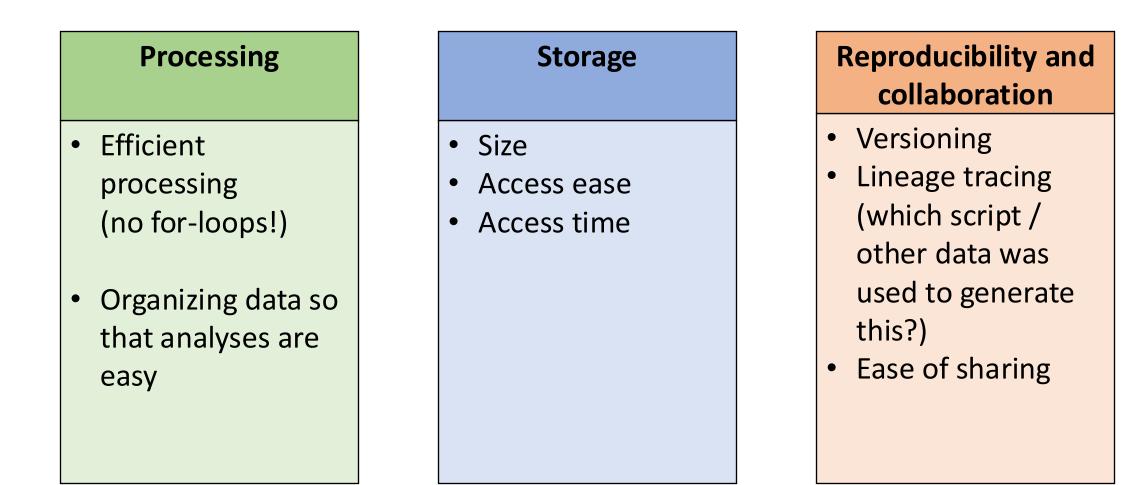
The data class

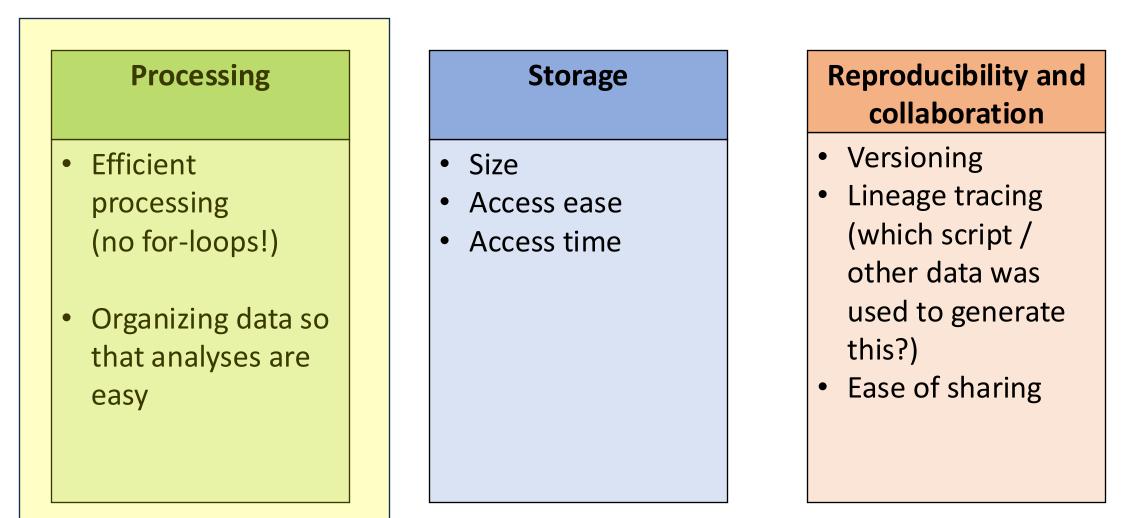
Pietro Berkes & Verjinia Metodieva



Things one thinks about when thinking about data



Things one thinks about when thinking about data

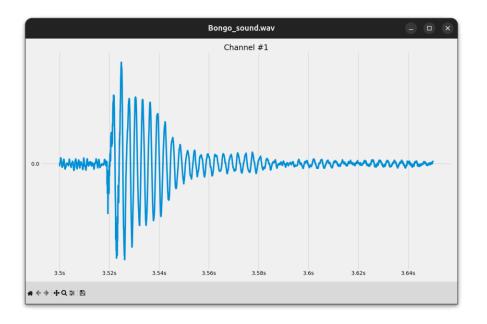


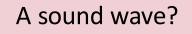
Hands-on

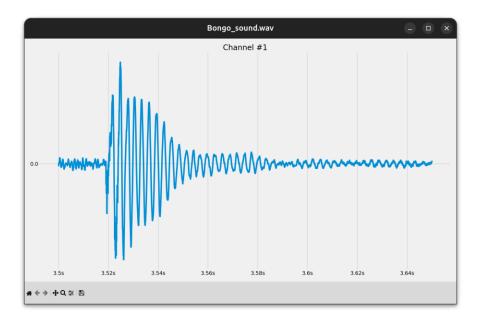
łĤł

What data structure would you use to represent...

A sound wave?







NumPy array

In [6]: sound_data

Out[6]:	0.75592186, 0.11718457, 0.81113341, 0.74382869, 0.91298397, 0.3602381, 0.67944923, 0.57444803, 0.95954499, 0.76332531, 0.15357459, 0.97231498, 0.67662718, 0.40815661, 0.64457074, 0.26389161,	0.25555136, 0.67261696, 0.25184725, 0.62055231, 0.64856368, 0.48290914, 0.07173351, 0.00930429, 0.25760187, 0.96272817, 0.96272817, 0.96055977, 0.1139344, 0.19233097, 0.97537645,	0.95416669, 0.72451477, 0.62847452, 0.9046905, 0.9046905, 0.80644398, 0.20847714, 0.8584085, 0.21714217, 0.43785728, 0.3616905, 0.57169277, 0.0642748, 0.74184693, 0.64942314, 0.95638066, 0.24012179, 0.14209784, 0.92983283,	0.2646681 , 0.06232598, 0.8103058 , 0.56664205, 0.46199345, 0.99162659, 0.32248766, 0.3810089, 0.39119371, 0.23896063, 0.50225193, 0.95013941, 0.26629893, 0.66487937, 0.87436447, 0.90399279, 0.75261696,	0.08694215, 0.20549438, 0.18100915, 0.73235338, 0.78516632, 0.26374781, 0.39167573, 0.17668711, 0.68268063, 0.61872801, 0.01361629, 0.38712684, 0.84672705, 0.86867536, 0.18407227, 0.39093908, 0.10078122,	
	0.87468408,	0.77990102,	0.92983283,	0.45841805,	•	

Hands-on



What data structure would you use to represent...

Phone book entries?

Can Francisco	415 margrave Fiduciary Advisors LLC	a block of the The	Uta
·····	415 3030 Bridgeway Sau 415 ARGREAVES David 276 Devon Dr S R	415 729-9283 415 448-5180	Harrington's Moving & Storage
Im Tax Preparation 6 School Frfx	4154 David & Becky 276 Devon Dr S R	415 479-3016	4415 Paradise Dr Tibrn A HARRIS Adam 106 Baltimore Ave C M
	415 Gordon 965 Magnolia Av Lrkspr	415 924-2582	Alan & Christine 4
	415% William	415 388-3439	Andrew & Mary 8 Via Capistrano Tibrn Anne 102 Ryan Av M Viy
	4159 William	415 388-4705	Anne 102 Ryan Av M Vly 2
	Tors Farnoosh 187 Cazneau Ave Sau	415 332-7533 415 454-3136	Anne 102 Ryan Av M Vly A
2	Is Kamila	415 454-3416	B
Innitree Wy S R	TS ARKER Howard 30 Raiston Av M Viy	415 383-9458	Harris Bail bonds 775 E Blithedale AV M Vly
literand & cupum chunich	APKIN John 20 Minor Ct C P	115 172-2/52	Barbra ABarry
Sica 88 Willow Frfx	ARKINS Edward 206 Evergreen Dr Kntfld	415 461-4116	Bernard & Bette 4
Indimortion Av M VIy	Bavid	415 888-2112	Bernice
Harf Rd Bins	Isi ARLE Jonathan Gabrielle	415 663-9283	Brent & Nanette 50 La Cuesta Lagntas



Phone book entries?

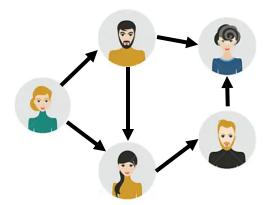
Pandas DataFrame

	15 7 argrave Fiduciary Advisors LLC	415 729-9283	Uta
an Tax Preparation 6 School Frfx	IS ARGREAVES David 276 Devon Dr S R IS David & Becky 276 Devon Dr S R IS Gordon 965 Magnolia Av Lrkspr	415 448-5180 415 479-3016 415 924-2582	4415 Paradise Dr Tibrn HARRIS Adam 106 Baltimore Ave C M
Imsarah Dr M Viy	15: S	415 464-0822	Alan & Christine Andrew & Mary 8 Via Capistrano Tibrn
Chiropractic 645 Tamalpais Dr C M	15 William	415 388-4705	Anne 102 Ryan Av M Vly
ay-sausalito Inc 669 Bridgeway Sau	ny Farnoosh 187 Cazneau Ave Sau	415 332-7533 415 454-3136	Anne 102 Ryan Av M Vly
Rundtree Wy S R	ARKER Howard 30 Raiston Av M Viy	415 383-9458	Harris Bail bonds 775 E Blithedale AV M Vly
limited Acupum chunich	APKIN John 20 Minor Ct C D	415 456-4818 415 472-2452	Barbra
	ARKINS Edward 206 Evergreen Dr Kntfld	415 669-7850	Bernice
Instantion AV W VIY	ARLAND C	415 663-9283 415 889-5334	Bourke Brent & Nanette 50 La Cuesta Lagntas

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
Alice	Johnson	555-8765	789 Pine St	54321	Lakeside
Bob	Brown	555-4321	321 Birch St	09876	Hilltop
Emma	Davis	555-7890	654 Elm St	11223	Greendale

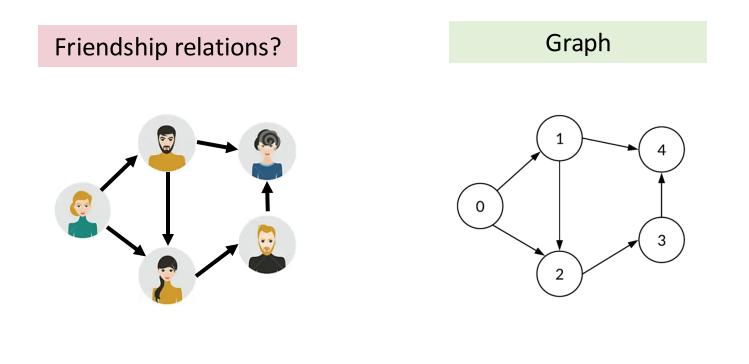


Friendship relations?



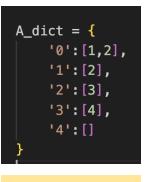


Implemented as



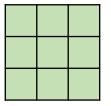
	0	1	2	3	4	
0	0	1	1	0	0	
1	0	0	1	0	1	
2	0	0	0	1	0	
3	0	0	0	0	1	
4	0	0	0	0	0	
•					_	

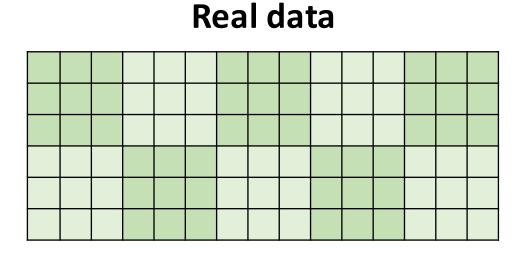
Adjacency matrix (array)



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

Development data



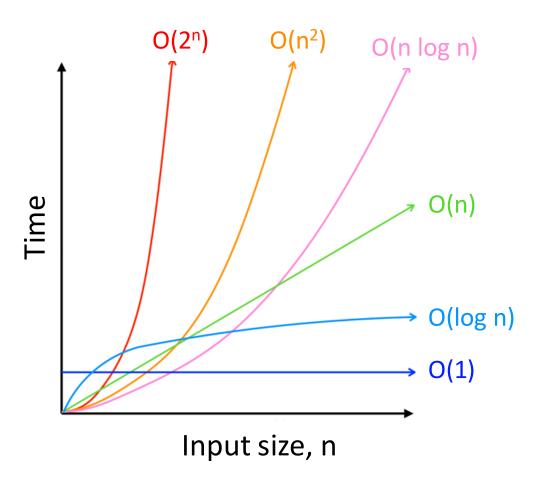


N data points, Processing time T 10x N data points **Processing time -> ?**

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

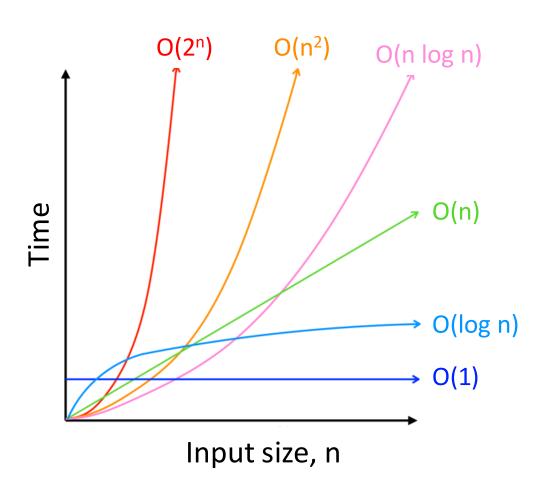


Hands-on: Operations on lists



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)	

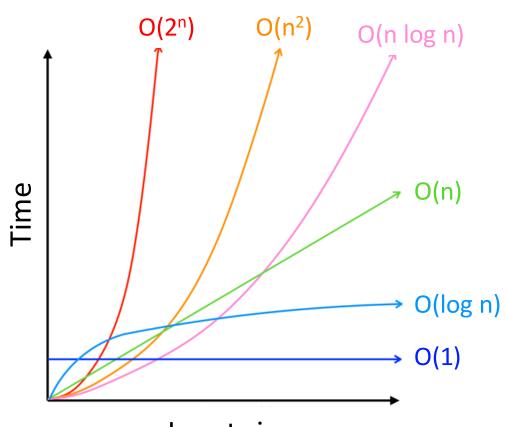


Hands-on: Operations on lists



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(n²)	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
July 2024, CC BY-SA	4.0 Data, v1.0



Input size, n

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']

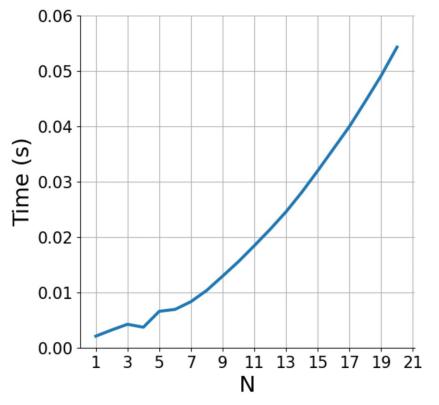
Implementation with two for-loops

```
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





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

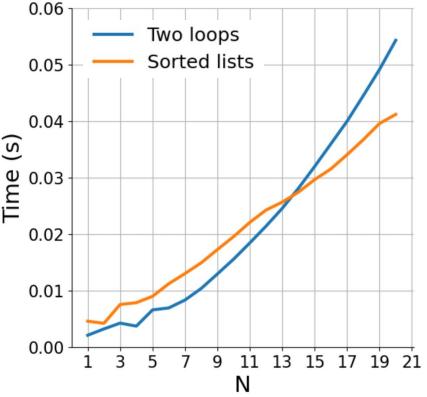
Implementation with sorted lists

```
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





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

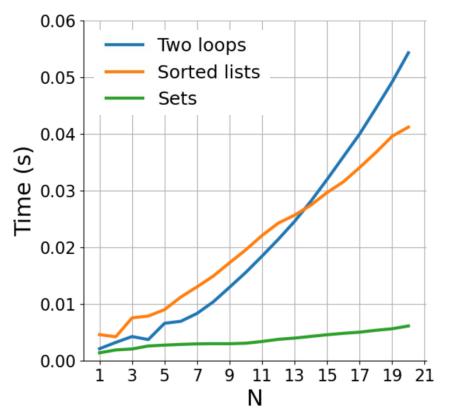
Implementation with sets

```
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? $N + N \sim O(N)$

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 (e.g., "if element in my_list:")	O(n)

Dictionaries ("hashmaps")

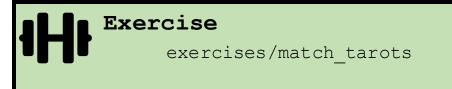
Inserting	O(1)
Finding a value by key (e.g., "if element in my_dict:")	O(1)

Sets: it's dictionaries without values

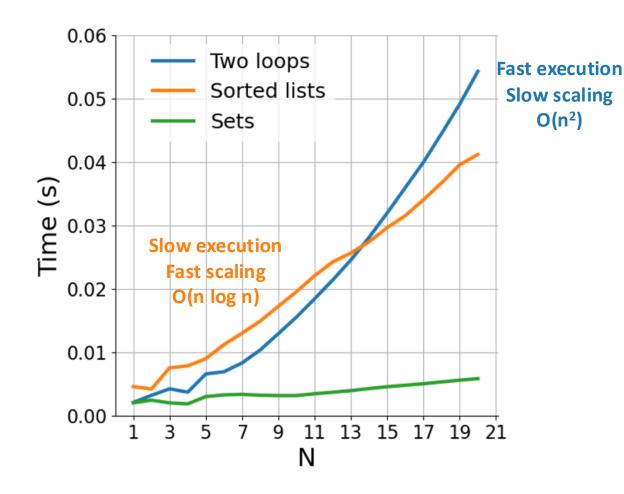
Inserting	O(1)
Finding a value by key (e.g. <i>,</i> "if element in my_set:")	O(1)

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

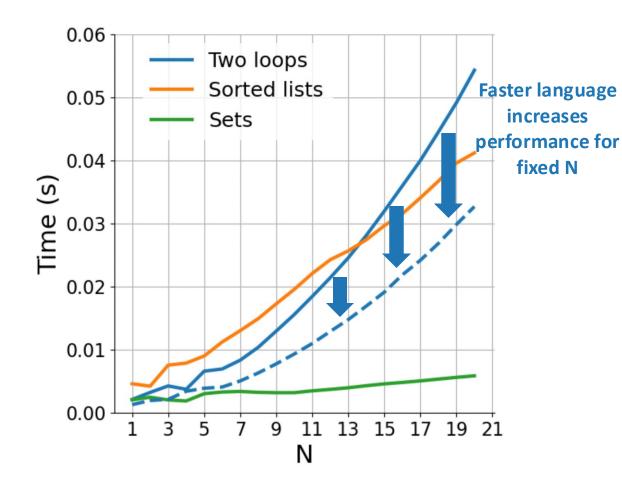




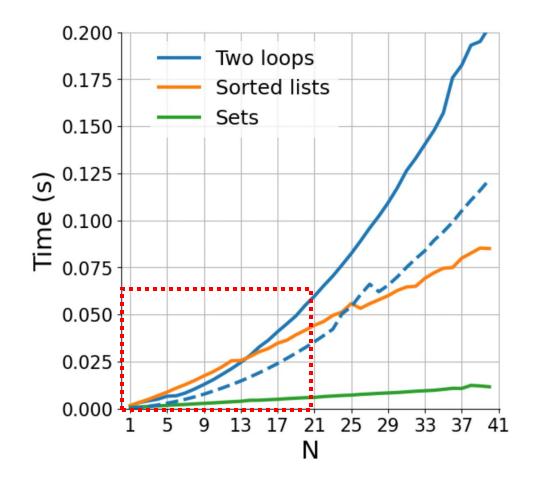
- Open the notebook match_tarots, and follow the instructions!
- Submit a PR for Issue #7 on GitHub



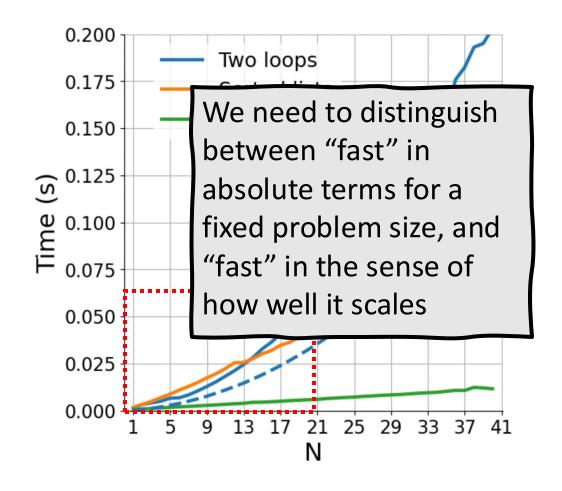






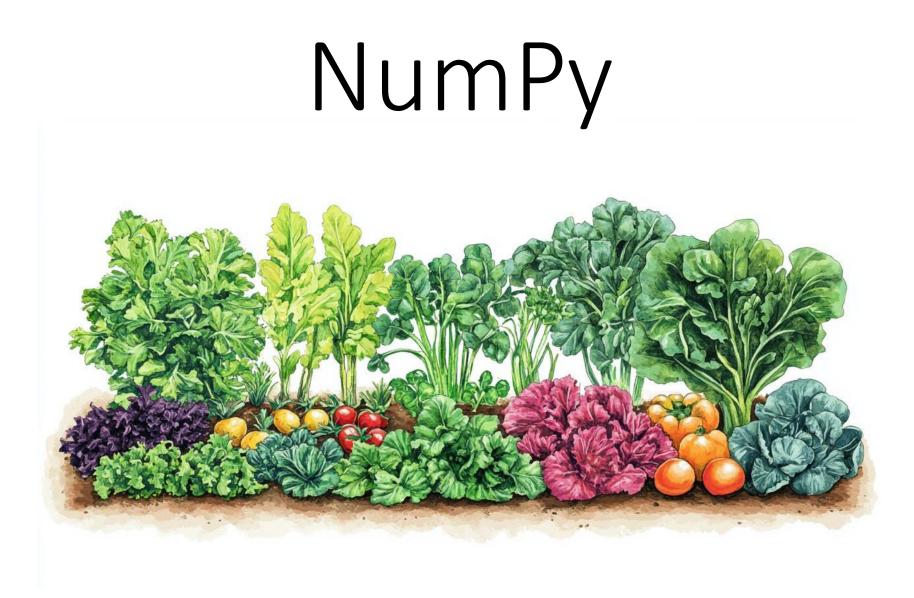








COMING UP NEXT: NumPy and the array data structure



NumPy – huh, yeah – what's it good for?

 Introduces new data structure: the array



An array is a regular, N-dimensional grid of data of the same type, typically numerical data

NumPy – huh, yeah – what's it good for?

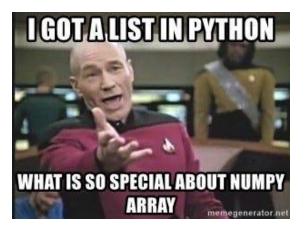
 Introduces new data structure: the array



An array is a regular, N-dimensional grid of data of the same type, typically numerical data

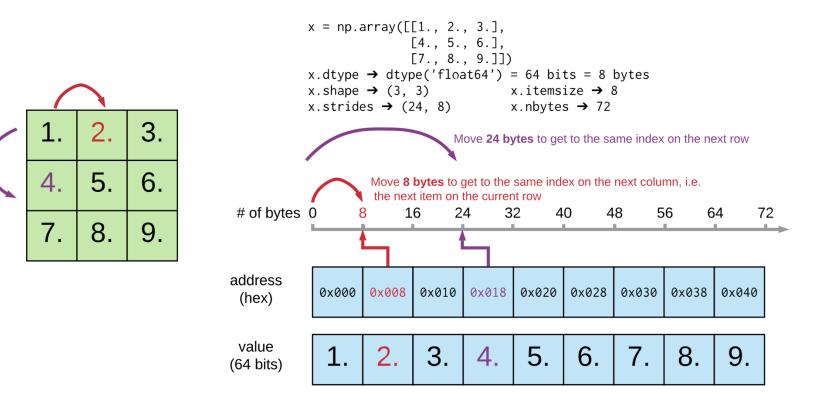
- An array could be represented as a list-of-lists
- Why are NumPy arrays better than a list-of-lists?

****Computer architecture class****



Efficiency of NumPy

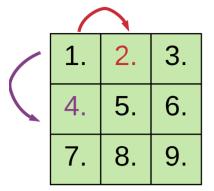
- 1) Memory:
 - data occupies the minimum amount of memory required
 - some operations can be done without touching the memory at all!



Efficiency of NumPy

1) Memory:

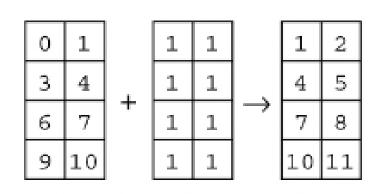
- data occupies the minimum amount of memory required
- some operations can be done without touching the memory at all!



2) Speed:

- Many operations can be done very efficiently in C. For this to be useful, we need to avoid Python forloops at all costs!
- operating on entire arrays rather than their individual elements
- \rightarrow "vectorize" the code

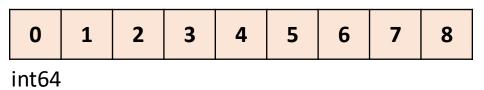
Vectorization



NumPy's memory efficiency

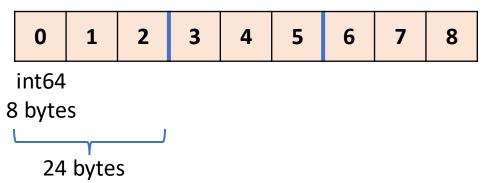


Memory block



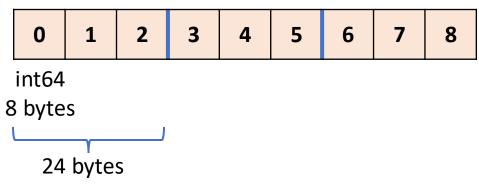
The array data is stored in a contiguous memory block, using native data types

Memory block



NumPy array metadata

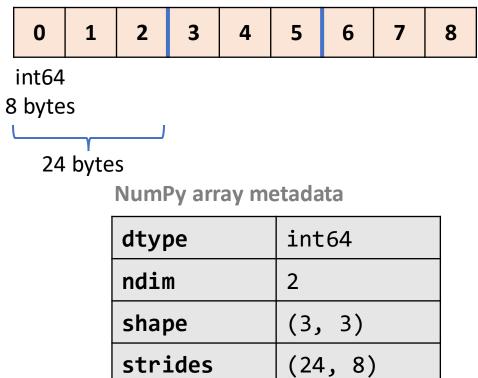
dtype	int64
ndim	2
shape	(3, 3)
strides	(24, 8)



NumPy array metadata

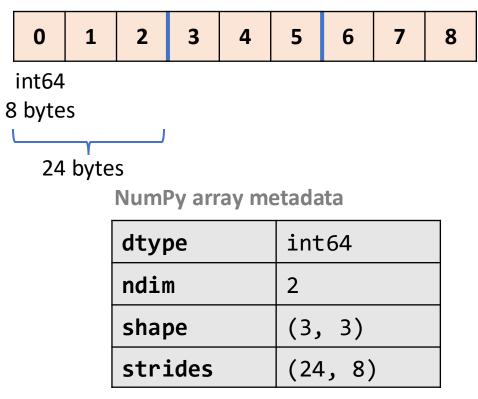
dtype	int64
ndim	2
shape	(3, 3)
strides	(24, 8)

Metadata tells NumPy how to interpret the memory block



Metadata tells NumPy how to interpret the memory block







Metadata tells NumPy how to interpret the memory block

NumPy view

0	1	2
3	4	5
6	7	8



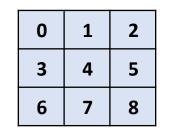
Х



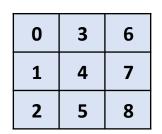
NumPy operation

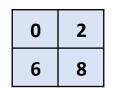
The same memory block can be interpreted in many ways

NumPy view









x.ravel()

x.T





NumPy operation



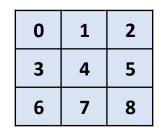






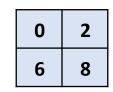
The same memory block can be interpreted in many ways

NumPy view





0	3	6
1	4	7
2	5	8



x[::2, ::2]

July 2024, CC BY-SA 4.0



NumPy operation

X

x.ravel()





July 2024, CC BY-SA 4.0

NumPy array metadata

	•
NumP	v view

The same memory block can be

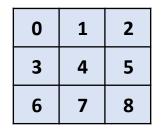
interpreted in many ways

dtype	int64
ndim	2
shape	(3, 3)
strides	(24, 8)

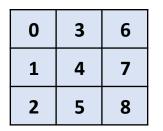
dtype	int64
ndim	1
shape	(9,)
strides	(8,)

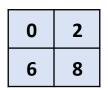
dtype	int64
ndim	2
shape	(3, 3)
strides	(8, 24)

dtype	int64
ndim	2
shape	(2, 2)
strides	(48, 16)



0 1 2 3 4 5 6 7 8







NumPy operation

very efficient --> O(1)



x.ravel()





July 2024, CC BY-SA 4.0

NumPy array metadata

dtype	int64
ndim	2
shape	(3, 3)
strides	(24, 8)

dtype	int64
ndim	1
shape	(9,)
strides	(8,)

dtype	int64
ndim	2
shape	(3, 3)
strides	(8, 24)

dtype	int64
ndim	2
shape	(2, 2)
strides	(48, 16)

There are NumPy operations that can be performed just by changing the metadata

0 3 6

0 1 2	3 4	56	7 8
-------	-----	----	-----

NumPy view

1

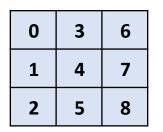
4

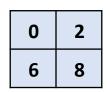
7

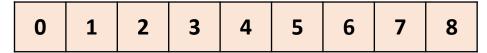
2

5

8







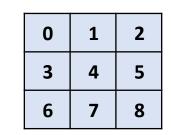
NumPy operation

X	
---	--

NumPy array metadata

dtype	int64
ndim	2
shape	(3, 3)
strides	(24, 8)

The same memory block can be interpreted in many ways



NumPy view

How does the metadata look in this case?

dtype	
ndim	
shape	
strides	

1	3	7
---	---	---

	_		_	_		_	_
/	$[\cap$	1	2],	1	\cap	11	
	Ο,	д,		11,	Ο,	_	
				L /		_	



NumPy operation

X

NumPy array metadata

dtype	int64
ndim	2
shape	(3, 3)
strides	(24, 8)

NumPy view

The same memory block can be

interpreted in many ways

0	1	2
3	4	5
6	7	8

Another memory block

1	3	7
---	---	---

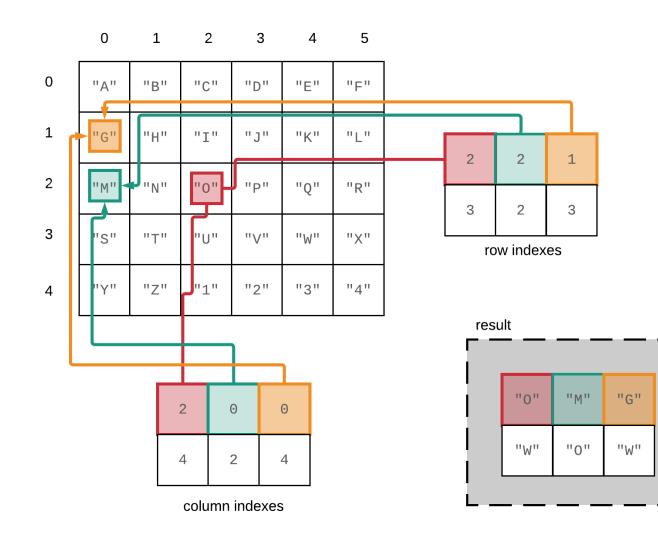
x[[0, 1, 2], [1, 0, 1]]

In this case new memory
needs to be allocated

dtype	
ndim	
shape	
strides	



Fancy indexing in NumPy – reference slide



Operations that only change the metadata return a "view " of the original memory block, otherwise a new memory block needs to be allocated, returning a "copy"



Live Coding notebooks/NumPy/NumPy_v

iews_and_copies.ipynb



NumPy views and copies



View

- accessing the array without changing the memory block
- slicing gives views
- in-place operations modify the memory block and all of its views

Сору

- when a copy of an array needs to be created, it allocates a separate memory block and associates it with a new metadata
- fancy indexing always gives copies
- a copy can be forced by method .copy()

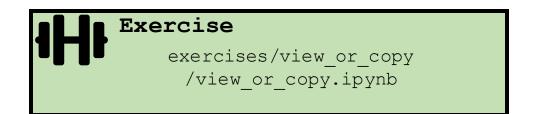
NumPy views and copies

View

- accessing the array without changing the memory block
- slicing gives views
- in-place operations modify the memory block and all of its views

Сору

- when a copy of an array needs to be created, it allocates a separate memory block and associates it with a new metadata
- fancy indexing always gives copies
- a copy can be forced by method .copy()

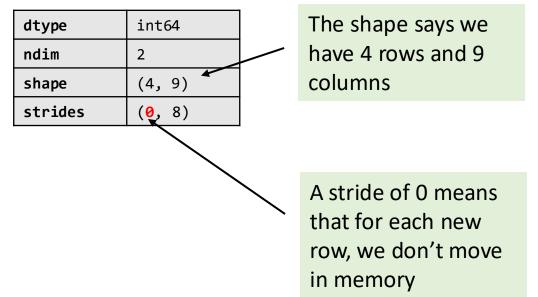


A special kind of view: broadcasting operations

Memory block



NumPy array metadata

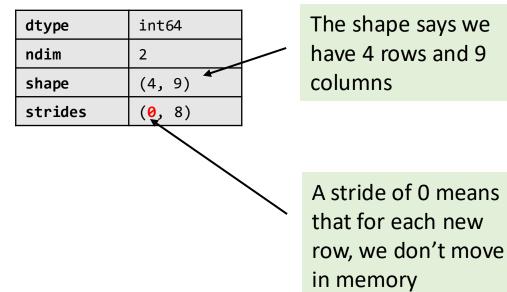


A special kind of view: broadcasting operations

Memory block



NumPy array metadata

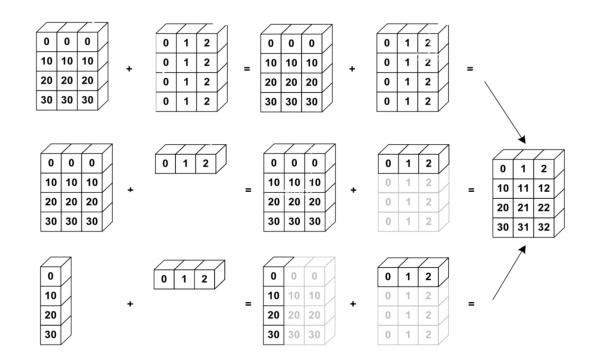


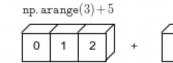
As a result, we obtain a view with duplicated rows, without using extra memory!

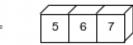
NumPy view

0	1	2	3	4	5	6	7	8
0	1	2	3	4	5	6	7	8
0	1	2	3	4	5	6	7	8
0	1	2	3	4	5	6	7	8

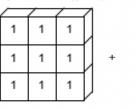
NumPy uses broadcasting to perform operation on arrays of different shape without having to allocate extra memory

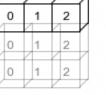






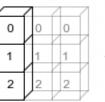
np.ones((3, 3)) + np.arange(3)





	/	/	
1	2	3	L
1	2	3	U
1	2	3	V

np. arange(3).reshape((3, 1)) + np. arange(3)





=

			Ζ
0	1	2	L
1	2	3	L
2	3	4	V



Broadcasting notebook summary



Dive in Broadcastig

notebooks/NumPy/broadcasting.ip ynb

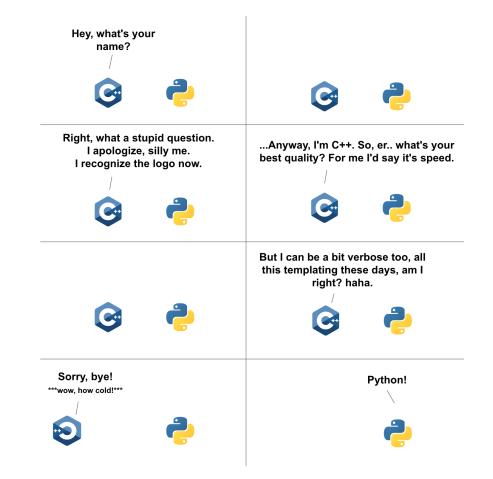
- how NumPy treats arrays with different shapes during arithmetic operations
- Rules of broadcasting
 - 1: If the two arrays differ in their number of dimensions, the shape of the one with fewer dimensions is *padded* with ones on its leading (left) side.
 - 2: If the shape of the two arrays does not match in any dimension, the array with shape equal to 1 in that dimension is stretched to match the other shape.
 - **3:** If in any dimension the sizes disagree and neither is equal to 1, an error is raised.

NumPy's speed efficiency



For-loops in Python vs in C

- Data is of a C numerical type → regular layout in memory
 - A C loop can jump from one memory location to the next by moving by "strides" bytes and accumulating the result
- To get that performance, one needs to vectorize! it's important to avoid for-loops at all costs



(with NumPy in Python)

Vectorization

operations performed on entire arrays at once

→Faster computation
 →no looping through each element individually



Vectorization



operations performed on entire arrays at once

→Faster computation
 →no looping through each element individually

Basic operators

Operator	rEquivalent ufunc	Description
+	np.add	Addition (e.g., $1 + 1 = 2$)
-	np.subtract	Subtraction (e.g., $3 - 2 = 1$)
-	np.negative	Unary negation (e.g., -2)
*	np.multiply	Multiplication (e.g., $2 * 3 = 6$)
/	np.divide	Division (e.g., 3 / 2 = 1.5)
//	np.floor_divide	e Floor division (e.g., 3 // 2 = 1)
**	np.power	Exponentiation (e.g., $2 ** 3 = 8$)
00	np.mod	Modulus/remainder (e.g., 9 % 4 =

Aggregation functions

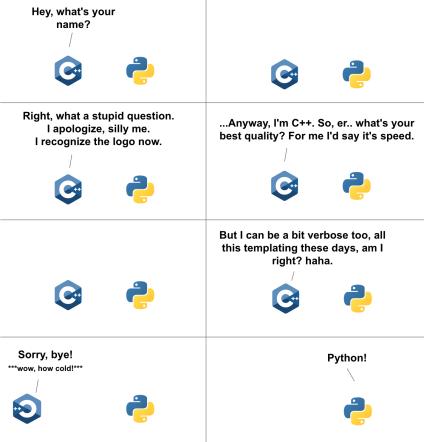
Function Name	NaN-safe Version	Description
np.sum	np.nansum	Compute sum of elements
np.prod	np.nanprod	Compute product of elements
np.mean	np.nanmean	Compute mean of elements
np.std	np.nanstd	Compute standard deviation
np.var	np.nanvar	Compute variance
np.min	np.nanmin	Find minimum value
np.max	np.nanmax	Find maximum value
np.argmin	np.nanargmin	Find index of minimum value
np.argmax	np.nanargmax	Find index of maximum value
np.median	np.nanmedian	Compute median of elements
np.percentile	np.nanpercentile	e Compute rank-based statistics of elements
np.any	N/A	Evaluate whether any elements are true
np.all	N/A	Evaluate whether all elements are true

= 1

For-loops in Python vs in C

- Data is of a C numerical type → regular layout in memory
 - A C loop can jump from one memory location to the next by moving by "strides" bytes and accumulating the result
- To get that performance, one needs to vectorize! it's important to <u>avoid for-loops at all costs</u>

How is efficiency of Python vs C in the Big-O sense?



(with NumPy in Python)

Exercise: vectorize the code





Exercise exercise

exercises/NumPy_vectorize /
 NumPy_vectorize.ipynb

Tabular data



Spreadsheets and databases rule the world!



What is tabular data?

Unlike arrays, each column can represent another type of value, with different data types

Date (index)	Wind speed	Wind direction	Rain fall (mm)	Hours of sun
7.3.2024	7.1	Ν	0.0	10
8.3.2024	0.3	NW	2.1	2
9.3.2024	1.1	SE	0.3	5

Subject ID (index)	Condition ID	Presentation nr	Response time (ms)	Response
VM	732	2	28	LEFT
VM	732	3	41	RIGHT
РВ	665	1	73	LEFT

What is tabular data?

Column and rows have meaningful labels (indices) that are attached to the data for each operation

Date (index)	Wind speed	Wind direction	Rain fall (mm)	Hours of sun
7.3.2024	7.1	Ν	0.0	10
8.3.2024	0.3	NW	2.1	2
9.3.2024	1.1	SE	0.3	5

Subject ID (index)	Condition ID	Presentation nr	Response time (ms)	Response
VM	732	2	28	LEFT
VM	732	3	41	RIGHT
PB	665	1	73	LEFT

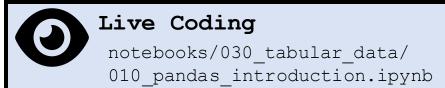
Many tools to handle tabular data

- Python tools
 - pandas: in-memory tabular data
 - dask: on-disk tabular data
- SQL databases
 - Optimized for retrieving rows (tree data structure for index)
 - Transactional: groups of operations are either all executed, or none
- Columnar DBs, Spark, Hadoop
 - Optimized for operations on columns
 - Ideal for data science tasks
 - Operations can be automatically distributed over multiple machines

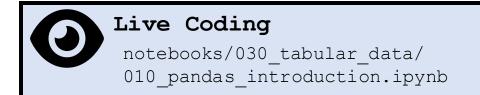
Tabular data ideas and operations are universal for all tabular data tools

- Pandas df.groupby('condition_id')['response_time'].mean()
- dask df.groupby('condition_id')['response_time'].mean()
- PySpark df.groupby('condition_id').avg('response_time')

Introduction to Pandas



Introduction to Pandas



Main points:

- A DataFrame is a tabular data structure
- DataFrames have labeled columns and rows ("indices")
- Columns can be of different C-native dtypes
- Operations are on columns by default
- NaNs are interpreted as missing data and ignored in most operations
- Strings (and dates) have a special accessor to perform vectorized string (or date) operations

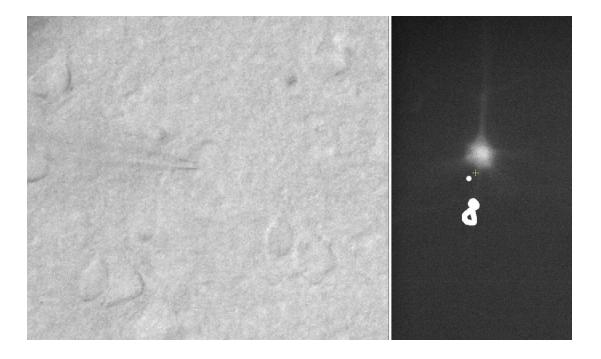
Basic Pandas reference slide

- Looking at data
 - df.head() : show the first 5 rows
 - df.tail() : show the last 5 rows
 - df.sample(n) : show n random rows
- Attributes
 - df.shape : size of the table
 - df.dtypes : print dtype of cols
 - df.columns : column index
 - df.index : rows index
- Indexing
 - df['age'] : get column 'age'
 - df[['age', 'name']] : multiple columns
 - df.iloc[0, 2] : one element, by position
- Exploration
 - df['name'].unique() : unique values
 - df['age'].describe() : summary stats
 - df['age'].value_counts(dropna=False) : number of rows per unique value in column

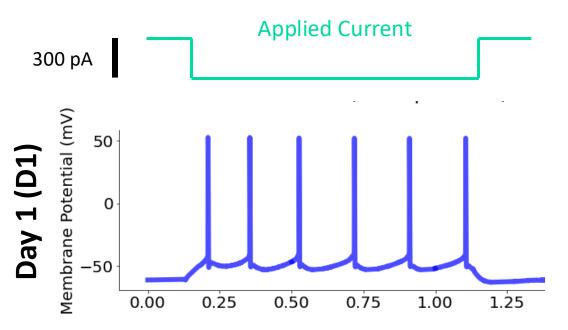
- Adding a column
 - df['new'] = df['age'] * 3.1 : add new column
- Filtering
 - df[df['age'] > 30] : select rows where condition is True
- Operations
 - df.min(), .max(), .mean(), .std(), etc. :
 column-wise operations
 - df.count() : count of non-NaN elements in columns
 - df.sort_values('name') : reorder rows by values of column 'name'
 - df.sort_index() : reorder rows by the index values
- String operations
 - df['name'].str : accessor for operations on the strings in a col
 - df['name'].str[2:4] : slice the strings in a col
 - df['name'].str.count('a') : count the letter 'a' in the string in a col

Tabular data example from the lab

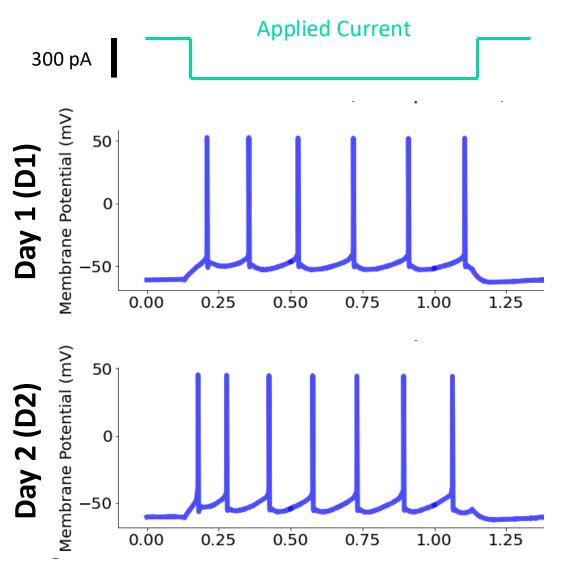
- Research question: Does neuronal activity change over time? Does this depend on the overall activity level of the neuronal network? The mainstream theory suggests that neural activity is self-regulating to maintain a baseline level ("homeostatic plasticity")
- Exp design: patch clamp recordings from the same cells (or different cells/ same slices) before and after prolonged incubation in high potassium (K)
- Potassium stimulates and TTX silences the entire network, allowing us to control the overall activity



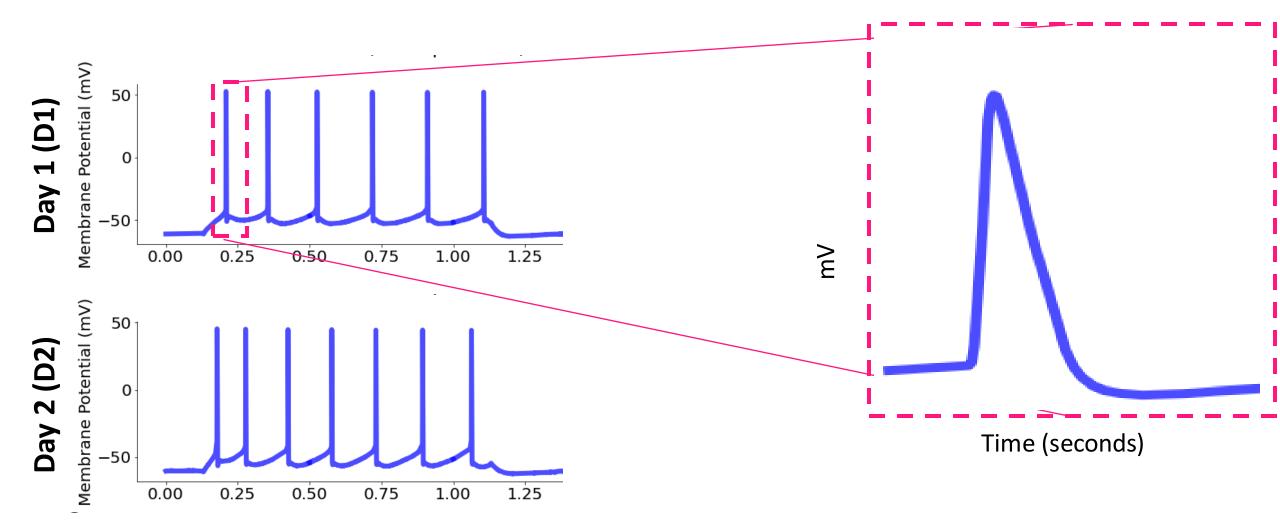
Variables



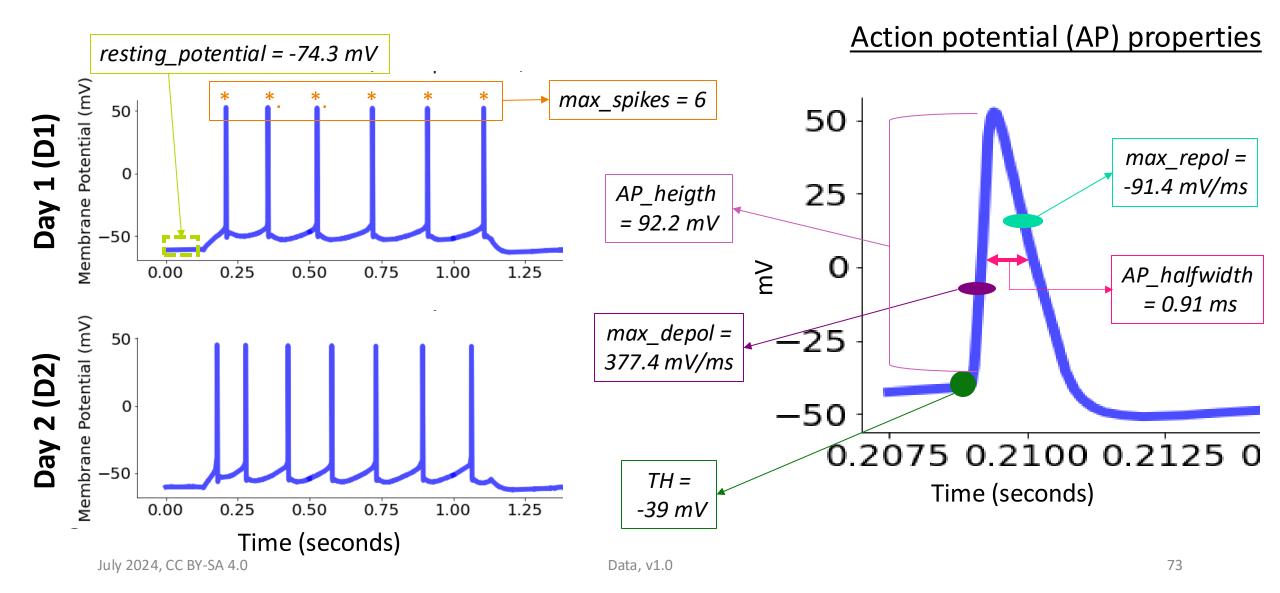
Variables



Variables



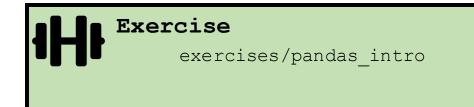
Variables



Hands-on

Let's have a look at the neural data

- Use Pandas to explore the neural data
- Submit a PR for Issue #2 on GitHub



TABULAR DATA OPERATIONS

Common operations on tabular data

- Tabular data has additional needs compared to arrays. Understanding how to vectorize these operations is critical for handling them
- Combine information across tables (join, anti-join)
 - Join: e.g., combine table with experiments results with table with experiments metadata (date, location, experimenter, free-form notes, ...)
 - Anti-join: e.g. student compiles list of outliers, exclude them from the table of experiments to analyze
- Summary tables (split-apply-combine)
 - E.g., compute average measurement and standard deviation by experimental condition and treatment dosage
- Window functions to vectorize complex computations over groups
 - E.g., compute the time distance between experiments by lab technician

Joins

Join operations: combining informations from multiple tables

subject_id	condition_id	response_time	response
312	A1	0.12	LEFT
312	A2	0.37	LEFT
312	C2	0.68	LEFT
313	A1	0.07	RIGHT
313	B1	0.08	RIGHT
314	A2	0.29	LEFT
314	B1	0.14	RIGHT
314	C2	0.73	RIGHT

	orientation	duration	surround	stimulus_type
A1	0	0.1	FULL	LINES
A2	0	0.01	NONE	DOTS
B1	45	0.1	NONE	PLAID
B2	45	0.01	FULL	PLAID
C1	90	0.2	FULL	WIGGLES

subject_id	condition_id	response_time	response	orientation	duration	surround	stimulus_type
312	A1	0.12	LEFT	0.0	0.10	FULL	LINES
312	A2	0.37	LEFT	0.0	0.01	NONE	DOTS
312	C2	0.68	LEFT	NaN	NaN	NaN	NaN
313	A1	0.07	RIGHT	0.0	0.10	FULL	LINES
313	B1	0.08	RIGHT	45.0	0.10	NONE	PLAID
314	A2	0.29	LEFT	0.0	0.01	NONE	DOTS
314	B1	0.14	RIGHT	45.0	0.10	NONE	PLAID
314	C2	0.73	RIGHT	NaN	NaN	NaN	NaN

Join operations



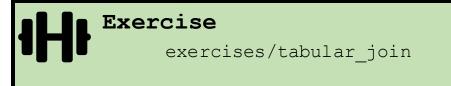
Join operations

Live Coding notebooks/tabular_data/ 020_join_operations.ipynb

Main points:

- Join operations can be used to combine two tables using the values of one or more columns
- Different types of join:
 - left/right: keep all the column values that are present in the first/second table
 - inner: keep all the column values that are present in both tables
 - outer: keep all the column values that are present in one or the other tables
- Anti-joins can be used to exclude the values that are present in one, but not the other table (filtering based on arbitrary criteria)

Hands-on



- Use joins to add experiment information to the neural data
- Use anti-joins to remove outliers
- Submit a PR for Issue #3 on GitHub

Split-apply-combine

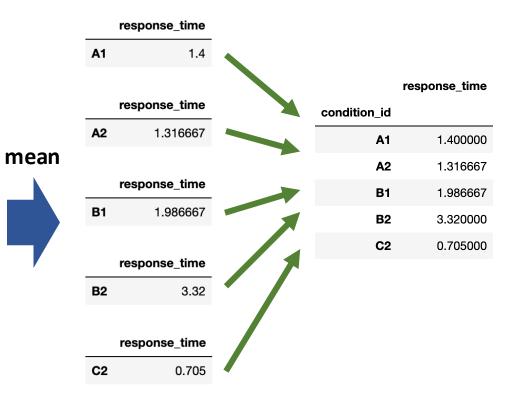
The basic structure of most numerical analyses

subject_id condition_id response_time response

combine

apply

split



	0	312	A1	0.12	LEFT
	3	313	A1	0.07	RIGHT
A1	8	711	A1	4.01	RIGHT
		subject_id	condition_id	response_time	response
A2 🛌	1	312	A2	0.37	LEFT
AZ	5	314	A2	0.29	LEFT
	9	712	A2	3.29	LEFT
B1					
DI					
DI		subject_id	condition_id	response_time	response
	4	subject_id 313	condition_id B1	response_time	response RIGHT
	4	· -			-
B1 B2		313	B1	0.08	RIGHT
	6	313 314	B1 B1	0.08	RIGHT
	6	313 314 713	B1 B1 B1	0.08	RIGHT RIGHT LEFT
	6	313 314 713	B1 B1 B1	0.08 0.14 5.74	RIGHT RIGHT LEFT

subject id condition id response time response

0.68

0.73

LEFT

RIGHT

C2

C2

	subject_id	condition_id	response_time	response
0	312	A1	0.12	LEFT
1	312	A2	0.37	LEFT
2	312	C2	0.68	LEFT
3	313	A1	0.07	RIGHT
4	313	B1	0.08	RIGHT
5	314	A2	0.29	LEFT
6	314	B1	0.14	RIGHT
7	314	C2	0.73	RIGHT
8	711	A1	4.01	RIGHT
9	712	A2	3.29	LEFT
10	713	B1	5.74	LEFT
11	714	B2	3.32	RIGHT

2

7

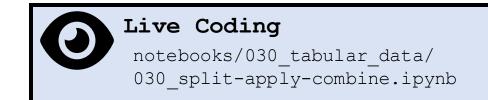
312

314

Split-apply-combine operations



Split-apply-combine operations



Main points:

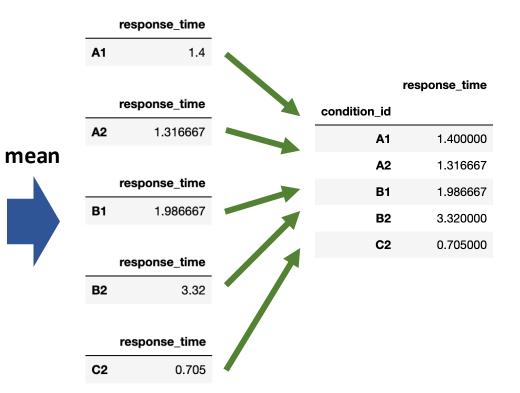
- Tabular data tools have a way to vectorize the standard split-apply-combine operations, using a "group-by" command
- In addition, Pandas has got a "pivot-table" command that can be used to simplify the creation of more complex summary tables

df.groupby('condition_id')['response_time'].mean()

combine

apply

split



		ounjootu			
	0	312	A1	0.12	LEFT
	3	313	A1	0.07	RIGHT
A1	8	711	A1	4.01	RIGHT
		subject_id	condition_id	response_time	response
A2	1	312	A2	0.37	LEFT
AZ	5	314	A2	0.29	LEFT
	9	712	A2	3.29	LEFT
B1					
		subject_id	condition_id	response_time	response
	4	313	B1	0.08	RIGHT
B2	6	314	B1	0.14	RIGHT
	10	713	B1	5.74	LEFT
C^{2}					
UZ Y		subject_id	condition_id	response_time	response

subject_id condition_id response_time response

subject_idcondition_idresponse_timeresponse0312A10.12LEFT1312A20.37LEFT2312C20.68LEFT3313A10.07RIGHT4313B10.08RIGHT5314A20.29LEFT6314B10.14RIGHT7314C20.73RIGHT8711A14.01RIGHT9712A23.29LEFT10713B15.74LEFT11714B23.32RIGHT
1 312 A2 0.37 LEFT 2 312 C2 0.68 LEFT 3 313 A1 0.07 RIGHT 4 313 B1 0.08 RIGHT 5 314 A2 0.29 LEFT 6 314 B1 0.14 RIGHT 7 314 C2 0.73 RIGHT 8 711 A1 4.01 RIGHT 9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
2 312 C2 0.68 LEFT 3 313 A1 0.07 RIGHT 4 313 B1 0.08 RIGHT 5 314 A2 0.29 LEFT 6 314 B1 0.14 RIGHT 7 314 C2 0.73 RIGHT 8 711 A1 4.01 RIGHT 9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
3 313 A1 0.07 RIGHT 4 313 B1 0.08 RIGHT 5 314 A2 0.29 LEFT 6 314 B1 0.14 RIGHT 7 314 C2 0.73 RIGHT 8 711 A1 4.01 RIGHT 9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
4 313 B1 0.08 RIGHT 5 314 A2 0.29 LEFT 6 314 B1 0.14 RIGHT 7 314 C2 0.73 RIGHT 8 711 A1 4.01 RIGHT 9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
5 314 A2 0.29 LEFT 6 314 B1 0.14 RIGHT 7 314 C2 0.73 RIGHT 8 711 A1 4.01 RIGHT 9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
6 314 B1 0.14 RIGHT 7 314 C2 0.73 RIGHT 8 711 A1 4.01 RIGHT 9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
7 314 C2 0.73 RIGHT 8 711 A1 4.01 RIGHT 9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
8 711 A1 4.01 RIGHT 9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
9 712 A2 3.29 LEFT 10 713 B1 5.74 LEFT
10 713 B1 5.74 LEFT
11 714 B2 3.32 RIGHT

data.pivot_table(index='condition_id', columns='response', values='response_time', aggfunc='mean',

split

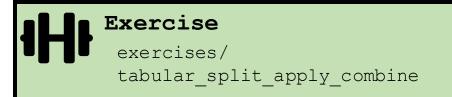
apply

combine

response	LEFT	RIGHT
ndition_id		
A1	0.12	2.04
A2	1.32	NaN
B1	5.74	0.11
B2	NaN	3.32
C2	0.68	0.73

	subject_id	condition_id	response_time	response
0	312	A1	0.12	LEFT
1	312	A2	0.37	LEFT
2	312	C2	0.68	LEFT
3	313	A1	0.07	RIGHT
4	313	B1	0.08	RIGHT
5	314	A2	0.29	LEFT
6	314	B1	0.14	RIGHT
7	314	C2	0.73	RIGHT
8	711	A1	4.01	RIGHT
9	712	A2	3.29	LEFT
10	713	B1	5.74	LEFT
11	714	B2	3.32	RIGHT

Hands-on



- Compute summary statistics for the neural data
- Submit a PR for Issue #4 on GitHub

Hands-on

Exercise exercises/tuberculosis

• Compute some summary tables for the WHO tuberculosis data



country year sp_m_014 sp_m_1524 sp_m_2534 ... sp_f_2534 sp_f_3544 sp_f_4554 sp_f_5564 sp_f_65

rownames

5551	San Marino	2009	NaN	NaN	NaN	 NaN	NaN	NaN	NaN	NaN
642	Belarus	2009	0.0	66.0	173.0	 52.0	52.0	41.0	25.0	68.0
7234	Zimbabwe	2007	138.0	500.0	3693.0	 3311.0	0.0	553.0	213.0	90.0
3471	Kuwait	2008	0.0	18.0	90.0	 47.0	27.0	7.0	5.0	6.0
3336	Jordan	2009	1.0	5.0	15.0	 14.0	8.0	3.0	7.0	12.0
2689	Grenada	2008	NaN	1.0	NaN	 NaN	NaN	NaN	NaN	NaN
634	Belarus	2001	2.0	NaN	NaN	 NaN	NaN	NaN	NaN	NaN

Tidy Data

Same data, different organization Which one is best for data analysis?

	John Smith	Jane Doe	Mary Johnson
treatmenta		16	3
treatmentb	2	11	1

name	trt	result
John Smith	a	
Jane Doe	a	16
Mary Johnson	\mathbf{a}	3
John Smith	b	2
Jane Doe	b	11
Mary Johnson	b	1

	treatmenta	treatmentb
John Smith		2
Jane Doe	16	11
Mary Johnson	3	1

Same data, different organization Which one is best for data analysis?

John Smit treatmenta — treatmentb	What do We war natural data an	tmenta — 16	treatmentb 2 11			
	name	trt	result	Mary Johnson	3	1
	John Smith	a				
	Jane Doe	a	16			
	Mary Johnson	a	3			
	John Smith	b	2			
	Jane Doe	b	11			

Tidy data

In tidy data:

- 1. Each variable forms a column
- 2. Each observation forms a row
- 3. Each type of observational unit forms a table

Variables (or features, attributes)

NS	S)
0	e
Ę	0
P	3
e z	Sa
S	
9	0

Subject ID	Condition ID	Trial nr	Response time (ms)	Response
VM	732	2	28	LEFT
VM	732	3	41	RIGHT
РВ	665	1	73	LEFT

Variables increase when new types of measurements are introduced

Observations increase when new units (dates, subjects, ...) are measured



Hands-on

Identify variables, observations, and values. What would a tidy version look like?

id	year	month	element	d1	d2	d3	d4	d5	d6	d7	d8
MX17004	2010	1	tmax								
MX17004	2010	1	tmin								
MX17004	2010	2	tmax		27.3	24.1					
MX17004	2010	2	tmin		14.4	14.4					
MX17004	2010	3	tmax					32.1			
MX17004	2010	3	tmin					14.2			
MX17004	2010	4	tmax								
MX17004	2010	4	tmin								
MX17004	2010	5	tmax								
MX17004	2010	5	tmin								

Table 11: Original weather dataset. There is a column for each possible day in the month. Columns d9 to d31 have been omitted to conserve space.

łĤł

Identify variables, observations, and values. What would a tidy version look like?

Hands-on

id	year	month	element	d1	d2	d3	d4	d5	d6	d7	d8
MX17004	2010	1	tmax								
MX17004	2010	1	tmin								
MX17004	2010	2	tmax		27.3	24.1					
MX17004	2010	2	tmin		14.4	14.4					
MX17004	2010	3	tmax					32.1			
MX17004	2010	3	tmin					14.2			
MX17004	2010	4	tmax								
MX17004	2010	4	tmin								
MX17004	2010	5	tmax								
MX17004	2010	5	tmin								

id	date	tmax	tmin
MX17004	2010-01-30	27.8	14.5
MX17004	2010-02-02	27.3	14.4
MX17004	2010-02-03	24.1	14.4
MX17004	2010-02-11	29.7	13.4
MX17004	2010-02-23	29.9	10.7
MX17004	2010-03-05	32.1	14.2
MX17004	2010-03-10	34.5	16.8
MX17004	2010-03-16	31.1	17.6
MX17004	2010-04-27	36.3	16.7
MX17004	2010-05-27	33.2	18.2

Table 11: Original weather dataset. There is a column for each possible day in the month. Columns d9 to d31 have been omitted to conserve space.

(b) Tidy data

Messy data

Variables are stored in both rows and columns



city	type	date	temperature
Bilbao	tmax	2024-07-03	34
Bilbao	tmin	2024-07-03	25
Bordeaux	tmax	2024-03-21	29
Bordeaux	tmin	2024-03-21	23
Berlin	tmax	2021-08-16	21
Berlin	tmin	2021-08-16	14
Heraklion	tmax	2021-09-01	30
Heraklion	tmin	2021-09-01	23

Column headers are values, not variable names

subject	date	Α	В
PB	2024-07-03	0.12	0.19
VM	2024-03-21	0.37	0.41
ΤZ	2021-08-16	0.68	0.73
LS	2021-09-01	0.07	0.08
ZS	2023-11-11	0.08	0.16

"Tidy datasets are all alike but every messy dataset is messy in its own way" – Hadley Wickham

Some variables are stored in the file names



2024-01_prices_DE.csv 2024-01_prices_FR.csv 2024-02_prices_DE.csv 2024-02_prices_FR.csv Multiple variables are stored in one column

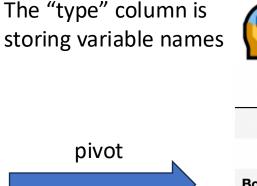


country	year	variable	cases
Angola	2000	sp_m_014	186.0
Angola	2001	sp_m_014	230.0
Angola	2002	sp_m_014	435.0
Angola	2003	sp_m_014	409.0
Angola	2004	sp_m_014	554.0
Angola	2005	sp_m_014	520.0
Angola	2006	sp_m_014	540.0

The life-changing magic of tidying up data

Pivoting – we know this one

city	type	date	temperature
Bilbao	tmax	2024-07-03	34
Bilbao	tmin	2024-07-03	25
Bordeaux	tmax	2024-03-21	29
Bordeaux	tmin	2024-03-21	23
Berlin	tmax	2021-08-16	21
Berlin	tmin	2021-08-16	14
Heraklion	tmax	2021-09-01	30
Heraklion	tmin	2021-09-01	23



city	date		
Berlin	2021-08-16	21	14
Bilbao	2024-07-03	34	25
Bordeaux	2024-03-21	29	23
Heraklion	2021-09-01	30	23

type tmax tmin



```
df.pivot_table(
    index=['city', 'date'], columns='type',
    values='temperature', aggfunc='max',
```

The life-changing magic of tidying up data

Melting – it's kind of the opposite of pivoting

The treatment values are stored as a column name

ubject	date	Α	В
PB	2024-07-03	0.12	0.19
VM	2024-03-21	0.37	0.41
ΤZ	2021-08-16	0.68	0.73
LS	2021-09-01	0.07	0.08
ZS	2023-11-11	0.08	0.16



pd.melt(data, id_vars=['subject', 'date'], value_name='response_time')

subject

PB 2024-07-03

VM 2024-03-21

date variable response_time

0.12

0.37

Α

Α

Split the columns in (A) "id_vars" and (B) non-"id_vars". The column names in (B) are used as new values in a new column "variable". The values in columns (B) go into a new column, "response_time".

The life-changing magic of tidying up data

pd.concat – add together tables with the same variables (columns)

Some variables are stored in the file names



2024-01_prices_DE.csv 2024-01_prices_FR.csv 2024-02_prices_DE.csv 2024-02_prices_FR.csv

```
tables = []
for filename in filenames:
    # Parse filename
    year_month, _, country = filename[:-4].split('_')
    # Read table and add columns for the variables
    df = pd.read_csv(filename)
    # Add the variables that were in the filename
    df['year_month'] = year_month
    df['country'] = country
    # Store table
    tables.append(df)
# Create complete table
```

```
tidy_df = pd.concat(tables)
```

Hands-on

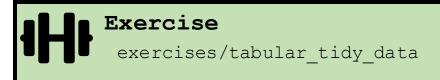
• Tidy up the data set in the tuberculosis exercise and compute the summary stats

Data, v1.0

Submit a PR for Issue #5 on GitHub

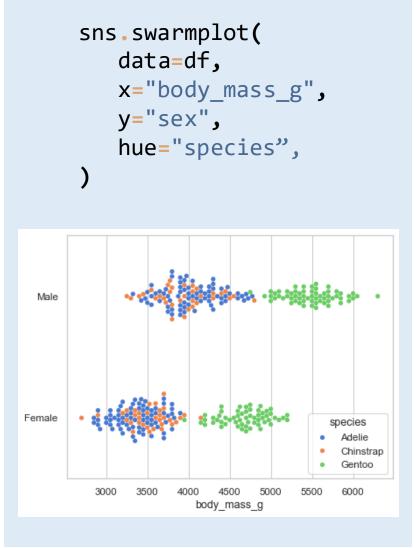
Multiple variables are stored in one column

year	variable	cases
2000	sp_m_014	186.0
2001	sp_m_014	230.0
2002	sp_m_014	435.0
2003	sp_m_014	409.0
2004	sp_m_014	554.0
2005	sp_m_014	520.0
2006	sp_m_014	540.0
	2000 2001 2002 2003 2004 2005	2000 sp_m_014 2001 sp_m_014 2002 sp_m_014 2003 sp_m_014 2004 sp_m_014 2005 sp_m_014



Why is tidy data good?

- Many analyses require a simple sequence of steps:
 - Filter by individual variables to discard data that is not needed
 - Group and summarize
 - Re-arrange (e.g. sort)
 - Visualize
- Joining tidy tables is easy!
- One can write generic code that takes tidy data as input.
 For example, seaborn relies on tidy data to make complex plots



Window functions

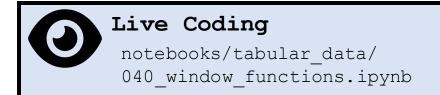
Window functions: grouped row-by-row operations

- "Window functions" are a kind of split-apply-combine operation, but instead of aggregating the data in a group and returning one value per group, they return one value per row
- Examples: ranking all entries in a group; computing the distance between timestamps per group; number the rows by group in chronological order
- In Pandas, most of these operations can be performed with a combination of sorting and grouping-by

Window functions



Window functions



- Main points:
 - Window functions perform row-by-row operations on grouped data
 - They are an advanced way of avoiding for loops with tabular data
 - In Pandas, they can be achieved with a combo of sorting and grouping-by

Window functions operations

df['nr_lefts'] = df.sort_values('time (ms)').groupby('subject_id')['is_left'].cumsum()

	subject_id	time (ms)	response	is_left		nr_lefts							
1602	1	43	RIGHT	False	1602	0							
785	1	121	LEFT	True	785	1			subject_id	time (ms)	response	is_left	nr_lefts
413	1	471	LEFT	True	413	2		1602	1	43	RIGHT	False	0
902	1	1093	LEFT	True	902	3		785	1	121	LEFT	True	1
								413	1	471	LEFT	True	2
	subject_id	time (ms)	response	is_left		nr_lefts		902	1	1093	LEFT	True	3
1486	2	3	RIGHT	False	1486	0		1486	2	3	RIGHT	False	0
629	2	353	LEFT	True	629	1		629	2	353	LEFT	True	1
1190	2	552	LEFT	True	1190	2		1190	2	552	LEFT	True	2
158	2	743	RIGHT	False	158	2		158	2	743	RIGHT	False	2
1393	2	903	RIGHT	False	1393	2		1393 1895	2	903 1036	RIGHT	False True	2 3
1895	2	1036	LEFT	True	1895	3		53	3	257	RIGHT	False	0
							1	574	3	540	RIGHT	False	0
	subject_id	time (ms)	response	is_left		nr_lefts		551	3	619	LEFT	True	1
53	3	257	RIGHT	False	53	0		1829	3	768	RIGHT	False	1
574	3	540	RIGHT	False	574	0							
551	3	619	LEFT	True	551	1							
1829	3	768	RIGHT	False	1829	1							

	subject_id	time (ms)	response	is_left
574	3	540	RIGHT	False
1190	2	552	LEFT	True
1895	2	1036	LEFT	True
53	3	257	RIGHT	False
158	2	743	RIGHT	False
551	3	619	LEFT	True
1602	1	43	RIGHT	False
413	1	471	LEFT	True
785	1	121	LEFT	True
1393	2	903	RIGHT	False
629	2	353	LEFT	True
1829	3	768	RIGHT	False
902	1	1093	LEFT	True
1486	2	3	RIGHT	False



	Exercise exercises/
П	exercises/
	tabular_window_functions

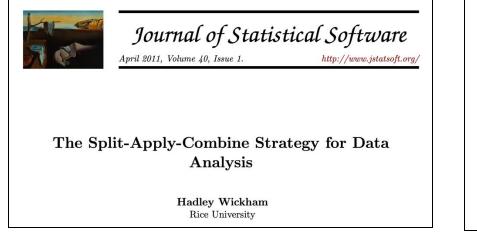
- Compute the average number of days each patcher waited between experiments
- Submit a PR for Issue #6 on GitHub

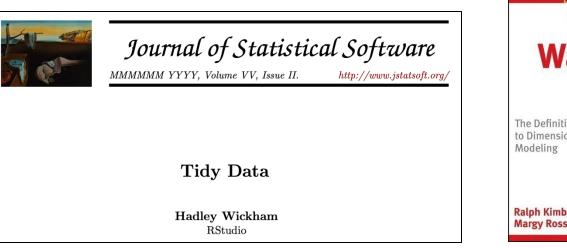
Global summary

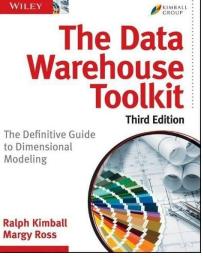
- There are many different data structures, each specialized in efficiently processing one type of data
- Code performance grows differently with data size: Big-O
- NumPy array efficiently store data in a C-native memory block, interpreted as an array using some metadata
- NumPy operations that only need to change the metadata do so, creating a view of the same memory block. These operations are O(1)!
- Tabular data can also be vectorized using joins, anti-joins, split-apply-combine operations, and window functions
- For these operations to be efficient and painless, data should be stored in a tidy data format

What we didn't talk about

- Other data structures: graphs, trees, priority queues, ...
- Options for working with large data on disk / remotely (instead of in-memory)
- Best practices in data handling: versioning, lineage, sharing
- Organizing a complex data set in multiple tables
- ... and a lot more!







Thank you!



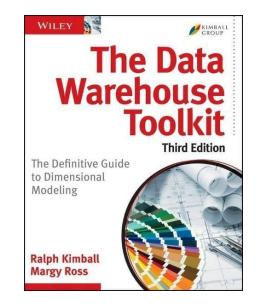
Data organization

- Data organization concepts:
 - tidy data
 - normalized data (star organization)
 - data science friendly data (denormalized)

Organizing multiple tables

- Dimension vs fact tables
- De-normalization (but for data analys flat tables are more convienent)

				-		
id	artist	track	time	id	date	rank
1	2 Pac	Baby Don't Cry	4:22	1	2000-02-26	87
2	2Ge+her	The Hardest Part Of	3:15	1	2000-03-04	82
3	3 Doors Down	Kryptonite	3:53	1	2000-03-11	72
4	3 Doors Down	Loser	4:24	1	2000-03-18	77
5	504 Boyz	Wobble Wobble	3:35	1	2000-03-25	87
6	98^0	Give Me Just One Nig	3:24	1	2000-04-01	94
7	A*Teens	Dancing Queen	3:44	1	2000-04-08	99
8	Aaliyah	I Don't Wanna	4:15	2	2000-09-02	91
9	Aaliyah	Try Again	4:03	2	2000-09-09	87
10	Adams, Yolanda	Open My Heart	5:30	2	2000-09-16	92
11	Adkins, Trace	More	3:05	3	2000-04-08	81
12	Aguilera, Christina	Come On Over Baby	3:38	3	2000-04-15	70
13	Aguilera, Christina	I Turn To You	4:00	3	2000-04-22	68
14	Aguilera, Christina	What A Girl Wants	3:18	3	2000-04-29	67
15	Alice Deejay	Better Off Alone	6:50	3	2000-05-06	66



Dealing with changes in the data

- Recommendations:
 - NEVER overwite a data file. Treat data files as immutable
 - Use versioning for changes in the data file, and load the latest version for new analyses, old versions to reproduce previous results
 - (pond is a library I'm working on to automatize this process)
- Like in computer code:
 - Adding new columns / rows is generally ok
 - Deleting/changing a column is not! Code will break! Add a new column instead