INTRODUCTION TO DATA SCIENCE

JOHN P DICKERSON

Lecture #5 – 9/10/2019
Lecture #6 – 9/12/2019

CMSC320
Tuesdays and Thursdays
5pm – 6:15pm

COMPUTER SCIENCE
UNIVERSITY OF MARYLAND

ANNOUNCEMENTS

Project 1 is posted!

- Current due date is September 25th (a bit over two weeks)
- https://github.com/cmsc320/fall2019/tree/master/project1
- Some people have run into an lxml problem – I've posted one solution on Piazza; please add to that/ask questions there.

Quiz 3 is due next Thursday at noon

- Same old, same old …

A guest lecture next Tuesday

- Candice Schumann will be covering version control systems and then giving a brief tutorial on best practices using git

REVIEW OF LAST LECTURES

Shift thinking from:

Imperative code to manipulate data structures

to:

Sequences/pipelines of operations on data

Two key questions:

1. **Data Representation**, i.e., what is the natural way to think about given data
2. **Data Processing Operations**, which take one or more datasets as input and produce

REVIEW OF LAST CLASS

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

- A powerful *n*-dimensional array object.
- Homogeneous arrays of fixed size
- Operations like: indexing, slicing, map, applying filters
- Also: Linear Algebra, Vector operations, etc.

- Many other libraries build on top of NumPy

TODAY/NEXT 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

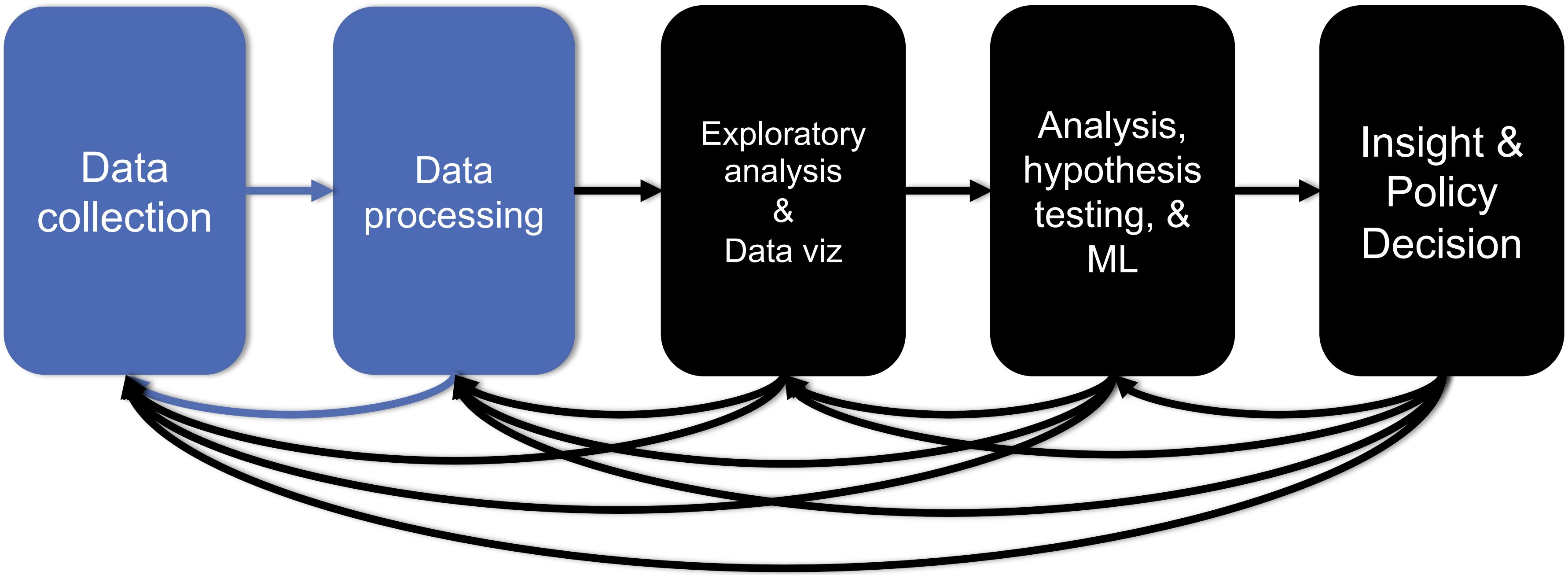
3. **Relational Databases**

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

4. **Apache Spark**

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

TODAY'S LECTURE



TODAY/NEXT CLASS

- **Tables**
  - Abstraction
  - Operations
- **Pandas**
- **Tidy Data**
- **SQL**

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

TABLES

ID	Address
1	College Park, MD, 20742
2	Washington, DC, 20001
3	Silver Spring, MD 20901

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

199.72.81.55 - - [01/Jul/1995:00:00:01 -0400] "GET /history/apollo/ HTTP/1.0" 200 6245
unicomp6.unicomp.net - - [01/Jul/1995:00:00:06 -0400] "GET /shuttle/countdown/ HTTP/1.0" 200 3985
199.120.110.21 - - [01/Jul/1995:00:00:09 -0400] "GET /shuttle/missions/sts-73/mission-sts-73.html HTTP/1.0" 200 4085

1. SELECT/SLICING

Select only some of the rows, or some of the columns, or a combination

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

Only columns
ID and Age

ID	age
1	12.2
2	11.0
3	15.6
4	35.1

Only rows
with wgt > 41

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

Both

ID	age
1	12.2
3	15.6
4	35.1

2. AGGREGATE/REDUCE

Combine values across a column into a single value

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

SUM

73.9	**232.6**	**640.0**

MAX

35.1	**84.2**	**185.8**

SUM(wgt_kg^2 - hgt_cm)

14167.66

What about ID/Index column?

Usually not meaningful to aggregate across it

May need to explicitly add an ID column

3. MAP

Apply a function to every row, possibly creating more or fewer columns

ID	Address
1	College Park, MD, 20742
2	Washington, DC, 20001
3	Silver Spring, MD 20901

ID	City	State	Zipcode
1	College Park	MD	20742
2	Washington	DC	20001
3	Silver Spring	MD	20901

Variations that allow one row to generate multiple rows in the output (sometimes called “flatmap”)

4. 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

By 'A' →

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

4. 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

By 'B' →

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

4. 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

By 'A', 'B' →

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

5. 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

5. GROUP BY AGGREGATE

Final result usually seen

As a table

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

Sum (C)
1.2

B = 2

Sum (C)
7.2

B = 3

Sum (C)
22.6

B = 4

Sum (C)
5.4

B	SUM(C)
1	1.2
2	7.2
3	22.6
4	5.4

6. UNION/INTERSECTION/DIFFERENCE

Set operations – only if the two tables have identical attributes/columns

ID	A	B	C
1	foo	3	6.6
2	bar	2	4.7
3	foo	4	3.1
4	foo	3	8.0

∪

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

→

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

Similarly Intersection and Set Difference manipulate tables as Sets

IDs may be treated in different ways, resulting in somewhat different behaviors

7. MERGE OR JOIN

Combine rows/tuples across two tables if they have the same key

ID	A	B
1	foo	3
2	bar	2
3	foo	4
4	foo	3

$\bowtie$

ID	C
1	1.2
2	2.5
3	2.3
5	8.0

$\rightarrow$

ID	A	B	C
1	foo	3	1.2
2	bar	2	2.5
3	foo	4	2.3

What about IDs not present in both tables?

Often need to keep them around

Can “pad” with NaN

7. MERGE OR JOIN

Combine rows/tuples across two tables if they have the same key

Outer joins can be used to ”pad” IDs that don’t appear in both tables

Three variants: LEFT, RIGHT, FULL

SQL Terminology -- Pandas has these operations as well

ID	A	B
1	foo	3
2	bar	2
3	foo	4
4	foo	3

⟗

ID	C
1	1.2
2	2.5
3	2.3
5	8.0

ID	A	B	C
1	foo	3	1.2
2	bar	2	2.5
3	foo	4	2.3
4	foo	3	NaN
5	NaN	NaN	8.0

SUMMARY

- **Tables: A simple, common abstraction**
  - Subsumes a set of “strings” – a common input
- **Operations**
  - Select, Map, Aggregate, Reduce, Join/Merge, Union/Concat, Group By
- **In a given system/language, the operations may be named differently**
  - E.g., SQL uses “join”, whereas Pandas uses “merge”
- **Subtle variations in the definitions, especially for more complex operations**

ID	A	B	C
1	foo	3	6.6
2	baz	2	4.7
3	foo	4	3.1
4	baz	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 'A' →

How many tuples in the answer?

A. 1
B. 3
C. 5
D. 8

ID	A	B	C
1	foo	3	6.6
2	baz	2	4.7
3	foo	4	3.1
4	baz	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 ‘A’, ‘B’ →

How many groups in the answer?

A. 1
B. 3
C. 4
D. 6

ID	A	B
1	foo	3
2	bar	2
4	foo	4
5	foo	3

$\bowtie$

ID	C
2	1.2
4	2.5
6	2.3
7	8.0

How many tuples in the answer?

A. 1
B. 2
C. 4
D. 6

ID	A	B
1	foo	3
2	bar	2
4	foo	4
5	foo	3

⟗

ID	C
2	1.2
4	2.5
6	2.3
7	8.0

FULL OUTER JOIN

All IDs will be present in the answer
With NaNs

How many tuples in the answer?

A. 1
B. 4
C. 6
D. 8

TODAY/NEXT CLASS

- **Tables**
  - Abstraction
  - Operations
- **Pandas**
- **Tidy Data**
- **SQL and Relational Databases**

PANDAS: HISTORY

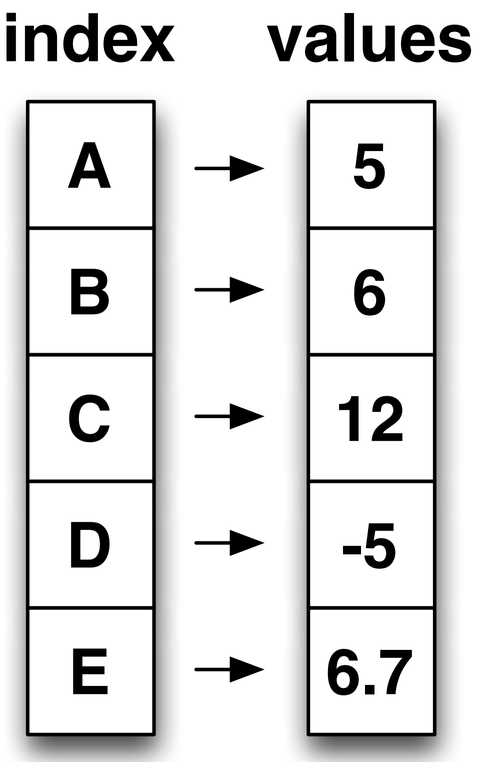
- **Written by: Wes McKinney**
  - Started in 2008 to get a high-performance, flexible tool to perform quantitative analysis on financial data

- **Highly optimized for performance, with critical code paths written in Cython or C**

- **Key constructs:**
  - Series (like a NumPy Array)
  - DataFrame (like a Table or Relation, or R data.frame)

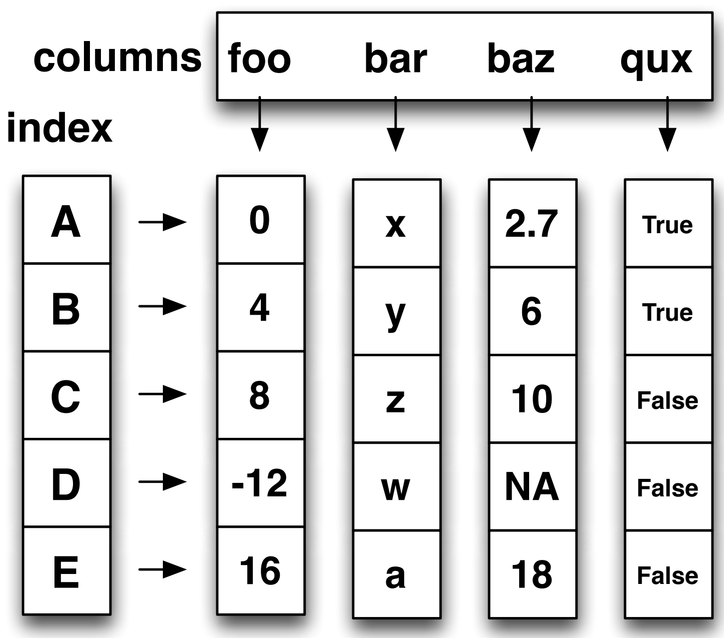
- **Foundation for Data Wrangling and Analysis in Python**

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

HIERARCHICAL INDEXES

Sometimes more intuitive organization of the data

Makes it easier to understand and analyze higher-dimensional data

e.g., instead of 3-D array, may only need a 2-D array

```
day              Fri    Sat    Sun    Thur
sex    smoker
Female No        3.125  2.725  3.329  2.460
       Yes       2.683  2.869  3.500  2.990
Male   No        2.500  3.257  3.115  2.942
       Yes       2.741  2.879  3.521  3.058
```

```
first   second
bar     one       0.469112
        two      -0.282863
baz     one      -1.509059
        two      -1.135632
foo     one       1.212112
        two      -0.173215
qux     one       0.119209
        two      -1.044236
dtype: float64
```

ESSENTIAL FUNCTIONALITY

Reindexing to change the index associated with a DataFrame

- Common usage to interpolate, fill in missing values

```
In [84]: obj3 = Series(['blue', 'purple', 'yellow'], index=[0, 2, 4])

In [85]: obj3.reindex(range(6), method='ffill')
Out[85]:
0      blue
1      blue
2    purple
3    purple
4    yellow
5    yellow
```

From: Python for Data Analysis; Wes McKinney

ESSENTIAL FUNCTIONALITY

"drop" to delete entire rows or columns

Indexing, Selection, Filtering: very similar to NumPy

Arithmetic Operations

- Result index union of the two input indexes
- Options to do "fill" while doing these operations

```
In [128]: s1
Out[128]:
a    7.3
c   -2.5
d    3.4
e    1.5
```

```
In [129]: s2
Out[129]:
a   -2.1
c    3.6
e   -1.5
f    4.0
g    3.1
```

```
In [130]: s1 + s2
Out[130]:
a    5.2
c    1.1
d    NaN
e    0.0
f    NaN
g    NaN
```

FUNCTION APPLICATION AND MAPPING

```
In [158]: frame = DataFrame(np.random.randn(4, 3), columns=list('bde'),
   .....:                   index=['Utah', 'Ohio', 'Texas', 'Oregon'])
```

```
In [159]: frame
Out[159]:
               b         d         e
Utah   -0.204708  0.478943 -0.519439
Ohio   -0.555730  1.965781  1.393406
Texas   0.092908  0.281746  0.769023
Oregon  1.246435  1.007189 -1.296221
```

```
In [160]: np.abs(frame)
Out[160]:
               b         d         e
Utah    0.204708  0.478943  0.519439
Ohio    0.555730  1.965781  1.393406
Texas   0.092908  0.281746  0.769023
Oregon  1.246435  1.007189  1.296221
```

```
In [161]: f = lambda x: x.max() - x.min()
```

```
In [162]: frame.apply(f)
Out[162]:
b    1.802165
d    1.684034
e    2.689627
```

```
In [163]: frame.apply(f, axis=1)
Out[163]:
Utah      0.998382
Ohio      2.521511
Texas     0.676115
Oregon    2.542656
```

From: Python for Data Analysis; Wes McKinney

SORTING AND RANKING

```
In [169]: obj = Series(range(4), index=['d', 'a', 'b', 'c'])

In [170]: obj.sort_index()
Out[170]:
a    1
b    2
c    3
d    0
```

```
In [187]: frame = DataFrame({'b': [4.3, 7, -3, 2], 'a': [0, 1, 0, 1],
   .....:                    'c': [-2, 5, 8, -2.5]})
```

```
In [188]: frame
Out[188]:
   a    b    c
0  0  4.3 -2.0
1  1  7.0  5.0
2  0 -3.0  8.0
3  1  2.0 -2.5
```

```
In [189]: frame.rank(axis=1)
Out[189]:
   a  b  c
0  2  3  1
1  1  3  2
2  2  1  3
3  2  3  1
```

From: *Python for Data Analysis; Wes McKinney*

DESCRIPTIVE AND SUMMARY STATISTICS

Table 5-10. Descriptive and summary statistics

Method	Description
`count`	Number of non-NA values
`describe`	Compute set of summary statistics for Series or each DataFrame column
`min, max`	Compute minimum and maximum values
`argmin, argmax`	Compute index locations (integers) at which minimum or maximum value obtained, respectively
`idxmin, idxmax`	Compute index values at which minimum or maximum value obtained, respectively
`quantile`	Compute sample quantile ranging from 0 to 1
`sum`	Sum of values
`mean`	Mean of values
`median`	Arithmetic median (50% quantile) of values
`mad`	Mean absolute deviation from mean value
`var`	Sample variance of values
`std`	Sample standard deviation of values
`skew`	Sample skewness (3rd moment) of values
`kurt`	Sample kurtosis (4th moment) of values
`cumsum`	Cumulative sum of values
`cummin, cummax`	Cumulative minimum or maximum of values, respectively
`cumprod`	Cumulative product of values
`diff`	Compute 1st arithmetic difference (useful for time series)
`pct_change`	Compute percent changes

From: Python for Data Analysis; Wes McKinney

CREATING DATAFRAMES

Directly from Dict or Series

From a Comma-Separated File – CSV file

- pandas.read_csv()
- Can infer headers/column names if present, otherwise may want to reindex

From an Excel File

- pandas.read_excel()

From a Database using SQL (see the reading for an example)

From Clipboard, URL, Google Analytics, …

…

From: Python for Data Analysis; Wes McKinney

MORE…

Unique values, Value counts

Correlation and Covariance

Functions for handling missing data – in a few classes

- dropna(), fillna()

Broadcasting

Pivoting

We will see some of these as we discuss data wrangling, cleaning, etc.

TODAY/NEXT CLASS

- **Tables**
  - Abstraction
  - Operations
- **Pandas**
- **Tidy Data**
- **SQL and Relational Databases**

TIDY DATA

Variables

Labels

Observations

age	wgt_kg	hgt_cm
12.2	42.3	145.1
11.0	40.8	143.8
15.6	65.3	165.3
35.1	84.2	185.8

But also:

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

EXAMPLE

Variable: measure or attribute:

- age, weight, height, sex

Value: measurement of attribute:

- 12.2, 42.3kg, 145.1cm, M/F

Observation: all measurements for an object

- A specific person is [12.2, 42.3, 145.1, F]

TIDYING DATA I

Name	Treatment A	Treatment B
John Smith	-	2
Jane Doe	16	11
Mary Johnson	3	1

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

Name	Treatment A	Treatment B	Treatment C	Treatment D
John Smith	-	2	-	-
Jane Doe	16	11	4	1
Mary Johnson	3	1	-	2

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

Thanks to http://jeannicholashould.com/tidy-data-in-python.html

TIDYING DATA II

In a few lectures …

Name	Treatment	Result
John Smith	A	-
John Smith	B	2
John Smith	C	-
John Smith	D	-
Jane Doe	A	16
Jane Doe	B	11
Jane Doe	C	4
Jane Doe	D	1
Mary Johnson	A	3
Mary Johnson	B	1
Mary Johnson	C	-
Mary Johnson	D	2

MELTING DATA I

religion	<$10k	$10-20k	$20-30k	$30-40k	$40-50k	$50-75k
Agnostic	27	34	60	81	76	137
Atheist	12	27	37	52	35	70
Buddhist	27	21	30	34	33	58
Catholic	418	617	732	670	638	1116
Dont know/refused	15	14	15	11	10	35
Evangelical Prot	575	869	1064	982	881	1486
Hindu	1	9	7	9	11	34
Historically Black Prot	228	244	236	238	197	223
Jehovahs Witness	20	27	24	24	21	30
Jewish	19	19	25	25	30	95

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

MELTING DATA II

```
f_df = pd.melt(df,
               ["religion"],
               var_name="income",
               value_name="freq")
f_df = f_df.sort_values(by=["religion"])
f_df.head(10)
```

religion	income	freq
Agnostic	<$10k	27
Agnostic	$30-40k	81
Agnostic	$40-50k	76
Agnostic	$50-75k	137
Agnostic	$10-20k	34
Agnostic	$20-30k	60
Atheist	$40-50k	35
Atheist	$20-30k	37
Atheist	$10-20k	27
Atheist	$30-40k	52

MORE COMPLICATED EXAMPLE

Billboard Top 100 data for songs, covering their position on the Top 100 for 75 weeks, with two "messy" bits:

- Column headers for each of the 75 weeks
- If a song didn't last 75 weeks, those columns have are null

year	artist.inverted	track	time	genre	date.entered	date.peaked	x1st.week	x2nd.week	...
2000	Destiny's Child	Independent Women Part I	3:38	Rock	2000-09-23	2000-11-18	78	63.0	...
2000	Santana	Maria, Maria	4:18	Rock	2000-02-12	2000-04-08	15	8.0	...
2000	Savage Garden	I Knew I Loved You	4:07	Rock	1999-10-23	2000-01-29	71	48.0	...
2000	Madonna	Music	3:45	Rock	2000-08-12	2000-09-16	41	23.0	...
2000	Aguilera, Christina	Come On Over Baby	3:38	Rock	2000-08-05	2000-10-14	57	47.0	...
2000	Janet	Doesn't Really Matter	4:17	Rock	2000-06-17	2000-08-26	59	52.0	...

Messy columns!

Thanks to http://jeannicholashould.com/tidy-data-in-python.html

MORE COMPLICATED EXAMPLE

```
# Keep identifier variables
id_vars = ["year",
           "artist.inverted",
           "track",
           "time",
           "genre",
           "date.entered",
           "date.peaked"]

# Melt the rest into week and rank columns
df = pd.melt(frame=df,
             id_vars=id_vars,
             var_name="week",
             value_name="rank")
```

Creates one row per week, per record, with its rank

MORE COMPLICATED EXAMPLE

```
# Formatting
df["week"] = df['week'].str.extract('(\d+)’,
                                    expand=False).astype(int)
df["rank"] = df["rank"].astype(int)
```

```
[…, “x2nd.week”, 63.0] → […, 2, 63]
```

```
# Cleaning out unnecessary rows
df = df.dropna()

# Create "date" columns
df['date'] = pd.to_datetime(
               df['date.entered']) +
               pd.to_timedelta(df['week'], unit='w') –
               pd.DateOffset(weeks=1)
```

MORE COMPLICATED EXAMPLE

```
# Ignore now-redundant, messy columns
df = df[["year",
         "artist.inverted",
         "track",
         "time",
         "genre",
         "week",
         "rank",
         "date"]]

df = df.sort_values(ascending=True,
 by=["year","artist.inverted","track","week","rank"])

# Keep tidy dataset for future usage
billboard = df

df.head(10)
```

MORE COMPLICATED EXAMPLE

year	artist.inverted	track	time	genre	week	rank	date
2000	2 Pac	Baby Don't Cry (Keep Ya Head Up II)	4:22	Rap	1	87	2000-02-26
2000	2 Pac	Baby Don't Cry (Keep Ya Head Up II)	4:22	Rap	2	82	2000-03-04
2000	2 Pac	Baby Don't Cry (Keep Ya Head Up II)	4:22	Rap	3	72	2000-03-11
2000	2 Pac	Baby Don't Cry (Keep Ya Head Up II)	4:22	Rap	4	77	2000-03-18
2000	2 Pac	Baby Don't Cry (Keep Ya Head Up II)	4:22	Rap	5	87	2000-03-25
2000	2 Pac	Baby Don't Cry (Keep Ya Head Up II)	4:22	Rap	6	94	2000-04-01
2000	2 Pac	Baby Don't Cry (Keep Ya Head Up II)	4:22	Rap	7	99	2000-04-08
2000	2Ge+her	The Hardest Part Of Breaking Up (Is Getting Ba...	3:15	R&B	1	91	2000-09-02
2000	2Ge+her	The Hardest Part Of Breaking Up (Is Getting Ba...	3:15	R&B	2	87	2000-09-09
2000	2Ge+her	The Hardest Part Of Breaking Up (Is Getting Ba...	3:15	R&B	3	92	2000-09-16

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

MORE TO DO?

Column headers are values, not variable names?

- Good to go!

Multiple variables are stored in one column?

- Maybe (depends on if genre text in raw data was multiple)

Variables are stored in both rows and columns?

- Good to go!

Multiple types of observational units in the same table?

- Good to go! One row per song’s week on the Top 100.

A single observational unit is stored in multiple tables?

- Don’t do this!

Repetition of data?

- Lots! Artist and song title’s text names. Which leads us to …

TODAY/NEXT CLASS

- **Tables**
  - Abstraction
  - Operations
- **Pandas**
- **Tidy Data**
- **SQL and Relational Databases**

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

Thanks to Zico Kolter for some structure for this lecture!

RELATION

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

Variables
(called attributes)

Labels

Observations
(called 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**

AREN'T THESE CALLED "INDEXES"?

Yes, in Pandas; but not in the database world

For most databases, an "index" is a data structure used to speed up retrieval of specific tuples

For example, to find all tuples with nat_id = 2:

- We can either scan the table – O(N)
- Or use an "index" (e.g., binary tree) – O(log N)

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**

RELATION SCHEMA

A list of all the attribute names, and their *domains*

create table department
    (dept_name **varchar**(20),
     building **varchar**(15),
     budget **numeric**(12,2) check (budget > 0),
     primary key (dept_name)
    );

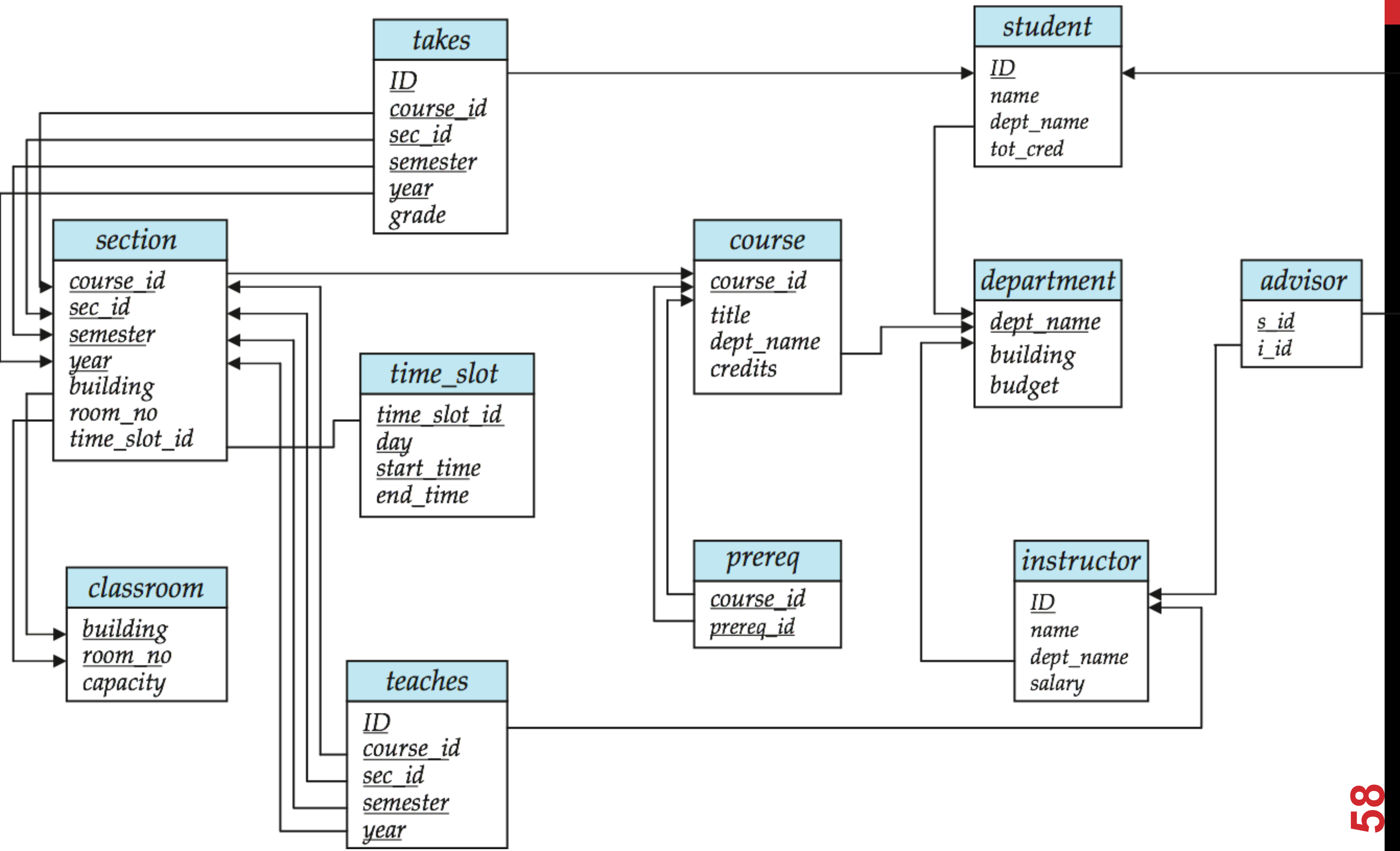
SQL Statements
To create Tables

create table *instructor* (

ID **char**(5),
name **varchar**(20) **not null,**
dept_name **varchar**(20),
salary **numeric**(8,2),

primary key (*ID*),
foreign key *(dept_name)* **references** *department*
)

SCHEMA DIAGRAMS



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.

Person — Nationality

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:

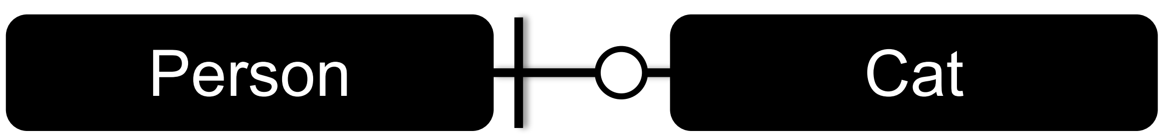
- Split a big row between SSD and HDD or distributed
- Restrict access to part of a row (some DBMSs allow column-level access control, but not all)
- Caching, partitioning, & serious stuff: take CMSC424

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

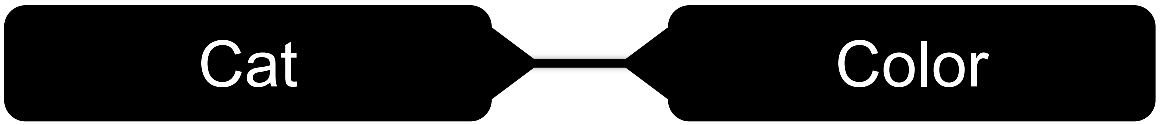
Say we want to keep track of people's cats' colorings:

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:

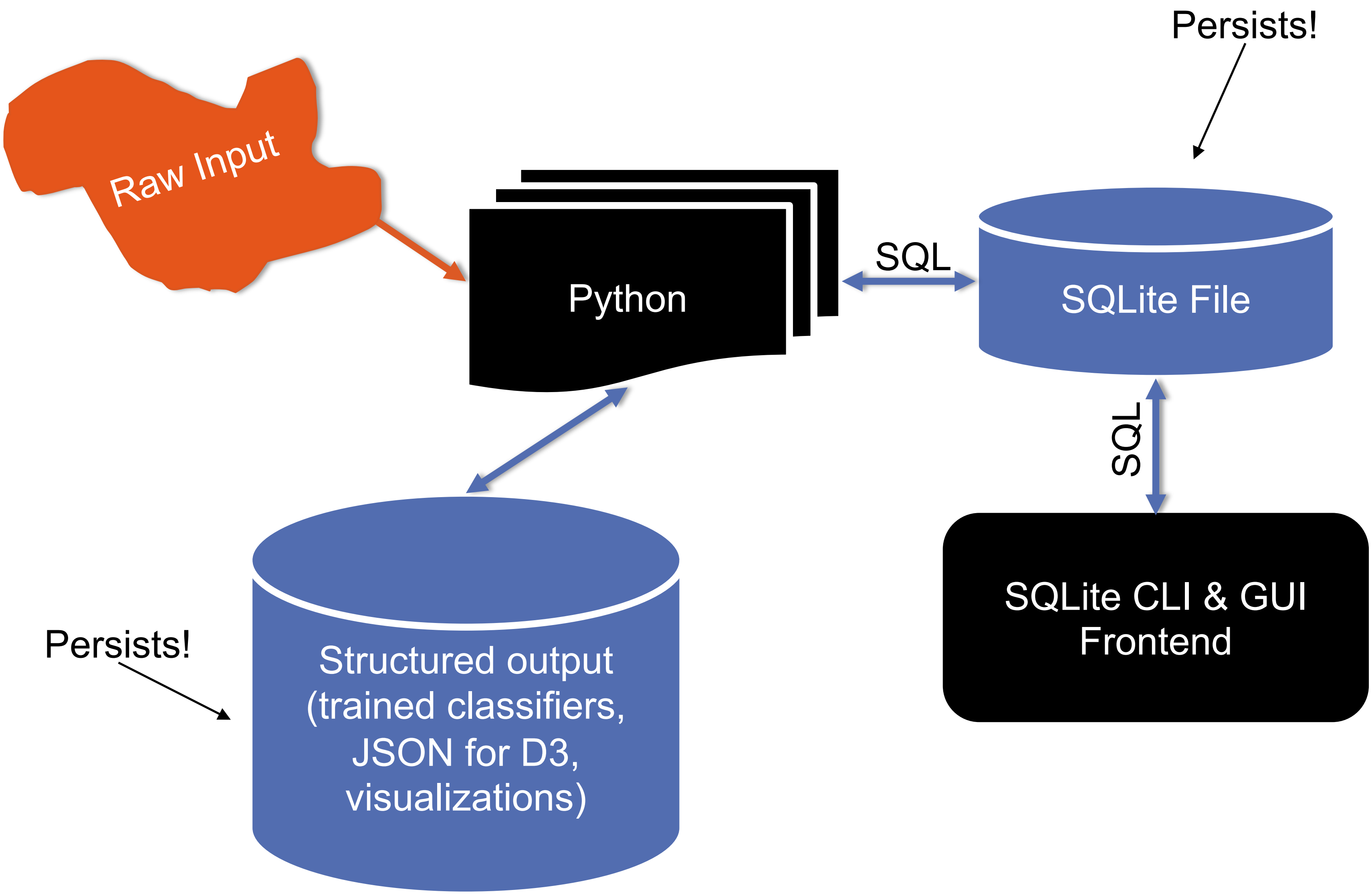
- Advantages include greater concurrency, less restrictive locking
- Disadvantages include, for this class, setup time ☺

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

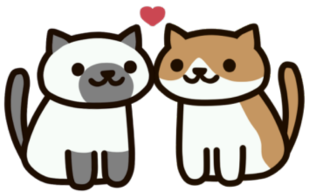
`cats`

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

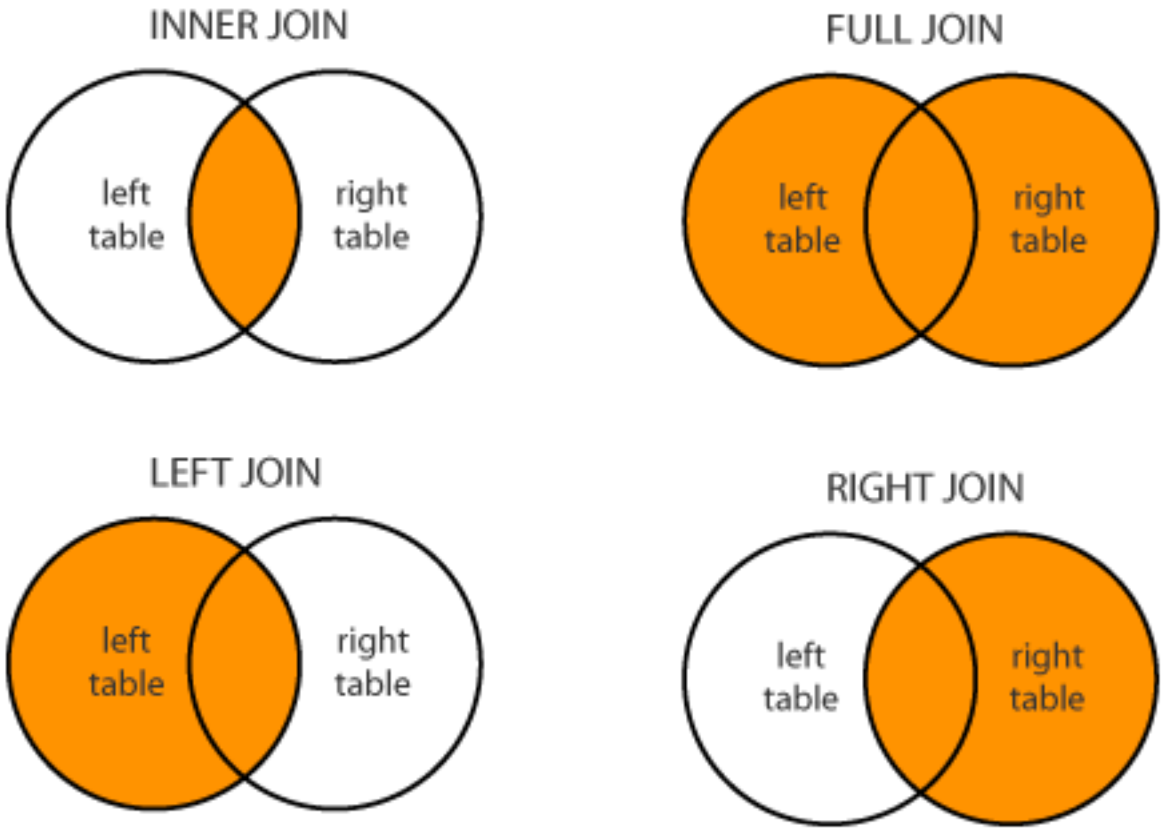


Image credit: http://www.dofactory.com/sql/join

GROUP BY AGGREGATES

```
SELECT nat_id, AVG(age) as average_age
FROM persons GROUP BY nat_id
```

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

nat_id	average_ age
1	19.48
2	15.6
3	18.1

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