Advanced Data Management (CSCI 640/490)

Data & Data Wrangling

Dr. David Koop

NumPy

- Fast **vectorized** array operations for data munging and cleaning, subsetting and filtering, transformation, and any other kinds of computations
- Common array algorithms like sorting, unique, and set operations
- Efficient descriptive statistics and aggregating/summarizing data
- Data alignment and relational data manipulations for merging and joining together heterogeneous data sets
- Expressing conditional logic as array expressions instead of loops with `if-elif-else` branches
- Group-wise data manipulations (aggregation, transformation, function application).

[W. McKinney, Python for Data Analysis]

pandas

- Contains high-level data structures and manipulation tools designed to make data analysis fast and easy in Python
- Built on top of NumPy
- Requirements:
  - Data structures with labeled axes (aligning data)
  - Time series data
  - Arithmetic operations that include metadata (labels)
  - Handle missing data
  - Merge and relational operations

Series

- A one-dimensional array (with a type) with an **index**
- Index defaults to numbers but can also be text (like a dictionary)
- Allows easier reference to specific items
- `obj = pd.Series([7,14,-2,1])`
- Basically two arrays: `obj.values` and `obj.index`
- Can specify the index explicitly and use strings
- ```
  obj2 = pd.Series([4, 7, -5, 3],
                   index=['d', 'b', 'a', 'c'])
  ```
- Kind of like fixed-length, ordered dictionary + can create from a dictionary
- ```
  obj3 = pd.Series({'Ohio': 35000, 'Texas': 71000,
                    'Oregon': 16000, 'Utah': 5000})
  ```

Indexing

- Same as with NumPy arrays but can use Series's index labels
- Slicing with labels: NumPy is **exclusive**, Pandas is **inclusive**!
  - `s = Series(np.arange(4))`
    `s[0:2] # gives two values like numpy`
  - `s = Series(np.arange(4), index=['a', 'b', 'c', 'd'])`
    `s['a':'c'] # gives three values, not two!`
- Obtaining data subsets
  - `[]`: get columns by label
  - `loc`: get rows/cols by label
  - `iloc`: get rows/cols by position (integer index)

- For single cells (scalars), also have `at` and `iat`

Filtering

- Same as with numpy arrays but allows use of column-based criteria
  - `data[data < 5] = 0`
  - `data[data['three'] > 5]`
- `data < 5` → boolean data frame, can be used to select specific elements

Data Frame

- A dictionary of Series (labels for each series)
- A spreadsheet with column headers
- Has an index shared with each series
- Allows easy reference to any cell
-
```
df = DataFrame({'state': ['Ohio', 'Ohio', 'Ohio', 'Nevada'],
                'year': [2000, 2001, 2002, 2001],
                'pop': [1.5, 1.7, 3.6, 2.4]})
```

- Index is automatically assigned just as with a series but can be passed in as well via index kwarg
- Can reassign column names by passing columns kwarg

Data Frame

```
df = pd.read_csv('penguins_lter.csv')
```

	studyName	Sample Number	Species	Region	Island	Stage	Individual ID	Clutch Completion	Date Egg	Culmen Length (mm)
0	PAL0708	1	Adelie Penguin (Pygoscelis adeliae)	Anvers	Torgersen	Adult, 1 Egg Stage	N1A1	Yes	11/11/07	39.1
1	PAL0708	2	Adelie Penguin (Pygoscelis adeliae)	Anvers	Torgersen	Adult, 1 Egg Stage	N1A2	Yes	11/11/07	39.5
2	PAL0708	3	Adelie Penguin (Pygoscelis adeliae)	Anvers	Torgersen	Adult, 1 Egg Stage	N2A1	Yes	11/16/07	40.3
3	PAL0708	4	Adelie Penguin (Pygoscelis adeliae)	Anvers	Torgersen	Adult, 1 Egg Stage	N2A2	Yes	11/16/07	NaN
4	PAL0708	5	Adelie Penguin (Pygoscelis adeliae)	Anvers	Torgersen	Adult, 1 Egg Stage	N3A1	Yes	11/16/07	36.7
...	...	...	...	...	...	...	...	...	...	...
339	PAL0910	120	Gentoo penguin (Pygoscelis papua)	Anvers	Biscoe	Adult, 1 Egg Stage	N38A2	No	12/1/09	NaN
340	PAL0910	121	Gentoo penguin (Pygoscelis papua)	Anvers	Biscoe	Adult, 1 Egg Stage	N39A1	Yes	11/22/09	46.8
341	PAL0910	122	Gentoo penguin (Pygoscelis papua)	Anvers	Biscoe	Adult, 1 Egg Stage	N39A2	Yes	11/22/09	50.4
342	PAL0910	123	Gentoo penguin (Pygoscelis papua)	Anvers	Biscoe	Adult, 1 Egg Stage	N43A1	Yes	11/22/09	45.2
343	PAL0910	124	Gentoo penguin (Pygoscelis papua)	Anvers	Biscoe	Adult, 1 Egg Stage	N43A2	Yes	11/22/09	49.9

344 rows × 17 columns

Data Frame

Column Names

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344 rows × 17 columns

Column: `df['Island']`

Data Frame

```
df = pd.read_csv('penguins_lter.csv')
```

Column Names

Row: `df.loc[2]`

Index

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344 rows × 17 columns

Row: `df.loc[2]`

Index

Cell: `df.loc[341,'Species']`

Column: `df['Island']`

Data Frame

```
df = pd.read_csv('penguins_lter.csv')
```

Column Names

	studyName	Sample Number	Species	Region	Island	Stage	Individual ID	Clutch Completion	Date Egg	Culmen Length (mm)
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...	...	...	...	...	...	...	...	...	...	...
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344 rows × 17 columns

Row: `df.loc[2]`

Index

Cell: `df.loc[341,'Species']`

Missing Data

Column: `df['Island']`

String Methods

- Can manipulate columns of strings
  - Use the `.str` modifier
- Most string and regex operations are available
- Examples:
  - `df.first_name.str.startswith("Jo")`
  - `df.name.str.split(' ')`

Mutating Dataframes

- assign allows new columns to be created, returns "new" dataframe
  - `df2 = df.assign(Total=df.Points1 + df.Points2)`
- More reusable:
  - `df2 = df.assign(Total=lambda df: df.Points1 + df.Points2)`
- If you have columns that are not proper identifiers, can use **kwargs
  - `df2 = df.assign(**{"Total Points": lambda df: df.Points1 + df.Points2})`

Assignment 2

- Assignment 1 Questions with pandas, DuckDB, and polars
- CS 640 students do all, CS 490 do pandas & DuckDB (polars is EC)
- Can work by framework or by query
- Most questions can be answered with a single statement… but that statement can take a while to write
  - Read documentation
  - Check hints

Next Week

- No in-person lectures
- You will work through courselets on data wrangling and data cleaning

Test 1

- Currently scheduled for Feb. 26
- Move to Wednesday, Feb. 28?
- Will cover topics through the courselets
- Format:
  - Multiple Choice
  - Free Response: longer-form questions that involve multiple steps, responding to readings
  - CSCI 640 students have an extra two pages

Reading

- Wednesday
- Discussing paper:
  - "Wrangler: Interactive Visual Specification of Data Transformation Scripts"
  - Kandel et al.
  - http://vis.stanford.edu/files/wrangler.pdf
- Read
- Come prepared with questions, thoughts
  - Compare with how things work in pandas

Chicago Food Inspections Exploration

- Using Pandas
- Using DuckDB
- Using Polars

Data

Data

- What is data?
  - Types
  - Semantics
- How is data structured?
  - Tables (Data Frames)
  - Databases
  - Data Cubes
- What formats is data stored in?
- Raw versus derived data

Data

- What is this data?

R011	42ND STREET & 8TH AVENUE	00228985	00008471	00000441	00001455	00000134	00033341	00071255
R170	14TH STREET-UNION SQUARE	00224603	00011051	00000827	00003026	00000660	00089367	00199841
R046	42ND STREET & GRAND CENTRAL	00207758	00007908	00000323	00001183	00003001	00040759	00096613

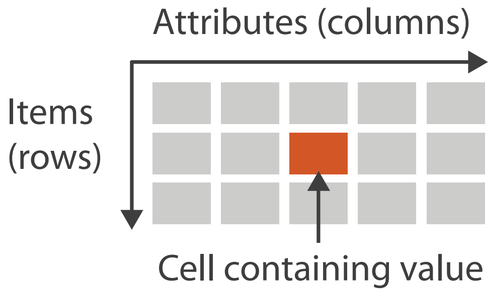
- Semantics: real-world meaning of the data
- Type: structural or mathematical interpretation
- Both often require metadata
  - Sometimes we can infer some of this information
  - Line between data and metadata isn't always clear

Data

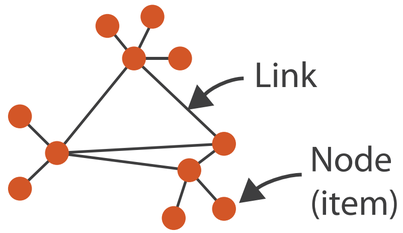
	REMOTE	STATION	FF	SEN/DIS	7-D AFAS UNL	D AFAS/RMF U	JOINT RR TKT	7-D UNL	30-D UNL
1	R011	42ND STREET & 8TH AVENUE	00228985	00008471	00000441	00001455	00000134	00033341	00071255
2	R170	14TH STREET-UNION SQUARE	00224603	00011051	00000827	00003026	00000660	00089367	00199841
3	R046	42ND STREET & GRAND CENTRAL	00207758	00007908	00000323	00001183	00003001	00040759	00096613
4	R012	34TH STREET & 8TH AVENUE	00188311	00006490	00000498	00001279	00003622	00035527	00067483
5	R293	34TH STREET - PENN STATION	00168768	00006155	00000523	00001065	00005031	00030645	00054376
6	R033	42ND STREET/TIMES SQUARE	00159382	00005945	00000378	00001205	00000690	00058931	00078644
7	R022	34TH STREET & 6TH AVENUE	00156008	00006276	00000487	00001543	00000712	00058910	00110466
8	R084	59TH STREET/COLUMBUS CIRCLE	00155262	00009484	00000589	00002071	00000542	00053397	00113966
9	R020	47-50 STREETS/ROCKEFELLER	00143500	00006402	00000384	00001159	00000723	00037978	00090745
10	R179	86TH STREET-LEXINGTON AVE	00142169	00010367	00000470	00001839	00000271	00050328	00125250
11	R023	34TH STREET & 6TH AVENUE	00134052	00005005	00000348	00001112	00000649	00031531	00075040
12	R029	PARK PLACE	00121614	00004311	00000287	00000931	00000792	00025404	00065362
13	R047	42ND STREET & GRAND CENTRAL	00100742	00004273	00000185	00000704	00001241	00022808	00068216
14	R031	34TH STREET & 7TH AVENUE	00095076	00003990	00000232	00000727	00001459	00024284	00038671
15	R017	LEXINGTON AVENUE	00094655	00004688	00000190	00000833	00000754	00020018	00055066
16	R175	8TH AVENUE-14TH STREET	00094313	00003907	00000286	00001144	00000256	00038272	00074661
17	R057	BARCLAYS CENTER	00093804	00004204	00000454	00001386	00001491	00039113	00068119
18	R138	WEST 4TH ST-WASHINGTON SQ	00093562	00004677	00000251	00000965	00000127	00031628	00074458

Dataset Types

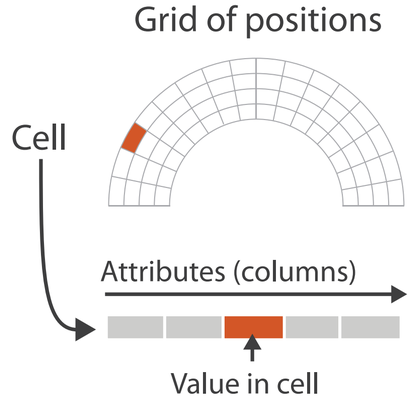
➔ Tables



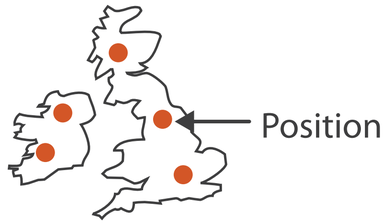
➔ Networks



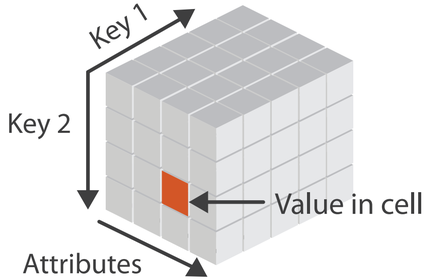
➔ Fields (Continuous)



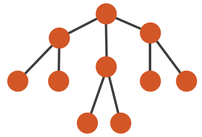
➔ Geometry (Spatial)



➔ *Multidimensional Table*



➔ *Trees*



[Munzner (ill. Maguire), 2014]

Data Terminology

- Items
  - An **item** is an individual discrete entity
  - e.g., a row in a table
- Attributes
  - An **attribute** is some specific property that can be measured, observed, or logged
  - a.k.a. variable, (data) dimension
  - e.g., a column in a table

Tables

A	B	C	S	T	U
Order ID	Order Date	Order Priority	Product Container	Product Base Margin	Ship Date
3	10/14/06	5-Low	Large Box	0.8	10/21/06
6	2/21/08	4-Not Specified	Small Pack	0.55	2/22/08
32	7/16/07	2-High	Small Pack	0.79	7/17/07
32	7/16/07	2-High	Jumbo Box		7/17/07
32	7/16/07	2-High	Medium Box		7/18/07
32	7/16/07	2-High	Medium Box		7/18/07
35	10/23/07	4-Not Specified	Wrap Bag	0.52	10/24/07
35	10/23/07	4-Not Specified	Small Box	0.58	10/25/07
36	11/3/07	1-Urgent	Small Box	0.55	11/3/07
65	3/18/07	1-Urgent	Small Pack	0.49	3/19/07
66	1/20/05	5-Low	Wrap Bag	0.56	1/20/05
69	6/6/05	4-Not Specified	Small Pack	0.44	6/6/05
69	6/6/05	4-Not Specified	Wrap Bag	0.6	6/6/05
70	12/18/06	5-Low	Small Box	0.59	12/23/06
70	12/18/06	5-Low	Wrap Bag	0.82	12/23/06
96	4/17/05	2-High	Small Box	0.55	4/19/05
97	1/29/06	3-Medium	Small Box	0.38	1/30/06
129	11/19/08	5-Low	Small Box	0.37	11/28/08
130	5/8/08	2-High	Small Box	0.37	5/9/08
130	5/8/08	2-High	Medium Box	0.38	5/10/08
130	5/8/08	2-High	Small Box	0.6	5/11/08
132	6/11/06	3-Medium	Medium Box	0.6	6/12/06
132	6/11/06	3-Medium	Jumbo Box	0.69	6/14/06
134	5/1/08	4-Not Specified	Large Box	0.82	5/3/08
135	10/21/07	4-Not Specified	Small Pack	0.64	10/23/07
166	9/12/07	2-High	Small Box	0.55	9/14/07
193	8/8/06	1-Urgent	Medium Box	0.57	8/10/06
194	4/5/08	3-Medium	Wrap Bag	0.42	4/7/08

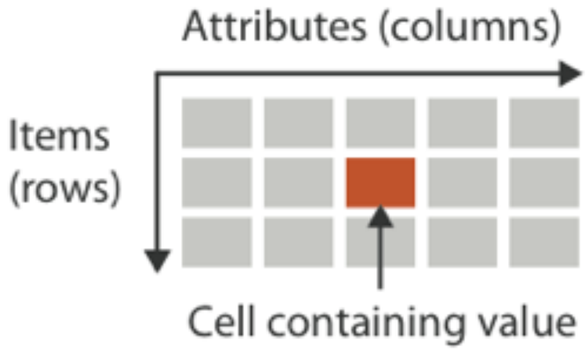
attribute

cell

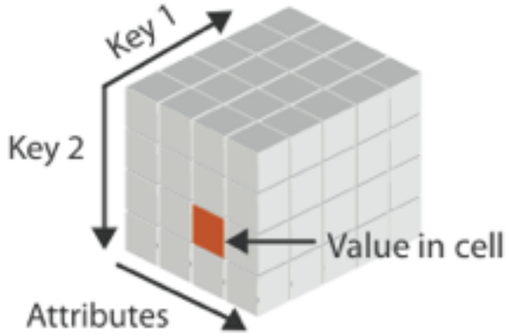
item

Tables

Flat



Multidimensional



- Data organized by rows & columns
  - row ~ item (usually)
  - column ~ attribute
  - label ~ attribute name
- Key: identifies each item (row), usually unique
  - Allows **join** of data from 2+ tables
  - Compound key: key split among multiple columns, e.g. (state, year) for population
- Multidimensional:
  - Split compound key
  - e.g. a data cube with (state, year)

[Munzner (ill. Maguire), 2014]

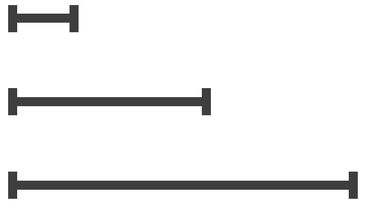
Attribute Types

➔ Categorical

➔ Ordered

➔ *Ordinal*

➔ *Quantitative*



[Munzner (ill. Maguire), 2014]

Categorial, Ordinal, and Quantitative

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32	7/16/07	2-High	Jumbo Box	0.72	7/17/07
32	7/16/07	2-High	Medium Box	0.6	7/18/07
32	7/16/07	2-High	Medium Box	0.65	7/18/07
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69	6/4/05	4-Not Spec		0.6	6/6/05
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70	12/18/06	5-Low		0.82	12/23/06
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193	8/8/06	1-Urgent	Medium Box	0.57	8/10/06
194	4/5/08	3-Medium	Wrap Bag	0.42	4/7/08

quantitative
ordinal
categorical

Categorial, Ordinal, and Quantitative

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194	4/5/08	3-Medium	Wrap Bag	0.42	4/7/08

quantitative
ordinal
categorical

Attribute Types

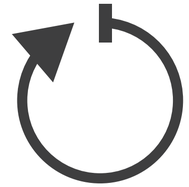
- May be further specified for computational storage/processing
  - **Categorical**: string, boolean, blood type
  - **Ordered**: enumeration, t-shirt size
  - **Quantitative**: integer, float, fixed decimal, datetime
- Sometimes, types can be **inferred** from the data
  - e.g. numbers and none have decimal points → integer
  - could be incorrect (data doesn't have floats, but could be)

Ordering Direction

➔ Sequential

➔ Diverging

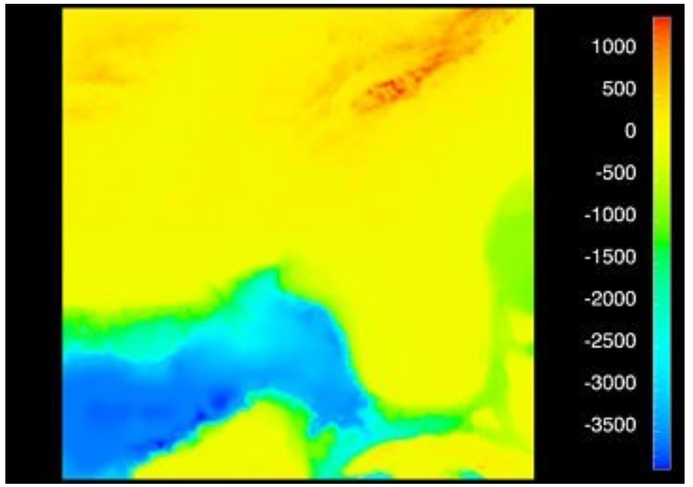
➔ Cyclic



[Munzner (ill. Maguire), 2014]

Sequential and Diverging Data

- Sequential: homogenous range from a minimum to a maximum
  - Examples: Land elevations, ocean depths
- Diverging: can be deconstructed into two sequences pointing in opposite directions
  - Has a **zero point** (not necessary 0)
  - Example: Map of both land elevation and ocean depth



[Rogowitz & Treinish, 1998]

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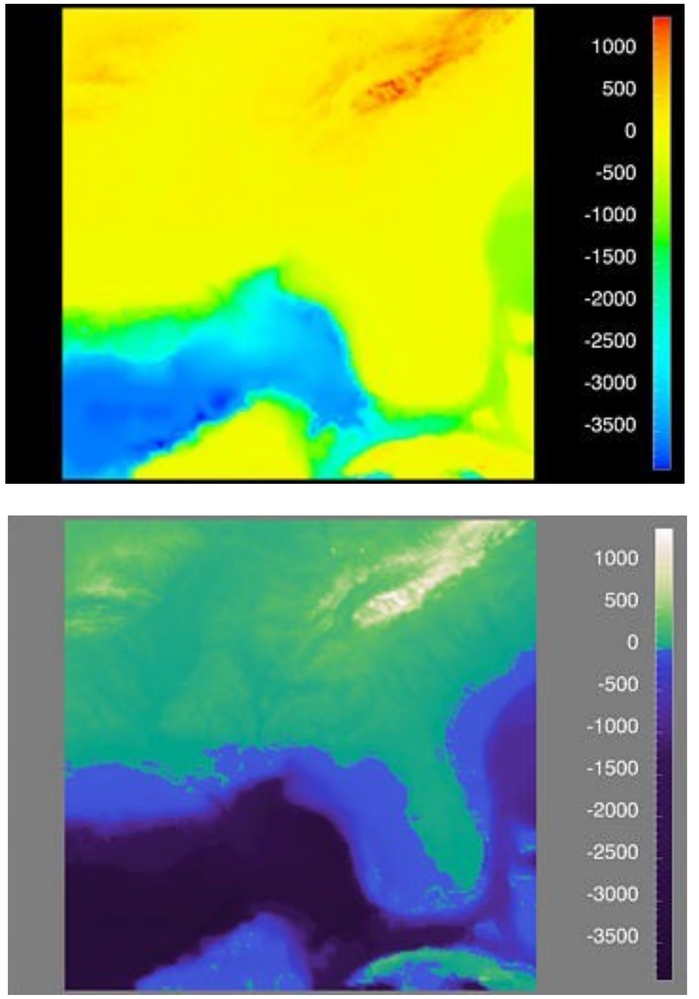
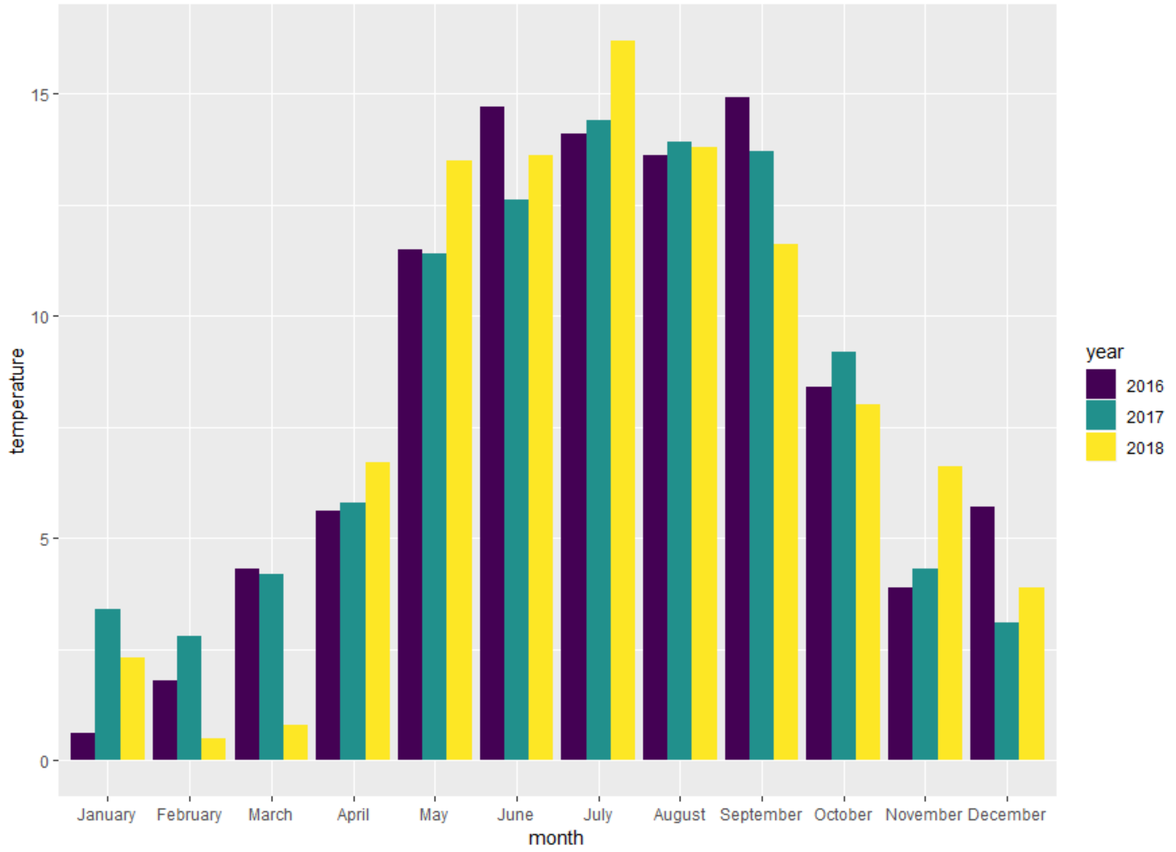
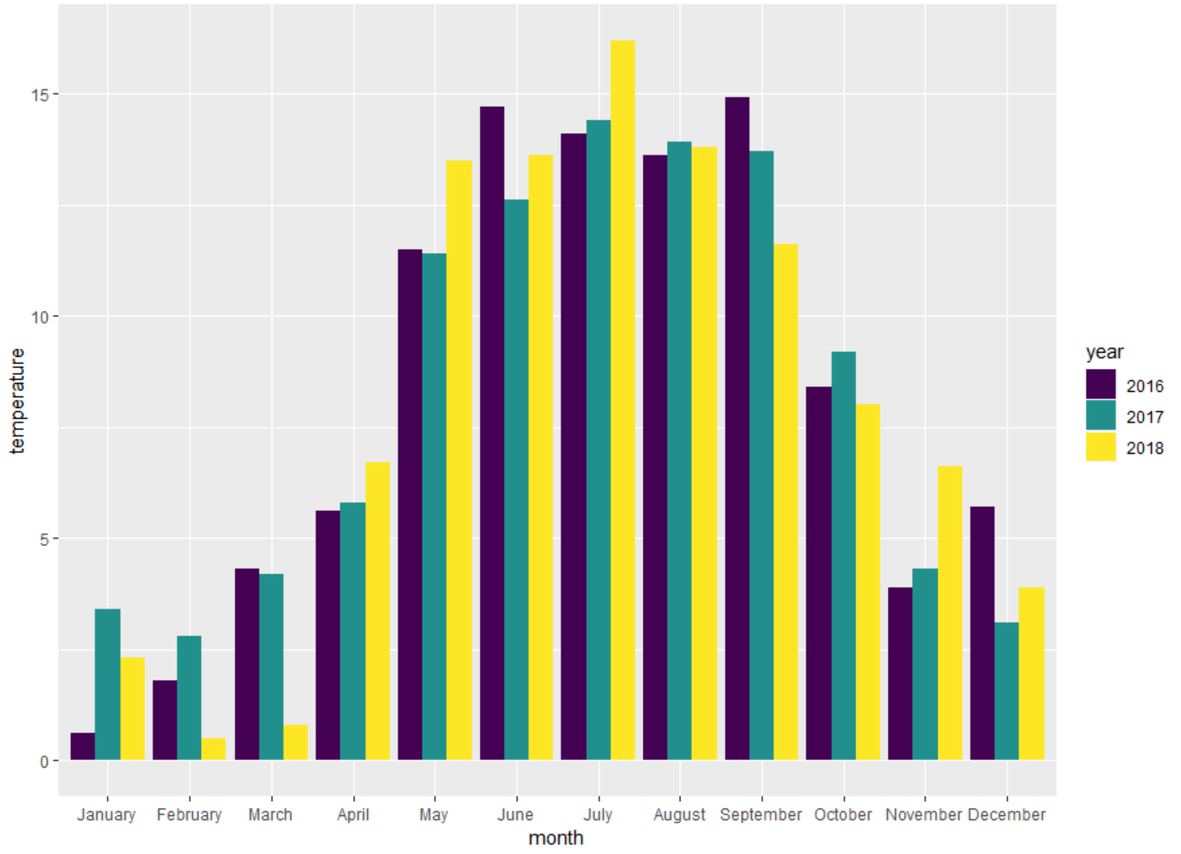


[Rogowitz & Treinish, 1998]

Cyclic Data


15
10
5
0
temperature
January
February
March
April
May
June
July
August
September
October
November
December
month
year
2016
2017
2018

Cyclic Data


temperature
15
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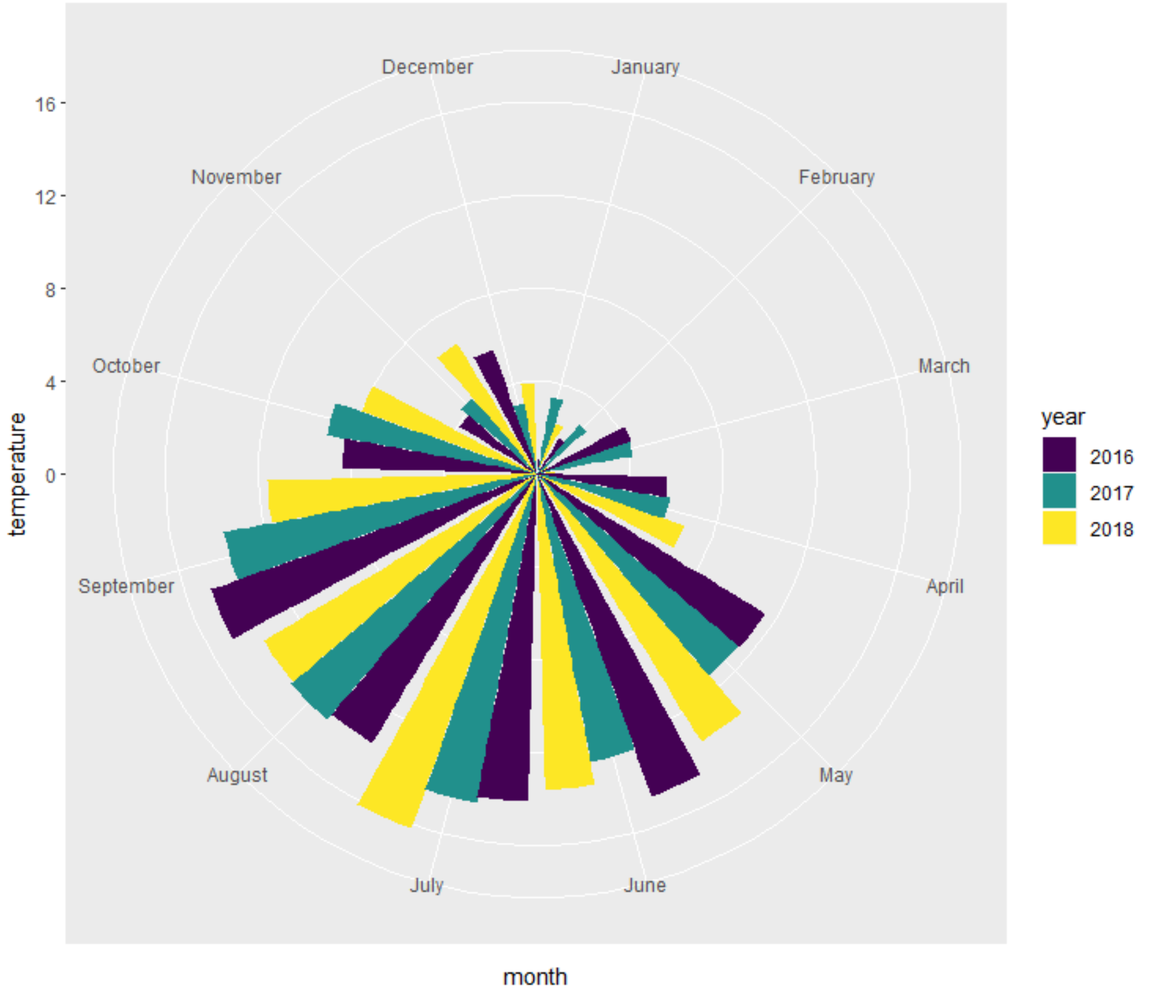
temperature
16
12
8
4
0
December
January
February
March
April
May
June
July
August
September
October
November
month
year
2016
2017
2018

Semantics

- The meaning of the data
- Example: 94023, 90210, 02747, 60115

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- Example: 94023, 90210, 02747, 60115
  - Attendance at college football games?
  - Salaries?
  - Zip codes?
- Cannot always infer based on what the data looks like
- Often require semantics to better understand data, column names help
- May also include rules about data: a zip code is part of an address that uniquely identifies a residence
- Useful for asking good questions about the data

Data Model vs. Conceptual Model

- Data Model: raw data that has a specific data type (e.g. floats):
  - Temperature Example: `[32.5, 54.0, -17.3]` (floats)
- Conceptual Model: how we think about the data
  - Includes semantics, reasoning
  - Temperature Example:
    - Quantitative: `[32.50, 54.00, -17.30]`

[via A. Lex, 2015]

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    - Ordered: `[warm, hot, cold]`
    - Categorical: `[not burned, burned, not burned]`

[via A. Lex, 2015]

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- Example 2: `Points, OpponentPoints`
  - Want to have a column indicating win/loss
  - `Win = True if (Points > OpponentPoints) else False`
- Example 3: `Points`
  - Want to have a column indicating how that point total ranks
  - `Rank = index in sorted list of all Point values`