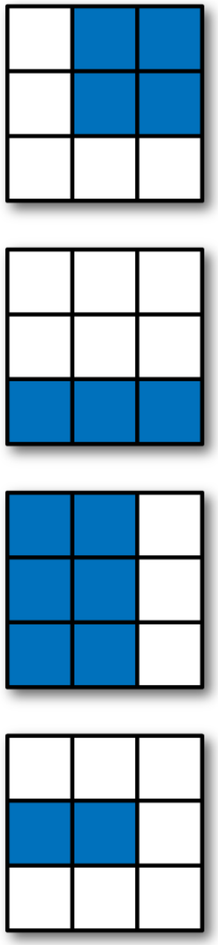
Programming Principles in Python (CSCI 503/490)

Data

Dr. David Koop

numpy Array Slicing

- Indexing is similar to lists
  - Even in 2D
  - `arr[2][2]` same as `arr[2,2]`
- Slicing is a bit different:
  - Slices are **views**
  - Dimensionality unchanged with pure slicing
  - `arr[1:3][:2] != arr[1:3,:2]`



Expression	Shape
`arr[:2, 1:]`	`(2, 2)`
`arr[2]`	`(3,)`
`arr[2, :]`	`(3,)`
`arr[2:, :]`	`(1, 3)`
`arr[:, :2]`	`(3, 2)`
`arr[1, :2]`	`(2,)`
`arr[1:2, :2]`	`(1, 2)`

[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
- Built with the following requirements:
  - Data structures with labeled axes (aligning data)
  - Support time series data
  - Do arithmetic operations that include metadata (labels)
  - Handle missing data
  - Add merge and relational operations

Documentation

- pandas documentation is pretty good
- Lots of recipes on stackoverflow for particular data manipulations/queries

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})
  ```

Arithmetic

- Add, subtract, multiply, and divide are element-wise like numpy
- …but use labels to align
- …and missing labels lead to `NaN` (not a number) values

```
In [28]: obj3
Out[28]:
Ohio      35000
Oregon    16000
Texas     71000
Utah       5000
dtype: int64
```

```
In [29]: obj4
Out[29]:
California      NaN
Ohio          35000
Oregon        16000
Texas         71000
dtype: float64
```

```
In [30]: obj3 + obj4
Out[30]:
California       NaN
Ohio           70000
Oregon         32000
Texas         142000
Utah             NaN
dtype: float64
```

- also have `.add`, `.subtract`, … that allow `fill_value` argument
- `obj3.add(obj4, fill_value=0)`

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
- Multiple criteria, use `&`, `|`, and `~`; remember parentheses!
  - `data[(data['three'] > 5) & (data['two'] < 10)]`
- Also can check for missing values via `isna()`/`isnull()`/`notnull()`
  - `data[data['three'].notnull() & data['two'].isnull()]`

Assignment 7

- Musical Artists Datasets
- Downloading and uncompressing files
- Finding files using OS libraries
- Load per-artist numpy arrays, each saved in the .npy format
- Store per-month dataframes, each in a csv file

Data Frame

- A dictionary of Series (labels for each series)
- A spreadsheet with row keys (the index) and 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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```

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...	...	...	...	...	...	...	...	...	...	...
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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

	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
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...	...	...	...	...	...	...	...	...	...	...
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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

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

	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
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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
...	...	...	...	...	...	...	...	...	...	...
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344 rows × 17 columns

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']`

Filtering

```
df[df['Culmen Length (mm)'] > 40]
```

	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
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344 rows × 17 columns

Filtering

```
df[df['Culmen Length (mm)'] > 40]
```

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344 rows × 17 columns

DataFrame Index

- Similar to index for Series
- Immutable
- Can be shared with multiple structures (DataFrames or Series)
- `in` operator works with: `'Ohio' in df.index`
- Can choose new index column(s) with `set_index()`
- `reindex` creates a new object with the data conformed to new index
  - `obj2 = obj.reindex(['a', 'b', 'c', 'd', 'e'])`
  - can fill in missing values in different ways

Sorting

- `sort_values` method on series
  - `obj.sort_values()`
- Missing values (`NaN`) are at the end by default (`na_position` controls, can be first)
- `sort_values` on DataFrame:
  - `df.sort_values(<list-of-columns>)`
  - `df.sort_values(by=['a', 'b'])`
- Also a `sort_index` method to sort by the index
  - `df.sort_index()`

Statistics

- `sum`: column sums (`axis=1` gives sums over rows)
- missing values are excluded unless the whole slice is `NaN`
- `idxmax, idxmin` are like argmax, argmin (return index)
- `describe`: shortcut for easy stats!

```
In [204]: df.describe()
Out[204]:
              one       two
count    3.000000  2.000000
mean     3.083333 -2.900000
std      3.493685  2.262742
min      0.750000 -4.500000
25%      1.075000 -3.700000
50%      1.400000 -2.900000
75%      4.250000 -2.100000
max      7.100000 -1.300000
```

```
In [205]: obj = Series(['a', 'a', 'b', 'c'] * 4)

In [206]: obj.describe()
Out[206]:
count     16
unique     3
top        a
freq       8
dtype: object
```

Unique Values and Value Counts

- `unique()` returns an array with only the unique values (no index)
  - `s = Series(['c','a','d','a','a','b','b','c','c'])`
    `s.unique() # array(['c', 'a', 'd', 'b'])`
- Also `nunique()` to count number of unique entries
- Data Frames use `drop_duplicates`
- `value_counts` returns a Series with index frequencies:
  - `s.value_counts() # Series({'c': 3,'a': 3,'b': 2,'d': 1})`

Reading & Writing Data in Pandas

Format	Data Description	Reader	Writer
text	CSV	read_csv	to_csv
text	Fixed-Width Text File	read_fwf	
text	JSON	read_json	to_json
text	HTML	read_html	to_html
text	Local clipboard	read_clipboard	to_clipboard
	MS Excel	read_excel	to_excel
binary	OpenDocument	read_excel	
binary	HDF5 Format	read_hdf	to_hdf
binary	Feather Format	read_feather	to_feather
binary	Parquet Format	read_parquet	to_parquet
binary	ORC Format	read_orc	
binary	Msgpack	read_msgpack	to_msgpack
binary	Stata	read_stata	to_stata
binary	SAS	read_sas	
binary	SPSS	read_spss	
binary	Python Pickle Format	read_pickle	to_pickle
SQL	SQL	read_sql	to_sql
SQL	Google BigQuery	read_gbq	to_gbq

[https://pandas.pydata.org/pandas-docs/stable/user_guide/io.html]

read_csv

- Convenient method to read csv files
- Lots of different options to help get data into the desired format
- Basic: `df = pd.read_csv(fname)`
- Parameters:
  - `path`: where to read the data from
  - `sep` (or `delimiter`): the delimiter (`','`, `' '`, `'\t'`, `'\s+'`)
  - `header`: if `None`, no header
  - `index_col`: which column to use as the row index
  - `names`: list of header names (e.g. if the file has no header)
  - `skiprows`: number of list of lines to skip

Writing CSV data with pandas

- Basic: `df.to_csv(<fname>)`
- Change delimiter with sep kwarg:
  - `df.to_csv('example.dsv', sep='|')`
- Change missing value representation
  - `df.to_csv('example.dsv', na_rep='NULL')`
- Don't write row or column labels:
  - `df.to_csv('example.csv', index=False, header=False)`
- Series may also be written to csv

Handling Missing Data

Argument	Description
`dropna`	Filter axis labels based on whether values for each label have missing data, with varying thresholds for how much missing data to tolerate.
`fillna`	Fill in missing data with some value or using an interpolation method such as `'ffill'` or `'bfill'`.
`isnull`	Return like-type object containing boolean values indicating which values are missing / NA.
`notnull`	Negation of `isnull`.

[W. McKinney, Python for Data Analysis]

Derived Data

- Create new columns from existing columns
  - `r["PctFail"] = r['Fail'] / r['Total']`
  - `r = r.assign(PctFail= r['Fail'] / r['Total'])`
- Note that operations are computed in a vectorized manner
- Similarities to functional paradigm (map/filter):
  - specify the operation once
  - no loops
  - interpreted as an operation on the entire column

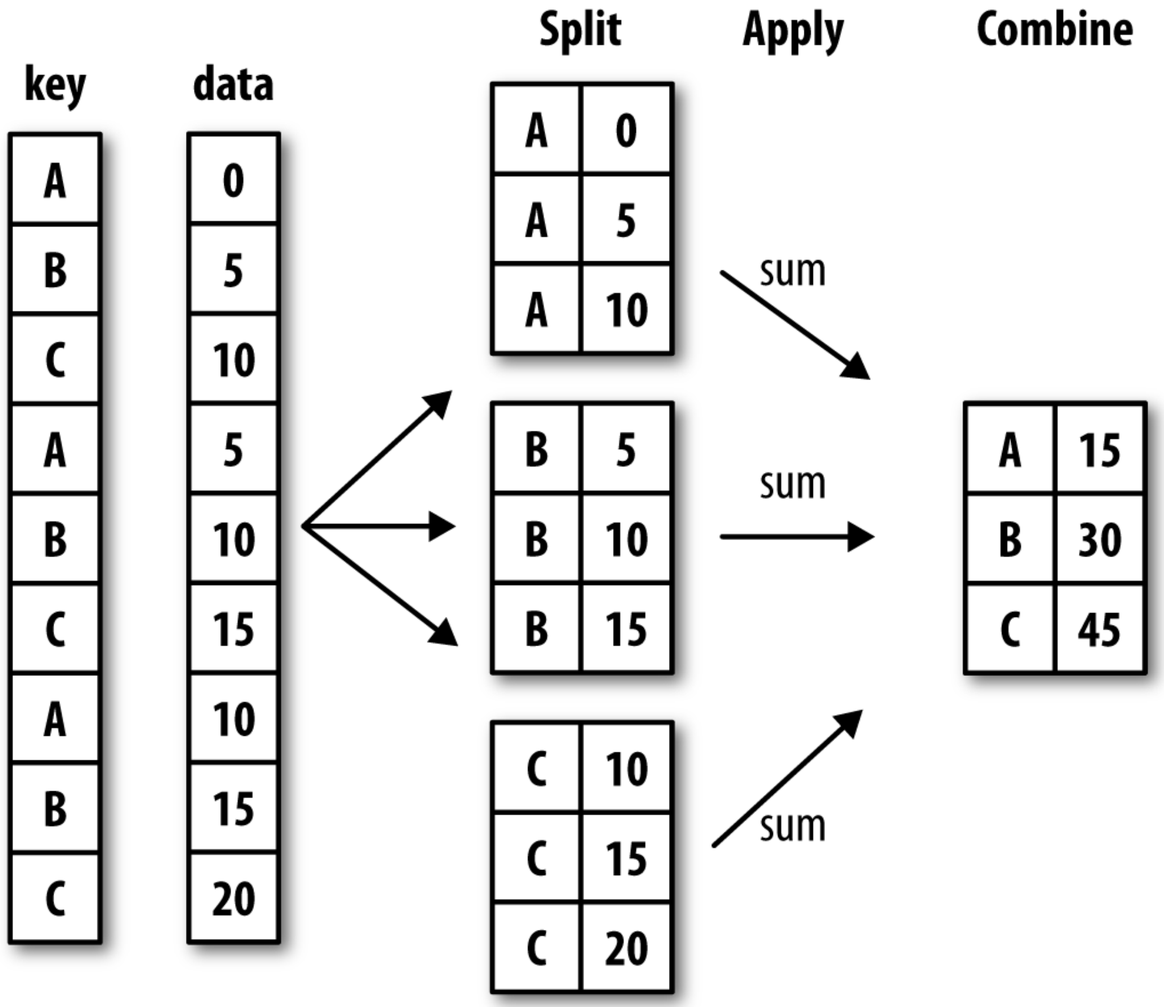
inplace

- Generally, when we modify a data frame, we reassign:
  - `rdf = df.reset_index()`
  - This is usually very **efficient**
  - Allows for method chaining
- There are versions where you can do this "inplace" (**try to avoid this**)
  - `df.reset_index(inplace=True)`
  - This means **no reassignment**, but it isn't usually any faster nor better
  - Sometimes still creates a copy
  - Will likely be deprecated

Aggregation

- Descriptive statistics
  - `df['Culmen Length (mm)'].mean()`
  - `.median()`
  - `.describe()`
  - `.count()`
  - `.min(), .max()`
- Also general methods
  - `.sum()`
  - `.product()`

Split-Apply-Combine



[W. McKinney, Python for Data Analysis]

Split-Apply-Combine

- Similar to Map (split+apply) Reduce (combine) paradigm
- The Pattern:
  1. **Split** the data by some grouping variable
  2. **Apply** some function to each group independently
  3. **Combine** the data into some output dataset
- The apply step is usually one of:
  - Aggregate
  - Transform
  - Filter

[T. Brandt]

In Pandas

- `groupby` method creates a `GroupBy` object
- `groupby` doesn't actually compute anything until there is an apply/aggregate step or we wish to examine the groups
- Choose keys (columns) to group by
- `size()` is the count of each group
- Other aggregates also work

Examples

- `df.groupby('Island')`
- `df.groupby('Island').size()`
- `df.groupby('Island')['Culmen Length (mm)'].mean()`

Split-Apply-Combine

- `df.groupby('Island')[['Culmen Length (mm)', 'Culmen Depth (mm)']].mean()`
- `df.groupby('Island').agg({'Culmen Length (mm)': 'mean', 'Culmen Depth (mm)': 'mean'})`
-
```
df.groupby('Island').agg(
    cul_length=('Culmen Length (mm)', 'mean'),
    cul_depth=('Culmen Depth (mm)', 'mean'))
```

Island	cul_length	cul_depth
Biscoe	45.257485	15.874850
Dream	44.167742	18.344355
Torgersen	38.950980	18.429412

Different Data Layouts

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

Initial Data

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

Transpose

name	trt	result
John Smith	a	—
Jane Doe	a	16
Mary Johnson	a	3
John Smith	b	2
Jane Doe	b	11
Mary Johnson	b	1

Tidy Data

[H. Wickham, 2014]

Problem: Variables stored in both rows & columns

Mexico Weather, Global Historical Climatology Network

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	—	—	—	—	—	—	—	—

[H. Wickham, 2014]

Problem: Variables stored in both rows & columns

Mexico Weather, Global Historical Climatology Network

id	year	month	element	d1	d2	d3	d4	d5	d6	d7	d8
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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	—	—	—	—	—	—	—	—

Variable in columns: day; Variable in rows: tmax/tmin

[H. Wickham, 2014]

Solution: Melting + Pivot

id	date	element	value
MX17004	2010-01-30	tmax	27.8
MX17004	2010-01-30	tmin	14.5
MX17004	2010-02-02	tmax	27.3
MX17004	2010-02-02	tmin	14.4
MX17004	2010-02-03	tmax	24.1
MX17004	2010-02-03	tmin	14.4
MX17004	2010-02-11	tmax	29.7
MX17004	2010-02-11	tmin	13.4
MX17004	2010-02-23	tmax	29.9
MX17004	2010-02-23	tmin	10.7

(a) Molten data

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

(b) Tidy data

[H. Wickham, 2014]

Melt

- Want to keep each observation separate (tidy), aka pivot_longer

	location	Temperature	Jan-2010	Feb-2010	Mar-2010
0	CityA	Predict	30	45	24
1	CityB	Actual	32	43	22

```
df.melt(id_vars=["location", "Temperature"],
        var_name="Date", value_name="Value")
```

	location	Temperature	Date	Value
0	CityA	Predict	Jan-2010	30
1	CityB	Actual	Jan-2010	32
2	CityA	Predict	Feb-2010	45
3	CityB	Actual	Feb-2010	43
4	CityA	Predict	Mar-2010	24
5	CityB	Actual	Mar-2010	22

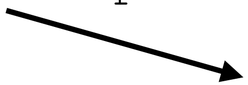
[AB Abhi]

Pivot

- Sometimes, we have data that is given in "long" format and we would like "wide" format (aka pivot_wider)
- Long format: column names are data values…
- Wide format: more like spreadsheet format
- Example:

```
         date     item     value
0  1959-03-31  realgdp  2710.349
1  1959-03-31     infl     0.000
2  1959-03-31    unemp     5.800
3  1959-06-30  realgdp  2778.801
4  1959-06-30     infl     2.340
5  1959-06-30    unemp     5.100
6  1959-09-30  realgdp  2775.488
7  1959-09-30     infl     2.740
8  1959-09-30    unemp     5.300
9  1959-12-31  realgdp  2785.204
```

```
.pivot('date', 'item', 'value')
```



```
item        infl   realgdp  unemp
date
1959-03-31  0.00  2710.349    5.8
1959-06-30  2.34  2778.801    5.1
1959-09-30  2.74  2775.488    5.3
1959-12-31  0.27  2785.204    5.6
1960-03-31  2.31  2847.699    5.2
```

[W. McKinney, Python for Data Analysis]

Reshaping Data

- Reshape/pivoting are fundamental operations
- Can have a nested index in pandas
- Example: Congressional Districts (Ohio's 1st, 2nd, 3rd, Colorado's 1st, 2nd, 3rd) and associated representative rankings
- Could write this in different ways:

number	one	two	three
state			
Ohio	0	1	2
Colorado	3	4	5

state	Ohio	Colorado
number		
one	0	3
two	1	4
three	2	5

state	number	
Ohio	one	0
	two	1
	three	2
Colorado	one	3
	two	4
	three	5

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number	one	two	three
state			
Ohio	0	1	2
Colorado	3	4	5

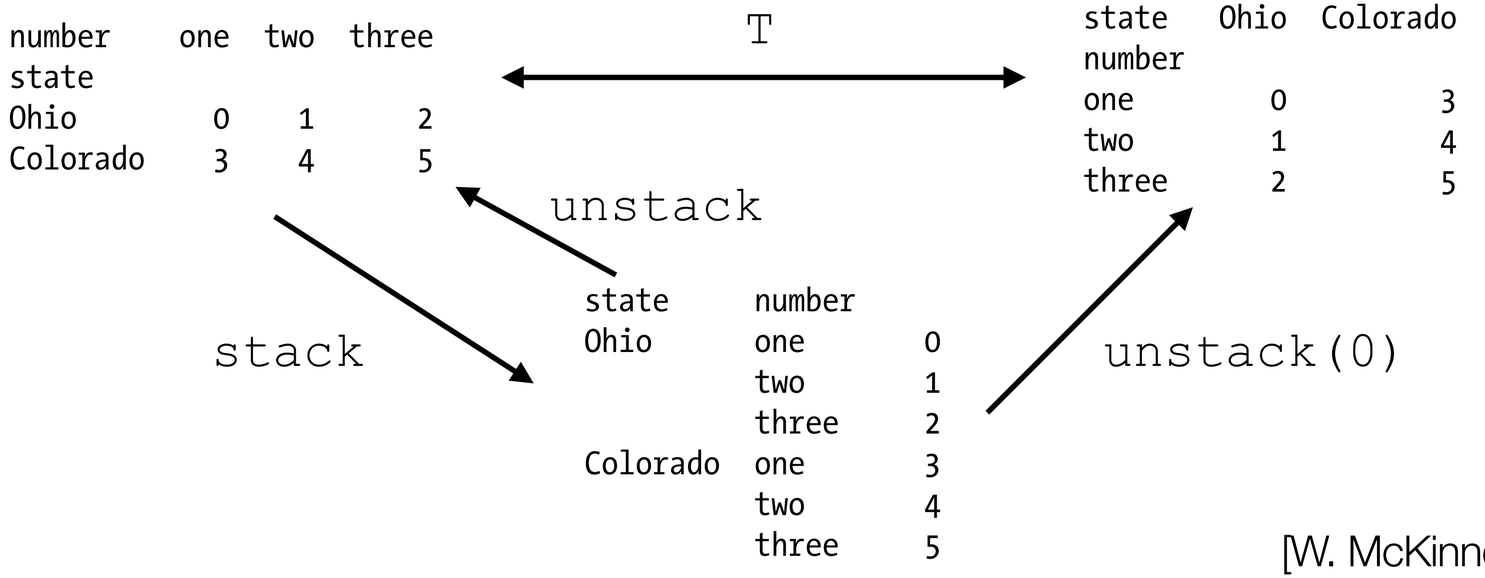
state	Ohio	Colorado
number		
one	0	3
two	1	4
three	2	5

MultiIndex

state	number	
Ohio	one	0
	two	1
	three	2
Colorado	one	3
	two	4
	three	5

Stack and Unstack

- `stack`: pivots from the columns into rows (may produce a Series!)
- `unstack`: pivots from rows into columns
- unstacking may add missing data
- stacking filters out missing data (unless `dropna=False`)
- can unstack at a different level by passing it (e.g. 0), defaults to innermost level



[W. McKinney, Python for Data Analysis]