

Python

Tools for Reproducible Research

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I’m a big proponent of the use of multiple programming languages: use different languages for different types of tasks.

Statisticians, in particular, should be proficient in some “scripting language” (e.g., Perl, Python, or Ruby). These types of languages give you far more flexibility for manipulating data files.

I’ve long used Perl, but I’ve switched to Ruby, and I’m trying to also be proficient in Python. I prefer Ruby to Python, but Python is much more widely used, and so if you’re going to just learn one such language, learn Python.

Why python?

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

2

For statisticians, the most important use of Python is for the manipulation of data files. This sort of script language is great for manipulating text, and data files are mostly plain text files.

In addition, I find a scripting language critical for performing simulations to evaluate others' command-line-based programs. They're also good for web-related stuff.

Python can also serve as an alternative to R for data analysis and graphics. And Jupyter notebooks are a big deal for reproducible research (and they can be used more broadly than Python).

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

3

The biggest annoyance about Python is the two competing versions, Python 2 and Python 3. For now, you should probably stick with Python 2.

Python 3 is much better than Python 2, but it hasn't penetrated the Python community sufficiently.

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

4

When you're just starting to learn, you can just stick with the pre-installed version of Python, if you are on some flavor of Unix.

Long term, I recommend Anaconda, which is an easy-to-install Python with basically all of the scientific packages you'd want. Installing these by hand seems really painful; installing Anaconda is easy.

Also, with Anaconda, it's easy to switch between Python 2 and Python 3.

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

5

It takes time to learn a new programming language. The only way you'll learn it is by forcing yourself to use it regularly. You need good, realistic problems to tackle. And it might take you just 30 minutes with the language you know but all afternoon in the new language. But if you don't force yourself, you'll never learn.

If you go away from it for a week, you'll be quite rusty when you come back. I've found it useful to develop a script that illustrates the various language features. ("How do I write a loop again? How do I define a function?") Looking through that, you'll pick it all up again quickly. It's harder to look back through a book in the same way.

Into the thick of it

Learn Python through one example

```
markers.txt  
families.txt    →    data.gen  
genotypes.txt
```

6

I can't really hope to teach you Python in 50 minutes, but I'll try. In this crash course, I'll go through a medium-sized script to combine a few data files and convert them into a different form.

`markers.txt` contains a list of ordered genetic markers.
`families.txt` contains information about subjects' familial relationships. `genotypes.txt` contains subjects' genotypes.

We're going to convert these data into the form used by the CRI-MAP program (an old program for constructing genetic maps).

Input: `markers.txt`

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

This is the `markers.txt` file. It just has one marker name per line.

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

8

This is the **families.txt** file; each line is one subject. In the **Father** and **Mother** columns, 0 indicates missing: a founding individual in that family. In the **Sex** column, 2 = female and 1 = male.

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	252		256/252	256/252	...
D20S478		267/263	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	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	...

The `genotypes.txt` file is a bit ugly. Rows are markers and individuals are in fixed-width columns, with the genotypes being two numeric alleles separated by a slash. Blank fields correspond to missing data.

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
...
```

10

The file we're converting to, **data.gen** in the format used by CRI-MAP, is a bit weird: Number of families, number of markers, the marker names in order, and then for each family, the family ID, the number of subjects in that family, and then the subjects. For each subject, there's a line with individual, mom, dad, and sex (0 = female, 1 = male), and then a line with genotype data, with two numbers for each marker, with 0's for missing values.

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 = {}
```

11

The first line (`#!/usr/bin/env python`) makes it so you can run this script from the command line by just typing its name. Using `/usr/bin/env` allows that Python might be located in a different place on different systems.

To make the script executable (on unix), type `chmod +x convert2.py`

In python, comments begin with `#` (as in R).

Instead of using braces to delineate blocks of code, Python uses indentation. I was initially turned off by this, but I've been converted to the idea (mostly from having written a lot of CoffeeScript code). You're going to indent anyway; why not have that indentation be meaningful?

You define functions with `def name (param):`

Unlike R, functions must have a `return` statement if you want to return a value.

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)
```

12

The `convert2.py` script is just a bunch of function definitions (and one class).

This bit at the bottom is executed only if the script is run from the command line. It does all of the real work: read in the data and then write it back out as a `.gen` file.

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

13

With Python (and R), there's a tendency to write a long mess of a script. It's better to focus on writing a set of reusable functions.

With the given example script, you can use `import convert2` to load the functions into python. This is similar to `library()` in R.

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()
```

14

If you type `convert2.py` from the command line, it will run the script and create the `data.gen` file, which you'll see (with `diff`) matches the target `data_save.gen` file.

Or you can type `python` (or `ipython`) at the command line and then import the module and run some of the functions by hand. You'll need to refer to the functions with the names preceded by `convert2.`, or you can use `from convert2 import *` and then skip the `convert2.` part.

The `read.markers` function reads in the ordered list of markers as a vector. (In Python, they call it a list.) Vectors in Python are indexed starting at 0. You can use the `len` function (like `length()` in R) to get the length.

You can grab slices with `:`, but note that they **don't** include the last element in the range.

And negative values are from the end, with `-1` being the **last** value.

Also, you can use `start:end:by`. Remember that `end` is **not** included.

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]
```

15

This is the function to read the ordered list of markers. It takes a single argument: the name of the file.

The first line (between the double-quotes) is a description that will be shown if you import the module and type `help(convert2.read_markers)`. Strings in Python can be defined using single- or double-quotes, just like in R.

The `with` business looks a bit odd, but it ensures that the file will be closed if anything goes wrong. I could just as well have written `lines=open(filename).readlines()` (The `'r'`, for reading, is the default.) After that bit of code, `lines` contains a vector with one marker name per line.

The last line contains a “list comprehension.” It’s a sort of one-line `for` loop, which applies the `strip()` function to each element of the `lines` vector (removing any end-of-line character).

`read_markers` and `open` are ordinary functions, much like those in R. `readlines` and `strip` are object-oriented “methods.” Think of them as functions where the first argument precedes the function name.

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")
```

16

I first define a class to contain the data for a single subject. It contains a function `__init__` for initializing an instance of the class (the data object for a single subject).

Within that function, `self` refers to the newly defined instance of the class, and `self.family`, etc., are the way to refer to the elements of the class object.

We create a new `Person` object by calling `Person(family, id, dad, mom, sex)`

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
```

17

This is the function to read the family information. I again use **with open() as file:** to open the file. If anything goes wrong, the file will be automatically “closed.”

I use **readline** to read (but ignore) the header line.

people = {} initializes a “hash.” This is like an unordered vector that is indexed by strings rather than numeric indices. (In Python, it’s called a “dictionary.”) I’m going to create a hash of **Person** objects, indicated by strings like “1-2” for individual 2 in family 1.

I use a **for** loop over lines in the file. For each line, I **strip** off any end-of-line character and then **split** it at the white space, into a vector.

I first call **Person** to define the **person** object, as then **person.famid** is defined, and I want to use that as the “hash key.”

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)])
```

18

The first function here cleans up a genotype string a bit. It strips off any white space, substitutes 0/0 in the case of a blank, and replaces the slash with a space. So a string like "78/125 " will be converted to "78 125". The `replace` function for strings is for doing text substitutions: it replaces every instance of its first argument with its second argument.

In the `read_genotypes` function, I grab all but the first element of the header line, which match what I'm using as the keys for my `people` hash. I then go through the rest of the file, one line at a time: I grab the marker name (getting rid of any spaces) and then go through the rest of the line, 7 characters at a time. `range(n)` returns the vector `[0, 1, ..., n-1]`.

If you look back at the `Person` class, you'll see that I'd initialized `gen` as a hash (with `self.gen = {}`). I'm filling this in, indexed by marker names. The `read_genotypes` function doesn't return anything, because it modifies the input `person` object (as a "side effect").

Note the backslash in the second-to-last line; this allows me to split a long line into two. If I left it off, Python would give an error.

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)
```

19

Here are a few helper functions that I use in the last `write_genfile` function.

`get_families` returns a vector of **distinct** family IDs. I use a **list comprehension** again, which gives a vector with all of the family names. Then `set` turns this into a “set” of distinct values. It acts here sort of like `unique()` in R.

`get_family_members` returns a vector of the famid codes for the family members in a given family. I’m using a list comprehension again, but with an additional `if` qualification.

`writeln` is just a little wrapper for the `write` function, to write a string to a file. Note that in this function, the `end` argument has a default value, much like in R functions.

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, "")
```

20

This is the function to write the CRI-MAP file. There are two interesting bits here.

First, `sorted()` returns a sorted version of a vector. I use it twice, the second time with `key=lambda famid: int(people[famid].id)` which is an anonymous function for sorting `Person` objects by their individual IDs (numerically).

The second interesting bit is

```
"%s %s %s %s" % (person.id, person.mom, person.dad,
person.sex)
```

which is like `sprintf`, in that I'm formatting a bunch of stuff as a string.

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)
```

21

We made it through the whole file; here's the bit at the bottom again. This bit is run only if you're executing the script from the command line.

I define the file names, read in the data, and then write it back out in a different form.

Basic types

- ▶ float

```
x = 0.3
```

- ▶ int

```
m = 5
```

- ▶ string

```
s = "blah"
```

- ▶ bool

```
x = True  
y = False
```

- ▶ None

```
x = None
```

- ▶ complex

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

22

These are the basic types. Python 2 also distinguishes between `int` and `long`, while Python 3 has just `int`.

`None` is a null object; you can use it as NA.

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
```

23

It's important to be able to convert between types, particularly for converting between strings and floats.

The `%` operator is particularly handy for formatted output, or just to convert things into strings. With `%s`, numbers will be converted to strings, but with `%d` and `%f`, strings will **not** automatically be converted to numbers – you'll get an error.

The `type` function returns the type of an object. The `dir` function returns a list of the methods

You can use `len` on strings, and you can subset them like a vector (aka list), and you can even loop over the characters in a string.

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])
```

24

Lists are like lists in R: they're ordered vectors whose elements can be basically anything.

Dictionaries are what I call hashes: an un-ordered list indexed by strings (called "keys").

Tuples are like lists, but the contents can't be changed. They're useful as return values from a function.

Sets are lists with only unique values.

matrices as lists of lists

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

25

The simplest way to handle a matrix is as a list of lists. They'd typically be stored by rows, as you'd then index the thing as `mat[row][col]`.

Also see [numpy \(numpy.org\)](http://numpy.org), for formal matrices and matrix methods.

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
```

26

for loops over lists successively take each possible value in the list. If you want the indices, you need to create a vector of indices with **range**. Or use **xrange**, which avoids actually creating the vector, but rather creates the elements when they're needed.

xrange is in Python2 only; in Python 3, just use **range**. The Python3 **range** is really the Python2 **xrange**. So actually in Python3, the first line needs to be `vec = list(range(4))`.

for loops over dictionaries (aka hashes) successively take each possible key. You can use **iteritems()** to iterate over key-value pairs or **itervalues()** to iterate over just the values. Like **xrange**, these generate the vector of iteracted values as needed rather than in advance. There's also a **iterkeys()** method, which is what is used as the default for **for** loops with dictionaries.

Note that these loops with dictionaries will be in arbitrary order. If you want a particular order, you first need to create a sorted vector of keys.

In Python3, use **.items()** and **.values()** in place of **.iteritems()** and **.itervalues()**, respectively.

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]]
```

27

List comprehensions are really useful for transformations or subsetting.

The `dict` function will convert a list of key-value pairs into a dictionary.

You can get by without them. But they can provide compact but readable code.

Note, again, that in Python3 you should use `.items()` in place of `.iteritems()`.

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()
```

28

Python has also sorts of methods for doing things with strings.

Use `dir` to get a list, eg `dir(str)`, `dir("")`, or `dir(x)` where `x` is a string.

Use `help` to get a description of one of the methods, eg `help(str.find)`, `help("").find`, or `help(x.find)`.

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)
```

29

A big reason to use scripting languages is for regular expression facilities. But I find regular expressions cumbersome in Python relative to Perl or Ruby.

There is some messiness about backslashes, so it's best with regular expressions to use “raw strings” by preceding the string with an `r`, as so: `r'blah'`.

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")
```

30

Unit tests are important for ensuring the correctness of Python code, as with any other programming effort.

Nose is simple tool for making Python unit tests. The above example is a minimal use of the tool.

At the command line, with tests in the file `nosetest_convert2.py`, you'd type `nosetests nosetest_convert2.py`

The `nose.tools` module contains a bunch of assertion functions. Here, I'm just using `assert_equal`.

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()
```

31

Python also has a built-in `unittest` module, but its use requires a bit more gunk. I don't totally understand all of this.

Like Nose, there are a variety of different assertion functions that you can use.

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

32

Applied statisticians need to be savvy with data file manipulation.

Don't let your scientific collaborators do any copy-paste to move data around; any data file manipulation should be done with a computer program.

In the long run, knowing Python, you'll be more self-sufficient and versatile.