

Python

Tools for Reproducible Research

Karl Broman

Biostatistics & Medical Informatics, UW–Madison

`biostat.wisc.edu/~kbroman`

`github.com/kbroman`

`@kwbroman`

Course web: bit.ly/tools4rr

Why python?

- ▶ Manipulating data files
- ▶ Simulations using others' programs

Why python?

- ▶ Manipulating data files
- ▶ Simulations using others' programs
- ▶ Web-related stuff

Why python?

- ▶ Manipulating data files
- ▶ Simulations using others' programs
- ▶ Web-related stuff
- ▶ Alternative to R for data analysis and graphics
- ▶ iPython notebooks

Python 2 vs Python 3

- ▶ Most people are using Python version 2.7
- ▶ Python 3 was introduced in 2008
 - A number of large changes
 - Some important Python programs haven't been ported
 - Few people seem to be using it day-to-day
- ▶ You should probably stick with Python 2
 - But be aware of differences

Installing Python

- ▶ On Mac or Unix, Python should be pre-installed

```
python --version
```

- ▶ For Windows (or to be current, or to alternate between Python 2 and 3), install **Anaconda**

Includes NumPy, SciPy, Pandas, iPython, Matplotlib, ...
continuum.io/downloads

Learning a new language

- ▶ Find a good book
- ▶ Have good example tasks/problems
- ▶ Play around
- ▶ Force yourself to use the new language
- ▶ Develop a script illustrating different language features

Into the thick of it

Learn Python through one example

markers.txt

families.txt

genotypes.txt

→

data.gen

Input: markers.txt

```
D20S103  
D20S482  
D20S851  
D20S604  
D20S1143  
D20S470  
D20S477  
D20S478  
D20S481  
D20S159  
D20S480  
D20S451  
D20S171  
D20S164
```

Input: families.txt

Family	Individual	Father	Mother	Sex
1	1	0	0	1
1	2	0	0	2
1	3	1	2	1
1	4	1	2	2
1	5	1	2	2
2	1	0	0	1
2	2	0	0	2
2	3	1	2	1
2	4	1	2	1
3	1	0	0	1
3	2	0	0	2
3	3	1	2	2
3	4	1	2	1
3	5	1	2	1
3	6	1	2	2
...				
5	6	1	2	2
5	7	1	2	1

Input: genotypes.txt

Marker	1-1	1-2	1-3	1-4	1-5	2-1	2-2	...
D20S103		100/98	98/98	98/98	98/98	100/100	100/96	...
D20S1143	176/172	180/176	176/180		172/180	172/176	172/172	...
D20S159	350/358	366/354	350/354	350/354	358/366	354/350	366/354	...
D20S164		191/207	207/207	215/191	215/207	191/207	207/215	...
D20S171	141/135	141/137	141/141	141/137	135/137	141/139	143/135	...
D20S451	324/308	320/316	324/316	308/320		308/324	312/316	...
D20S470	306/302	302/306	302/306	306/302	302/302	302/294	310/266	...
D20S477	256/252	260/252	252/252		256/252	256/252		...
D20S478		267/263	263/263	263/263	263/267	255/271	263/247	...
D20S480		304/284		304/284	304/284	296/296	300/300	...
D20S481	229/237	241/237	237/237	229/237	237/237	245/245		...
D20S482	155/159	159/167	159/159	155/167	159/167	147/155	159/155	...
D20S604	151/147		147/135	151/143	151/143		147/143	...
D20S851	132/140	148/144	132/144	132/148	132/148		144/140	...

Output: data.gen

```
5
14
D20S103
D20S482
...
D20S171
D20S164
1
5
1 0 0 1
0 0 155 159 132 140 151 147 176 172 306 302 256 252 0 0 ...
2 0 0 0
100 98 159 167 148 144 0 0 180 176 302 306 260 252 267 ...
3 2 1 1
98 98 159 159 132 144 147 135 176 180 302 306 252 252 ...
4 2 1 0
98 98 155 167 132 148 151 143 0 0 306 302 0 0 263 263 ...
5 2 1 0
98 98 159 167 132 148 151 143 172 180 302 302 256 252 ...
2
4
...
```

The top of the Python script

```
#!/usr/bin/env python
# Combine the data in "genotypes.txt", "markers.txt" and
# "families.txt" and convert them into a CRI-MAP .gen file
#
# This is the python 2 version

def read_markers (filename):
    "Read an ordered list of marker names from a file."
    with open(filename, 'r') as f:
        lines = f.readlines()
    return [line.strip() for line in lines]

class Person:
    "Person class, to contain the data on a subject."
    def __init__ (self,family, id, dad, mom, sex):
        self.family = family
        self.id = id
        self.dad = dad
        self.mom = mom
        self.sex = "0" if sex == "2" else sex # convert 1/2 -> 1/0
        self.famid = family + '-' + id
        self.gen = {}
```

The bottom of the Python script

```
if __name__ == '__main__':  
    # file names  
    gfile = "genotypes.txt" # genotype data  
    mfile = "markers.txt"   # list of markers, in order  
    ffile = "families.txt"  # family information  
    ofile = "data.gen"      # output file  
  
    # read the data  
    markers = read_markers(mfile)  
    people = read_families(ffile)  
    read_genotypes(gfile, people)  
  
    # write the data  
    write_genfile(ofile, people, markers)
```

Write functions & modules not scripts

- ▶ Write a set of reusable functions
- ▶ Your code will be easier to read
- ▶ You may actually reuse the code, this way

Try it out

```
$ convert2.py
$ diff data.gen data_save.gen
```

```
$ python          # (or ipython)

>>> import convert2

>>> help(convert2)
>>> help(convert2.read_markers)

>>> markers = convert2.read.markers("markers.txt")
>>> markers[0]
>>> len(markers)
>>> markers[-1]
>>> markers[0:2]
>>> markers[0:-1]
>>> markers[5:]
>>> markers[:5]
>>> markers[0:7:2]

>>> quit()
```


Read the marker names

```
def read_markers (filename):  
    "Read an ordered list of marker names from a file."  
    with open(filename, 'r') as f:  
        lines = f.readlines()  
    return [line.strip() for line in lines]
```

class Person

```
class Person:
    "Person class, to contain the data on a subject."
    def __init__(self, family, id, dad, mom, sex):
        self.family = family
        self.id = id
        self.dad = dad
        self.mom = mom
        self.sex = "0" if sex == "2" else sex # convert 1/2 -> 1/0
        self.famid = family + '-' + id
        self.gen = {}
```

Example use:

```
ind = Person("1", "3", "1", "2", "2")
```

read_families

```
def read_families (filename):  
    "Read family info and return a hash of people."  
    with open(filename, 'r') as file:  
        file.readline() # header row  
        people = {}  
        for line in file:  
            vals = line.strip().split()  
            person = Person(vals[0],vals[1],vals[2],vals[3],vals[4])  
            people[person.famid] = person  
    return people
```

read_genotypes

```
def parse_genotype (string):
    "Clean up string -> genotype"
    string = string.replace(' ', '')
    string = "0/0" if string == "" else string
    return string.replace('/', ' ')

def read_genotypes (filename, people):
    "Read genotype data, fill in genotypes within people hash"
    with open(filename, 'r') as file:

        header = file.readline().strip().split()
        header = header[1:] # omit the first field, "Marker"

        for line in file:
            marker = line[:9].replace(' ', '')
            line = line[9:]
            for i in range(len(header)):
                person = header[i]
                start = i*7
                people[person].gen[marker] = \
                    parse_genotype(line[start:(start+7)])
```

Some helper functions

```
def get_families (people):  
    "Return a vector of distinct families"  
    return set([people[key].family for key in people])  
  
def get_family_members (people, family):  
    "Return a vector of famids for subjects within a family."  
    return [key for key in people \  
            if people[key].family == family]  
  
def writeln (file, line, end="\n"):  
    "Write a single line to a file."  
    file.write(str(line) + end)
```

write_genfile

```
def write_genfile (filename, people, markers):
    "Write genotype data to a file, in CRI-MAP format."
    with open(filename, 'w') as file:
        families = sorted(get_families(people))
        writeln(file, len(families))

        writeln(file, len(markers))
        for marker in markers:
            writeln(file, marker)

        for family in families:
            writeln(file, family)
            members = sorted(get_family_members(people, family), \
                             key=lambda famid: int(people[famid].id))
            writeln(file, len(members))

            for famid in members:
                person = people[famid]
                writeln(file, "%s %s %s %s" % (person.id, \
                                                person.mom, person.dad, person.sex))

            for marker in markers:
                writeln(file, person.gen[marker], " ")
            writeln(file, "")
```

The bottom of the Python script

```
if __name__ == '__main__':  
    # file names  
    gfile = "genotypes.txt" # genotype data  
    mfile = "markers.txt"   # list of markers, in order  
    ffile = "families.txt"  # family information  
    ofile = "data.gen"      # output file  
  
    # read the data  
    markers = read_markers(mfile)  
    people = read_families(ffile)  
    read_genotypes(gfile, people)  
  
    # write the data  
    write_genfile(ofile, people, markers)
```

Basic types

- ▶ float

```
x = 0.3
```

- ▶ int

```
m = 5
```

- ▶ string

```
s = "blah"
```

- ▶ bool

```
x = True
```

```
y = False
```

- ▶ None

```
x = None
```

- ▶ complex

```
x = 5+0j
```


Converting between types, and such

```
n = 5
type(n)

s = str(n)
x = float(n)

"%s %s %s" % (n, s, x)
"%d %d %d" % (n, int(s), x)
"%f %f %f" % (n, float(s), x)

dir(s)
dir(x)

s = "blah"
len(s)
s[2:]
s[:-1]
for ch in s:
    print ch
```

Multi-element types

- ▶ list

```
x = [1, 2, 3, None, "blah"]  
y = [ [ 1, 2 ], [ 3, 4, 5 ], 6 ]
```

- ▶ dictionary

```
h = {'x': 3, 'y': 5, 'name':"Karl"}
```

- ▶ tuple

```
x = (1, [2,3])
```

- ▶ set

```
S = set([5, 3, 5, 1, 2, 1])
```

matrices as lists of lists

```
x = [ [1, 2, 3, 4], [5, 6, 7, 8], [9, 10, 11, 12] ]  
x[1][3]
```

for loops

```
vec = range(4)
for x in vec:
    print (x+1)**2

import math
for i in xrange(len(vec)):
    print math.log( vec[i] + 1 )

h = {'x':3, 'y':4, 'z':2}
for k in h:
    print k, h[k]

for k in sorted(h.keys()):
    print k, h[k]

for k,v in h.iteritems():
    print k, v

for v in h.itervalues():
    print v
```

list comprehensions

```
vec = range(10)
[v**2 for v in vec if v > 5]

h = {'x':3, 'y':4, 'zz':2}
[h[k]**2 for k in h]
[h[k]**2 for k in h if len(k) == 1]
[[k, v**3] for k,v in h.iteritems()]
dict( [[k, v**3] for k,v in h.iteritems()] )

x = [k+1 for k in range(6)]
y = [True, False, True, False, False, False]
[x[i] for i in range(len(x)) if y[i]]
```

More with strings

```
x = "bread and jam"
y = x.split(" ")
z = " ".join(y)

dir(x)
help(x.index)

x.endswith("jam")
x.startswith("bre")
x.count("a")
x.find("and")
x.find("jelly")
x.index("and")
x.index("jelly")

x.replace("jam", "jelly")

x.capitalize()
x.title()
x.upper()
x.upper().lower()
```

Regular expressions

```
import re

x = "Bread and Jam"
re.findall(r'[A-Z]', x)
re.split(r'[A-Z]', x)
re.sub(r'[A-Z]', '', x)

ph = "555-12-3456"
re.findall(r'-', ph)
re.findall(r'\d+', ph)
re.split(r'\D', ph)
re.sub(r'\D', '', ph)
```

Unit tests: Nose

```
# This is nosetest_convert2.py
#
# At command line, type "nosetests nosetest_convert2.py"

from nose.tools import assert_equal
from convert2 import *

def test_parse_genotype():
    assert_equal(parse_genotype("      "), "0 0")
    assert_equal(parse_genotype("100/98 "), "100 98")
    assert_equal(parse_genotype("90/96  "), "90 96")
    assert_equal(parse_genotype("90/ 96  "), "90 96")
    assert_equal(parse_genotype(" 3 / 8  "), "3 8")
```


Unit tests: unittest

```
#!/usr/bin/env python
# Test one of the functions in convert2.py
#
# on the command line, type "test_convert2.py"

import unittest
from convert2 import *

class check_parse_genotype(unittest.TestCase):
    def test_parse_genotype(self):
        self.assertEqual(parse_genotype("      "), "0 0")
        self.assertEqual(parse_genotype("100/98 "), "100 98")
        self.assertEqual(parse_genotype("90/96  "), "90 96")
        self.assertEqual(parse_genotype("90/ 96  "), "90 96")
        self.assertEqual(parse_genotype(" 3 / 8  "), "3 8")

if __name__ == '__main__':
    unittest.main()
```

Summary

- ▶ Learn a scripting language, like Python
 - Not just for manipulating data files, but worth the effort just for that.
- ▶ Force yourself to use it