tabular-data

October 17, 2023

0.1 Tabular Data and Graphing lesson

tabular data is generally presented in rows and columns. You might have to analyzed this type of data in a spreadsheet program before.

[1]: import numpy

[2]: help(numpy.genfromtxt)

Help on function genfromtxt in module numpy:

genfromtxt(fname, dtype=<class 'float'>, comments='#', delimiter=None,
skip_header=0, skip_footer=0, converters=None, missing_values=None,
filling_values=None, usecols=None, names=None, excludelist=None, deletechars="
!#\$%&'()*+,-./:;<=>?@[\\]^{|}~", replace_space='_', autostrip=False,
case_sensitive=True, defaultfmt='f%i', unpack=None, usemask=False, loose=True,
invalid_raise=True, max_rows=None, encoding='bytes', *, like=None)

Load data from a text file, with missing values handled as specified.

Each line past the first `skip_header` lines is split at the `delimiter` character, and characters following the `comments` character are discarded.

Parameters

fname : file, str, pathlib.Path, list of str, generator
 File, filename, list, or generator to read. If the filename
 extension is ``.gz`` or ``.bz2``, the file is first decompressed. Note
 that generators must return bytes or strings. The strings
 in a list or produced by a generator are treated as lines.

dtype : dtype, optional

Data type of the resulting array.

If None, the dtypes will be determined by the contents of each column, individually.

comments : str, optional

The character used to indicate the start of a comment.

All the characters occurring on a line after a comment are discarded.

delimiter: str, int, or sequence, optional

The string used to separate values. By default, any consecutive whitespaces act as delimiter. An integer or sequence of integers

can also be provided as width(s) of each field.

skiprows : int, optional

`skiprows` was removed in numpy 1.10. Please use `skip_header` instead.

skip_header : int, optional

The number of lines to skip at the beginning of the file.

skip_footer : int, optional

The number of lines to skip at the end of the file.

converters : variable, optional

The set of functions that convert the data of a column to a value.

The converters can also be used to provide a default value

for missing data: ``converters = {3: lambda s: float(s or 0)}``.

missing : variable, optional

`missing` was removed in numpy 1.10. Please use `missing_values` instead.

missing_values : variable, optional

The set of strings corresponding to missing data.

filling_values : variable, optional

The set of values to be used as default when the data are missing.

usecols : sequence, optional

Which columns to read, with 0 being the first. For example,

``usecols = (1, 4, 5)`` will extract the 2nd, 5th and 6th columns.

names : {None, True, str, sequence}, optional

If `names` is True, the field names are read from the first line after the first `skip_header` lines. This line can optionally be preceded by a comment delimiter. If `names` is a sequence or a single-string of comma-separated names, the names will be used to define the field names in a structured dtype. If `names` is None, the names of the dtype fields will be used, if any.

excludelist : sequence, optional

A list of names to exclude. This list is appended to the default list ['return','file','print']. Excluded names are appended with an underscore: for example, `file` would become `file_`.

deletechars : str, optional

 \boldsymbol{A} string combining invalid characters that must be deleted from the names.

defaultfmt : str, optional

A format used to define default field names, such as "f%i" or "f $_{0}$ 02i". autostrip : bool, optional

Whether to automatically strip white spaces from the variables.

replace_space : char, optional

Character(s) used in replacement of white spaces in the variable names. By default, use a '_'.

case_sensitive : {True, False, 'upper', 'lower'}, optional

If True, field names are case sensitive.

If False or 'upper', field names are converted to upper case.

If 'lower', field names are converted to lower case.

unpack : bool, optional

If True, the returned array is transposed, so that arguments may be

unpacked using ``x, y, z = genfromtxt(…)``. When used with a structured data-type, arrays are returned for each field.

Default is False.

usemask : bool, optional

If True, return a masked array.

If False, return a regular array.

loose : bool, optional

If True, do not raise errors for invalid values.

invalid_raise : bool, optional

If True, an exception is raised if an inconsistency is detected in the number of columns.

If False, a warning is emitted and the offending lines are skipped.

max_rows : int, optional

The maximum number of rows to read. Must not be used with skip_footer at the same time. If given, the value must be at least 1. Default is to read the entire file.

.. versionadded:: 1.10.0

encoding : str, optional

Encoding used to decode the inputfile. Does not apply when `fname` is a file object. The special value 'bytes' enables backward compatibility workarounds that ensure that you receive byte arrays when possible and passes latin1 encoded strings to converters. Override this value to receive unicode arrays and pass strings as input to converters. If set to None the system default is used. The default value is 'bytes'.

.. versionadded:: 1.14.0

like : array_like

Reference object to allow the creation of arrays which are not NumPy arrays. If an array-like passed in as ``like`` supports the ``_array_function__`` protocol, the result will be defined by it. In this case, it ensures the creation of an array object compatible with that passed in via this argument.

.. versionadded:: 1.20.0

Returns

out : ndarray

Data read from the text file. If `usemask` is True, this is a masked array.

See Also

numpy.loadtxt : equivalent function when no data is missing.

Notes

- * When spaces are used as delimiters, or when no delimiter has been given as input, there should not be any missing data between two fields.
- * When the variables are named (either by a flexible dtype or with `names`), there must not be any header in the file (else a ValueError exception is raised).
- * Individual values are not stripped of spaces by default. When using a custom converter, make sure the function does remove spaces.

References

```
.. [1] NumPy User Guide, section `I/O with NumPy
```

```
<https://docs.scipy.org/doc/numpy/user/basics.io.genfromtxt.html>`..
Examples
_____
>>> from io import StringIO
>>> import numpy as np
Comma delimited file with mixed dtype
>>> s = StringIO(u"1,1.3,abcde")
>>> data = np.genfromtxt(s, dtype=[('myint','i8'),('myfloat','f8'),
... ('mystring','S5')], delimiter=",")
>>> data
array((1, 1.3, b'abcde'),
      dtype=[('myint', '<i8'), ('myfloat', '<f8'), ('mystring', 'S5')])</pre>
Using dtype = None
>>> _ = s.seek(0) # needed for StringIO example only
>>> data = np.genfromtxt(s, dtype=None,
... names = ['myint','myfloat','mystring'], delimiter=",")
>>> data
array((1, 1.3, b'abcde'),
      dtype=[('myint', '<i8'), ('myfloat', '<f8'), ('mystring', 'S5')])</pre>
Specifying dtype and names
>>> _ = s.seek(0)
>>> data = np.genfromtxt(s, dtype="i8,f8,S5",
... names=['myint','myfloat','mystring'], delimiter=",")
>>> data
array((1, 1.3, b'abcde'),
      dtype=[('myint', '<i8'), ('myfloat', '<f8'), ('mystring', 'S5')])</pre>
An example with fixed-width columns
>>> s = StringIO(u"11.3abcde")
```

```
>>> data = np.genfromtxt(s, dtype=None, names=['intvar','fltvar','strvar'],
              delimiter=[1,3,5])
        >>> data
        array((1, 1.3, b'abcde'),
              dtype=[('intvar', '<i8'), ('fltvar', '<f8'), ('strvar', 'S5')])</pre>
        An example to show comments
        >>> f = StringIO('''
        ... text,# of chars
        ... hello world,11
        ... numpy,5''')
        >>> np.genfromtxt(f, dtype='S12,S12', delimiter=',')
        array([(b'text', b''), (b'hello world', b'11'), (b'numpy', b'5')],
          dtype=[('f0', 'S12'), ('f1', 'S12')])
[3]: filepath = 'data/distance_data_headers.csv'
     distances = numpy.genfromtxt(fname=filepath, delimiter=',',dtype= 'unicode')
[4]: print(distances)
    [['Frame' 'THR4_ATP' 'THR4_ASP' 'TYR6_ATP' 'TYR6_ASP']
     ['1' '8.9542' '5.8024' '11.5478' '9.9557']
     ['2' '8.6181' '6.0942' '13.9594' '11.6945']
     ['9998' '8.6625' '7.7306' '9.5469' '10.3063']
     ['9999' '9.2456' '7.8886' '9.8151' '10.7564']
     ['10000' '8.8135' '7.917' '9.9517' '10.7848']]
[5]: headers= distances[0]
[6]: print(headers)
    ['Frame' 'THR4_ATP' 'THR4_ASP' 'TYR6_ATP' 'TYR6_ASP']
[7]: data = distances[1:]
     print(data)
    [['1' '8.9542' '5.8024' '11.5478' '9.9557']
     ['2' '8.6181' '6.0942' '13.9594' '11.6945']
     ['3' '9.0066' '6.0637' '13.0924' '11.3043']
     ['9998' '8.6625' '7.7306' '9.5469' '10.3063']
     ['9999' '9.2456' '7.8886' '9.8151' '10.7564']
     ['10000' '8.8135' '7.917' '9.9517' '10.7848']]
```

```
[8]: data = data.astype(float
 [9]: print(data)
     [[1.00000e+00 8.95420e+00 5.80240e+00 1.15478e+01 9.95570e+00]
      [2.00000e+00 8.61810e+00 6.09420e+00 1.39594e+01 1.16945e+01]
      [3.00000e+00 9.00660e+00 6.06370e+00 1.30924e+01 1.13043e+01]
      [9.99800e+03 8.66250e+00 7.73060e+00 9.54690e+00 1.03063e+01]
      [9.99900e+03 9.24560e+00 7.88860e+00 9.81510e+00 1.07564e+01]
      [1.00000e+04 8.81350e+00 7.91700e+00 9.95170e+00 1.07848e+01]]
[10]: # To access a specific element of an array, array name[row,colum]
[11]: print(data[2,1])
     9.0066
[12]: point1 = data[0,1]
      point2 = data[1,0]
[13]: print(F'point1 is {point1}')
     point1 is 8.9542
[14]: print(F'point2 is {point2}')
     point2 is 2.0
[15]: small_data = data[0:10, 0:3]
      print(small_data)
     [[ 1.
                8.9542 5.8024]
      [ 2.
                8.6181 6.0942]
      Г3.
                9.0066 6.0637]
      Г4.
                9.2002 6.0227]
      [ 5.
                9.1294 5.9365]
      [ 6.
                9.0462 6.2553]
      Г7.
                8.8657 5.9186]
      Г8.
                9.3256 6.2351]
      [ 9.
                9.4184 6.1993]
      Γ10.
                9.06
                        6.0478]]
[16]: set1 = small_data[5,:]
      set2 = small_data[:,1:]
      print(F'set1 is {set1}')
```

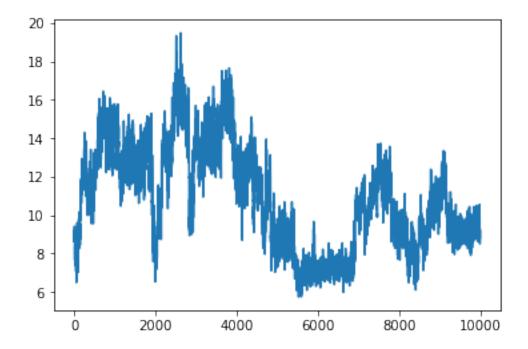
```
9.0462 6.25531
     set1 is [6.
[17]: print(set2)
     [[8.9542 5.8024]
      [8.6181 6.0942]
      [9.0066 6.0637]
      [9.2002 6.0227]
      [9.1294 5.9365]
      [9.0462 6.2553]
      [8.8657 5.9186]
      [9.3256 6.2351]
      [9.4184 6.1993]
      [9.06
             6.0478]]
[18]: # To trake an average numpy, mean(data_set)
      thr4_atp_data = data[:,1]
      print(thr4_atp_data)
     [8.9542 8.6181 9.0066 ... 8.6625 9.2456 8.8135]
[19]: average = numpy.mean(thr4_atp_data)
      print(average)
     10.876950930000001
[20]: average = numpy.mean(data[:,1]) # its the same thing as line [26]
      print(average)
     10.876950930000001
[21]: #range for Loop does an operation a particular number of times
      #range (start, end)
[22]: # How do I find the number of colums?
      # Using skills you already know, think about how you could find the number of L
       ⇔colums
      num_columns = len(data[200,:])
      print(num_columns)
[23]: for i in range(1,num_columns):
          data_column = data[:,i]
          average = numpy.mean(data_column)
          print(F'{headers[i]} : {average: .4f}')
```

THR4_ATP : 10.8770 THR4_ASP : 7.3423 TYR6_ATP : 11.2098 TYR6_ASP : 10.9934

```
[24]: import matplotlib.pyplot as plt
```

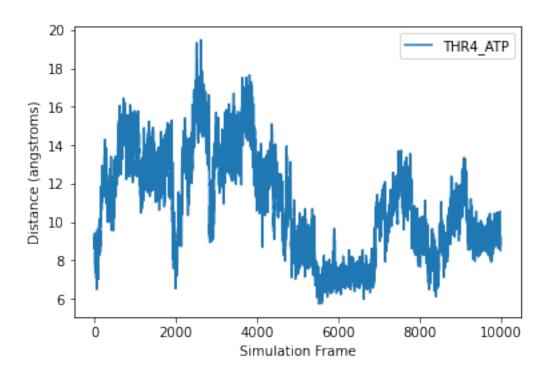
```
[25]: plt.figure()
   plt.plot(data[:,0], data[:,1])
```

[25]: [<matplotlib.lines.Line2D at 0x7f93aa98eeb0>]



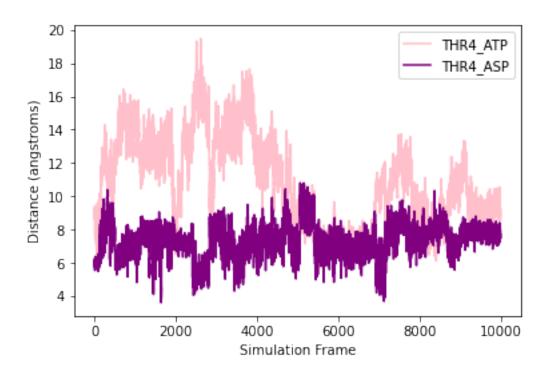
```
[26]: plt.figure()
   plt.plot(data[:,1], label=F'{headers[1]}')
   plt.xlabel('Simulation Frame')
   plt.ylabel('Distance (angstroms)')
   plt.legend()

plt.savefig(F'{headers[1]}')
```



```
[28]: plt.figure()
  plt.plot(data[:,1], label=F'{headers[1]}', color='pink')
  plt.plot(data[:,2], label=F'{headers[2]}', color='purple')
  plt.xlabel('Simulation Frame')
  plt.ylabel('Distance (angstroms)')
  plt.legend()

plt.savefig(F'{headers[1]}.png', dpi=300)
```

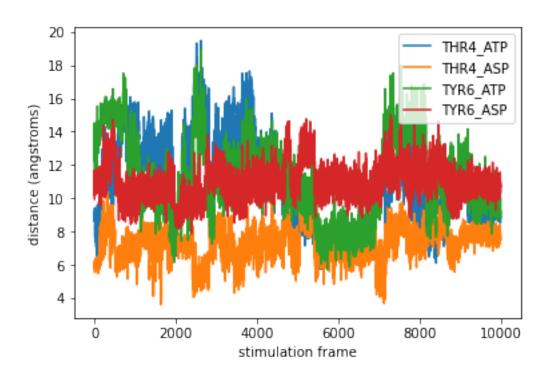


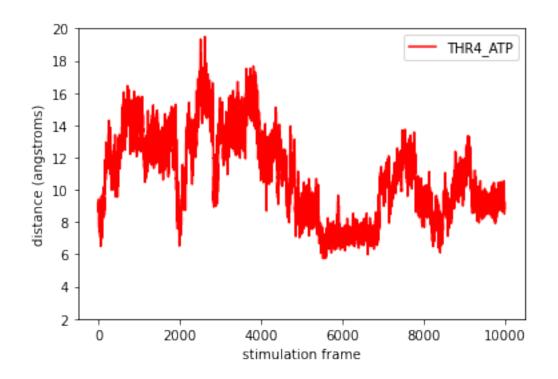
```
[]: #using tje example ablove use a range for loo[ to make a plot with all of the columns of data]
```

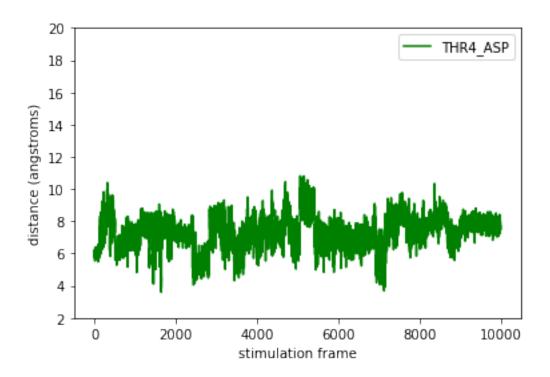
```
[31]: plt.figure()

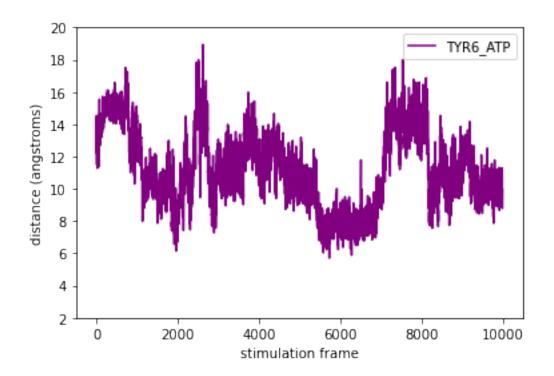
for i in range(1,num_columns):
    plt.plot(data[:,i], label=F'{headers[i]}')
    plt.legend()

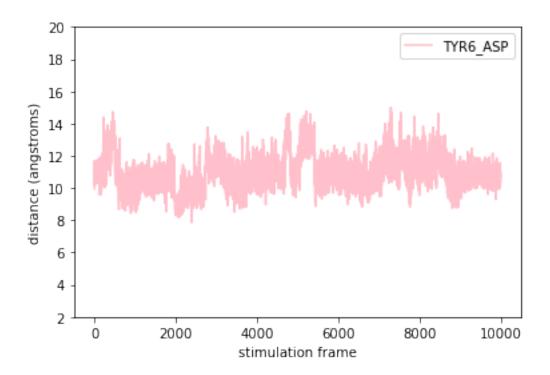
plt.xlabel('stimulation frame')
    plt.ylabel('distance (angstroms)')
```











[]: