9 Data Analysis with pandas

9.1 Introduction to pandas

9.1.1 What is pandas?

pandas is a widely-used, open-source Python library for data manipulation and analysis. Unlike NumPy, its basic array-like data structure, the DataFrame object, can contain heterogeneous data types (floats, integers, strings, dates, etc.) that may be structured in a hierarchy and indexed. It provides a large number of vectorized functions for cleaning, transforming and aggregating data efficiently using similar idioms to those used by NumPy. Its name derives from the term "panel data" (otherwise known as "longitudinal data"), which refers to data sets of several variables followed over multiple time periods for the same individual.

The pandas homepage, https://pandas.pydata.org/, contains details of the latest release and how to download and install pandas. In this chapter we follow the common convention of importing the library as the alias pd:

```
import pandas as pd
```

The key pandas data structures are Series and DataFrame, representing a onedimensional sequence of values and a data table, respectively. Their basic properties and use will be described in this section, followed by more advanced features and applications to examples in subsequent sections. pandas is a large, complex library with a lot of functionality; this chapter aims to cover the basics: more detailed examples are provided on the website accompanying the book.

9.1.2 Series

In its simplest form, a Series may be created in the same way as a one-dimensional NumPy array:

```
In [x]: river_lengths = pd.Series([6300, 6650, 6275, 6400])
In [x]: river_lengths
Out[x]:
0    6300
1    6650
2    6275
3    6400
dtype: int64
```

The Series can be given a name and dtype:

Unlike a NumPy array, however, each element in a pandas Series is associated with an *index*. Since we did not set the index explicitly here, a default integer sequence (starting at 0) is used for the index:

```
In [x]: river_lengths.index
Out[x]: RangeIndex(start=0, stop=4, step=1)
```

RangeIndex is a pandas object that works in a memory-efficient way like Python's range built-in to provide a monotonic integer sequence. It is often useful to refer to the rows of a Series with some other label than an integer index. Explicit indexing of the entries can be achieved by passing a sequence as the index argument or by creating the Series from a dictionary:

```
In [x]: river_lengths = pd.Series(data=[6300, 6650, 6275, 6400],
                          index=['Yangtze', 'Nile', 'Mississippi', 'Amazon'],
                           name='Length /km')
   . . . :
or:
In [x]: river_lengths = pd.Series(data={'Yangtze': 6300, 'Nile': 6650,
                                        'Mississippi': 6275, 'Amazon': 6400},
  . . . :
   . . . :
                                  name='Length /km')
In [x]: river_lengths
Out[x]:
Yangtze
              6300
Nile
              6650
Mississippi 6275
               6400
Name: Length /km, dtype: int64
```

This allows a nicely expressive way of referring to Series entries using the index labels instead of integers; either individually:

```
In [x]: river_lengths['Nile']
Out[x]: 6650
instead of river_lengths[1]; or from another sequence:
```

```
In [x]: river_lengths[['Amazon', 'Nile', 'Yangtze']]
Out[x]:
Amazon 6400
Nile 6650
Yangtze 6300
Name: Length /km, dtype: int64
```

instead of river_lengths[[3, 1, 0]]. Python-style slicing also works as expected:

```
In [x]: river_lengths[2::-1]
Out[x]:
Mississippi 6275
Nile 6650
Yangtze 6300
Name: Length /km, dtype: int64
```

It is even possible to use a slice-like notation for the index labels, but note that in this case the endpoint is *inclusive*:

Providing the index label is a valid Python identifier, one can refer to a row as an *attribute* of the Series:

```
In [x]: river_lengths.Mississippi
Out[x]: 6275
```

It is, of course, possible to do numerical operations on Series data, in a vectorized fashion, as for NumPy arrays:

In the above we have also chosen to update the Series object's name attribute. Note that the dtype has also changed appropriately from int64 to float64 to accommodate the new values.

Comparison operations and filtering a Series with a boolean operation creates a new Series:

```
In [x]: river_lengths > 4000
Out[x]:
Nile
               True
              False
Amazon
              False
Mississippi False
Name: Length /miles, dtype: bool
In [x]: river_lengths[river_lengths <= 4000]</pre>
Out[x]:
             3976.774400
Amazon
Yangtze
             3914.637300
Mississippi 3899.103025
Name: Length /miles, dtype: float64
```

Tests for membership of a Series examine the *index*, not the *values*:

```
In [x]: 'Yangtze' in river_lengths
Out[x]: True
```

Series can be *sorted*, either by their index or their values, using Series.sort_index and Series.sort_values, respectively. By default these methods return a new Series, but they can also be used to update the original Series with the argument inplace=True. A further argument, ascending, can be True (the default) or False to set the ordering:

```
In [x]: river_lengths.sort_index()
Out[x]:
Amazon
              3976.774400
Mississippi 3899.103025
Nile
             4132.117150
Yangtze
             3914.637300
Name: Length /miles, dtype: float64
In [x]: river_lengths.sort_values(ascending=False, inplace=True)
In [x]: river_lengths
Out[x]:
Nile
             4132.117150
              3976.774400
Amazon
Yangtze
              3914.637300
            3899.103025
Mississippi
Name: Length /miles, dtype: float64
```

When two series are combined, they are aligned by index label.

```
In [x]: masses = pd.Series({'Ganymede': 1.482e23,
                            'Callisto': 1.076e23,
                            'Io': 8.932e22,
                            'Europa': 4.800e22,
                            'Moon': 7.342e22,
                            'Earth': 5.972e24}, name='mass /kg')
In [x]: radii = pd.Series({'Ganymede': 2.634e6,
                           'Io': 1.822e6,
                           'Moon': 1.737e6,
                           'Earth': 6.371e6}, name='radius /m')
In [x]: from scipy.constants import G
In [x]: surface_g = G * masses / radii**2
In [x]: surface_g.name = 'surface gravity /m.s-2'
In [x]: surface_g.index.name = 'Body'
In [x]: surface_g
Body
Callisto
                 NaN
Earth
           9.819650
Europa
                 NaN
Ganymede 1.425634
           1.795740
Ιo
Moon
           1.624075
Name: surface gravity /m.s-2, dtype: float64
```

Note that where no correspondence can be made within the indexes (an index label in one Series that is missing from the other), the result is "Not a Number" (NaN). The methods is null and not null test for this:

```
In [x]: surface_g.isnull()
Out[x]:
Body
Callisto
            True
Earth
            False
            True
Europa
Ganymede
            False
            False
Ιo
Moon
            False
Name: surface gravity /m.s-2, dtype: bool
```

To return a list without any missing values, either filter with surface_g[surface_g.notnull()] or use the dropna method:

Finally, to convert a Series into a NumPy ndarray (dropping the index and other metadata), use the values property:

Example E9.1 NaN entries can be replaced in a pandas Series with a specified value using the fillna method:

```
In [x]: ser1 = pd.Series({'b': 2, 'c': -5, 'd': 6.5}, index=list('abcd'))
In [x]: ser1
Out[x]:
а
    NaN
b
    2.0
   -5.0
C
   6.5
dtype: float64
In [x]: ser1.fillna(1, inplace=True)
In [x]: ser1
Out[x]:
a
    1.0
b
    2.0
   -5.0
c
    6.5
dtype: float64
```

Infinities (represented by the floating-point inf value) can be replaced with the replace method, which takes a scalar or sequence of values and substitutes them with another, single value:

```
In [x]: ser2 = pd.Series([-3.4, 0, 0, 1], index=ser1.index)
In [x]: ser2
Out[x]:
   -3.4
    0.0
b
c 0.0
d
   1.0
dtype: float64
In [x]: ser3 = ser1 / ser2
In [x]: ser3
Out[x]:
   -0.294118
b
         inf
         -inf
С
d
    6.500000
dtype: float64
In [x]: ser3.replace([np.inf, -np.inf], 0)
Out[x]:
   -0.294118
b
    0.000000
    0.000000
С
   6.500000
dtype: float64
```

(Assuming NumPy has been imported with import numpy as np.)

9.1.3 DataFrame

Creating a DataFrame

A DataFrame is a two-dimensional table of data that can be thought of as an ordered set of Series columns, which all have the same index. To create a simple DataFrame from a dictionary, assign value sequences¹ to column name keys:

```
In [x]: data = {'mass': [1.482e23, 1.076e23, 8.932e22, 4.800e22, 7.342e22],
               'radius': [2.634e6, None, 1.822e6, None, 1.737e6],
               'parent': ['Jupiter', 'Jupiter', 'Jupiter', 'Jupiter', 'Earth']
In [x]: index = ['Ganymede', 'Callisto', 'Io', 'Europa', 'Moon']
In [x]: df = pd.DataFrame(data, index=index)
In [x]: df
Out[x]:
                mass radius parent
Ganymede 1.482000e+23 2634000.0 Jupiter
Callisto 1.076000e+23
                       NaN Jupiter
         8.932000e+22 1822000.0 Jupiter
Europa
         4.800000e+22
                           NaN Jupiter
         7.342000e+22 1737000.0
                                   Earth
```

Values which were None in the data have been assigned to NaN in the DataFrame. We may wish to rename a column or index row: to do this, call rename, declaring which

 $^{^{1}\,}$ The (unspecified) units here are SI units: kg and m.

axis ('index' [the same as 'rows', and the default] or 'columns'²) contains the label(s) to be renamed, and passing a dictionary mapping each original label to its replacement. Remember to set inplace=True if you want the original DataFrame modified rather than a new copy returned. For example,

This last statement has returned a new DataFrame but not altered the original one, df.

Accessing Rows, Columns and Cells

An individual column can be obtained by indexing or by attribute (if its name is a valid Python identifier):

```
In [x]: df['mass']  # or df.mass
Out[x]:
Ganymede    1.482000e+23
Callisto    1.076000e+23
Io     8.932000e+22
Europa    4.800000e+22
Moon    7.342000e+22
Name: mass, dtype: float64
```

Since this column is just a pandas Series, individual values can be retrieved by position or reference to the index label:

```
In [x]: df['mass'][2]
Out[x]: 8.932e+22
In [x]: df['mass']['Io']  # or df['mass'].Io or df.mass.Io
Out[x]: 8.932e+22
```

Now, for retrieving columns and individual values this is fine, but assignment raises a warning:

```
In [x]: df['radius']['Callisto'] = 2.410e6
/Users/christian/envs/py37/bin/ipython:1: SettingWithCopyWarning:
A value is trying to be set on a copy of a slice from a DataFrame
...
```

In this case, it has worked:

```
In [x]: df['radius']['Callisto']
Out[x]: 2410000.0
```

but the message is a general warning that "chained indexing" ([..][..]) can lead to unpredictable results when used for assignment: depending on how the data are stored

 $^{^2}$ One can also refer to the rows and columns of a DataFrame with axis=0 and axis=1, respectively.

in memory, it is possible for the indexing expression to yield a *copy* of the data rather than a view. Assigning to the copy rather than modifying the data in-place is what the SettingWithCopyWarning is warning could happen. *Chained indexing for assignment operations should be avoided.*

Two DataFrame methods, loc and iloc, can be used to reliably access and assign to columns, rows and cells; using them is strongly recommended. loc selects by row and column *labels*:

The single row of data indexed by the label Europa is returned as a Series. If only a subset of the columns are required, pass their names in a sequence to the second axis:³

```
In [x]: df.loc['Europa', ['mass', 'planet']]
Out[x]:
mass     4.8e+22
planet    Jupiter
Name: Europa, dtype: object
```

Slicing, "fancy" indexing and boolean indexing are all supported by loc:

```
In [x]: df.loc[:, 'mass'] # the same as df['mass'] - returns a Series
Out[x]:
Ganymede
          1.482000e+23
Callisto 1.076000e+23
           8.932000e+22
Ιo
           4.800000e+22
           7.342000e+22
Moon
Name: mass, dtype: float64
In [x]: df.loc['Ganymede':'Io', ['mass', 'radius']]
Out[x]:
                 mass
                          radius
Ganymede 1.482000e+23 2634000.0
Callisto 1.076000e+23 2410000.0
         8.932000e+22 1822000.0
In [x]: df.loc[['Moon', 'Europa'], 'planet']
Out[x]:
Moon
           Earth
Europa
        Jupiter
Name: planet, dtype: object
In [x]: df.loc[df.planet=='Jupiter', 'radius']
Out[x]:
           2634000.0
Ganymede
Callisto
           2410000.0
```

³ Note that whilst chained indexing refers to a cell in column, row order: df[col][row], loc locates cells the other way round: df.loc[row, col] or df.loc[row][col].

```
Io 1822000.0
Europa NaN
Name: radius, dtype: float64
```

The value of a single cell can therefore be retrieved from the row and column labels:

```
In [x]: df.loc['Europa', 'mass']
Out[x]: 4.8e+22
```

This is the safe way to modify data in a DataFrame:

```
In [x]: df.loc['Europa', 'radius'] = 1.561e6  # no warning, data changed in place
In [x]: df.loc['Europa']
Out[x]:
mass     4.8e+22
radius    1.561e+06
parent     Jupiter
Name: Europa, dtype: object
```

It is common to use loc in combination with boolean indexing to filter rows by column values. For example, the masses of Jupiter's moons:

The rows corresponding to moons with radii less than 2000 km:

The second method, iloc, retrieves data by numerical index position:

```
In [x]: df.iloc[1]
                           # the second row
Out[x]:
mass
         1.076e+23
radius
         2.41e+06
parent
          Jupiter
Name: Callisto, dtype: object
In [x]: df.iloc[:, [1, 2]]
                            # all rows, second and third columns
Out[x]:
            radius planet
Ganymede 2634000.0 Jupiter
Callisto 2410000.0 Jupiter
         1822000.0 Jupiter
Ιo
       1561000.0 Jupiter
Europa
        1737000.0 Earth
In [x]: df.iloc[-1, 1]
                          # last row, second column
Out[x]: 1737000.0
```

For single scalar values, there are also at and iat:

```
In [x]: df.at['Moon', 'mass']  # same as df.loc['Moon', 'mass']  
Out[x]: 7.342e+22  
In [x]: df.iat[-1, 0]  # same as df.iloc[-1, 0]  
Out[x]: 7.342e+22
```

Example E9.2 There is a potential source of confusion when using loc for a Series or DataFrame with an integer index: it is important to remember that *loc always refers* to the index labels, whereas iloc takes a (zero-based) integer location index:

```
In [x]: df = pd.DataFrame(np.arange(12).reshape(4, 3) + 10,
                        index=[1, 2, 3, 4], columns=list('abc'))
In [x]: df
Out[x]:
  a b
1 10 11 12
2 13 14 15
3 16 17 18
4 19 20 21
In [x]: df.loc[1] # the row with index *label* 1 (the first row)
Out[x]:
a
   10
С
   12
Name: 1, dtype: int64
In [x]: df.iloc[1] # the row with index *location* 1 (the row labeled 2)
a
   13
b
    14
    15
Name: 2, dtype: int64
  Note also that index labels do not have to be unique:
In [x]: df.index = [1, 2, 2, 3] # change the index labels
   a b
          С
```

```
In [x]: df
Out[x]:
1 10 11 12
2 13 14 15
2 16 17 18
3 19 20 21
In [x]: df.loc[2]
                   # a DataFrame: all rows labeled 2
Out[x]:
  a b
2 13 14 15
2 16 17 18
In [x]: df.iloc[2]
                  # a Series: there is only one row located at index 2
Out[x]:
a 16
b
    17
```

```
c 18
Name: 2, dtype: int64
```

Combining Series and DataFrames

Another way to create a DataFrame is from a nested dictionary or from a dictionary of Series. In each case, the outer dictionary keys contain the *column* names; Series and inner dictionaries end up as rows:

```
boeing_wingspan = pd.Series({'B747-8': 68.4, 'B777-9': 64.8, 'B787-10': 60.12},
                           name='wingspan')
boeing_length = pd.Series({'B747-8': 76.3, 'B777-9': 76.7, 'B787-10': 68.28},
                            name='length')
boeing_range = pd.Series({'B777-9': 13940, 'B787-10': 11910},
                            name='range', dtype=float)
# Create a DataFrame from a dictionary of Series.
df_boeing = pd.DataFrame({'wingspan': boeing_wingspan, 'length': boeing_length,
                          'range': boeing_range})
# Create a DataFrame from a dictionary of dictionaries.
df_airbus = pd.DataFrame({'range': {'A350-1000': 16100, 'A380-800': 14800},
                          'wingspan': {'A350-1000': 64.75, 'A380-800': 79.75},
                          'length': {'A350-1000': 73.8, 'A380-800': 72.72} })
In [x]: df_boeing
Out[x]:
         wingspan length
                             range
B747-8
            68.40
                   76.30
B777-9
           64.80
                   76.70 13940.0
B787-10
            60.12
                    68.28 11910.0
In [x]: df_airbus
Out[x]:
           range wingspan length
A350-1000 16100
                     64.75
                            73.80
A380-800
          14800
                     79.75
                            72.72
```

Note that missing values in the columns become NaN in the DataFrame. To concatenate two DataFrames, use $pd.concat:^4$

```
In [x]: pd.concat((df_airbus, df_boeing))
Out[x]:
          length
                    range wingspan
A350-1000
           73.80 16100.0
                              64.75
A380-800
           72.72 14800.0
                              79.75
                              68.40
B747-8
           76.30
                      NaN
B777-9
           76.70 13940.0
                              64.80
           68.28 11910.0
                              60.12
```

⁴ Note that the concat and append functions require data to be copied into a new DataFrame and for large data sets can be slow and memory-inefficient. In this case, if at all possible, it is better to pre-allocate an empty DataFrame of the right size and to insert data directly into it.

(df_airbus.append(df_boeing) would give the same result.)

To add a single column to a DataFrame, assign a sequence of values or a Series object:

Concatenating DataFrames with different columns fills the unknown values with NaN:

```
In [x]: df_aircraft = pd.concat((df_airbus, df_boeing))
In [x]: df_aircraft
Out[x]:
          length
                   range speed wingspan
A350-1000 73.80 16100.0 950.0
                                   64.75
A380-800
         72.72 14800.0 903.0
                                   79.75
B747-8
          76.30
                   NaN
                          NaN
                                   68.40
B777-9
           76.70 13940.0
                           NaN
                                   64.80
B787-10
           68.28 11910.0
                           NaN
                                    60.12
```

Note that retrieving a Series as a row or column returns a *view* on the DataFrame, so changes to this Series will be reflected in it:

```
In [x]: speeds = df_aircraft['speed']
In [x]: speeds['B747-8','B787-10'] = 903, 956
                                             # changes df_aircraft data
In [x]: jumbo = df_aircraft.loc['B747-8']
                                            # changes df aircraft data
In [x]: jumbo.range = 15000
In [x]: df_aircraft
Out[x]:
          length
                   range speed wingspan
A350-1000 73.80 16100.0 950.0
                                  64.75
           72.72 14800.0 903.0
A380-800
                                    79.75
B747-8
           76.30 15000.0 903.0
                                   68.40
B777-9
           76.70 13940.0
                           NaN
                                    64.80
B787-10
           68.28 11910.0 956.0
                                    60.12
```

To remove a column from a DataFrame, call Python's del keyword:

```
In [x]: del df_aircraft['speed']
                                        # NB but not del df_aircraft.speed
In [x]: df_aircraft
Out[x]:
          length
                    range wingspan
A350-1000 73.80 16100.0
                              64.75
A380-800
           72.72 14800.0
                              79.75
B747-8
           76.30 15000.0
                              68.40
B777-9
           76.70 13940.0
                              64.80
B787-10
           68.28 11910.0
                              60.12
```

The drop function can be used to selectively remove rows and columns from a DataFrame. A new object is returned unless inplace=True is specified:

```
In [x]: df_aircraft.drop(['A350-1000', 'A380-800'])
                                                    # drop rows by default
Out[x]:
        length
                range wingspan
B747-8
         76.30 15000.0
B777-9
         76.70 13940.0
                            64.80
B787-10 68.28 11910.0
                           60.12
In [x]: df_aircraft.drop(['length', 'wingspan'], axis='columns', inplace=True)
In [x]: df_aircraft
Out[x]:
            range
A350-1000 16100.0
          14800.0
A380-800
B747-8
          15000.0
B777-9
         13940.0
B787-10
         11910.0
```

9.1.4 Sorting, Arithmetic and Statistics

As might be expected, many of the most useful functions for data analysis are available from within pandas.

Example E9.3 The file india-data.csv, available at https://scipython.com/eg/bak, contains columns of demographic data on the 36 states and union territories (UTs) of India. When read in with:

```
In [x]: df = pd.read_csv('india-data.csv', index_col=0)
```

(more on this method in the next section), the DataFrame produced contains an Index of State/UT name and columns:

We can quickly inspect the DataFrame with df.head(n), which outputs the first n rows (or five rows if n is not specified):

```
46809027 ...
West Bengal
                                                   71.16
Madhya Pradesh
                     37612306 ...
                                                   60.02
[5 rows x 5 columns]
pandas makes it straightforward to compute new columns for our DataFrame:
In [x]: df['Population'] = df['Male Population'] + df['Female Population']
In [x]: total_pop = df['Population'].sum()
In [x]: print(f'Total population: {total_pop:,d}')
Total population: 1,210,754,977
In [x]: df['Population Density (km-2)'] = df['Population'] / df['Area (km2)']
In [x]: df.loc['West Bengal', 'Population Density (km-2)']
Out[x]: 1028.440091490896
                              # population density of West Bengal
```

Maximum and minimum values are obtained in the same way as in NumPy, for example:

mean population density

```
In [x]: df['Male Literacy (%)'].min()
Out[x]: 73.39
```

Out[x]: 368.3195047153525

In [x]: total_pop / df['Area (km2)'].sum()

Perhaps more usefully, idxmin and idxmax return the index *label(s)* of the minimum and maximum values, respectively:

```
In [x]: df['Area (km2)'].idxmax() # largest state/UT by area
Out[x]: 'Rajasthan'
```

Naturally, the value returned can be passed to df.loc to obtain the entire row. For example, the row corresponding to the most densely populated state / UT:

```
In [x]: df.loc[df['Population Density (km-2)'].idxmax()]
Out[x]:
Male Population
Female Population
                           7800615
                           1484
Area (km2)
Male Literacy (%)
                           91.03
                           80.93
Female Literacy (%)
                            16687940
Population
Population Density (km-2)
                          1.124524e+04
Name: Delhi, dtype: float64
```

Correlation statistics between DataFrames or Series can be calculated with the corr function:

```
In [x]: df['Female Literacy (%)'].corr(df['Fertility Rate'])
Out[x]: -0.7361949271996956
```

In this case (two columns of data being compared), a single correlation coefficient is produced. More generally, the correlation *matrix* is returned as a new DataFrame. pandas can be used to quickly produce a variety of simple, labeled plots and charts from a DataFrame with a family of df.plot methods. By default, these use the Matplotlib backend, so the syntax is the same as presented in Chapter 7. For example,

```
In [x]: df.plot.scatter('Female Literacy (%)', 'Fertility Rate')
```

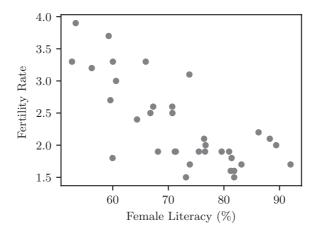


Figure 9.1 Scatter plot of fertility rate against female literacy for the 36 states and UTs of India.

Figure 9.1 shows the resulting plot.

9.2 Reading and Writing Series and DataFrames

9.2.1 Reading Text Files

Delimited Text Files

The core method for reading text files of data into a DataFrame is pd.read_csv. This works in much the same way as NumPy's genfromtxt method, but with additional functionality for naming columns and setting the DataFrame index. It takes no fewer than 49 possible arguments, but the most important are described below.⁵

- filepath_or_buffer (required): The path to the file to read: this can be a local file or a URL for fetching data across the internet.
- sep: The column delimiter; by default ',', but use '\s+' for whitespace-delimited columns, '\t' for tab-delimiters, or None to force pandas to try to infer the delimiter. See also delim_whitespace.
- delimiter: An alias for sep.
- header: The row numbers (indices) to use for the column names. The default is header=0: use the first row for the column names. *Note*: if the file does not have a header, specify header=None and set the column names with the names argument.

⁵ See the documentation at https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.read_csv.html for a complete description.

- names: A sequence of unique column names to use. If the file contains no header, set header=None in addition to setting names.
- index_col: The column(s) to use as the row labels in the DataFrame.
- usecols: A sequence of column indices (as for NumPy's loadtxt method) or column names identifying the columns to be read into the DataFrame.
- squeeze: If the data required consist of a single column, then squeeze=True will return a Series instead of the default, a DataFrame.
- converters: A dictionary of functions for converting the values in specified columns in the input file into data values for the DataFrame. The dictionary keys can be column indices or column names.
- skiprows: An integer giving the number of lines at the start of the file to skip over before reading the data or a sequence giving the indices of rows to skip.
- skipfooter: The number of rows at the bottom of the file to skip (by default, 0).
- nrows: The number of rows of the file to read: this is useful for reading a subset of lines from a very large file for testing or exploring its data.
- na_values: A string or sequence of strings to treat as NaN values, in addition to the default values which include 'NaN', 'NA', 'NULL' and '#N/A' (see the documentation for a full list).
- parse_dates: Set to True to parse the index column(s) as a sequence of datetime objects (see Section 9.3.2); other options are available for this argument (see the online documentation).
- comment: Specify a single character, such as '#', which, when found at the start of a line, signals that the whole line is to be ignored.
- skip_blank_lines: The default, True, skips over blank lines in the input file; set to False to interpret these as a row of NaN values instead.
- delim_whitespace: Can be set to True instead of specifying sep='\s+' to indicate that the data columns are separated by whitespace.

Example E9.4 The file ionization-energies.csv, available to download at https://scipython.com/eg/baq, contains the ionization energies (in eV) of some of the elements of the periodic table:

```
Ionization Energies (eV) of the first few elements of the periodic table Element, IE1, IE2, IE3, IE4, IE5
H, 13.59844
He, 24.58741, 54.41778
Li, 5.39172, 75.64018, 122.45429
Be, 9.3227, 18.21116, 153.89661, 217.71865
B, 8.29803, 25.15484, 37.93064, 259.37521, 340.22580
C, 11.26030, 24.38332, 47.8878, 64.4939, 392.087
N, 14.53414, 29.6013, 47.44924, 77.4735, 97.8902
O, 13.61806, 35.11730, 54.9355, 77.41353, 113.8990
F, 17.42282, 34.97082, 62.7084, 87.1398, 114.2428
Ne, 21.5646, 40.96328, 63.45, 97.12, 126.21
Na, 5.13908, 47.2864, 71.6200, 98.91, 138.40
```

These data can be read into a DataFrame as follows. Here, we suppose that we are only interested in the first two periods of the periodic table and the first four ionization energies:

- Note that the usecols argument includes the column we want to set to the DataFrame index and nrows includes the column headers (but not the skipped rows).
- **2** The whitespace around the column names is not automatically removed. pandas provides a variety of methods for manipulating strings within the str "accessor" namespace, which can be applied to all the column names in one statement; this is faster than using rename:

```
df.rename(columns=lambda s: s.strip(), inplace=True)
```

Example E9.5 The following text file, available at https://scipython.com/eg/bao, contains data concerning 13 vitamins important for human health.

```
List of vitamins, their solubility (in fat or water) and recommended dietary allowances for men / women.

Data from the US Food and Nutrition Board, Institute of Medicine, National Academies
```

```
Vitamin B1 Water
                  1.2mg/1.1mg
Vitamin B2
           Water
                   1.3 mg / 1.1 mg
Vitamin B3 Water
                   16mg/14mg
Vitamin B5 Water
                   5mg
Vitamin B6 Water
                  1.5mg/1.4mg
Vitamin B7
           Water
                   30ug
Vitamin B9 Water
                   400 ua
Vitamin B12 Water 2.4ug
Vitamin C
           Water
                   90ma/75ma
Vitamin D
           Fat
                   15ug
Vitamin E Fat
                   15ma
                   110ug/120ug
Vitamin K Fat
--- Data for guidance only, consult your physician ---
```

900ug/700ug

Vitamin A Fat

The recommended (daily) dietary allowances are listed in either of two units in the final column; sometimes these are different for men and women. If we wish to parse this column into an average value in μg , we can use a converter function as in the following code.

Listing 9.1 Reading in a text table of vitamin data

In this code, the four header rows and one footer row are skipped (blank lines are skipped automatically); the Index is set to the first *used* column (index_col=0, identifying the vitamin). The converter function averages the numerical values encountered (after conversion to μg), where multiple values are assumed to be separated by a solidus character (/).

Fixed-Width Text Files

The method read_fwf reads fixed-width formatted files. The field widths are passed as a list of tuples to the argument colspecs, giving the half-open intervals of the fields to read in from each line; i.e. (i, j) refers to the field from index i to index j - 1. Alternatively, if the intervals are contiguous, a list of field widths can be passed to the argument widths.

We return to the np.genfromtxt example of Section 6.2.3. The following short file, data.txt, consists of four columns with widths 2, 1, 9 and 3 characters (spaces are indicated with '..'):

```
_12__100.231.03
_11_1201.842.04
_11___99.324.02
  To read in this file with pandas, use either:
df = pd.read_fwf('data.txt',
                 colspecs=[(0, 2), (2, 3), (3, 12), (12, 15)], header=None)
or, since the intervals are contiguous:
df = pd.read_fwf('data.txt', widths=(2, 1, 9, 3), header=None)
to give the DataFrame:
   0 1
               2
0 1 2
         100.231 0.03
1 1 1 1201.842 0.04
2 1 1
         99.324 0.02
```

9.2.2 Writing Text Files

The DataFrame method to_csv outputs its data to a text file, formatted according to the arguments summarized below. 6

- path_or_buf: A file path or file object to output to; if None, the DataFrame is returned as string.
- sep: The single-character field-delimiter (defaults to ', ').
- na_rep: The string to use to represent missing data (defaults to the empty string, '').
- float_format: The C-style format specifier (see Section 2.3.7) for floating-point numbers.
- columns: A sequence identifying the columns to output.
- header: By default, True, indicating that column names should be output; can be set to False or a list of column names.
- index: By default, True, indicating that row names should be output.
- compression: One of 'infer', 'gzip', 'bz2', 'zip', 'xz', None to specify whether and how to compress the output file. The default is 'infer': pandas determines the intended compression method from the filename extension.

Example E9.6 To write a comma-separated file containing data on vitamins from the DataFrame created in Example E9.5 to_csv can be used as follows:

```
df.to_csv('vitamins.csv', float_format='%.1f', columns=['Solubility', 'RDA'])
```

The file written is:

```
Vitamin, Solubility, RDA
A,Fat,800.0
B1,Water,1150.0
B2,Water,1200.0
B3,Water,15000.0
B5,Water,5000.0
B6,Water,1450.0
B7,Water,30.0
B9,Water,400.0
B12,Water,2.4
C,Water,82500.0
D,Fat,15.0
E,Fat,15000.0
K,Fat,115.0
```

⁶ Full documentation is available at https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas. DataFrame.to_csv.html

4	А	В	С	D	E	F	G
1		Structural properties of some diatomic molecules					
2	Molecule	Bond length /A	we /cm-1	wexe /cm-1	De /kJ.mol-1		
3	I ₂	2.666	214.5	0.614	224.1042237		
4	O ₂	1.20752	1580.19	11.98	623.3408948		
5	CI ₂	1.987	559.7	2.67	350.8836826		
6	F ₂	1.41193	916.64	11.236	223.640111		
7	N ₂	1.09768	2358.57	14.324	1161.440719		
8	СО	1.128323	2169.81358	13.28831	1059.592595		
9	NO	1.15077	1904.20	14.075	770.4430432		
10	Data from the NIST	Chemistry WebBoo	k: Constants of Dia	tomic Molecules			
11	https://webbook.nis	t.gov					
12							
13							
14							
15							
16							
17							

Figure 9.2 An Excel sheet containing data concerning the structural properties of some diatomic molecules.

9.2.3 Microsoft Excel Files

pandas is able to read DataFrames from Excel files with both .xls and .xlsx extensions with the function pd.read_excel. You may need to install the xlrd package⁷ separately from your Python package manager or using pip on the command line with, for example:

pip install xlrd

The file path to the Excel document is passed as the first argument to read_excel. Most of the additional arguments already described for read_csv function in the same way, except that usecols can be passed either a list of column indices or a string giving the range of Excel column labels: for example: 'B:K', 'A,D,G:K'.

By default, only the first sheet of the file is used; to read in from a different sheet or more than one sheet, pass one or more indexes or sheet names to the argument sheet_name.

Example E9.7 The Excel file bond-lengths.xlsx, available online at https://scipython.com/eg/bbk, contains data on the bond lengths, vibrational constants and dissociation energies of some diatomic molecules. The single sheet is named 'Diatomics'. Column A contains the molecular formula; the first row is a title, and the second row contains the column names. There is also a footer of two lines, as shown in Figure 9.2.

The following statement can be used to read in a DataFrame containing these data:

⁷ https://pypi.org/project/xlrd/

```
df = pd.read_excel('bond-lengths.xlsx',
       index_col=0, # the first column contains the index labels
                              # ignore the last two lines of the sheet
# take the column names from the second row
       skipfooter=2,
       header=1,
       usecols='A:E',
                              # use Excel columns labeled A-E
       sheet_name='Diatomics' # take data from this sheet
print(df)
         Bond length /A
                           we /cm-1 wexe /cm-1 De /kJ.mol-1
Molecule
               2.666000
                         214.50000
                                       0.61400
               1.207520 1580.19000 11.98000
                                                 623.340895
02
                                     2.67000
C12
               1.987000 559.70000
                                                350.883683
F2
               1.411930 916.64000
                                     11.23600
                                                 223.640111
                                     14.32400
               1.097680 2358.57000
                                                 1161.440719
                                      13.28831 1059.592595
               1.128323 2169.81358
CO
NO
               1.150770 1904.20000
                                     14.07500
                                                 770.443043
```

Should you be in the unfortunate position of needing to *write* to an Excel spreadsheet file, use to_excel, as in the following example. Again, there may be a dependency to resolve: if the openpyxl module⁸ is not available, you can install through your package manager or using pip:

```
pip install openpyxl
```

Example E9.8 To create some data to write to a file, the following program generates a DataFrame with the height of a projectile launched at three different angles (in the columns) as a function of time (rows):

Listing 9.2 The height of a projectile as a function of time

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt

# Acceleration due to gravity, m.s-2.
g = 9.81

# Time grid, s.
t = np.linspace(0, 5, 500)
# Projectile launch angles, deg.
theta0 = np.array([30, 45, 80])
# Projectile launch speen, m.s-1.
v0 = 20

def z(t, v0, theta0):
    """Return the height of the projectile at time t > 0."""
    return -g/2 * t**2 + v0*t*np.sin(theta0)
```

⁸ https://pypi.org/project/openpyxl/

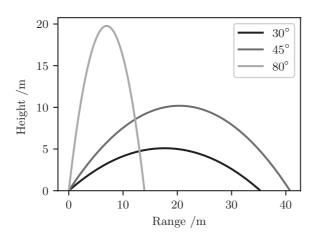


Figure 9.3 Trajectories of a projectile launched with $v_0 = 20 \text{ m s}^{-1}$ at three different angles.

```
def x(t, v0, theta0):
    """Return the range of the projectile at time t > 0."""
    return v0 * t * np.cos(theta0)
# An empty DataFrame with columns for the different launch angles.
df = pd.DataFrame(columns=theta0, index=t)
# Populate df with the projectile heights as a function of time.
for theta in theta0:
    df[theta] = z(t, v0, np.radians(theta))
# Once the projectile has landed (z <= 0), set the height data as invalid.
df[df <= 0] = np.nan
# Create a Matplotlib figure with the trajectories plotted.
fig, ax = plt.subplots()
for theta in theta0:
    ax.plot(x(t, v0, np.radians(theta)), df[theta], label=f'$\{theta\}^\circ circ$')
# The maximum height obtained by the projectile for each value of theta0.
heights = df.max()
print(heights)
# Set the y-limits with a bit of padding at the top; label the axes.
ax.set_ylim(0, heights.max()*1.05)
ax.set_xlabel('Range /m')
ax.set_ylabel('Height /m')
ax.legend()
plt.show()
```

Figure 9.3 shows the plot of the trajectories that is produced by this code. To save the DataFrame df to an Excel file in a single sheet, use to_excel:

```
df.to_excel('projectile.xlsx', sheet_name='Dependence on angle')
```

To write an Excel file with more than one sheet, create a pd.ExcelWriter object and call to_excel for each pandas object to output:

```
with pd.ExcelWriter('projectile2.xlsx') as writer:
    for theta in theta0:
        # Only retain the valid data for each trajectory.
        ser = df[theta].dropna()
        # Change the Series index to be the range instead of time.
        ser.index = x(ser.index, v0, np.radians(theta))
        ser.to_excel(writer, sheet_name=f'{theta} deg')
```

9.2.4 Web Scraping

The pandas function read_html can be used to parse web pages for data contained in HTML tables. A list of DataFrames is returned, and the default arguments for this function do a pretty good job on most well-formed pages. The most useful arguments are listed below.

- io: A URL, filepath or file object from which to parse the HTML
- match: An optional string to search for within the table: only tables containing this string are parsed and returned.⁹
- header: The row index to be used for the column headers; the default, None, uses the HTML > header cells, if present.
- index_col: The column(s) to use as the row labels in the DataFrame.
- attrs: A dictionary of HTML attributes to identify the required table; for example, attrs={'id': 'data-table'}.
- thousands: The separator used in grouping the digits of large numbers; defaults to ','.
- decimal: The character used in denoting the decimal point; the default is '.', as used in the United States, United Kingdom, Australia, Japan, China and South Korea; non-British European countries often use ','.
- na_values: String(s) used to denote NaN data, as for read_csv.

Example E9.9 At the time of writing, the first table on the Wikipedia page https: //en.wikipedia.org/wiki/List_of_wine-producing_regions contains columns of the rank, country name and wine production for the principal wine-producing countries in the world. To parse it with pandas:

 $^{^{9}}$ match can be a regular expression.

Italy	1	4796900
France	2	4607850
Spain	3	4293466
United States	4	3300000
China	5	1700000

- In this case, the table is identified by a match to the text inside the <caption> element of the first on the page.
- **2** dfs is a list containing a single item, the DataFrame parsed from the matching table.

9.2.5 Exercises

Problems

P9.2.1 The web page at https://scipython.com/ex/bab gives tables for the total ozone column amounts in October in "Dobson units," and the concentrations of two chlorofluorocarbon (CFC) compounds, "F11" and "F12", in parts per trillion by volume (pptv) for the years 1957 – 1984; see Farman *et al.*, *Nature* **315**, 207 (1985).

Read in and parse these data, and plot them on a suitable chart.

P9.2.2 At https://en.wikipedia.org/wiki/Abundances_of_the_elements_(data_page) Wikipedia gives a list of element abundances for the Sun and solar system in an HTML table (amongst other, similar data). Use pandas' read_html method to read in and parse the Kaye and Laby data (column headed "Y1") and plot a bar chart demonstrating *Oddo-Harkins rule*: that elements with even atomic numbers are more abundant than those with neighboring odd atomic numbers.

P9.2.3 The *Hertzsprung–Russell diagram* classifies stars on a scatter plot: each star is represented as a point with an *x*-coordinate of effective temperature and a *y*-coordinate of *luminosity*, a measure of the star's radiated electromagnetic power. The page at https://scipython.com/ex/bak can be used to obtain a version of the HYG-database, which provides data on 119614 stars. Read in these data with pandas and plot a Hertzsprung–Russell diagram. The luminosity column is identified as 'lum' in the header and the star temperature can be calculated from its *color index* (also referred to as (B-V) and identified as the column labeled 'ci') using the Ballesteros formula:

$$T/K = 4600 \left(\frac{1}{0.92(B-V) + 1.7} + \frac{1}{0.92(B-V) + 0.62} \right).$$

¹⁰ The Dobson unit is defined as the thickness, in units of 0.01 mm, that a layer of pure gas would form at standard conditions for temperature and pressure from its total column amount in the atmosphere above a region of the Earth's surface.

¹¹ https://github.com/astronexus/HYG-Database, released under a Creative Commons Attribution-ShareAlike license

Note that the luminosity is best visualized on a logarithmic scale and the temperature axis is usually plotted in reverse (decreasing temperature towards the right-hand side of the diagram).

P9.2.4 Transport for London (TfL) is the UK local government body responsible for the public transport system of Greater London; they make available an Excel document, available from the link at https://scipython.com/ex/bam, which provides statistics about the usage of the underground network (the Tube) in the form of entry and exit passenger numbers for a "typical" day at each station over the years 2007–2017.

Read in this document with pandas, and analyze it to determine: (a) the busiest station on a typical weekday in 2017; (b) the station with the greatest percentage increase in passengers over the period 2007–2017; (c) the station with the largest relative difference in passenger numbers between the working week and a typical Sunday in 2017.

P9.2.5 The HITRAN database (https://hitran.org) provides a list of molecular line intensities for modeling radiative transmission in planetary atmospheres. Its native format consists of 160-character records of fixed-width fields.

Use pandas to read in the file CO2-transitions.par, available from https://scipython.com/ex/ban (where a description of the fields can also be found). Plot line intensity against wavelength for these transitions in the infrared region of the spectrum ($\lambda = 10 \text{ mm}$ to 700 nm, corresponding to wavenumber $\tilde{v} = 1 \text{ cm}^{-1}$ to about 14 000 cm⁻¹), where carbon dioxide (CO₂) is responsible for a significant fraction of the greenhouse effect in Earth's atmosphere.

9.3 More Advanced Indexing

9.3.1 Hierarchical Indexes with MultiIndex

A DataFrame is an intrinsically two-dimensional array of data: to represent data in higher dimensions, it is common to use hierarchical indexing to represent multiple *levels* within a single index. If the data are sparse or heterogeneous, this is much more efficient than creating a multidimensional NumPy array. For example, consider a data set concerning the mean monthly temperature and rainfall in five European cities. This could be considered three-dimensional, the dimensions being "city," "month" and "data type" (this last meaning either temperature or rainfall). For five cities (Paris, Berlin, Vienna, London, Madrid) and four months (Jan, Apr, Jul, Oct), there would therefore be 40 data points in total.

We *could* create a conventional single-level index consisting of (city, month) tuples, but it wouldn't be very convenient or flexible. Instead, we can create a hierarchical index with two levels from a sequence of two-item tuples using pd.MultiIndex.from_tuples:

```
In [x]: cities = ('Paris', 'Berlin', 'Vienna', 'London', 'Madrid')
In [x]: months = ('Jan', 'Apr', 'Jul', 'Oct')
In [x]: index = pd.MultiIndex.from_tuples(
```

MultiIndexes of this form (the Cartesian product of two or more sequences) are so common that there is a convenience function, from_product, for their creation:

```
index = pd.MultiIndex.from_product((cities, months))
```

We can create a DataFrame with this index by assigning an array of data in the shape (20, 2):

```
In [x]: index.names = ['City', 'Month']
In [x]: # Mean monthly temperature (degC) for each city in each of Jan, Apr, Jul,
Oct.
In [x]: temps = [[4.9, 11.5, 20.5, 13.0], [0.1, 9.0, 19.1, 9.4],
                [0.3, 10.7, 20.8, 10.2], [5.2, 9.9, 18.7, 12.0],
   ...:
                [6.3, 12.9, 25.6, 15.1]
               1
   . . . :
In [x]: # Mean monthly rainfall (mm) for each city in each of Jan, Apr, Jul,
In [x]: rainfall = [[51.0, 51.8, 62.3, 61.5], [37.2, 33.7, 52.5, 32.2],
  ...:
                   [38., 45., 70., 38.], [55.2, 43.7, 44.5, 68.5],
                   [33., 45., 12., 60.]
   ...:
In [x]: arr = np.array((temps, rainfall)).reshape((2, 20)).T
In [x]: df = pd.DataFrame(arr, index=index, columns=['Mean temperature /degC',
                                                     'Mean rainfall /mm'])
In [x]: df
Out[x]:
              Mean temperature /degC Mean rainfall /mm
City Month
Paris Jan
                                                   51.0
                                4.9
                                11.5
                                                   51.8
       Apr
                                20.5
                                                   62.3
      Jul
                                13.0
                                                   61.5
      0ct
Berlin Jan
                                0.1
                                                  37.2
                                9.0
                                                  33.7
      Apr
      1111
                               19.1
                                                  52.5
      0ct
                                9.4
                                                   32.2
Vienna Jan
                                0.3
                                                   38.0
                               10.7
                                                  45.0
      Apr
       Jul
                                20.8
                                                  70.0
      0ct
                               10.2
                                                  38.0
London Jan
                                5.2
                                                   55.2
                                9.9
                                                  43.7
      Apr
       Jul
                                18.7
                                                  44.5
      0ct
                                12.0
                                                  68.5
```

Madrid	Jan	6.3	33.0
	Apr	12.9	45.0
	Jul	25.6	12.0
	0ct	15.1	60.0

The loc method can be used to index into the DataFrame's MultiIndex:

```
In [x]: df.loc['Vienna']
Out[x]:
      Mean temperature /degC Mean rainfall /mm
Month
Jan
                         0.3
                                           38.0
Apr
                        10.7
                                           45.0
                        20.8
                                           70.0
1111
0ct
                        10.2
                                           38.0
In [x]: df.loc[('Paris', 'Jul')]
Out[x]:
Mean temperature /degC 20.5
Mean rainfall /mm
                        62.3
Name: (Paris, Jul), dtype: float64
In [x]: df.loc[('Paris', 'Jul'), 'Mean rainfall /mm']
Out[x]: 62.3
```

To slice a MultiIndex, however, it must first be sorted:

```
In [x]: df['Berlin':'London']
Out[x]: ...
UnsortedIndexError: 'Key length (1) was greater than MultiIndex lexsort depth (0)'
```

This somewhat cryptic error message is a result of the way pandas is optimized to slice only indexes which are in lexicographical order. There are several methods to sort a MultiIndex, but the simplest is to use sort_index as we did previously:

```
In [x]: df.sort_index(inplace=True)
In [x]: df['Berlin':'London']
Out[x]:
             Mean temperature /degC Mean rainfall /mm
City Month
                                9.0
                                                 33.7
Berlin Apr
      Jan
                                0.1
                                                 37.2
                               19.1
      1111
                                                 52.5
      0ct
                                9.4
                                                 32.2
                               9.9
                                                 43.7
London Apr
      Jan
                               5.2
                                                 55.2
      Jul
                               18.7
                                                 44.5
                               12.0
                                                 68.5
```

Note that this has sorted the months into alphabetical order as well. To keep them in chronological order, one approach would be to number the months instead by relabeling the index:

```
In [x]: df2 = df.rename({'Jan': 1, 'Apr': 4, 'Jul': 7, 'Oct': 10})
In [x]: df2.sort_index(inplace=True)
In [x]: df2.loc['Vienna', 'Mean temperature /degC']
Out[x]:
Month
```

```
1     0.3
4     10.7
7     20.8
10     10.2
Name: Mean temperature /degC, dtype: float64
```

The useful xs function makes selecting data indexed at different levels of a MultiIndex easier, and does not require the index to be sorted. For example, to retrieve the climate data for January in all cities:

```
In [x]: df.xs('Jan', level=1)
                                 # look in second level of the MultiIndex for 'Jan'
Out[x]:
        Mean temperature /degC Mean rainfall /mm
City
                           0.1
                                              37.2
Berlin
London
                           5.2
                                              55.2
Madrid
                           6.3
                                              33.0
Paris
                            4.9
                                              51.0
Vienna
                            0.3
                                              38.0
```

A Series or DataFrame with a hierarchical row index can be reshaped so as to create a MultiIndex on the columns instead by using the unstack() function:

```
In [x]: df.unstack()
Out[x]:
      Mean temperature /degC
                                       ... Mean rainfall /mm
Month
                        Apr Jan Jul ...
                                                             Jul
                                                                  0ct
                                                       Jan
City
                        9.0 0.1 19.1 ...
Berlin
                                                      37.2 52.5 32.2
London
                        9.9 5.2
                                 18.7
                                      . . .
                                                      55.2 44.5
                                                                  68.5
                       12.9 6.3 25.6 ...
                                                      33.0 12.0 60.0
Madrid
Paris
                       11.5 4.9 20.5 ...
                                                      51.0 62.3 61.5
Vienna
                       10.7 0.3 20.8 ...
                                                      38.0 70.0 38.0
[5 rows x 8 columns]
```

9.3.2 Timestamps and Time Series

pandas provides a Timestamp object, representing an instant in time to some precision. The to_datetime method provides a powerful and flexible way of parsing a human-readable string into a Timestamp. The following examples all evaluate to a timestamp representing midnight on the 12th of March, 2020: Timestamp('2020-03-12 00:00:00'). Note that where the date is ambiguous, by default it is resolved in favor of the US convention: MM/DD/YY: to force a string to be interpreted as DD/MM/YY set dayfirst=True.

```
pd.to_datetime('2020-03-12')
pd.to_datetime('12/3/20', dayfirst=True)
pd.to_datetime('3/12/20')
pd.to_datetime('12 March, 2020')
pd.to_datetime('12th of March 2020')
pd.to_datetime('Mar 12, 2020')
```

Times are also handled gracefully:

Table 9.1 Some string codes for pandas time frequencies and offsets

Code	Description	
A	Year end	
M	Month end	
W	Week	
D	Calendar day	
H	Hour	
T	Minute	
S	Second	
L	Millisecond	
U	Microsecond	

```
In [x]: pd.to_datetime('9:05 21 August 2017')
Out[x]: Timestamp('2017-08-21 09:05:00')
In [x]: pd.to_datetime('21 August 2017 09:05:23')
Out[x]: Timestamp('2017-08-21 09:05:23')
```

Indexes can be constructed as a range of regularly spaced Timestamps with the date_range function. Ranges can be specified by passing the start and end date, or by passing the start date and the number of *periods*. The range interval is one day by default, but this can be controlled with the freq argument (see Table 9.1 for valid values).

- By defaults, monthly ranges specified with freq='M' are marked at the end of the month. The same is true for annual ranges (freq='A').
- **②** To set timestamps at the start of each month use freq='MS' (and freq='AS' for annual ranges).

pandas makes a distinction between a timestamp (represented by a Timestamp object) and a *time period*: an interval of time between two points in time. A time period is represented by the Period object and its start and end points are accessed through its attributes start_time and end_time. The syntax for creating time periods is similar to date ranges:

```
In [x]: p = pd.Period('2020-04', freq='M')
In [x]: t = pd.Timestamp('2020-04-03 14:30')
In [x]: p.start_time < t < p.end_time
Out[x]: True</pre>
```

It is often necessary to resample a time series at a different (higher or lower) frequency. The resample method assists with this: it returns a Resampler object which can be used to aggregate the data in some appropriate way. For example, in *downsampling* (resampling the data to a wider time frame), it may be appropriate to take the mean, minimum, maximum or sum of the values in the resampling interval. The following example should make this clearer.

Example E9.10 The file river-level.csv, available at https://scipython.com/eg/bal, lists the height in meters above sea level of Chitterne Brook, a small river in Wiltshire, England. Heights are given as minimum, average, and maximum values for each day between 1 January 2014 and 31 December 2016.

The following code reads in the data and plots the daily river height along with its monthly average, minimum and maximum values.

```
import pandas as pd
import matplotlib.pyplot as plt

df = pd.read_csv('river-level.csv', index_col=0, comment='#', parse_dates=True)

rs_monthly = df.resample('M')

df['avg_level'].plot(label='Daily average')

rs_monthly['avg_level'].mean().plot(label='Monthly average')

rs_monthly['min_level'].min().plot(label='Monthly minimum')

rs_monthly['max_level'].max().plot(label='Monthly maximum')

plt.xlabel('Date')

plt.ylabel('River level /m')

plt.gca().legend()

plt.show()
```

• Note that we need to set parse_dates=True to force pandas to interpret the first column as a DatetimeIndex.

Figure 9.4 shows the resulting plot.

9.3.3 Exercises

Problems

P9.3.1 Use pandas to read in the file, tb-cases.txt, available from https://scipython.com/ex/bao, which provides numbers of cases of tuberculosis in the USA, broken down by state for the years 1993–2018. Create a DataFrame with a hierarchical index (MultiIndex) consisting of the state name and year. Plot these data appropriately and determine the state with the greatest relative decrease in tuberculosis over the time period considered.

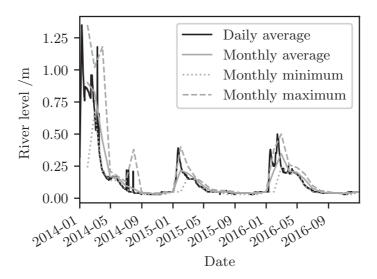


Figure 9.4 The level of Chitterne Brook in meters over the period 2014–2016.

P9.3.2 The populations of each state in the USA over the years 1993–2018 are given in the file US-populations.txt, available from https://scipython.com/ex/bap. Read these data into a pandas DataFrame with a suitable index, and analyze them for any interesting trends. Then combine these data with those of Problem P9.3.1 to determine the states with the greatest and least prevalence of tuberculosis per head of population in 2018.

9.4 Data Cleaning and Exploration

Any scientific research, particularly experimental research, will generate data sets containing invalid or missing values. Data points can be dropped or fall outside the detectable range of the measuring instrument, may get transcribed incorrectly, or are obtained incompletely from various sources. pandas provides a variety of methods for dealing with such missing values, including functions for removing them or replacing them with average or default values.

This book does not attempt to provide a guide to the scientific method, but the reader should be aware that the way in which one deals with missing or invalid data can bias the subsequent analysis towards a particular set of conclusions.

9.4.1 Missing Values

The default *sentinel value* indicating missing data is NaN. In Section 9.1.2 we have already used the methods isnull() and notnull() to test for the presence or absence of such values, and the method dropna(), which returns a new DataFrame with rows containing only non-null data:

```
In [x]: df = pd.DataFrame([[
                           1.1, np.nan, np.nan,
                          0.8, np.nan, 3.6,
                                               2.91.
  ...:
                       Γ
   . . . :
                       [ 1.2, 2.5, 1.6,
                                               2.7],
  ...:
                       [np.nan, np.nan, np.nan, np.nan],
                       [np.nan, np.nan, 3.6,
  . . . :
                       columns=list('ABCD'))
In [x]: df
            C
       В
   Α
 1.1 NaN NaN 10.3
1 0.8 NaN 3.6 2.9
2 1.2 2.5 1.6
3 NaN NaN NaN
                NaN
4 NaN NaN 3.6
In [x]: df.dropna()
Out[x]:
        В
            C
   Α
2 1.2 2.5 1.6 2.7
```

You may wish to drop only rows (or columns) which consist entirely of NaN. In that case, pass the argument how='all' instead of using the default, how='any':

It is also possible to specify a threshold number of NaN values to trigger the drop of a column or row:

An alternative to dropping the NaN values is to replace them with valid data according to some process. This is the purpose of the fillna() method. Common options are given in the following examples.

Replace all NaN values with a single value:

```
In [x]: df.fillna(3.6)
```

```
Out[x]:

A B C D

0 1.1 3.6 3.6 10.3
1 0.8 3.6 3.6 2.9
2 1.2 2.5 1.6 2.7
3 3.6 3.6 3.6 3.6
4 3.6 3.6 5.3
```

Replace NaN values with the last encountered valid value down the columns ("fill forward"):

Replace NaN values with the last encountered valid value along the rows:

```
In [x]: df.fillna(method='ffill', axis=1)
Out[x]:
         A     B     C     D
0    1.1    1.1    1.1    10.3
1    0.8    0.8    3.6    2.9
2    1.2    2.5    1.6    2.7
3    NaN    NaN    NaN    NaN
4    NaN    NaN    3.6    5.3
```

Passing a dictionary of column or index names enables close control over the filling values; chaining calls can then give a powerful and flexible way to clean data. For example, to fill in the missing data in columns A and C with their means:

A further example:

It may be that the data set being used uses a different sentinel value to indicate invalid data, for example -1 or -99. The replace method can canonicalize such data:

```
In [x]: ser = pd.Series([1.2, 3.5, -99, -99, 4.0, -99, -0.5])
In [x]: ser.replace(-99, np.nan)
Out[x]:
0     1.2
1     3.5
2     NaN
3     NaN
4     4.0
5     NaN
6     -0.5
dtype: float64
```

replace can also take a dictionary mapping values to their replacements:

```
In [x]: ser.replace({-99: 0, -0.5: np.nan})
Out[x]:
0    1.2
1    3.5
2    0.0
3    0.0
4    4.0
5    0.0
6    NaN
dtype: float64
```

9.4.2 Duplicate Values

The DataFrame method duplicated() returns a Series of boolean values indicating whether each row is a duplicate of a previous row; drop_duplicates() drops such rows. By default, both methods consider all columns; to remove rows with duplicate entries in a single column or several columns, pass a column name or a sequence of column names explicitly. A further argument, keep, determines whether the first encountered row ('first', the default) or last encountered row ('last') is retained.

```
In [x]: df = pd.DataFrame([['Lithium', 'Li', 3, 6, 0.0759],
                         ['Lithium', 'Li', 3, 7, 0.9241],
   . . . :
                         ['Sodium', 'Na', 11, 23, 1],
   ...:
                         ['Potassium', 'K', 19, 39, 0.932581],
   . . . :
                         ['Potassium', 'K', 19, 40, 1.17e-4],
                         ['Potassium', 'K', 19, 41, 0.067302]],
   . . . :
                        columns=['Element', 'Symbol', 'Z', 'A', 'Abundance'])
   ...:
In [x]: df
Out[x]:
    Element Symbol Z A Abundance
0
   Lithium Li 3 6 0.075900
               Li 3 7 0.924100
Na 11 23 1.000000
   Lithium
1
2
    Sodium
               K 19 39 0.932581
3 Potassium
4 Potassium
               K 19 40 0.000117
5 Potassium
               K 19 41 0.067302
In [x]: df.drop_duplicates(['Symbol'])
Out[x]:
    Element Symbol Z A Abundance
    Lithium Li 3 6 0.075900
```

```
2    Sodium    Na    11    23    1.000000
3    Potassium    K    19    39    0.932581

In [x]: df.drop_duplicates(['Symbol', 'Z'], keep='last')
Out[x]:
        Element Symbol         Z          A Abundance
1        Lithium         Li         3         7    0.924100
2        Sodium         Na    11    23         1.000000
5        Potassium          K    19    41    0.067302
```

9.4.3 Binning Data

It is often necessary to bin together large amounts of continuous data, either to reduce it to a manageable size or to categorize it based on value. The pandas function cut can be used to do this in a similar way to NumPy's histogram function (Section 6.3.3):

```
In [x]: marks = [67, 80, 34, 55, 77, 66, 59, 52, 70, 67, 58, 63, 49, 72]
In [x]: bins = [0, 40, 60, 70, 80, 100]
In [x]: dist = pd.cut(marks, bins)
In [x]: dist
[(60, 70], (70, 80], (0, 40], (40, 60], ..., (60, 70], (40, 60], (70, 80]]
Length: 14
Categories (5, interval): [(0, 40] < (40, 60] < (60, 70] < (70, 80] < (80, 100]]</pre>
```

Each mark is placed in a bin with edges defined by the sequence bins. The number of values in each bin is returned by value_counts:

By default, the right side of each interval is closed (values equal to this side are included in the bin, indicated by ']') and the left side is open (indicated by '('); this can be swapped by setting the argument right=False:

The bins can also be named by passing a sequence of strings to the labels argument:

```
In [x]: dist = pd.cut(marks, bins, labels=list(reversed('ABCDE')), right=False)
In [x]: dist
[C, A, E, D, B, ..., C, D, C, D, B]
Length: 14
```

```
Categories (5, object): [E < D < C < B < A]
In [x]: pd.value_counts(dist)
Out[x]:
D      5
C      4
B      3
A      1
E      1
dtype: int64</pre>
```

Note that the categories do not have any particular order. To put the counts in order of decreasing grade, we can sort the Series index:

9.4.4 Dealing with Outliers

Detecting and filtering outliers is, like dealing with missing values or invalid data, a potentially subtle process and careful thought should be given to the assumptions behind the expected underlying distribution. However, often, outlying values are expected based on detector failure (sticky pixels, cosmic rays, and the like), obvious errors, or well-understood exceptional cases. Filtering them automatically can be achieved with NumPy-like array operations.

For example, consider a simulated village in which the 200 houses have normally-distributed prices ($\mu = \$250\,000$, $\sigma = \$55\,000$), with the exception of a couple of mansions worth many times more than the average home:

```
In [x]: nhouses = 200
   In [x]: mu, sigma = 250, 55
                                     # mean, standard deviation in $1000s
In [x]: prices = np.clip(np.random.randn(nhouses)*sigma + mu, 0, None).astype(int)
   In [x]: prices[-2] = 1.e3
   In [x]: prices[-1] = 2.e3
   In [x]: df = pd.DataFrame(prices, columns=['price, $1000s'])
   In [x]: df.tail()
   Out[x]:
        price, $1000s
   195
                  247
   196
                  218
   197
                  236
   198
                 1000
   199
                 2000
```

• np.clip(arr, min, max) constrains the values of arr to fall within min and max, here to prevent negative house prices being produced by the random sampling. This is itself a type of outlier filtering!

These outliers distort the mean and (especially) the standard deviation of the house price distribution:

```
In [x]: df.median()
                            # the median is a robust measure of central tendency
Out[x]:
price, $1000s
                 247.8
dtype: float64
In [x]: df.mean()
                            # the mean is affected more by the outliers
Out[x]:
price, $1000s
                 258.775
dtype: float64
In [x]: df.std()
                            # the standard deviation is greatly affected
Out[x]:
price, $1000s
                 145.796907
dtype: float64
```

We may be interested in analyzing the prices of "ordinary" houses in the village, ignoring the mansions. One way to do this is to identify the mansions as deviating from the mean house price by, say, three standard deviations and setting their prices to NaN:

```
In [x]: df[df > 3*df.std()+df.mean()] = np.nan
In [x]: df.tail()
    price, $1000s
195      247.0
196      218.0
197      236.0
198      NaN
199      NaN
```

Now we find values closer to the (non-mansion) house price distribution:

```
In [x]: df.mean()
Out[x]:
price, $1000s     246.237374
dtype: float64

In [x]: df.std()
Out[x]:
price, $1000s     55.995279
dtype: float64
```

Example E9.11 Robert Millikan's famous oil-drop experiments were carried out at the University of Chicago from 1909 to determine the magnitude of the charge of the electron. In a single experiment, an electrically charged oil droplet was observed to fall a known distance, d, between two uncharged plates at its terminal velocity, v_g : from the time taken, t_g , the droplet's radius, a, can be deduced. Next, a voltage was applied to the plates, inducing an electric field between them. As the droplet rises under the resulting net force, the time taken, t_e , for it to move back up through the same distance, d, can be used to deduce its total charge, q, which is observed to be an integer multiple of the same base value, e, that is: q = Ne.

 $^{^{12}}$ Since May 2019, this quantity has been fixed by definition at 1.602176634 \times 10⁻¹⁹ C.

For the free-fall part of the experiment,¹³ when the droplet falls at constant terminal velocity $v_g = -d/t_g$ there is no net force on it: the sum of the gravitational and drag forces is zero:

$$F_g + F_d = 0 \implies -m'g - 6\pi\eta a v_g = 0,$$

where $m'=\frac{4}{3}\pi a^3\rho'=\frac{4}{3}\pi a^3(\rho_{\rm oil}-\rho_{\rm air})$ is the effective mass of the droplet (after the mass of air it displaces is taken into account), $g=9.803~{\rm m\,s^{-1}}$ is the acceleration due to gravity in Chicago, and $\eta=1.859\times 10^{-5}~{\rm kg\,m^{-1}\,s^{-1}}$ is the air viscosity under the experimental conditions (temperature, humidity, etc.). Rearranging, we get the following expression for the droplet radius:

$$a = \sqrt{\frac{-9\eta v_g}{2\rho' g}}.$$

When a suitable voltage is applied to the plates and the droplet moves upwards at a constant velocity $v_e = d/t_e$, the force due to the electric field is balanced by gravity and the drag force (at this new velocity):

$$F_e + F_g + F'_d = 0 \Rightarrow qE + 6\pi \eta a v_g - 6\pi \eta a v_e = 0$$

$$\Rightarrow q = \frac{6\pi \eta a (v_e - v_g)}{E} = \frac{6\pi \eta a d}{E} \left(\frac{1}{t_g} + \frac{1}{t_e}\right)$$

Each droplet (labeled A–H) was observed three times for each different charge, q, acquired by exposure to X-rays (up to seven experiments per droplet).

The data at https://scipython.com/eg/bam give the time data for a number of such experiments conducted with an oil of density $\rho_{\text{oil}} = 917.3 \text{ kg m}^{-3}$ on a day for which $\rho_{\text{air}} = 1.17 \text{ kg m}^{-3}$. The magnitude of the electric field was $E = 322.1 \text{ kN C}^{-1}$ and the distance the drops move, d = 11.09 mm. We can use these data to estimate e (assuming it is not fixed by definition) as follows.

dron	expt	+ ~	+0	+ a	+0	+ a	te
urop	•	tg	te	tg	te	tg	
Α	1	13.102	46.822	12.941	46.896	13.086	46.681
Α	2	12.938	86.767	13.032	86.952	13.086	86.746
Α	3	13.023	61.082	12.958	60.826	12.998	60.860
Α	4	12.943	86.747	12.922	86.840	13.054	86.899
В	1	11.434	56.305	11.350	56.097	11.246	56.282
В	2	11.402	75.823	11.584	75.819	11.487	76.063
В	3	11.591	44.717	11.397	44.851	11.364	44.776
В	4	11.443	75.905	11.368	75.975	11.457	76.041
В	5	11.434	75.939	11.414	75.880	11.444	75.929
В	6	11.559	75.892	11.414	75.924	11.292	75.985
В	7	11.394	44.716	11.589	44.753	11.401	44.794
C	1	16.197	100.458	16.010	100.486	16.329	100.461
C	2	16.241	47.727	16.106	47.714	16.177	47.625
C	3	16.133	37.879	16.267	37.746	16.203	37.709
C	4	16.170	64.765	16.136	64.649	16.229	64.508
D	1	16.176	38.017	16.127	37.910	16.282	38.020

 $^{^{13}}$ In this example we adopt a coordinate system in which the droplet's vertical position, z, increases in the "up" direction.

```
D
       2 16.275 38.280 16.092 38.208 16.133
                                                   38.092
D
         16.422 48.327 16.073 48.284 16.212
                                                   48.184
                                         16.105
          16.134
                  38.202 16.258 38.270
D
                                                   38.229
       4
D
          16.164 102.562
                           16.217 102.673
                                           16.194
                                                  102.696
                                          12.307
                          12.116
          12.275
                  55.020
Ε
       1
                                  54.962
                                                   54.978
          12.157
                  54.772
                          12.183
                                   54.967
                                          12.046
                                                   55.219
Ε
       2
Ε
       3
          12.146
                  55.004
                          12.118
                                  54.938
                                          12.346
                                                   54.869
E
          12.319
                  43.635
                           12.243
                                   43.552
                                           12.073
       4
                                                   43.582
F
       1
          14.172
                  61.946
                          14.174
                                   61.970
                                           14.069
                                                   61.959
          14.145
                  90.718 13.955
                                  90.707
                                          14.075
                                                   90.866
F
       2
F
       3
         14.070
                  62.147
                         14.074
                                  61.961
                                          14.247
                                                   61.892
                                          14.106
F
          14.017
                  61.968 14.101
                                   61.921
       4
                                                   62.174
G
           9.723
                   50.375
                            9.527
                                   50.482
                                            9.502
                                                   50.508
           9.463
                  63.755
                                  63.853
                            9.670
                                            9.509
G
       2
                                                   63.827
G
           9.448
                  63.804
                            9.407
                                   63.899
                                            9.563
                                                   63.768
G
       4
           9.327
                  63.855
                           9.518
                                  63.967
                                           9.533
                                                   63.824
Н
       1
          13.192
                  73.375
                          13.167
                                   73.338
                                           13.316
                                                   73.449
                                          13.334
Η
       2
          13.042
                  42.642
                          13.387
                                   42.428
                                                   42.459
Н
         13.389
                  42.379 13.244 42.373 13.055
                                                   42.610
Н
          13.114
                  73.161
                         13.226 73.384
                                          13.207
                                                   73.257
                  73.295
Н
          13.030
                          13.022 73.419
                                          13.438
                                                   73.512
```

First, define the necessary parameters:

Next, read in the data, assigning the first two columns to a MultiIndex:

```
In [x]: import pandas as pd
In [x]: df = pd.read_csv('eg10-millikan-data.txt', delim_whitespace=True,
                       index_col=[0, 1])
In [x]: df.head()
Out[x]:
              tg
                           tg.1
                                   te.1
                                          tg.2
drop expt
          13.102 46.822 12.941 46.896 13.086 46.681
          12.938 86.767 13.032 86.952 13.086 86.746
    2
          13.023
                 61.082
                         12.958
                                 60.826
                                        12.998
          12.943 86.747 12.922 86.840 13.054 86.899
          11.434 56.305 11.350 56.097 11.246 56.282
```

Note that pandas has added a counting integer to the column names to make them distinct.

We will start with just a single droplet, taking the transpose of its data:

```
te.1 46.896 86.952 60.826 86.840
tg.2 13.086 13.086 12.998 13.054
te.2 46.681 86.746 60.860 86.899
```

We would prefer to label each row as simply 'tg' or 'te':

```
In [x]: dropA.index = dropA.index.str.slice(0, 2)
In [x]: dropA
Out[x]:
expt
          1
                  2
                          3
     13.102 12.938 13.023 12.943
tg
   46.822 86.767 61.082 86.747
     12.941 13.032 12.958 12.922
46.896 86.952 60.826 86.840
tq
te
    13.086 13.086 12.998 13.054
ta
     46.681 86.746 60.860 86.899
```

We require the average of all of the values of t_g (in the absence of the electric field the droplet takes the same time to fall the distance d) and the average value of t_e for each column (each experiment may have a different droplet charge, but the fall–rise times are measured three times for each experiment):

```
In [x]: tg = dropA.loc['tg'].values.mean()
In [x]: te = dropA.loc['te'].mean()
In [x]: tg
Out[x]: 13.00691666666667
In [x]: te
Out[x]:
expt
1     46.799667
2     86.821667
3     60.922667
4     86.828667
dtype: float64
```

Now use the value of t_g to calculate the droplet's radius:

```
In [x]: a = np.sqrt(9*eta*d/tg/2/rhop/g)
In [x]: a
Out[x]: 2.8181654881967875e-06
```

or about 2.82 µm. The charge we deduce for each experiment is:

```
In [x]: q = 6 * np.pi * eta * a * d / E * (1/tg + 1/te)
In [x]: q
Out[x]:
expt
1    -3.340563e-18
2    -3.005663e-18
3    -3.172143e-18
4    -3.005631e-18
dtype: float64
```

Repeating this for all the droplets, we can add a column, q to the DataFrame df:

```
for drop in df.index.levels[0]:
    drop_df = df.loc[drop].T
    drop_df.index = drop_df.index.str.slice(0, 2)
```

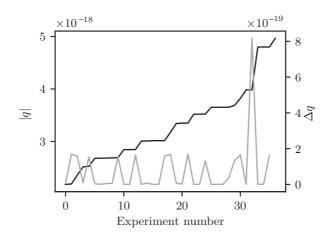


Figure 9.5 Sorted droplet charges, q, and neighbouring differences, Δq .

```
tg = drop_df.loc['tg'].values.mean()
te = drop_df.loc['te'].mean()
a = np.sqrt(9*eta*d/tg/2/rhop/g)
q = 6 * np.pi * eta * a * d / E * (1/tg + 1/te)
df.loc[drop, 'q'] = q.values
```

It is now helpful to sort the droplet charges by magnitude and to plot the sorted array and its differences (Figure 9.5):

```
In [x]: sorted_q = sorted(-df.loc[:, 'q'])
In [x]: plt.plot(sorted_q)
In [x]: plt.ylabel('$|q|$')
In [x]: plt.twinx()
In [x]: dq = np.diff(sorted_q)
In [x]: plt.plot(dq)
In [x]: plt.ylabel(r'$\Delta q$')
In [x]: plt.show()
```

It certainly seems possible that the droplet charge is always a multiple of some value between 1×10^{-19} C and 2×10^{-19} C. We can therefore estimate the value of |e|:

```
In [x]: e_estimate = dq[(dq>1.e-19) & (dq<2.e-19)].mean() In [x]: e_estimate  
Out[x]: 1.5697150510604604e-19
```

We can now add a column to df for the number of elementary charges we hypothesise for each experiment:

```
In [x]: df['N'] = (df['q'] / e_estimate).astype(int)
```

Considering all the data then gives us our estimate for the magnitude of the electron charge:

```
In [x]: (df['q']/df['N']).mean()
Out[x]: 1.5923552150386455e-19
within 1% of the defined value.
```

9.4.5 Exercises

Problems

P9.4.1 Use pandas' cut method to classify the stars in the data set of Problem P9.2.3 according to their temperature by placing them into the bins labeled M, K, G, F, A, B, and O with left edges (in K) at 2400, 3700, 5200, 6000, 7500, 10000, and 30000.

Hence modify the code in the solution to this problem to plot the stars in a color appropriate to their temperature by establishing the following mapping:

Hint: pandas provides a map method for mapping input values from an existing column to output values in a new column using a dictionary.

P9.4.2 Reanalyze the data from Example E9.11, concerning Millikan's oil-drop experiment, to use a more accurate approximation for the effective air viscosity:

$$\eta = \frac{\eta_0}{1 + \frac{b}{ap}},$$

where p=100.82 kPa is the air pressure, $\eta_0=1.859\times 10^{-5}$ kg m⁻¹ s⁻¹, $b=7.88\times 10^{-3}$ Pa m, and a is the droplet radius.

P9.4.3 The Cambridge University Digital Technology Group have been recording the weather from the roof of their department building since 1995 and make the data available to download at www.cl.cam.ac.uk/research/dtg/weather/.

Read in the entire data set and parse it with pandas to determine (a) the most common wind direction; (b) the fastest wind speed measured; (c) the year with the sunniest June; (d) the day with the highest rainfall; (e) the coldest temperature measured. Note that there are occasional missing and invalid data points in the data set.

P9.4.4 The data set at https://scipython.com/ex/baq lists the following quantities, in US dollars over time: (a) the price of gold; (b) the S&P 500 US stock market index; and (c) the price of the cryptocurrency Bitcoin. Compare the performance of these indexes over the period 2010–2020 with respect to the regular investment of \$100 per month.

9.5 Data Grouping and Aggregation

9.5.1 DataFrame Grouping with groupby

The powerful pandas method groupby can be used to analyze data in a Series or DataFrame based on their categorization according to some key row (or column) values. The term *split-apply-combine* describes the process succinctly: first, the data is split according to its categorization; next, the analysis technique or statistical method required (for example, summing values or finding their mean) is applied to the split

groups; finally, the results of the analysis are combined into a result object. Figure 9.6 depicts a simple example of the process.

Example E9.12 Consider the following table of the yields of three compounds, A, B and C, attained in a synthesis experiment by three students, Anu, Jenny and Tom.

```
In [x]: data = [['Anu', 'A', 5.4], ['Anu', 'B', 6.7], ['Anu', 'C', 10.1],
                   ['Jenny', 'A', 6.5], ['Jenny', 'B', 5.9], ['Jenny', 'C', 12.2], ['Tom', 'A', 4.0], ['Tom', 'B', None], ['Tom', 'C', 9.5]
   . . . :
   . . . :
In [x]: df = pd.DataFrame(data, columns=['Student', 'Compound', 'Yield /g'])
In [x]: print(df)
  Student Compound Yield /g
       Anu
                               5.4
                    Α
1
       Anu
                     В
                               6.7
2
                             10.1
       Anu
                    C
     Jenny
4
     Jenny
                     В
                              5.9
     Jenny
                     C
                             12.2
6
       Tom
                              4.0
                     Α
       Tom
                               NaN
```

One way of analyzing these data is to group them by compound ("split" into separate data structures, each with a common value of 'Compound') and then apply some operation (say, finding the mean) to each group, before recombining into a single DataFrame, as illustrated in Figure 9.6.

In [x]: grouped = df.groupby('Compound')

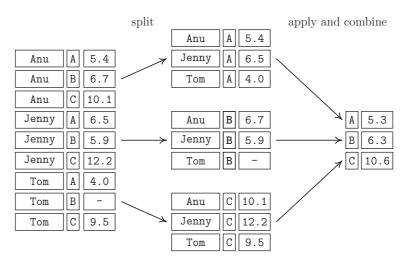


Figure 9.6 An illustration of the *split-apply-combine* paradigm for analyzing data with grouped data in pandas: the DataFrame is split into groups by compound (A, B and C); the mean function is applied to the groups; these values are combined into the returned object.

Here, the 'Student' column has been ignored as a so-called "nuisance" column: there is no helpful way to take the mean of a string. The max() and min() functions, however, consider the strings' lexigraphical ordering:

Note that max() has returned 'Tom' for every row, since this name is lexigraphically last ('greatest') in the 'Student' column. The column 'Yield /g' consists of the maximum yields for each compound, across all students. To apply the function to a subset of the columns only (which may be necessary for very large DataFrames), select them before the function call, for example:

```
In [x]: grouped['Yield /g'].min()
Out[x]:
Compound
A     4.0
B    5.9
C    9.5
Name: Yield /g, dtype: float64
```

The object returned by groupby() can be iterated over:

```
In [x]: for compound, group in grouped:
  ...: print('Compound:', compound)
          print(group)
  . . . :
Compound: A
 Student Compound Yield /g
   Anu
           Α
                    5.4
3
  Jenny
               Α
                      6.5
6
   Tom
               Α
                      4.0
Compound: B
 Student Compound Yield /g
    Anu
             В
                      6.7
  Jenny
               В
                      5.9
4
    Tom
               В
                      NaN
Compound: C
 Student Compound Yield /g
2
    Anu
            C 10.1
5
   Jenny
               C
                     12.2
8
    Tom
              C
                     9.5
```

We can also group by the 'Student' column:

Another powerful feature is the ability to group on the basis of a specified mapping, provided, for example, by a dictionary. Suppose each student is undertaking a different degree programme:

First, turn the 'Student' column into an Index and then group, not by the Index itself but using the provided mapping:

That is, the average yield for students of chemistry was 7.8 g, whereas for pharmacology it was only 6.75 g.

9.5.2 Exercises

Problems

P9.5.1 The Organisation for Economic Co-operation and Development (OECD), within its Programme for International Student Assessment (PISA), publishes an evaluation of the educational systems around the world by measuring the performance of 15-year-old school pupils on mathematics, science, and reading. The evaluation is carried out every three years.

Historical PISA data can be downloaded from https://scipython.com/ex/bza. Read these data in to a pandas DataFrame and use its grouping functionality to determine and visualize (a) the overall performance of all studied countries over time; (b) the gender disparity (if any) in each of reading, mathematics and science; and (c) the correlation between the performances in each of these areas across all countries.

P9.5.2 Read in the data at https://scipython.com/ex/bar concerning recent Formula One Grands Prix seasons, and rank (a) the drivers by their number of wins; (b) the constructors by their number of wins; and (c) the circuits by their average fastest lap per race.

9.6 Examples

The following examples demonstrate the practical use of pandas in two case studies involving the analysis and visualization of real data.

Example E9.13 The file nuclear-explosion-data.csv, available to download at https://scipython.com/eg/ban, contains data on all nuclear explosions between 1945 and 1998. We will use pandas to analyze it in various ways.

Inspection of the file in a text editor shows that it contains a header line naming the columns, so we can load it straight away with pd.read_csv and inspect its key features:

```
In [x]: import pandas as pd
In [x]: df = pd.read_csv('nuclear-explosion-data.csv')
In [x]: df.head()
Out[x]:
      date
               time
                      id country ... yield_upper purpose
                                                              name
 19450716 123000.0 45001 USA ... 21.0 WR
                                                          TRINITY
                                                                      TOWER
1 19450805 231500.0 45002
                              USA ...
                                            15.0 COMBAT LITTLEBOY AIRDROP
                              USA ...
2 19450809
            15800.0 45003
                                            21.0 COMBAT
                                                          FATMAN AIRDROP
                              USA ...
  19460630 220100.0 46001
                                            21.0
                                                   WE
                                                             ABLE AIRDROP
4 19460724 213500.0 46002 USA ...
                                           21.0
                                                     WE
                                                             BAKER
                                                                         UW
[5 rows x 16 columns]
In [x]: df.index
Out[x]: RangeIndex(start=0, stop=2051, step=1)
In [x]: df.columns
Out[x]:
Index(['date', 'time', 'id', 'country', 'region', 'source', 'lat', 'long',
      'mb', 'Ms', 'depth', 'yield_lower', 'yield_upper', 'purpose', 'name',
      'type'],
     dtype='object')
```

There are 16 columns; here we will be concerned with those described in Table 9.2.

It is natural to assign the date and time of the explosion to the DataFrame index. Some helper functions facilitate this:

¹⁴ from N.-O. Bergkvist and R. Ferm, *Nuclear Explosions 1945–1998*, Swedish Defence Research Establishment/SIPRI, Stockholm, July 2000.

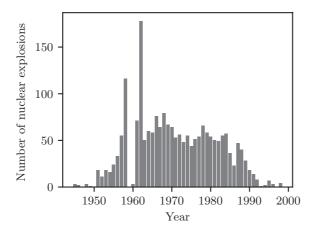


Figure 9.7 Bar chart of the number of nuclear explosions by year between 1945 and 1998.

We can plot the number of explosions in each year by grouping on index.year and finding the size of each group; a regular Matplotlib bar chart can then be produced:

```
explosion_number = df.groupby(df.index.year).size()
import matplotlib.pyplot as plt
fig, ax = plt.subplots()
ax.bar(explosion_number.index, explosion_number.values)
ax.set_xlabel('Year')
ax.set_ylabel('Number of nuclear explosions')
plt.show()
```

Figure 9.7 shows the resulting plot.

Table 9.2 Important columns of nuclear explosion data in file nuclear-explosion-data.csv

Column	Description		
date	Date of explosion in format YYYYMMDD		
time	Time of explosion in format HHMMSS.Z, where Z represents		
	tenths of seconds		
country	The state that carried out the explosion		
lat	The latitude of the explosion in degrees, relative to the equator		
long	The longitude of the explosion in degrees, relative to the prime meridian		
yield_lower	Lower estimate of the yield in kilotons (kt) of TNT		
yield_upper	Upper estimate of the yield in kilotons (kt) of TNT		
type	The method of deployment of the nuclear device		

A stacked bar chart can break down the annual count of explosions by country. First, group by both year and country and get the explosion counts for this grouping with size():

```
df2 = df.groupby([df.index.year, df.country])
explosions_by_country = df2.size()
print(explosions_by_country.head(7))
     country
1945 USA
1946 USA
                 2
1948 USA
1949 USSR
                1
1951 USA
                16
     USSR
                 2
1952 UK
                 1
dtype: int64
```

Next, unstack the second index into columns, filling the empty entries with zeros:

```
explosions_by_country = explosions_by_country.unstack().fillna(0)
print(explosions_by_country.head(7))
```

country	CHINA	FRANCE	INDIA	PAKISTAN	UK	USA	USSR
1945	0.0	0.0	0.0	0.0	0.0	3.0	0.0
1946	0.0	0.0	0.0	0.0	0.0	2.0	0.0
1948	0.0	0.0	0.0	0.0	0.0	3.0	0.0
1949	0.0	0.0	0.0	0.0	0.0	0.0	1.0
1951	0.0	0.0	0.0	0.0	0.0	16.0	2.0
1952	0.0	0.0	0.0	0.0	1.0	10.0	0.0
1953	0.0	0.0	0.0	0.0	2.0	11.0	5.0

Each row in this DataFrame can then be plotted as stacked bars on a Matplotlib chart:

```
countries = ['USA', 'USSR', 'UK', 'FRANCE', 'CHINA', 'INDIA', 'PAKISTAN']
bottom = np.zeros(len(explosions_by_country))
fig, ax = plt.subplots()
for country in countries:
    ax.bar(explosions_by_country.index, explosions_by_country[country],
        bottom=bottom, label=country)
    bottom += explosions_by_country[country].values

ax.set_xlabel('Year')
ax.set_ylabel('Number of nuclear explosions')
ax.legend()
plt.show()
```

Figure 9.8 shows the resulting stacked bar chart.

The geopandas package provides a convenient way to plot the yield data on a world map. A full description of geographic information systems (GIS) is beyond the scope of this book, but geopandas is relatively self-contained and easy to use. First, read in the DataFrame for a low-resolution earth map (included with geopandas), and plot it on a Matplotlib Axes object. We'll accept the default equirectangular projection but customize the borders and fill the land areas in gray:

```
import geopandas
```

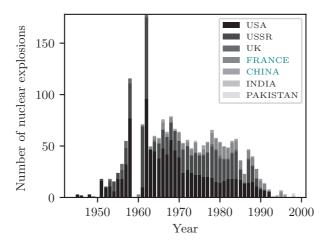


Figure 9.8 Stacked bar chart of the number of nuclear explosions by year caused by different countries between 1945 and 1998.

```
world = geopandas.read_file(geopandas.datasets.get_path('naturalearth_lowres'))
fig, ax = plt.subplots()
world.plot(ax=ax, color="0.8", edgecolor='black', linewidth=0.5)
```

The data provide lower and upper estimates of the explosion yield, so take the average and add circles as a scatter plot at the explosions' latitudes and longitudes. There is quite a large dynamic range from a few kilotons of TNT up to 50 million tons for the Tsar Bomba hydrogen bomb test of 1961, so clip the lower circle size to ensure that the smaller explosions are visible on the map:

```
df['yield_estimate'] = df[['yield_lower','yield_upper']].mean(axis=1)
sizes = (df['yield_estimate'] / 120).clip(10)
ax.scatter(df['long'], df['lat'], s=sizes, fc='r', ec='none', alpha=0.5)
ax.set_ylim(-60, 90)
plt.axis('off')
plt.show()
```

The result is Figure 9.9.

Example E9.14 The file volcanic-eruptions.csv, available to download at https://scipython.com/eg/bap, contains data concerning 822 significant volcanic events on Earth between 1750 BCE and 2020 CE from the US National Centres for Environmental Information (NCEI). The information on each event is given in commaseparated fields and includes date, volcano name, location, type, estimated number of human deaths and "Volcanic Explosivity Index" (VEI).

¹⁵ https://www.ngdc.noaa.gov/hazard/volcano.shtml.



Figure 9.9 A map of nuclear explosions, showing the blast yield, between 1945 and 1998.

The data are readily parsed into a DataFrame with:

```
In [x]: df = pd.read_csv('volcanic-eruptions.csv', index_col=0)
```

The most deadly volcanic eruption in the database is that of Ilopango, around the middle of the fifth century CE:

```
In [x]: df.loc[df['Deaths'].idxmax()]
Out[x]:
                    450
Year
Month
                    NaN
Day
                    NaN
Name
               Ilopango
           El Salvador
Location
           El Salvador
Country
Latitude
                13.672
                -89.053
Longitude
Elevation
                    450
                Caldera
Type
VEI
                  30000
Deaths
Name: 25, dtype: object
```

It would be helpful to have a column with the day, month and year of the explosion parsed into a string. Define a helper function, get_date:

```
def get_date(year, month, day):
    if year < 0:
        s_year = f'{-year} BCE'
    else:
        s_year = str(year)
    if pd.isnull(month):
        return s_year
    s_date = f'{int(month)}/{s_year}'
    if pd.isnull(day):
        return s_date
    return f'{int(day)}/{s_date}'</pre>
```

and apply it to the DataFrame:

Simple filtering can give us a list of eruptions with a VEI of at least 6 since the start of the nineteenth century:

```
In [x]: df[(df['VEI'] >= 6) & (df['Year'] >= 1800)]
Out[x]:
    Year Month Day
                           Name ...
                                             Type VEI
218 1815
          4.0 10.0
                        Tambora ... Stratovolcano 7.0 11000.0
                                                                10/4/1815
    1883
           8.0 27.0
                       Krakatau ...
                                      Caldera 6.0
                                                        2000.0
                                                                27/8/1883
365 1902
          10.0 25.0 Santa Maria ...
                                     Stratovolcano 6.0
                                                        2500.0 25/10/1902
          9.0
                                                         2.0
                                                               6/9/1912
386 1912
               6.0
                     Novarupta ...
                                      Caldera 6.0
650 1991
           6.0 15.0
                       Pinatubo ... Stratovolcano 6.0
                                                         350.0
                                                                15/6/1991
```

To find the 10 most explosive eruptions, we could filter out those with unknown VEI values before sorting:

```
In [x]: df[pd.notnull(df['VEI'])].sort_values('VEI').tail(10)[
                 ['date', 'Name', 'Type', 'Country', 'VEI']]
Out[x]:
         date
                       Name
                                      Type
                                                    Country VEI
         653
                    Dakataua
                                   Caldera Papua New Guinea
2.5
         450
                   Ilopango
                                  Caldera
                                              El Salvador 6.0
                                                    Russia 6.0
22
         240
                    Ksudach Stratovolcano
21
         230
                      Taupo
                                  Caldera
                                               New Zealand 6.0
                                           United States 6.0
         60 Bona-Churchill Stratovolcano
18
99
    19/2/1600
              Huaynaputina
                             Stratovolcano
                                                      Peru
                Veniaminof Stratovolcano
                                              United States 6.0
    1750 BCE
1
40
         1000
                Changbaishan Stratovolcano
                                              North Korea 7.0
218 10/4/1815
                    Tambora
                             Stratovolcano
                                                 Indonesia 7.0
                   Santorini Shield volcano
     1610 BCE
```

However, there are many entries with a VEI of 6 and their ordering here is not clear. A better approach might be to sort first by VEI and next by deaths, setting na_position='first' to ensure that the null values are placed before numerical values (and therefore effectively rank lowest):

```
In [x]: df.sort_values(['VEI', 'Deaths'], na_position='first').tail(10)[
                  ['date', 'Name', 'Type', 'Country', 'VEI', 'Deaths']]
Out[x]:
                                                   Country VEI
                      Name
     6/9/1912
                                              United States 6.0
386
                 Novarupta
                                  Caldera
                                                                  2.0
    15/6/1991
                             Stratovolcano
                                               Philippines
                                                            6.0
650
                 Pinatubo
                                                                  350.0
                            Stratovolcano
     19/2/1600 Huaynaputina
99
                                                      Peru 6.0
                                                                 1500.0
120
        1660 Long Island Complex volcano Papua New Guinea 6.0
322
    27/8/1883
                 Krakatau
                                 Caldera
                                                Indonesia 6.0
                                                                 2000.0
                            Stratovolcano
365 25/10/1902
               Santa Maria
                                                 Guatemala 6.0
                                                                 2500.0
25
          450
                  Ilopango
                                  Caldera
                                                El Salvador 6.0 30000.0
      1610 BCE
                  Santorini Shield volcano
                                                   Greece 7.0
3
                                                                  NaN
40
         1000 Changbaishan Stratovolcano
                                                North Korea 7.0
                                                                    NaN
     10/4/1815
                            Stratovolcano
                                                Indonesia 7.0 11000.0
                   Tambora
```

We can also plot some histograms summarizing the data (Figure 9.10):

```
fig, axes = plt.subplots(nrows=2, ncols=2)
df['Day'].hist(bins=31, ax=axes[0][0], grid=False)
```

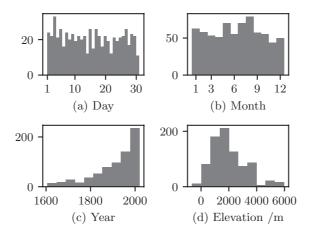


Figure 9.10 Histograms summarizing some of the columns of volcanic event data: (a) day of month; (b) month of year; (c) frequency by year since 1600 – hopefully, volcanic events have been progressively better recorded since 1600 and have not actually increased in frequency; (d) volcano elevation.

```
axes[0][0].set_xlabel('(a) Day')
df['Month'].hist(bins=np.arange(1, 14) - 0.5, ax=axes[0][1], grid=False)
axes[0][1].set_xticks(range(1, 13))
axes[0][1].set_xlabel('(b) Month')
df[df['Year']>1600]['Year'].hist(ax=axes[1][0], grid=False)
axes[1][0].set_xlabel('(c) Year')
df['Elevation'].hist(ax=axes[1][1], grid=False)
axes[1][1].set_xlabel('(d) Elevation /m')
plt.tight_layout()
plt.show()
```