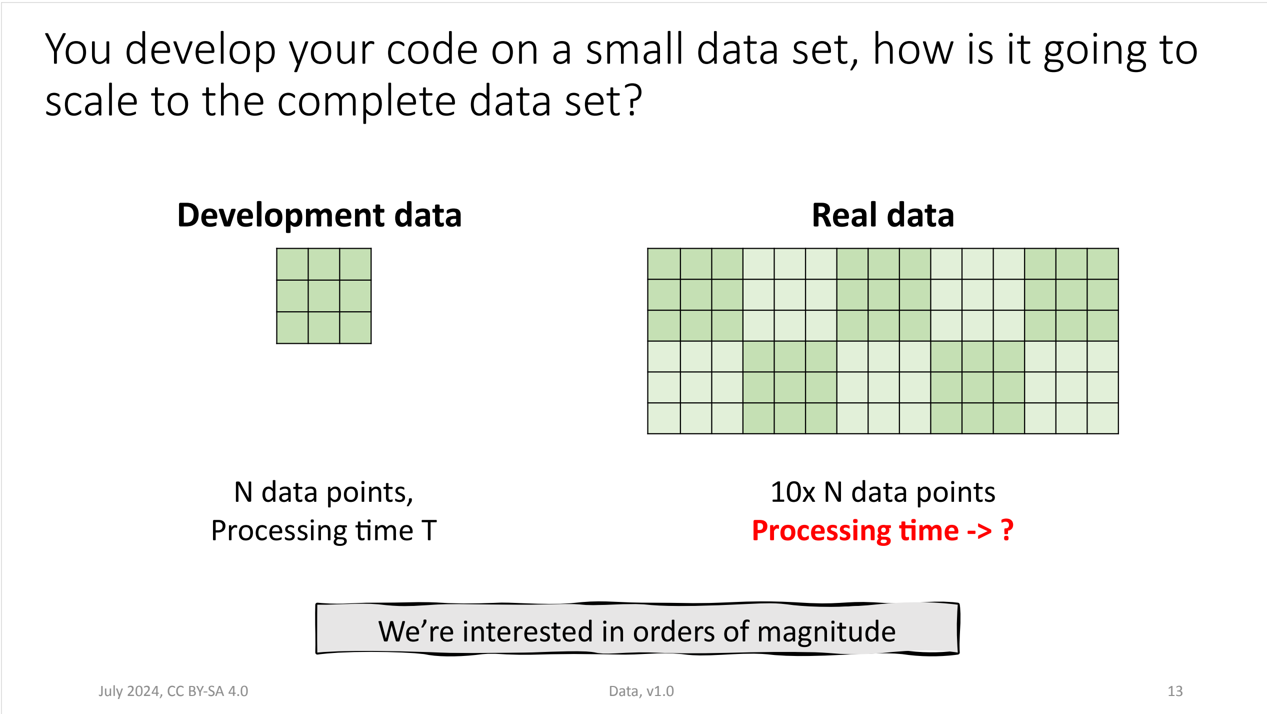

Dictionary



Data and code are related.

Nice transition from the last question. In extreme case, when the relations in the graph are dynamic/ changing a lot, using a dictionary is not a good solution. Instead, when small dataset and we are mainly interested in visualizing the relations, it might be.
The NumPy array solutions, scales much better, in case there are hundreds of dynamically changing relations to inspect.

How performance scales: big-O

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O(1)	constant	1x time
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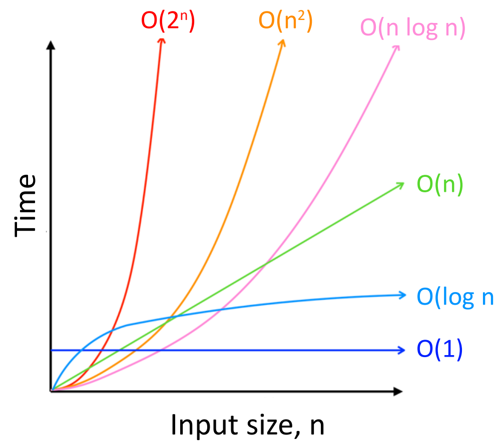
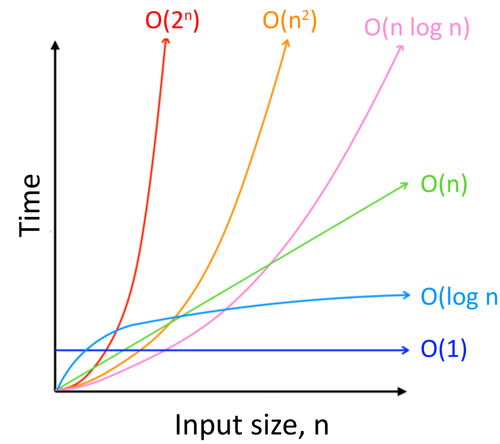
O(n * log n)	linearithmic	~10-20x time
O(log n)	logarithmic	~1-2x time



Hands-on: Operations on lists

Big-O class	What we call it	Time increase, when data increases 10x
O(1)	constant	1x time
O(n)	linear	10x time
O(n^2)	quadratic	100x time
O(n * log n)	linearithmic	~10-20x time
O(log n)	logarithmic	~1-2x time

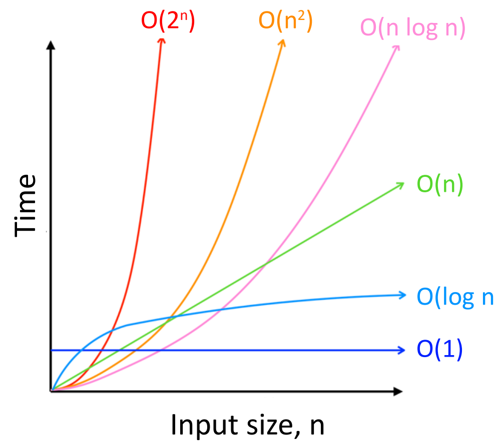
Big-O class	Operation on lists that scales this way
O(1)	
O(n)	
O(n^2)	
O(n * log n)	
O(log n)	



Hands-on: Operations on lists

Big-O class	What we call it	Time increase, when data increases 10x
$O(1)$	constant	1x time
$O(n)$	linear	10x time
$O(n^2)$	quadratic	100x time
$O(n * \log n)$	linearithmic	~10-20x time
$O(\log n)$	logarithmic	~1-2x time

Big-O class	Operation on lists that scales this way
$O(1)$	Getting an element by its index
$O(n)$	Summing elements in list
$O(n^2)$	Computing distance between all pairs of elements in the list
$O(n * \log n)$	Sorting the list
$O(\log n)$	Searching an element in a sorted list



Example: Find common words

Given two lists of words, extract all the words that are in common

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']
```

Expected result: `['apple', 'orange', 'banana']`

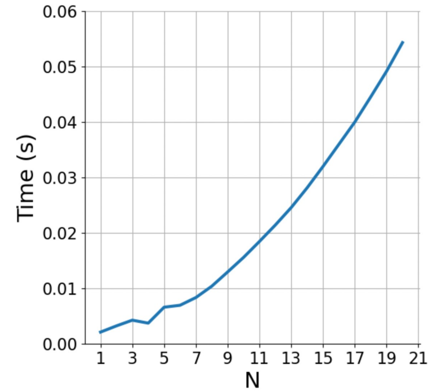
Implementation with two for-loops

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

common = []
for w in words1:
    if w in words2:
        common.append(w)
```

What is the big-O complexity of this implementation?

Implementation with two for-loops

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

common = []
for w in words1:          # O(N)
    if w in words2:        # O(N)
        common.append(w)   # O(1)
```



What is the big-O complexity of this implementation?
N * N ~ **$O(N^2)$**

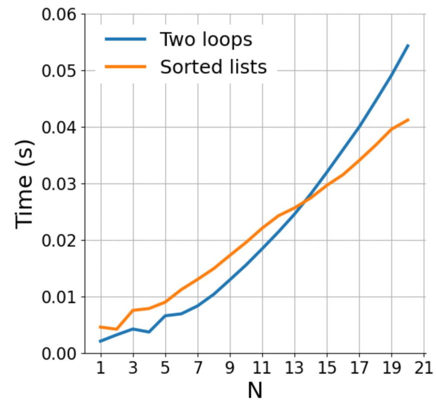
Implementation with sorted lists

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

words1 = sorted(words1) # ['apple', 'banana', 'melon', 'orange', 'peach']
words2 = sorted(words2) # ['apple', 'avocado', 'banana', 'kiwi', 'orange']

common = []
idx2 = 0
for w in words1:
    while idx2 < len(words2) and words2[idx2] < w:
        idx2 += 1

    if idx2 >= len(words2):
        break

    if words2[idx2] == w:
        common.append(w)
```

What is the big-O complexity of this implementation?

Implementation with sorted lists

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

words1 = sorted(words1)     # O(N * log(N))
words2 = sorted(words2)     # O(N * log(N))

common = []
idx2 = 0
for w in words1:                                    # O(N)
    while idx2 < len(words2) and words2[idx2] < w:  # O(N) in total
        idx2 += 1

    if idx2 >= len(words2): # O(1)
        break

    if words2[idx2] == w:   # O(1)
        common.append(w)
```



What is the big-O complexity of this implementation?

2 * (N * log(N)) + 2 * N ~ **O(N log N)**

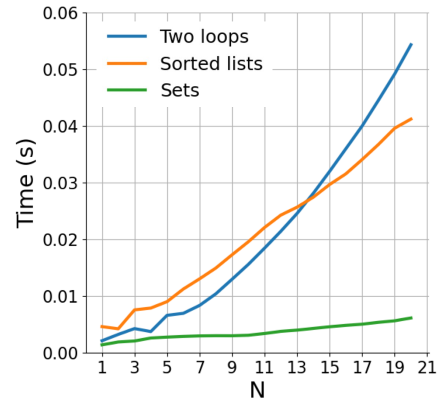
Implementation with sets

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

words2 = set(words2)

common = []
for w in words1:
    if w in words2:
        common.append(w)
```

What is the big-O complexity of this implementation?

Implementation with sets

```
words1 = ['apple', 'orange', 'banana', 'melon', 'peach']
words2 = ['orange', 'kiwi', 'avocado', 'apple', 'banana']

words2 = set(words2)      # O(N)

common = []
for w in words1:          # O(N)
    if w in words2:           # O(1)
        common.append(w)      # O(1)
```



What is the big-O complexity of this implementation?

N + N ~ **O(N)**

Basic reference sheet about Python data structures

Lists: collection of ordered, arbitrary data

Getting an element by index	O(1)
Appending	O(1)
Inserting an element at index	O(n)
Sorting	O(n log n)
Finding an element by value (e.g., "if element in my_list: …", list.index, etc.)	O(n)
Copy a list	O(n)

Dictionaries ("hashmaps")

Inserting	O(1)
Finding a value by key (e.g., "if element in my_dict: …")	O(1)
Create dictionary from lists	O(n)

Sets: it's dictionaries without values

Inserting	O(1)
Finding a value by key (e.g., "if element in my_set: …")	O(1)
Create set from list	O(n)

See also: https://wiki.python.org/moin/TimeComplexity

Note that there may be different implementations of these data structures with different complexities, these are for the Python implementation.

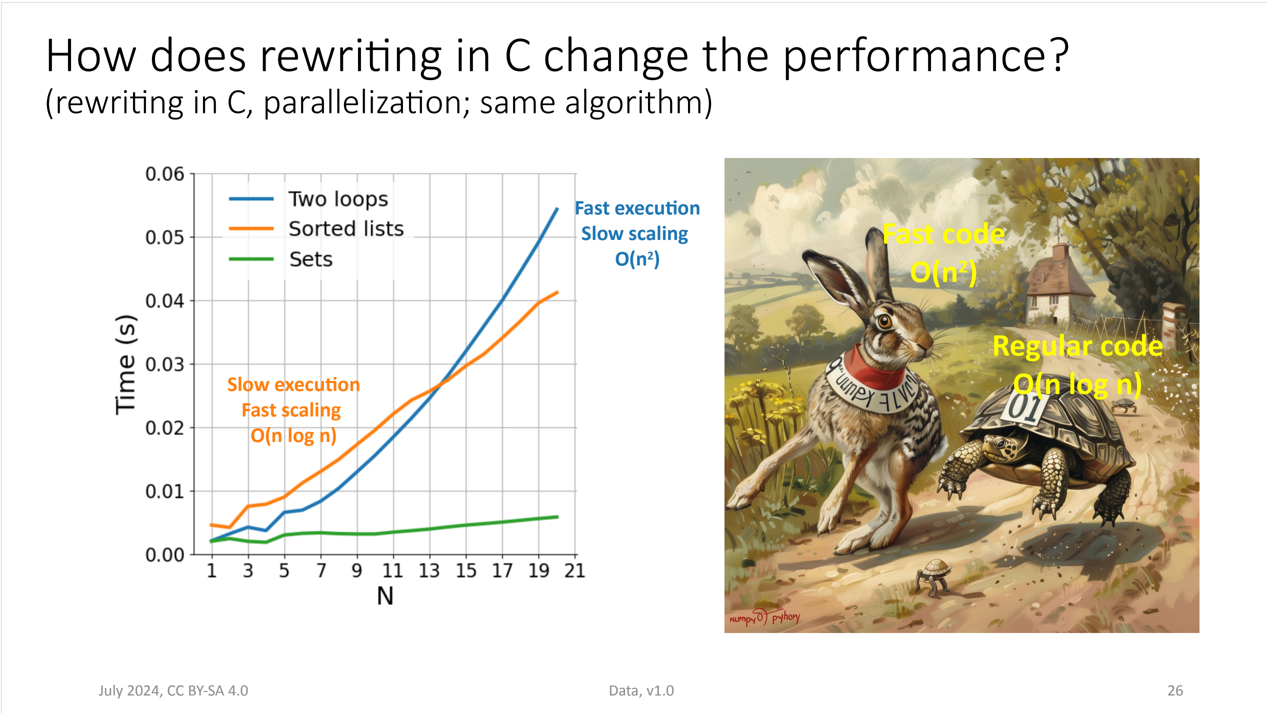
E.g., if finding an element in a list is important, one could implement it as two dictionaries, one mapping indices to data, one mapping data to indices. Finding out the complexities of all the operations with this implementation is left as a homework.

Hands-on

Exercise
exercises/match_tarots

- Open the notebook `match_tarots`, and follow the instructions!

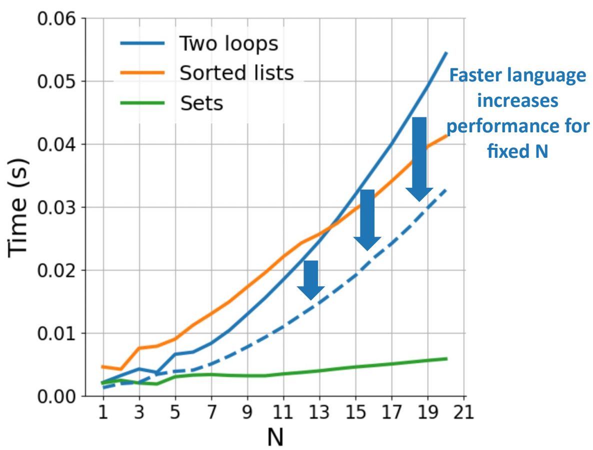
- Submit a PR for Issue #1 on `git.aspp.school/ASPP/2025-plovdiv-data`



Parallelization lowers the curves.
For a fixed code, linear code is no necessarily faster.
Important when n is growing
Parallelization/ optimization ✉ you can make the code faster for any fixed N, but the shape (of growth) can never change

How does rewriting in C change the performance?

(rewriting in C, parallelization; same algorithm)



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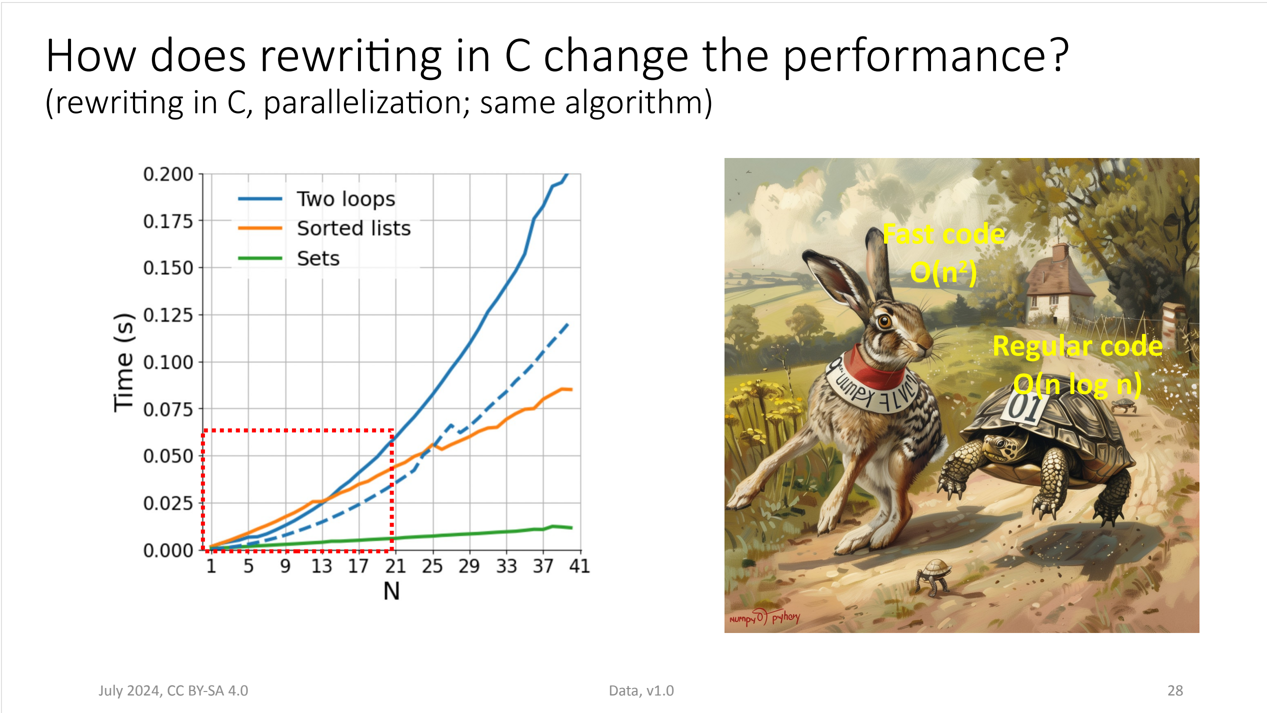

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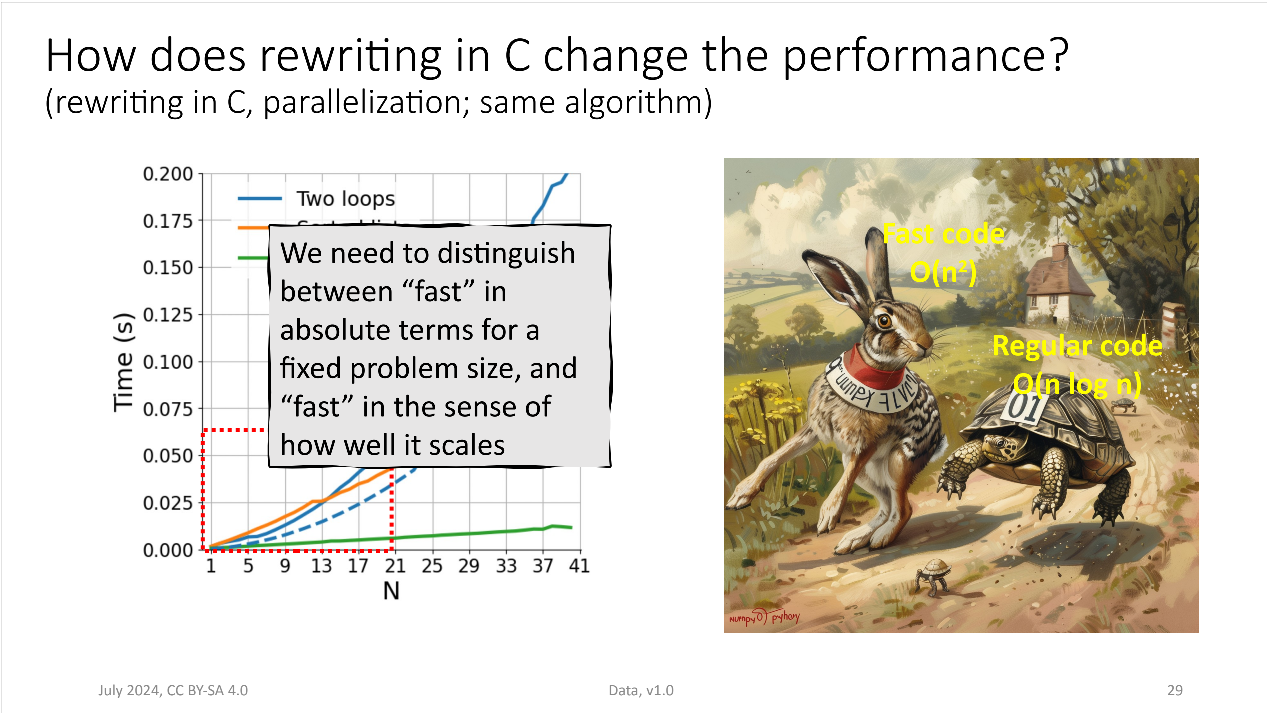

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COMING UP NEXT:
NumPy and the array data structure

Some data structures

- list: ordered, heterogeneous storage, stack/queue, fast access by index, slow search
- set: unordered
- dictionary
- arrays: e.g. numpy, HDF5
- tables: e.g. pandas, dask, spark, SQL
- graph: social network structure
- tree: to rapidly search a dataset
- heap
- stack
- queue
- priority queue