

# WorkingWithStructuredData

February 21, 2015

```
In [1]: %matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
%precision 4
import os, sys, glob
```

## 0.1 Using SQLite3

Will change this to use the same example for queries and schema design

- Subjects - Ann, Bob, Charlie
- Tests - Liver function, Complete blood count
- Test parameters - AST, ALT, RBC, platelets, WBC (may perform all or only subset of parameters)
- Different number of visits, different number of tests per visit

### 0.1.1 Working example dataset

This data contains the survival time after receiving a heart transplant, the age of the patient and whether or not the survival time was censored

- Number of Observations - 69
- Number of Variables - 3

Variable name definitions:: \* death - Days after surgery until death \* age - age at the time of surgery \* censored - indicates if an observation is censored. 1 is uncensored

```
In [2]: import statsmodels.api as sm
heart = sm.datasets.heart.load_pandas().data
heart.take(np.random.choice(len(heart), 6))
```

```
Out[2]:
```

	survival	censors	age
66	110	0	23.7
24	1367	0	48.6
30	897	1	46.1
67	13	0	28.9
49	499	0	52.2
35	322	1	48.1

```
In [3]: import sqlite3
conn = sqlite3.connect('heart.db')
```

### 0.1.2 Creating and populating a table

```
In [4]: c = conn.cursor()
```

```
    c.execute('''CREATE TABLE IF NOT EXISTS transplant
                (survival integer, censors integer, age real)''')
```

```
    c.executemany("insert into transplant(survival, censors, age) values (?, ?, ?)", heart.values);
```

### 0.1.3 SQL queries

SQL Queries take the form

```
select (distinct) ... from ... (limit ...)
where ...
groupby ..
order by ...
```

where most of the query apart from the `select ... from ...` are optional.

Selecting all columns, first 10 rows

```
In [5]: for row in c.execute('''select * from transplant limit 5;'''):
        print row
```

```
(15, 1, 54.3)
(3, 1, 40.4)
(624, 1, 51.0)
(46, 1, 42.5)
(127, 1, 48.0)
```

Using where to filter rows

```
In [6]: # only find censored data for subjects < 40 years old
        for row in c.execute('''
            select * from transplant
            where censors=0 and age < 40 limit 5;'''):
            print row
```

```
(1775, 0, 33.3)
(1106, 0, 36.8)
(875, 0, 38.9)
(815, 0, 32.7)
(592, 0, 26.7)
```

Using SQL functions

```
In [7]: for row in c.execute('''select count(*), avg(age) from transplant where censors=0 and age < 40;
        print row
```

```
(9, 31.433333333333333)
```

Using groupby to find number of censored and uncensored subjects and their average age

```
In [8]: query = '''
        select censors, count(*), avg(age) from transplant
        group by censors;
        '''
        for row in c.execute(query):
            print row

(0, 24, 41.729166666666664)
(1, 45, 48.4844444444444456)
```

Using having to filter grouped results

```
In [9]: query = '''
        select censors, count(*), avg(age) from transplant
        group by censors
        having avg(age) < 45;
        '''
        for row in c.execute(query):
            print row

(0, 24, 41.729166666666664)
```

Using order by to sort results

```
In [10]: query = '''
        select * from transplant
        where age < 40
        order by age desc;
        '''
        for row in c.execute(query):
            print row

(875, 0, 38.9)
(1106, 0, 36.8)
(44, 1, 36.2)
(1, 0, 35.2)
(1775, 0, 33.3)
(815, 0, 32.7)
(12, 1, 29.2)
(13, 0, 28.9)
(592, 0, 26.7)
(167, 0, 26.7)
(110, 0, 23.7)
(228, 1, 19.7)
```

Reading into a numpy structured array

```
In [11]: result = c.execute(query).fetchall()
        arr = np.fromiter(result, dtype='i4,i4,f4')
        arr.dtype.names = ['survival', 'censors', 'age']
        print '\n'.join(map(str, arr))
```

```

(875, 0, 38.900001525878906)
(1106, 0, 36.79999923706055)
(44, 1, 36.20000076293945)
(1, 0, 35.20000076293945)
(1775, 0, 33.29999923706055)
(815, 0, 32.70000076293945)
(12, 1, 29.200000762939453)
(13, 0, 28.899999618530273)
(592, 0, 26.700000762939453)
(167, 0, 26.700000762939453)
(110, 0, 23.700000762939453)
(228, 1, 19.700000762939453)

```

### Reading into a numpy regular array

```

In [12]: from itertools import chain
         result = c.execute(query).fetchall()
         arr = np.fromiter(chain.from_iterable(result), dtype=np.float)
         print arr.reshape(-1,3)

```

```

[[ 8.7500e+02  0.0000e+00  3.8900e+01]
 [ 1.1060e+03  0.0000e+00  3.6800e+01]
 [ 4.4000e+01  1.0000e+00  3.6200e+01]
 [ 1.0000e+00  0.0000e+00  3.5200e+01]
 [ 1.7750e+03  0.0000e+00  3.3300e+01]
 [ 8.1500e+02  0.0000e+00  3.2700e+01]
 [ 1.2000e+01  1.0000e+00  2.9200e+01]
 [ 1.3000e+01  0.0000e+00  2.8900e+01]
 [ 5.9200e+02  0.0000e+00  2.6700e+01]
 [ 1.6700e+02  0.0000e+00  2.6700e+01]
 [ 1.1000e+02  0.0000e+00  2.3700e+01]
 [ 2.2800e+02  1.0000e+00  1.9700e+01]]

```

### 0.1.4 Working with multiple tables in SQL

We will construct a new database with 2 tables to illustrate the concept of joins.

```

In [13]: conn1 = sqlite3.connect('samples.db')
         c1 = conn1.cursor()

         c1.execute(
             '''
             CREATE TABLE IF NOT EXISTS t1(
                 ID TEXT,
                 Name TEXT,
                 Value Real);
             '''
         )

         c1.execute('''
         CREATE TABLE IF NOT EXISTS t2(
             ID TEXT,
             Name TEXT,
             Value Real,
             Age INTEGER);
         ''');

```

```

from string import ascii_lowercase
for i in range(5):
    c1.execute('''insert into t1(ID, Name, Value) values (%d, '%s', %.2f)''' % (i, ascii_lower
    c1.execute('''insert into t2(ID, Name, Value, Age) values (%d, '%s', %.2f, %d)''' % (i*2,

```

## Cartesian product

In [14]: *# Without specifying a join, the result is all possible combinations*

```

query = '''
select t1.ID, t2.ID from t1, t2;
'''

for row in c1.execute(query):
    print row

```

```

(u'0', u'0')
(u'0', u'2')
(u'0', u'4')
(u'0', u'6')
(u'0', u'8')
(u'1', u'0')
(u'1', u'2')
(u'1', u'4')
(u'1', u'6')
(u'1', u'8')
(u'2', u'0')
(u'2', u'2')
(u'2', u'4')
(u'2', u'6')
(u'2', u'8')
(u'3', u'0')
(u'3', u'2')
(u'3', u'4')
(u'3', u'6')
(u'3', u'8')
(u'4', u'0')
(u'4', u'2')
(u'4', u'4')
(u'4', u'6')
(u'4', u'8')

```

## Inner joins

In [15]: *# Inner join (intersection)*

```

query = '''
select t1.ID, t2.ID, t1.value, t2.value, t1.value * t2.value from t1, t2
where t1.ID = t2.ID;
'''

for row in c1.execute(query):
    print row

```

```

(u'0', u'0', 0.0, 5.0, 0.0)
(u'2', u'2', 4.0, 6.0, 24.0)
(u'4', u'4', 16.0, 9.0, 144.0)

```

```
In [16]: # left join keeps all values from the left table (t2)
# and values from the right (t1) where there is a match
query = '''
select t1.id, t2.ID, t1.value, t2.value from t2 left join t1 on t1.ID = t2.ID
'''

for row in c1.execute(query):
    print row

(u'0', u'0', 0.0, 5.0)
(u'2', u'2', 4.0, 6.0)
(u'4', u'4', 16.0, 9.0)
(None, u'6', None, 14.0)
(None, u'8', None, 21.0)
```

```
In [17]: # same join but we switch left and right tables
query = '''
select t1.ID, t2.ID, t1.value, t2.value from t1 left join t2 on t1.ID = t2.ID
'''

for row in c1.execute(query):
    print row

(u'0', u'0', 0.0, 5.0)
(u'1', None, 1.0, None)
(u'2', u'2', 4.0, 6.0)
(u'3', None, 9.0, None)
(u'4', u'4', 16.0, 9.0)
```

## Self-joins

```
In [18]: # we can join a table to itself by using aliases
# lets add a few more rows to t1 which may have the same id and name but different values

for i in range(5):
    c1.execute('''insert into t1(ID, Name, Value) values (%d, '%s', %.2f)''' % (i, ascii_lower(
        chr(97 + i)))

for row in c1.execute('select * from t1;'):
    print row

(u'0', u'a', 0.0)
(u'1', u'b', 1.0)
(u'2', u'c', 4.0)
(u'3', u'd', 9.0)
(u'4', u'e', 16.0)
(u'0', u'a', 0.0)
(u'1', u'b', 1.0)
(u'2', u'c', 8.0)
(u'3', u'd', 27.0)
(u'4', u'e', 64.0)
```

```
In [19]: # Now use a self-join to find paired values for the same ID and name

query = '''
select t1a.ID, t1a.Name, t1a.value, t1b.value from t1 as t1a, t1 as t1b
where t1a.Name = t1b.Name and t1a.Value < t1b.Value
order by t1a.ID ASC;
```

```

'''
for row in c1.execute(query):
    print row

(u'2', u'c', 4.0, 8.0)
(u'3', u'd', 9.0, 27.0)
(u'4', u'e', 16.0, 64.0)

```

### 0.1.5 Basic concepts of database normalization

In which we convert a dataframe into a normalized database.

```

In [127]: names = ['ann', 'bob', 'ann', 'bob', 'carl', 'delia', 'ann']
         tests = ['wbc', 'wbc', 'rbc', 'rbc', 'wbc', 'rbc', 'platelets']
         values1 = [10, 11.2, 300, 204, 9.8, 340, 125]
         values2 = [10.6, 13.2, 322, 214, 10.3, 343, 145]
         df = pd.DataFrame([names, tests, values1, values2]).T
         df.columns = ['names', 'tests', 'values1', 'values2']
         df

```

```

Out[127]:
   names  tests  values1  values2
0   ann    wbc        10     10.6
1   bob    wbc       11.2     13.2
2   ann    rbc       300     322
3   bob    rbc       204     214
4  carl    wbc        9.8     10.3
5  delia    rbc       340     343
6   ann  platelets     125     145

```

In [129]: *# names are put into their own table so there is no duplication*

```

name_table = pd.DataFrame(df['names'].unique(), columns=['name'])
name_table['name_id'] = name_table.index
columns = ['name_id', 'name']
name_table[columns]

```

```

Out[129]:
   name_id  name
0         0   ann
1         1   bob
2         2  carl
3         3  delia

```

In [130]: *# tests are put into their own table so there is no duplication*

```

test_table = pd.DataFrame(df['tests'].unique(), columns=['test'])
test_table['test_id'] = test_table.index
columns = ['test_id', 'test']
test_table[columns]

```

```

Out[130]:
   test_id  test
0         0   wbc
1         1   rbc
2         2  platelets

```

In [132]: *# the values1 and values2 correspond to visit 1 and 2, so  
# we create a visits table*

```

visit_table = pd.DataFrame([1,2], columns=['visit'])
visit_table['visit_id'] = visit_table.index
columns = ['visit_id', 'visit']
visit_table[columns]

```

```

Out[132]:
   visit_id  visit
0         0      1
1         1      2

```

In [97]: *# finally, we link each value to a triple(name\_id, test\_id, visit\_id)*

```

value_table = pd.DataFrame([
    [0,0,0,10], [1,0,0,11.2], [0,1,0,300], [1,1,0,204], [2,0,0,9.8], [3,1,0,340], [0,2,0,125],
    [0,0,1,10.6], [1,0,1,13.2], [0,1,1,322], [1,1,1,214], [2,0,1,10.3], [3,1,1,343], [0,2,1,145.0]
], columns=['name_id', 'test_id', 'visit_id', 'value'])
value_table

```

```

Out[97]:
   name_id  test_id  visit_id  value
0         0         0         0    10.0
1         1         0         0    11.2
2         0         1         0   300.0
3         1         1         0   204.0
4         2         0         0    9.8
5         3         1         0   340.0
6         0         2         0   125.0
7         0         0         1   10.6
8         1         0         1   13.2
9         0         1         1   322.0
10        1         1         1   214.0
11        2         0         1   10.3
12        3         1         1   343.0
13        0         2         1  145.0

```

At the end of the normalization, we have gone from 1 dataframe with multiple redundancies to 4 tables with unique entries in each row. This organization helps maintain data integrity and is necessary for efficiency as the number of test values grows, possibly into millions of rows. As we have seen, we can use SQL queries to recreate the original data format if that is more convenient for analysis.

### 0.1.6 Using HDF5

When your data consists of many numerical and matrices, each of which is relatively independent, relational databases offer little benefit, and it is more efficient to use HDF5 (Hierarchical Data Format) for storage. For example, your data may come from a simulation which generates a 3D matrix and a list of count data at every iteration.

In [44]: `import h5py`

```

f = h5py.File('simulation.h5')

```

```

In [45]: for i in range(10): # iterations in simulation
          xs = np.random.random((100,100,100))
          ys = np.random.randint(0,100,(i+1)*10)
          group = f.create_group('Iteration%03d' % i)
          group.create_dataset('xs', data=xs)
          group.create_dataset('ys', data=ys)

```



```
In [46]: f.keys()
```

```
Out[46]: [u'Iteration000',
          u'Iteration001',
          u'Iteration002',
          u'Iteration003',
          u'Iteration004',
          u'Iteration005',
          u'Iteration006',
          u'Iteration007',
          u'Iteration008',
          u'Iteration009']
```

```
In [47]: f['Iteration008'].keys()
```

```
Out[47]: [u'xs', u'ys']
```

```
In [48]: g8 = f['Iteration008']
          print g8['xs'][2:5,2:5,2:5]
          print g8['ys'][-10:]
```

```
[[[ 0.0367  0.2883  0.5562]
   [ 0.9494  0.5614  0.1159]
   [ 0.8887  0.7396  0.891 ]]]
```

```
[[ 0.7552  0.1539  0.216 ]
 [ 0.6671  0.4682  0.9107]
 [ 0.5565  0.5443  0.1665]]
```

```
[[ 0.3972  0.1205  0.9487]
 [ 0.7874  0.3466  0.2818]
 [ 0.1248  0.0161  0.6898]]]
[37 69  5 15 10 44 20 73 74 24]
```

### 0.1.7 Interfacing withPandas

```
In [26]: import pandas as pd
```

```
In [27]: df = pd.read_sql('select * from transplant;', conn)
```

```
In [28]: df.take(np.random.randint(0, len(df), 6))
```

```
Out[28]:      survival  censors   age
         8          23         1  56.9
        38         815         0  32.7
        12         730         1  58.4
        58         339         0  54.4
        53         439         0  52.9
        27         994         1  48.6
```

```
In [29]: df1 = pd.read_sql('select t1.name, t2.value, t2.age from t1, t2 where t1.name = t2.name;', conn)
```

```
In [30]: df1
```

```
Out[30]:   Name  Value  Age
         0     a      5    0
         1     c      6   10
```

2	e	9	20
3	a	5	0
4	c	6	10
5	e	9	20

```
In [31]: c.close()
         c1.close()
         conn.close()
         conn1.close()
```

```
In [60]: store = pd.HDFStore('dump.h5')
         store['transplant'] = df
         store['tables'] = df1
         store.close()
```

/Users/cliburn/anaconda/lib/python2.7/site-packages/pandas/io/pytables.py:2453: PerformanceWarning: your performance may suffer as PyTables will pickle object types that it cannot map directly to c-types [inferred.type->unicode,key->block2\_values] [items->['Name']]

```
warnings.warn(ws, PerformanceWarning)
```

```
In [62]: transplant_df = pd.read_hdf('dump.h5', 'transplant')
         transplant_df.take(np.random.randint(0, len(df), 6))
```

```
Out[62]:
```

	survival	censors	age
50	305	0	49.3
3	46	1	42.5
0	15	1	54.3
22	1	1	41.5
47	63	1	56.4
19	1549	0	40.6

```
In [64]: table_df = pd.read_hdf('dump.h5', 'tables')
         table_df
```

```
Out[64]:
```

	Name	Value	Age
0	a	5	0
1	c	6	10
2	e	9	20
3	a	5	0
4	c	6	10
5	e	9	20

```
In [65]: store
```

```
Out[65]: <class 'pandas.io.pytables.HDFStore'>
         File path: dump.h5
         File is CLOSED
```

```
In [66]: store = pd.HDFStore('dump.h5')
```

```
In [67]: store.keys()
```

```
Out[67]: ['/tables', '/transplant']
```

```
In [68]: store.close()
```

```
In []:
```