INTRODUCTION TO DATA SCIENCE

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Lecture #6 – 9/17/2018

CMSC320
Mondays and Wednesdays
2pm – 3:15pm

COMPUTER SCIENCE
UNIVERSITY OF MARYLAND

ANNOUNCEMENTS

Project 1 is out!

- Announced on ELMS and Piazza
- https://github.com/JohnDickerson/cmsc320-fall2018/tree/master/project1
- Due date is September 28th

LAST CLASS/THIS CLASS

1. **NumPy: Python Library for Manipulating nD Arrays**

   Multidimensional Arrays, and a variety of operations including Linear Algebra

2. **Pandas: Python Library for Manipulating Tabular Data**

   Series, Tables (also called **DataFrames**)
   Many operations to manipulate and combine tables/series

3. **Relational Databases**

   Tables/Relations, and SQL (similar to Pandas operations)

4. **Apache Spark**

   Sets of objects or key-value pairs
   MapReduce and SQL-like operations

TABLES

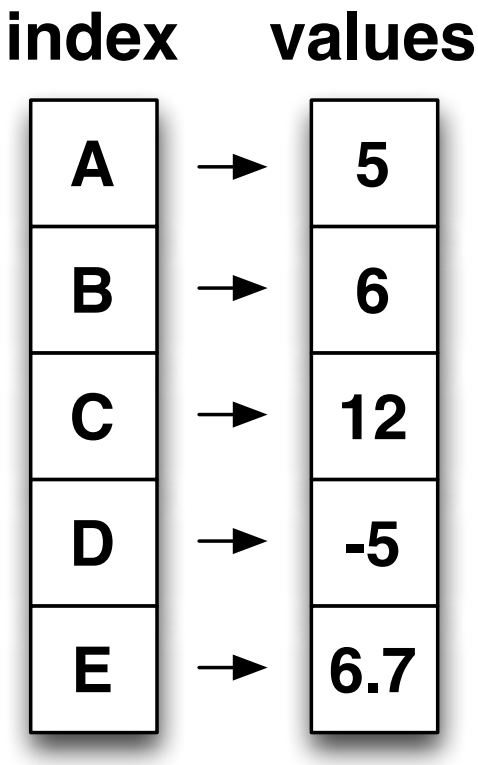
Special Column, called “Index”, or “ID”, or “Key”
Usually, no duplicates Allowed

Variables
(also called Attributes, or Columns, or Labels)

Observations, Rows, or Tuples

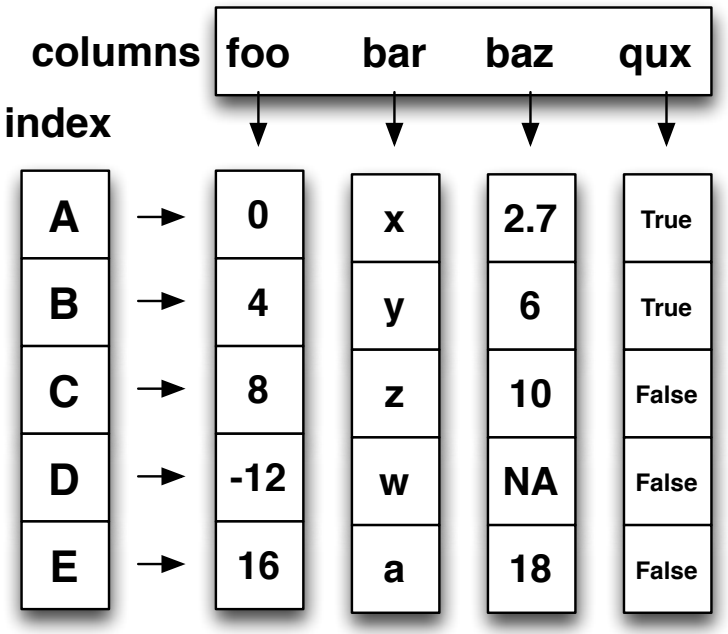
ID	age	wgt_kg	hgt_cm
1	12.2	42.3	145.1
2	11.0	40.8	143.8
3	15.6	65.3	165.3
4	35.1	84.2	185.8

PANDAS: SERIES



- Subclass of numpy.ndarray
- Data: any type
- Index labels need not be ordered
- Duplicates possible but result in reduced functionality

PANDAS: DATAFRAME



- Each column can have a different type
- Row and Column index
- Mutable size: insert and delete columns

- Note the use of word “index” for what we called “key”
  - Relational databases use “index” to mean something else
- Non-unique index values allowed
  - May raise an exception for some operations

RECAP: GROUP BY

Group tuples together by column/dimension

ID	A	B	C
1	foo	3	6.6
2	bar	2	4.7
3	foo	4	3.1
4	foo	3	8.0
5	bar	1	1.2
6	bar	2	2.5
7	foo	4	2.3
8	foo	3	8.0

A = foo

ID	B	C
1	3	6.6
3	4	3.1
4	3	8.0
7	4	2.3
8	3	8.0

A = bar

ID	B	C
2	2	4.7
5	1	1.2
6	2	2.5

RECAP: GROUP BY

Group tuples together by column/dimension

ID	A	B	C
1	foo	3	6.6
2	bar	2	4.7
3	foo	4	3.1
4	foo	3	8.0
5	bar	1	1.2
6	bar	2	2.5
7	foo	4	2.3
8	foo	3	8.0

B = 1

ID	A	C
5	bar	1.2

B = 2

ID	A	C
2	bar	4.7
6	bar	2.5

B = 3

ID	A	C
1	foo	6.6
4	foo	8.0
8	foo	8.0

B = 4

ID	A	C
3	foo	3.1
7	foo	2.3

RECAP: GROUP BY

Group tuples together by column/dimension

ID	A	B	C
1	foo	3	6.6
2	bar	2	4.7
3	foo	4	3.1
4	foo	3	8.0
5	bar	1	1.2
6	bar	2	2.5
7	foo	4	2.3
8	foo	3	8.0

A = bar, B = 1

ID	C
5	1.2

A = bar, B = 2

ID	C
2	4.7
6	2.5

A = foo, B = 3

ID	C
1	6.6
4	8.0
8	8.0

A = foo, B = 4

ID	C
3	3.1
7	2.3

RECAP: GROUP BY AGGREGATE

Compute one aggregate

Per group

ID	A	B	C
1	foo	3	6.6
2	bar	2	4.7
3	foo	4	3.1
4	foo	3	8.0
5	bar	1	1.2
6	bar	2	2.5
7	foo	4	2.3
8	foo	3	8.0

Group by ‘B’
Sum on C

B = 1

ID	A	C
5	bar	1.2

B = 1

Sum (C)
1.2

B = 2

ID	A	C
2	bar	4.7
6	bar	2.5

B = 2

Sum (C)
7.2

B = 3

ID	A	C
1	foo	6.6
4	foo	8.0
8	foo	8.0

B = 3

Sum (C)
22.6

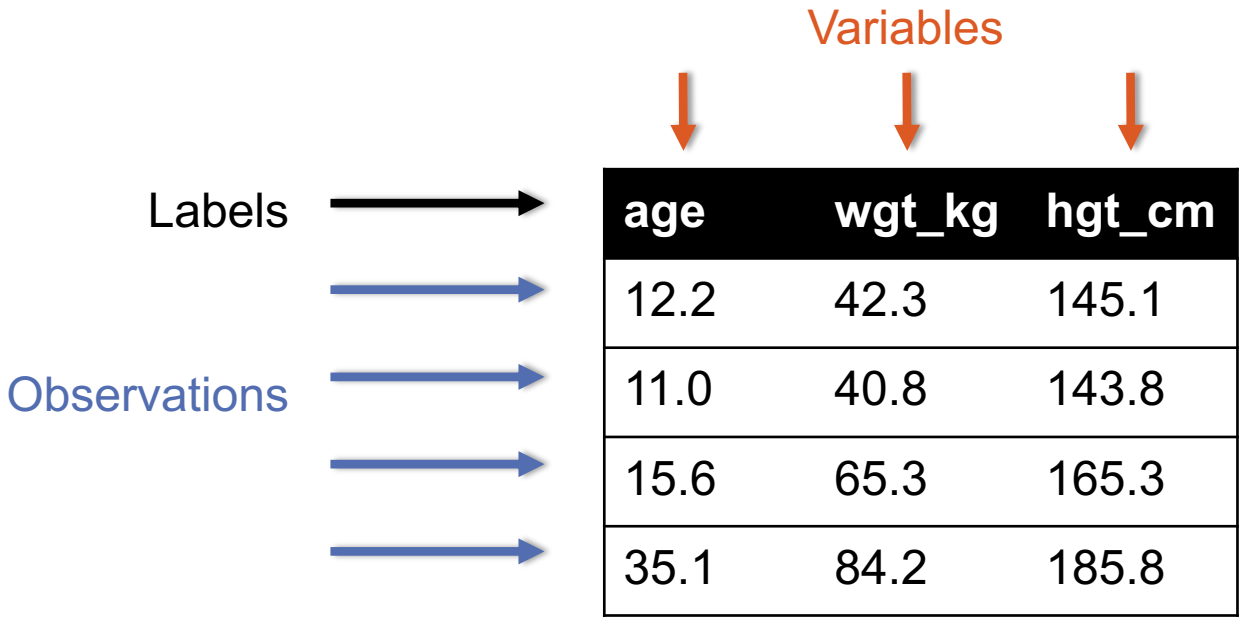
B = 4

ID	A	C
3	foo	3.1
7	foo	2.3

B = 4

Sum (C)
5.4

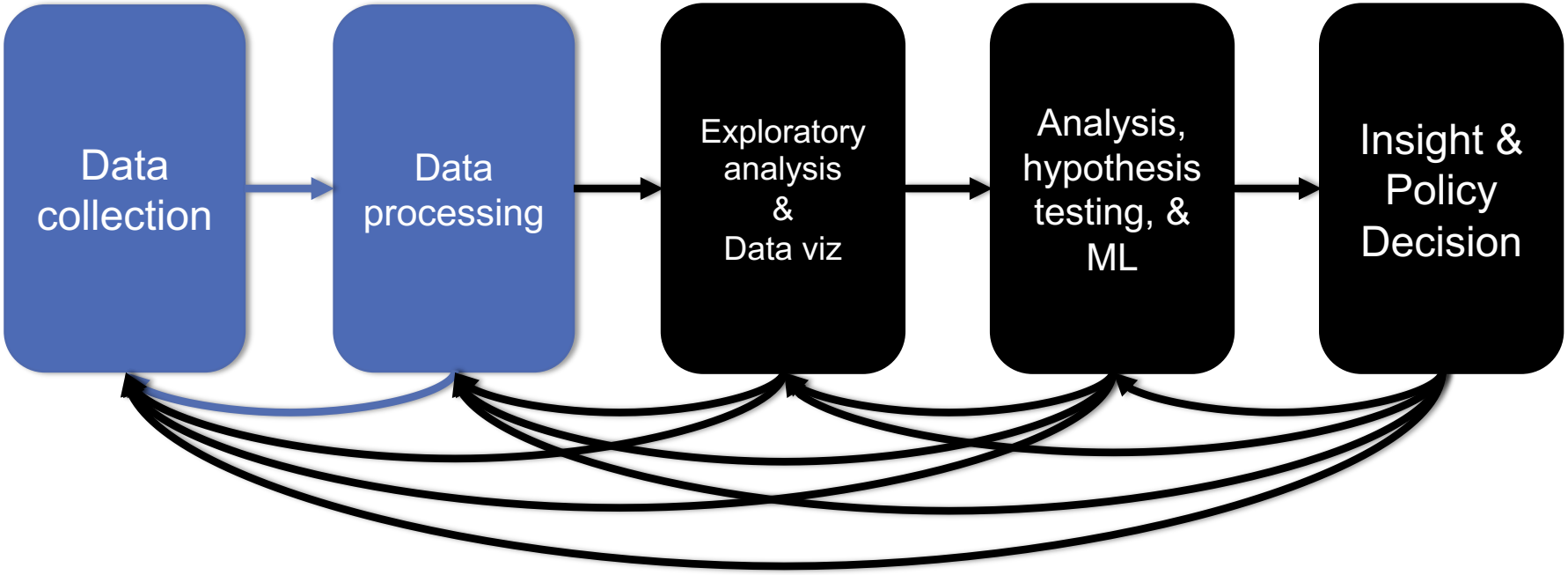
TIDY DATA



But also:

- **Names of files/DataFrames = description of one dataset**
- **Enforce one data type per dataset (ish)**

TODAY'S LECTURE



TODAY'S LECTURE

Relational data:

- What is a relation, and how do they interact?

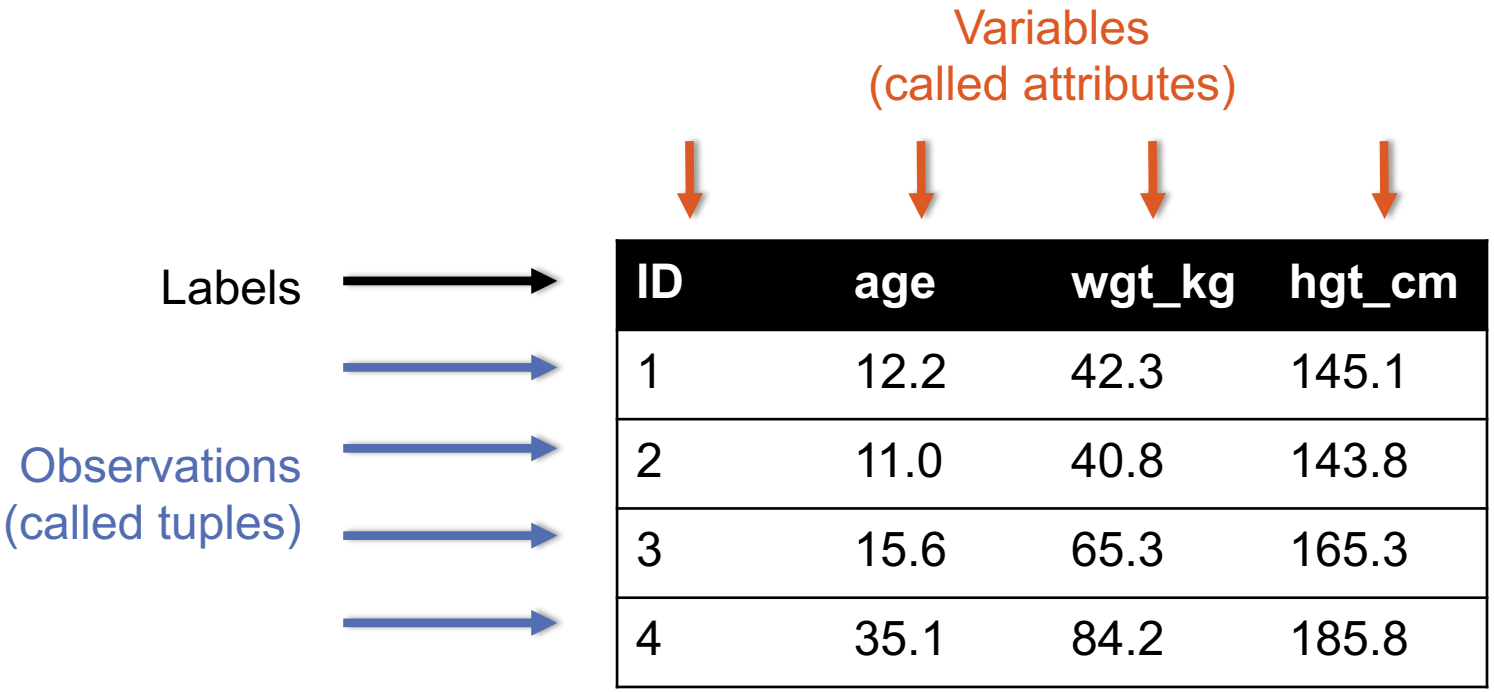
Querying databases:

- SQL
- SQLite
- How does this relate to `pandas`?

Joins

RELATION

Simplest relation: a table aka tabular data full of unique tuples



ID	age	wgt_kg	hgt_cm
1	12.2	42.3	145.1
2	11.0	40.8	143.8
3	15.6	65.3	165.3
4	35.1	84.2	185.8

PRIMARY KEYS

ID	age	wgt_kg	hgt_cm	nat_id
1	12.2	42.3	145.1	1
2	11.0	40.8	143.8	1
3	15.6	65.3	165.3	2
4	35.1	84.2	185.8	1
5	18.1	62.2	176.2	3
6	19.6	82.1	180.1	1

ID	Nationality
1	USA
2	Canada
3	Mexico

The primary key is a unique identifier for every tuple in a relation

- **Each tuple has exactly one primary key**

FOREIGN KEYS

ID	age	wgt_kg	hgt_cm	nat_id
1	12.2	42.3	145.1	1
2	11.0	40.8	143.8	1
3	15.6	65.3	165.3	2
4	35.1	84.2	185.8	1
5	18.1	62.2	176.2	3
6	19.6	82.1	180.1	1

ID	Nationality
1	USA
2	Canada
3	Mexico

Foreign keys are attributes (columns) that point to a different table's primary key

- **A table can have multiple foreign keys**

SEARCHING FOR ELEMENTS

Find all people with nationality Canada (nat_id = 2):

??????????????

ID	age	wgt_kg	hgt_cm	nat_id
1	12.2	42.3	145.1	1
2	11.0	40.8	143.8	1
3	15.6	65.3	165.3	2
4	35.1	84.2	185.8	1
5	18.1	62.2	176.2	3
6	19.6	82.1	180.1	1

O(n) 

INDEXES

Like a hidden sorted map of references to a specific attribute (column) in a table; allows O(log n) lookup instead of O(n)

loc	ID	age	wgt_kg	hgt_cm	nat_id
0	1	12.2	42.3	145.1	1
128	2	11.0	40.8	143.8	2
256	3	15.6	65.3	165.3	2
384	4	35.1	84.2	185.8	1
512	5	18.1	62.2	176.2	3
640	6	19.6	82.1	180.1	1

nat_id	locs
1	0, 384, 640
2	128, 256
3	512

INDEXES

Actually implemented with data structures like B-trees

- (Take courses like CMSC424 or CMSC420)

But: indexes are not free

- Takes memory to store
- Takes time to build
- Takes time to update (add/delete a row, update the column)

But, but: one index is (mostly) free

- Index will be built automatically on the primary key

Think before you build/maintain an index on other attributes!

RELATIONSHIPS

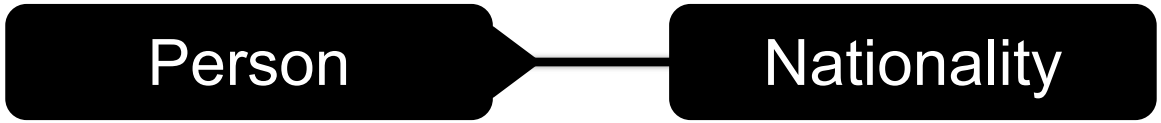
Primary keys and foreign keys define interactions between different tables aka entities. Four types:

- One-to-one
- One-to-one-or-none
- One-to-many and many-to-one
- Many-to-many

Connects (one, many) of the rows in one table to (one, many) of the rows in another table

ONE-TO-MANY & MANY-TO-ONE

One person can have one nationality in this example, but one nationality can include many people.



ID	age	wgt_kg	hgt_cm	nat_id
1	12.2	42.3	145.1	1
2	11.0	40.8	143.8	1
3	15.6	65.3	165.3	2
4	35.1	84.2	185.8	1
5	18.1	62.2	176.2	3
6	19.6	82.1	180.1	1

ID	Nationality
1	USA
2	Canada
3	Mexico

ONE-TO-ONE

Two tables have a one-to-one relationship if every tuple in the first tables corresponds to exactly one entry in the other

In general, you won't be using these (why not just merge the rows into one table?) unless:

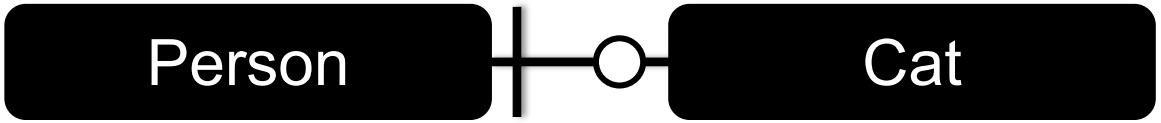
- Split a big row between SSD and HDD or distributed
- Restrict access to part of a row (some DBMSs allow column-level access control, but not all)
- Caching, partitioning, & serious stuff: take CMSC424

ONE-TO-ONE-OR-NONE

Say we want to keep track of people's cats:

Person ID	Cat1	Cat2
1	Chairman Meow	Fuzz Aldrin
4	Anderson Pooper	Meowly Cyrus
5	Gigabyte	Megabyte

People with IDs 2 and 3 do not own cats*, and are not in the table. Each person has at most one entry in the table.



Is this data tidy?

*nor do they have hearts, apparently.

MANY-TO-MANY

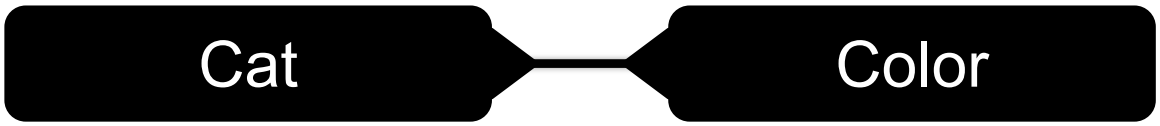
Say we want to keep track of people's cats' colorings:

ID	Name
1	Megabyte
2	Meowly Cyrus
3	Fuzz Aldrin
4	Chairman Meow
5	Anderson Pooper
6	Gigabyte

Cat ID	Color ID	Amount
1	1	50
1	2	50
2	2	20
2	4	40
2	5	40
3	1	100

One column per color, too many columns, too many nulls

Each cat can have many colors, and each color many cats



ASSOCIATIVE TABLES

Cats

ID	Name
1	Megabyte
2	Meowly Cyrus
3	Fuzz Aldrin
4	Chairman Meow
5	Anderson Pooper
6	Gigabyte

Cat ID	Color ID	Amount
1	1	50
1	2	50
2	2	20
2	4	40
2	5	40
3	1	100

Colors

ID	Name
1	Black
2	Brown
3	White
4	Orange
5	Neon Green
6	Invisible

Primary key ??????????

- [Cat ID, Color ID] (+ [Color ID, Cat ID], case-dependent)

Foreign key(s) ??????????

- Cat ID and Color ID

ASIDE: PANDAS

So, this kinda feels like pandas …

- And pandas kinda feels like a relational data system …

Pandas is not strictly a relational data system:

- No notion of primary / foreign keys

It does have indexes (and multi-column indexes):

- pandas.Index: ordered, sliceable set storing axis labels
- pandas.MultiIndex: hierarchical index

Rule of thumb: do heavy, rough lifting at the relational DB level, then fine-grained slicing and dicing and viz with pandas

SQLITE

On-disk relational database management system (RDMS)

- Applications connect directly to a file

Most RDMSs have applications connect to a server:

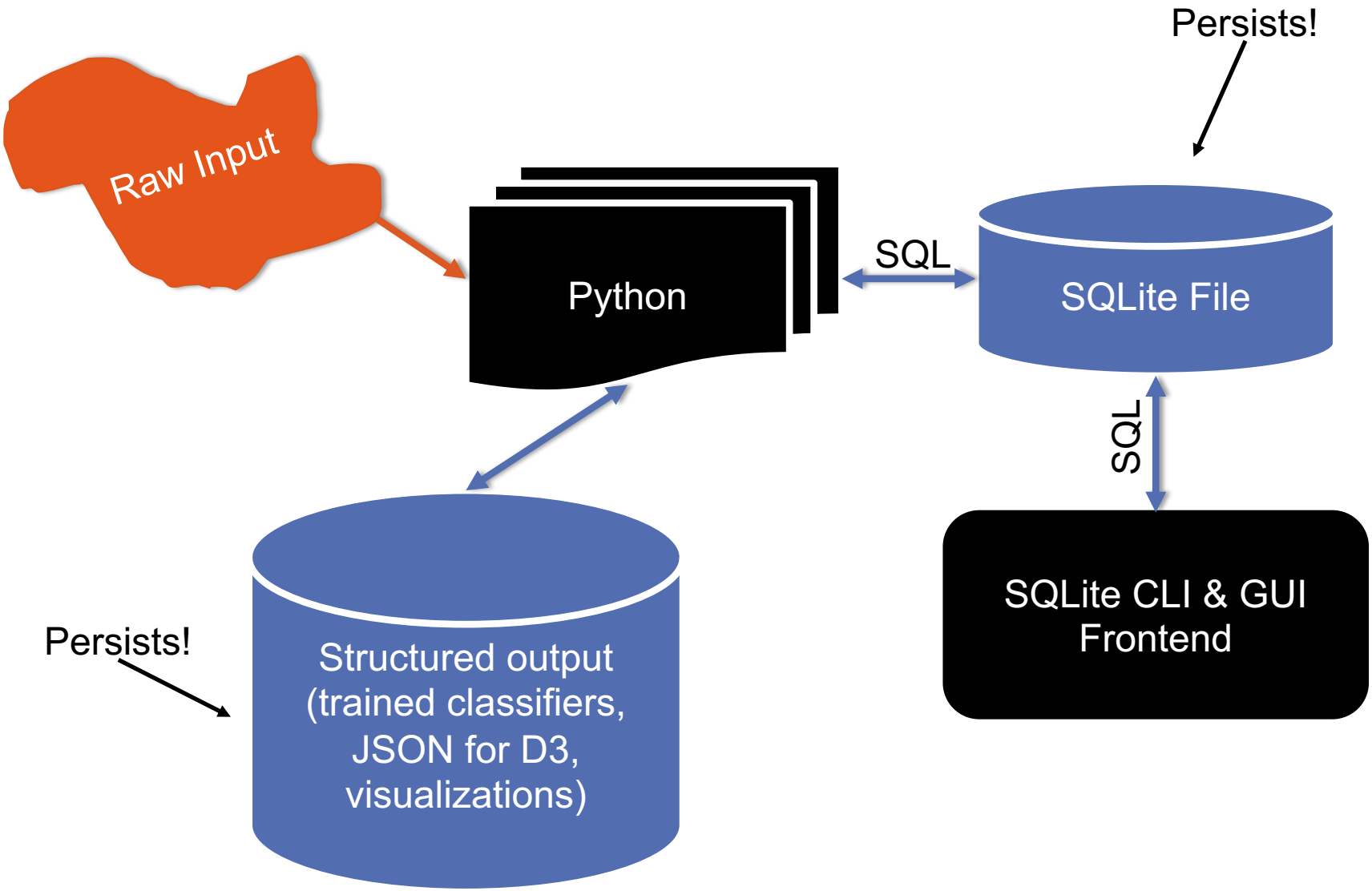
- Advantages include greater concurrency, less restrictive locking
- Disadvantages include, for this class, setup time ☺

Installation:

- `conda install -c anaconda sqlite`
- (Should come preinstalled, I think?)

All interactions use Structured Query Language (SQL)

HOW A RELATIONAL DB FITS INTO YOUR WORKFLOW



CRASH COURSE IN SQL (IN PYTHON)

```
import sqlite3

# Create a database and connect to it
conn = sqlite3.connect("cmsc320.db")
cursor = conn.cursor()

# do cool stuff
conn.close()
```

Cursor: temporary work area in system memory for manipulating SQL statements and return values

If you do not close the connection (`conn.close()`), any outstanding transaction is rolled back

- (More on this in a bit.)

CRASH COURSE IN SQL (IN PYTHON)

```
# Make a table
cursor.execute("""
CREATE TABLE cats (
    id INTEGER PRIMARY KEY,
    name TEXT
)""")
```

????????

id	name

cats

Capitalization doesn't matter for SQL reserved words

- **SELECT = select = SeLeCt**

Rule of thumb: capitalize keywords for readability

CRASH COURSE IN SQL (IN PYTHON)

```
# Insert into the table
cursor.execute("INSERT INTO cats VALUE (1, 'Megabyte')")
cursor.execute("INSERT INTO cats VALUE (2, 'Meowly Cyrus')")
cursor.execute("INSERT INTO cats VALUE (3, 'Fuzz Aldrin')")
conn.commit()
```

id	name
1	Megabyte
2	Meowly Cyrus
3	Fuzz Aldrin

```
# Delete row(s) from the table
cursor.execute("DELETE FROM cats WHERE id == 2");
conn.commit()
```

id	name
1	Megabyte
3	Fuzz Aldrin

CRASH COURSE IN SQL (IN PYTHON)

```
# Read all rows from a table
for row in cursor.execute("SELECT * FROM cats"):
    print(row)
```

```
# Read all rows into pandas DataFrame
pd.read_sql_query("SELECT * FROM cats", conn, index_col="id")
```

id	name
1	Megabyte
3	Fuzz Aldrin

index_col="id": treat column with label "id" as an index

index_col=1: treat column #1 (i.e., "name") as an index

(Can also do multi-indexing.)

JOINING DATA

A join operation merges two or more tables into a single relation. Different ways of doing this:

- Inner
- Left
- Right
- Full Outer

Join operations are done on columns that explicitly link the tables together

INNER JOINS

id	name
1	Megabyte
2	Meowly Cyrus
3	Fuzz Aldrin
4	Chairman Meow
5	Anderson Pooper
6	Gigabyte

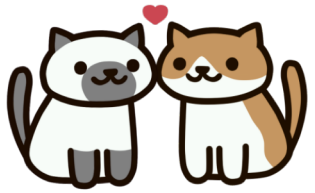
`cats`

cat_id	last_visit
1	02-16-2017
2	02-14-2017
5	02-03-2017

`visits`

Inner join returns merged rows that share the same value in the column they are being joined on (`id` and `cat_id`).

id	name	last_visit
1	Megabyte	02-16-2017
2	Meowly Cyrus	02-14-2017
5	Anderson Pooper	02-03-2017



INNER JOINS

```
# Inner join in pandas
df_cats = pd.read_sql_query("SELECT * from cats", conn)
df_visits = pd.read_sql_query("SELECT * from visits", conn)
df_cats.merge(df_visits, how = "inner",
              left_on = "id", right_on = "cat_id")
```

```
# Inner join in SQL / SQLite via Python
cursor.execute("""
                SELECT
                    *
                FROM
                    cats, visits
                WHERE
                    cats.id == visits.cat_id
                """)
```

LEFT JOINS

Inner joins are the most common type of joins (get results that appear in both tables)

Left joins: all the results from the left table, only some matching results from the right table

Left join (`cats`, `visits`) on (`id`, `cat_id`) ??????????

id	name	last_visit
1	Megabyte	02-16-2017
2	Meowly Cyrus	02-14-2017
3	Fuzz Aldrin	NULL
4	Chairman Meow	NULL
5	Anderson Pooper	02-03-2017
6	Gigabyte	NULL

RIGHT JOINS

Take a guess!

Right join
(`cats`, `visits`)
on
(`id`, `cat_id`)
`??????????`

id	name
1	Megabyte
2	Meowly Cyrus
3	Fuzz Aldrin
4	Chairman Meow
5	Anderson Pooper
6	Gigabyte

`cats`

cat_id	last_visit
1	02-16-2017
2	02-14-2017
5	02-03-2017
7	02-19-2017
12	02-21-2017

`visits`

id	name	last_visit
1	Megabyte	02-16-2017
2	Meowly Cyrus	02-14-2017
5	Anderson Pooper	02-03-2017
7	NULL	02-19-2017
12	NULL	02-21-2017

LEFT/RIGHT JOINS

```
# Left join in pandas
df_cats.merge(df_visits, how = “left”,
              left_on = “id”, right_on = ”cat_id”)
```

```
# Left join in SQL / SQLite via Python
cursor.execute(“SELECT * FROM cats LEFT JOIN visits ON
                    cats.id == visits.cat_id”)
```

```
# Right join in pandas
df_cats.merge(df_visits, how = “right”,
              left_on = “id”, right_on = ”cat_id”)
```

```
# Right join in SQL / SQLite via Python
☹
```

FULL OUTER JOIN

Combines the left and the right join ???????????

id	name	last_visit
1	Megabyte	02-16-2017
2	Meowly Cyrus	02-14-2017
3	Fuzz Aldrin	NULL
4	Chairman Meow	NULL
5	Anderson Pooper	02-03-2017
6	Gigabyte	NULL
7	NULL	02-19-2017
12	NULL	02-21-2017

```
# Outer join in pandas
df_cats.merge(df_visits, how = "outer",
              left_on = "id", right_on = "cat_id")
```

GOOGLE IMAGE SEARCH ONE SLIDE SQL JOIN VISUAL

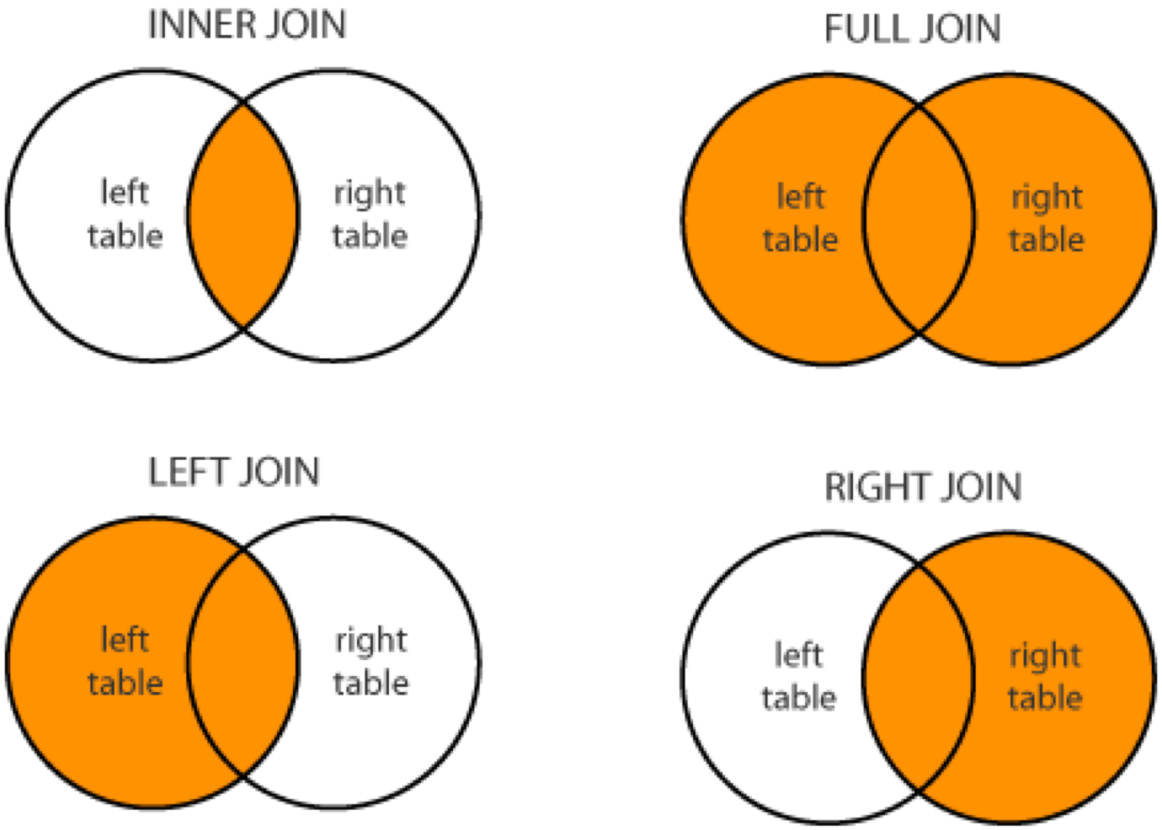


Image credit: http://www.dofactory.com/sql/join

RAW SQL IN PANDAS

If you "think in SQL" already, you'll be fine with pandas:

- `conda install -c anaconda pandasql`
- Info: http://pandas.pydata.org/pandas-docs/stable/comparison_with_sql.html

```
# Write the query text
q = """
    SELECT
        *
    FROM
        cats
    LIMIT 10;"""

# Store in a DataFrame
df = sqldf(q, locals())
```

NEXT CLASS:

EXPLORATORY ANALYSIS