PoL Physics of Life TU Dresden

CENTER FOR SYSTEMS BIOLOGY DRESDEN

Python programming basics

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With material from

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Till Korten

Who has programming experience?

I have never programmed

I have adjusted existing scripts/macros

I have written my own script

Working with variables

- Variables can hold numeric values and you can do math with them

```
# initialize parameters
room_width = 5
room_length = 6

# run algorithm on given parameters
room_area = room_width * room_length

print(room_area)
```

```
30
```

Working with variables and string values

- Also text (called strings) as values for variables are supported

Single and double quotes allowed

```
first_name = "Robert"
last_name = 'Haase'

print("Hello " + first_name + " " + last_name)
```

```
Hello Robert Haase
```

f-Strings

- String formatting is made easy using f-strings.

```
f"This is an f-string. a's value is {a}. Doubling the value of a gives {2*a}."
```

```
"This is an f-string. a's value is 5. Doubling the value of a gives 10."
```

Comments

Comments should contain additional information such as

- User documentation
  - What does the program do?
  - How can this program be used?
- Your name / institute in case a reader has a question
- Comment why things are done.
- Do not comment what is written in the code already!

```
#
# This program sums up two numbers.
#
# Usage:
# * Run it in Python 3.8
#
# Author: Robert Haase, PoL TUD
#         Robert.haase@tu-dresden.de
# April 2021

# initialise program
a = 1
b = 2.5

# run complicated algorithm
final_result = a + b

# print the final result
print( final_result )
```

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Handling many items: lists

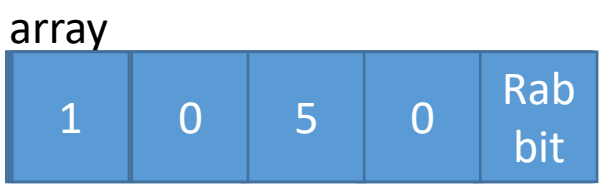
Lists

- Lists are variables, where you can store multiple values

Give me a “0”, five times!

```
array = [0] * 5
```

Computer memory



Arrays in Python

- Modifying lists entries

```
numbers = [0, 1, 2, 3, 4]

# write in one array element
numbers[1] = 5

print(numbers)
```

```
[0, 5, 2, 3, 4]
```

Note: The first element has index 0!

- Creating lists of defined size

What?

How many?

```
zeros = [0] * 10
print(zeros)
```

```
[0, 0, 0, 0, 0, 0, 0, 0, 0, 0]
```

- Concatenating lists

```
ones = [1, 1, 1]
twos = [2, 2, 2, 2]

# concatenate arrays
numbers = ones + twos

print(numbers)
```

```
[1, 1, 1, 2, 2, 2, 2]
```

+ means appending

Subsets

```
# Arrays
numbers = [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
print(numbers)
```

```
[0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

- Creating subsets of lists

Start

End

```
subset = numbers[2:4]
print(subset)
```

```
[2, 3]
```

Step

```
subset_with_gaps = arr[1:8:2]
print(subset_with_gaps)
```

```
[1, 3, 5, 7]
```

data[start:stop:step]

Indexing, cropping, subsets

- “Indexing” is addressing certain elements in lists. The first element is “0” away from the start.

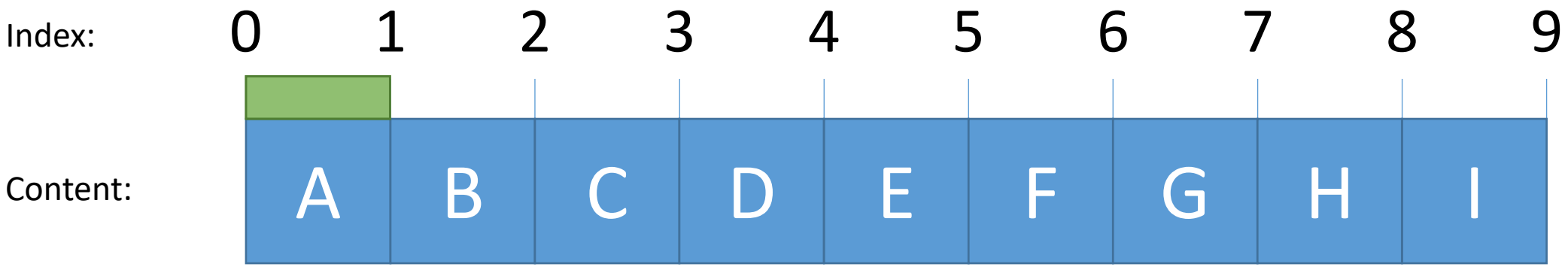
```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```

Index:	0	1	2	3	4	5	6	7	8	9
Content:	A	B	C	D	E	F	G	H	I	

Indexing, cropping, subsets

- “Indexing” is addressing certain elements in lists. The first element is “0” away from the start.

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```



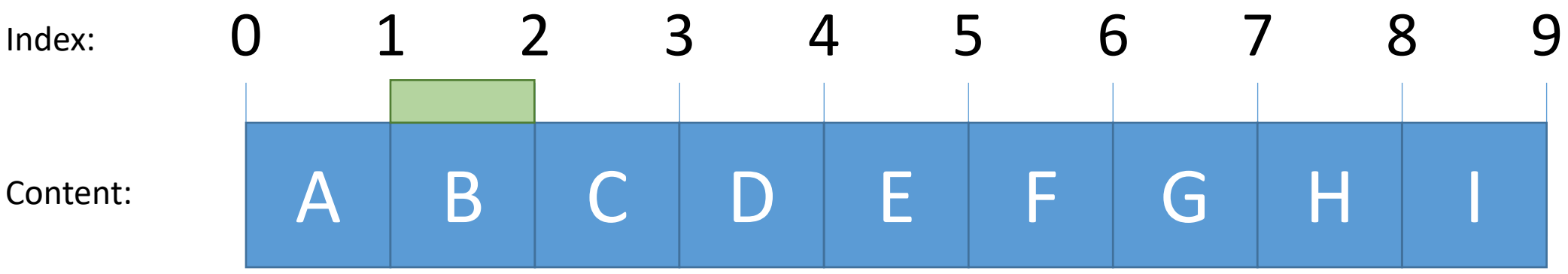

```
data[0]
```

```
'A'
```

Indexing, cropping, subsets

- “Indexing” is addressing certain elements in lists. The first element is “0” away from the start.

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[0]
```

```
'A'
```

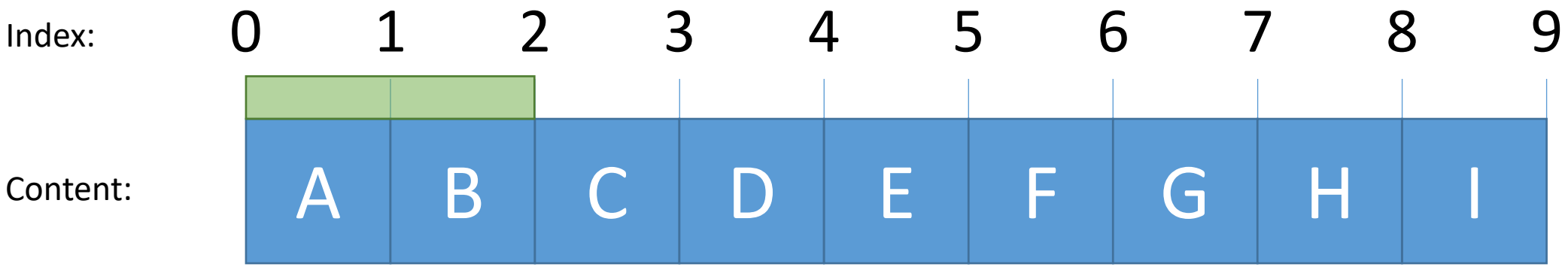
```
data[1]
```

```
'B'
```

Indexing, cropping, subsets

- “Indexing” is addressing certain elements in lists. The first element is “0” away from the start.

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[0]
```

```
'A'
```

```
data[1]
```

```
'B'
```

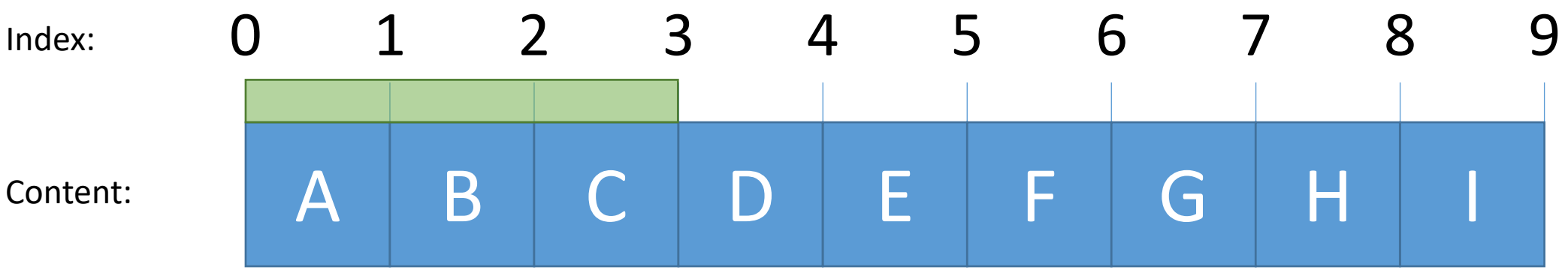
```
data[0:2]
```

```
['A', 'B']
```

Indexing, cropping, subsets

- “Indexing” is addressing certain elements in lists. The first element is “0” away from the start.

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[0]
```

```
'A'
```

```
data[1]
```

```
'B'
```

```
data[0:2]
```

```
['A', 'B']
```

```
data[0:3]
```

```
['A', 'B', 'C']
```

```
data[1:2]
```

```
['B']
```

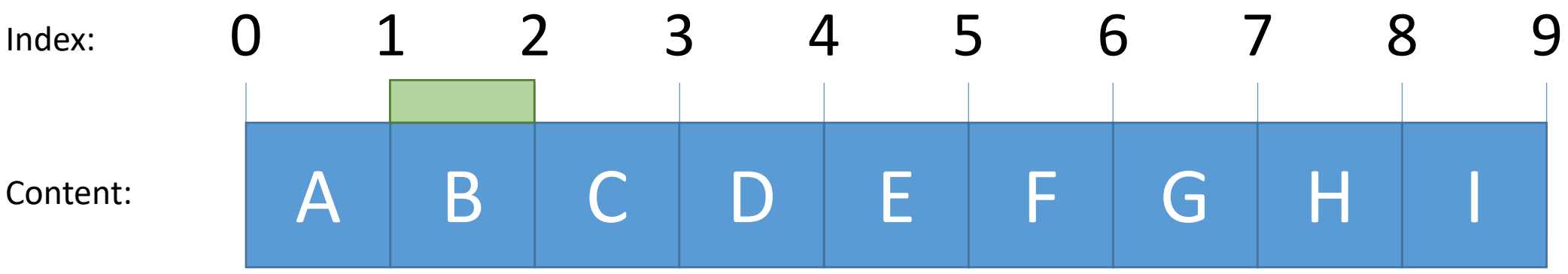
```
len(data)
```

```
9
```

Indexing, cropping, subsets

- “Indexing” is addressing certain elements in lists. The first element is “0” away from the start.

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[0]
```

```
'A'
```

```
data[1]
```

```
'B'
```

```
data[0:2]
```

```
['A', 'B']
```

```
data[0:3]
```

```
['A', 'B', 'C']
```

```
data[1:2]
```

```
['B']
```

Indexing, cropping, subsets

- “Indexing” is addressing certain elements in lists. The first element is “0” away from the start.

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```

Index:	0	1	2	3	4	5	6	7	8	9
Content:	A	B	C	D	E	F	G	H	I	

```
data[0]
```

```
'A'
```

```
data[1]
```

```
'B'
```

```
data[0:2]
```

```
['A', 'B']
```

```
data[0:3]
```

```
['A', 'B', 'C']
```

```
data[1:2]
```

```
['B']
```

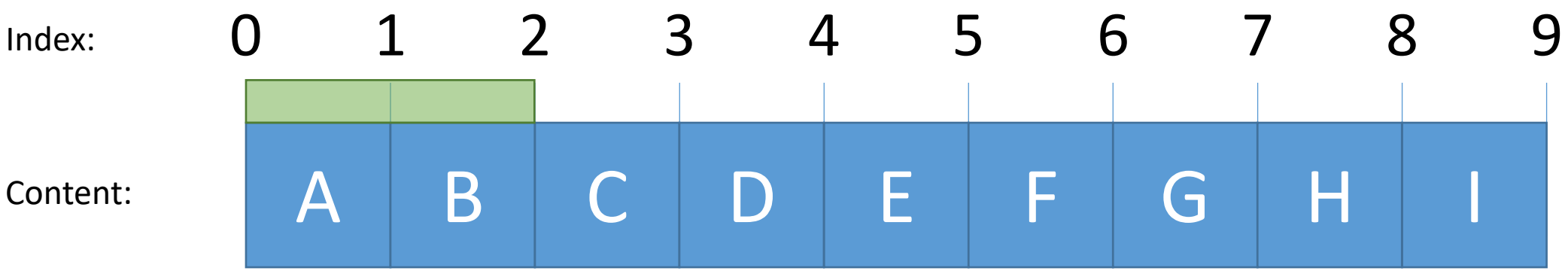
```
len(data)
```

```
9
```

Indexing, cropping, subsets

- You can leave start and end out when specifying index ranges

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```



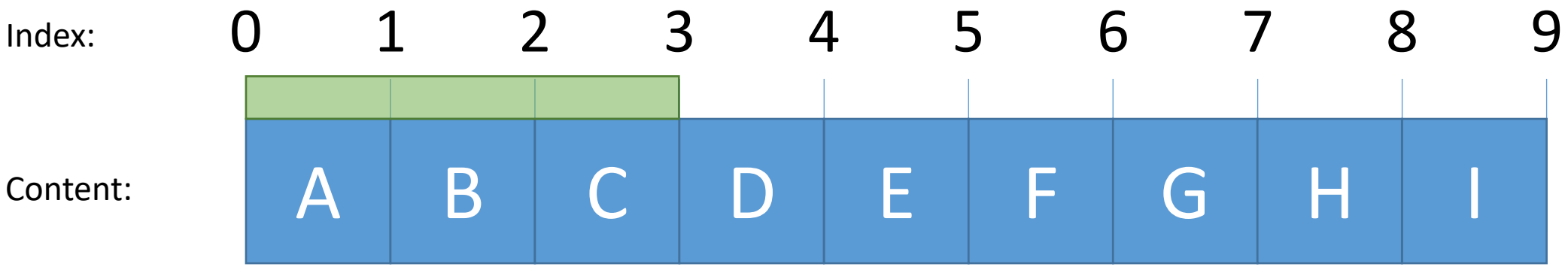

```
data[:2]
```

```
['A', 'B']
```

Indexing, cropping, subsets

- You can leave start and end out when specifying index ranges

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[:2]
```

```
['A', 'B']
```

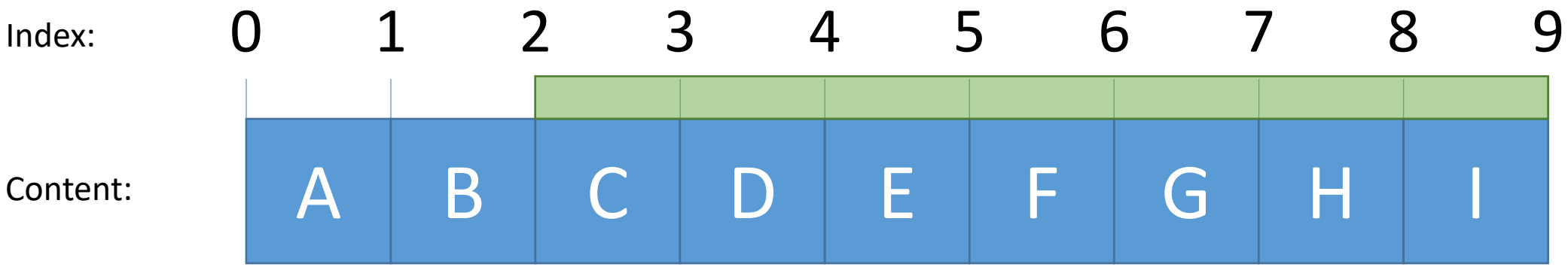
```
data[:3]
```

```
['A', 'B', 'C']
```

Indexing, cropping, subsets

- You can leave start and end out when specifying index ranges

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[:2]
```

```
['A', 'B']
```

```
data[:3]
```

```
['A', 'B', 'C']
```

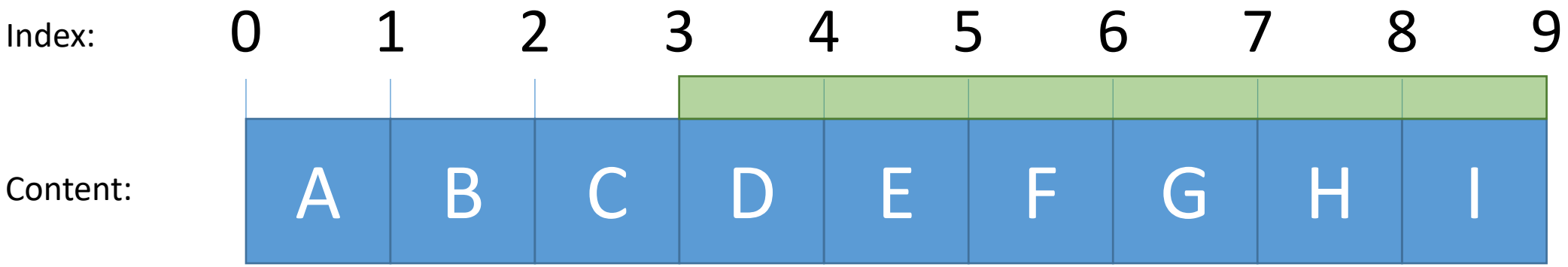
```
data[2:]
```

```
['C', 'D', 'E', 'F', 'G', 'H', 'I']
```

Indexing, cropping, subsets

- You can leave start and end out when specifying index ranges

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[:2]
```

```
['A', 'B']
```

```
data[:3]
```

```
['A', 'B', 'C']
```

```
data[2:]
```

```
['C', 'D', 'E', 'F', 'G', 'H', 'I']
```

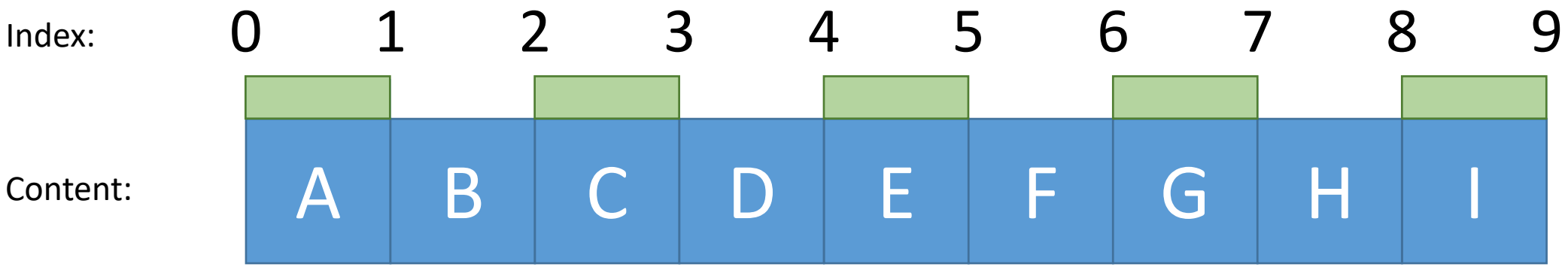
```
data[3:]
```

```
['D', 'E', 'F', 'G', 'H', 'I']
```

Indexing, cropping, subsets

- The step-size allows skipping elements

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```



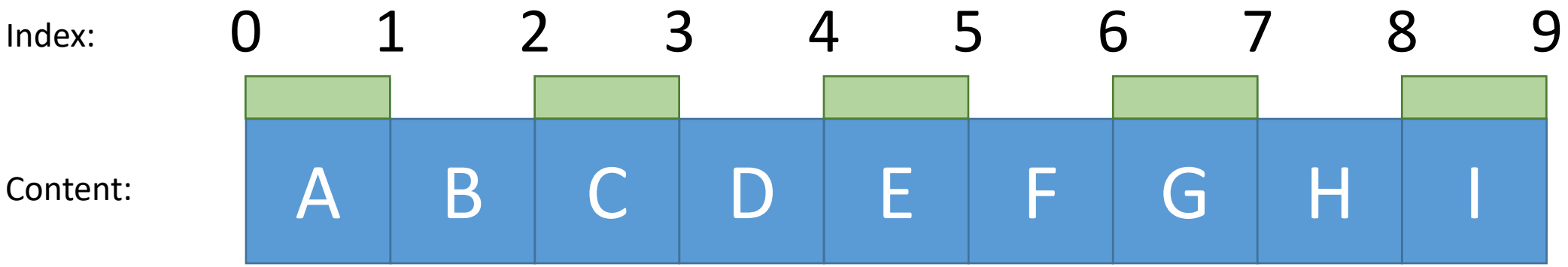

```
data[0:10:2]
```

```
['A', 'C', 'E', 'G', 'I']
```

Indexing, cropping, subsets

- The step-size allows skipping elements

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[0:10:2]
```

```
['A', 'C', 'E', 'G', 'I']
```

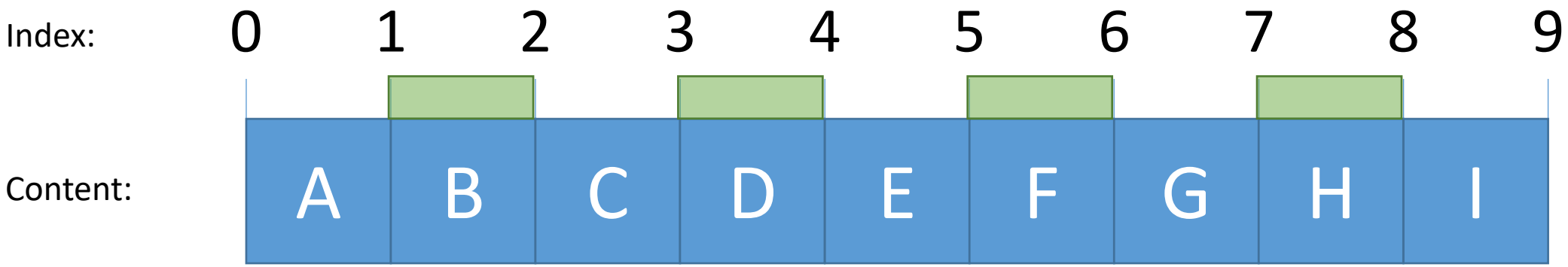
```
data[::2]
```

```
['A', 'C', 'E', 'G', 'I']
```

Indexing, cropping, subsets

- The step-size allows skipping elements

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```




```
data[0:10:2]
```

```
['A', 'C', 'E', 'G', 'I']
```

```
data[::2]
```

```
['A', 'C', 'E', 'G', 'I']
```

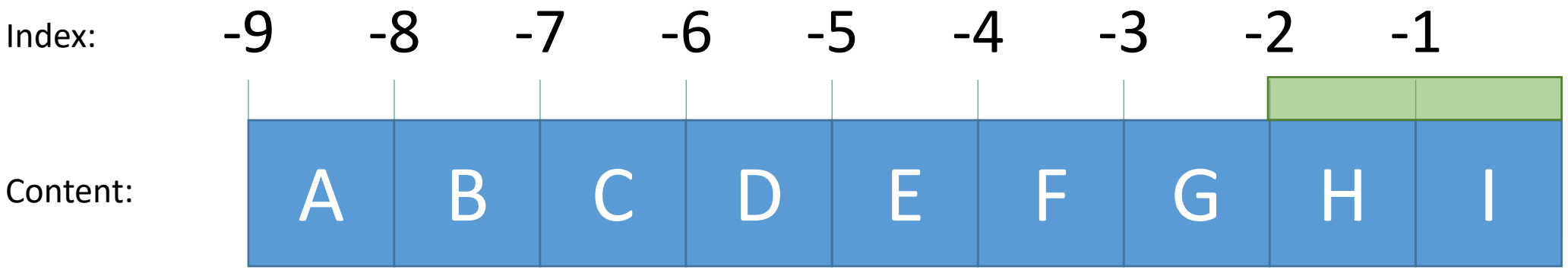
```
data[1::2]
```

```
['B', 'D', 'F', 'H']
```

Indexing, cropping, subsets

- Indexing also works with negative indices

```
data = ['A', 'B', 'C', 'D', 'E', 'F', 'G', 'H', 'I']
```



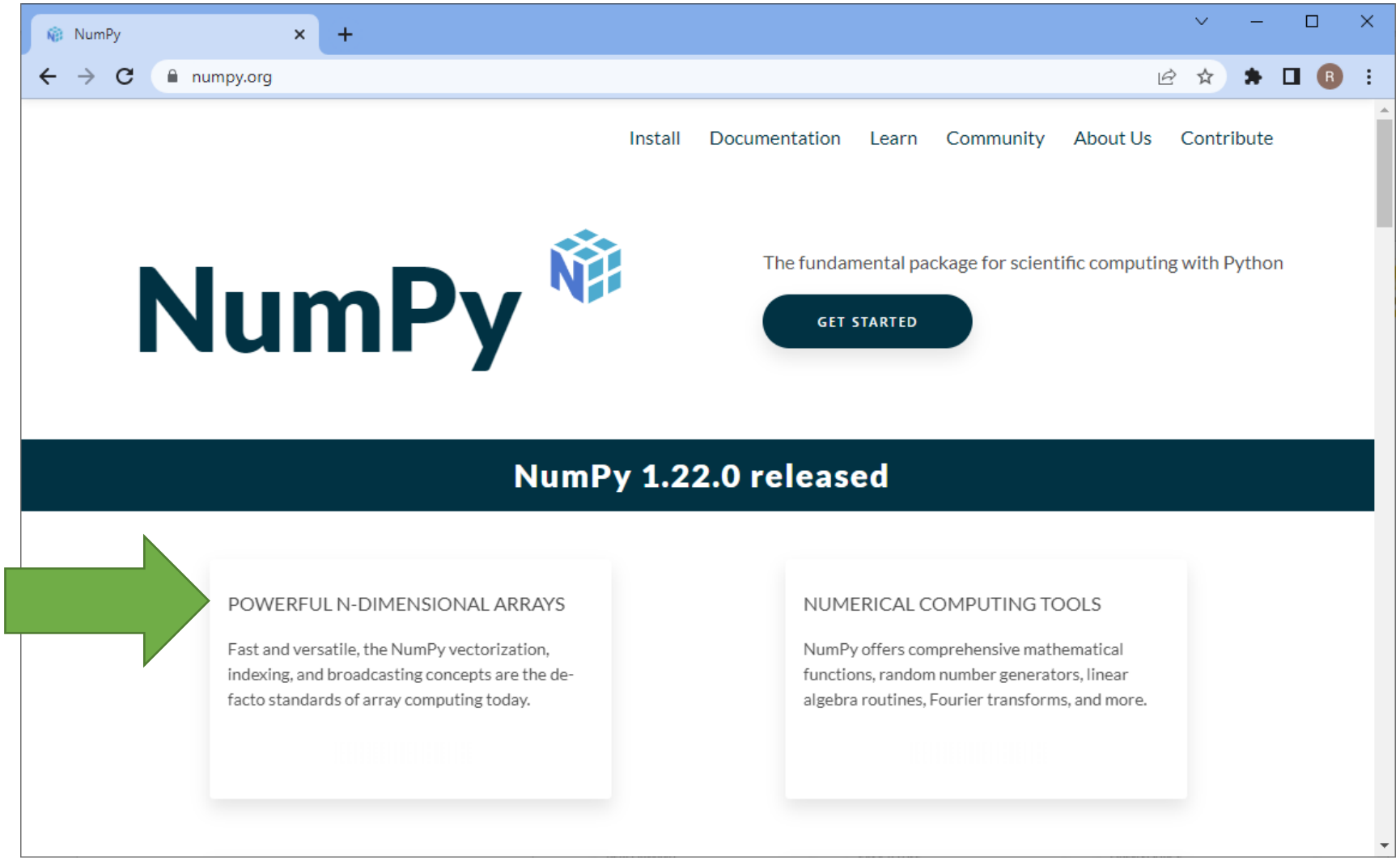

```
data[-2:]
```

```
['H', 'I']
```

numpy

- The fundamental package for scientific computing with python.

- `conda install numpy`



https://numpy.org/

numpy

- Simplifying mathematical operations on n-dimensional arrays

Tell python that you want to use a library called numpy

- Python arrays of arrays (lists of lists)

```
# multidimensional arrays
matrix = [
    [1, 2, 3],
    [2, 3, 4],
    [3, 4, 5]
]

print(matrix)
```

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

```
result = matrix * 2
print(result)
```

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

- numpy arrays

```
import numpy as np

np_matrix = np.asarray(matrix)

print(np_matrix)
```

If “numpy” is to long, you can give an alias “np”

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

```
np_result = np_matrix * 2
print(np_result)
```

```
[[ 2  4  6]
 [ 4  6  8]
 [ 6  8 10]]
```

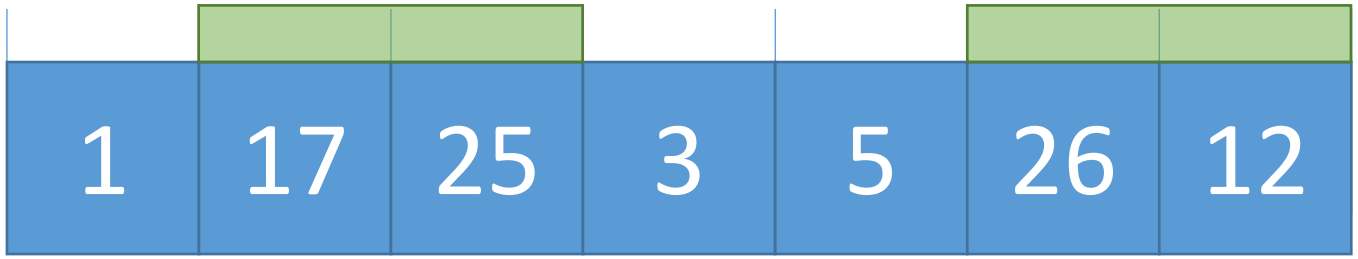
Masking

- “Masking” is addressing certain elements in numpy arrays, e.g. depending on their content

```
import numpy
measurements = numpy.asarray([1, 17, 25, 3, 5, 26, 12])
measurements
```

```
array([ 1, 17, 25,  3,  5, 26, 12])
```

Content:




```
mask = measurements > 10
mask
```

```
array([False,  True,  True, False, False,  True,  True])
```

```
measurements[mask]
```

```
array([17, 25, 26, 12])
```

Basic descriptive statistics using numpy

- Basic descriptive statistics

```python
import numpy as np

measurements = [1, 4, 6, 7, 2]

mean = np.mean(measurements)
print("Mean: " + str(mean))
```

```
Mean: 4.0
```

numpy.mean — NumPy v1.18 M

numpy.org/doc/1.18/reference/generated/numpy.mean.html?highlight=mean#numpy.mean

NumPy

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numpy.average

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numpy.mean

numpy.mean(*a, axis=None, dtype=None, out=None, keepdims=<no value>*) [source]

Compute the arithmetic mean along the specified axis.

Returns the average of the array elements. The average is taken over the flattened array by default, otherwise over the specified axis. **float64** intermediate and return values are used for integer inputs.

Parameters:

a : *array_like*

Array containing numbers whose mean is desired. If *a* is not an array, a conversion is attempted.

axis : *None or int or tuple of ints, optional*

Axis or axes along which the means are computed. The default is to compute the mean of the flattened array.

New in version 1.7.0.

If this is a tuple of ints, a mean is performed over multiple axes, instead of a single axis or all the axes as before.

dtype : *data-type, optional*

Type to use in computing the mean. For integer inputs, the default is **float64**; for floating point inputs, it is the same as the input dtype.

out : *ndarray, optional*

Alternate output array in which to place the result. The default is `None`; if provided, it must have the same shape as the expected output, but the type will be cast if necessary. See *ufuncs-output-type* for more details.

keepdims : *bool, optional*