

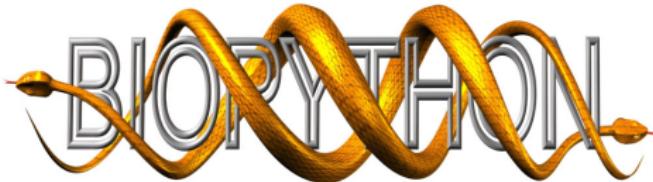
Advanced Topics: Biopython

Day Three

Peter J. A. Cock

The James Hutton Institute, Invergowrie, Dundee, DD2 5DA, Scotland, UK

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Talk Outline

1 Optimization and Profiling

2 Profiling in Python

3 Testing

Optimization and Profiling

- Once you've got some working code, you may want or need it to run faster
- With experience you may be able to guess what is slow
- If in doubt, profile it (measure it)

Premature optimization

“We should forget about small efficiencies, say about 97% of the time: premature optimization is the root of all evil”

Donald Knuth

(author of ‘The Art of Computer Programming’, etc)

Optimization Costs

- Optimization is *not* free
- Efforts to speed code up may be wasted
- You risk breaking things (unit tests help)
- Beware of trading speed for higher memory

If you double the speed, will it actually save you any time?

Only optimize if you need to

- ➊ Get it right
- ➋ Test really is right
- ➌ Profile if slow
- ➍ Optimize
- ➎ Repeat from 2

Profiling in Python

- Try the `profile` module
<http://docs.python.org/library/profile.html>
- Can be run 'live'
- Can be run with profiling logged to a file

Example: Counting FASTQ with SeqIO.parse

```
from Bio import SeqIO

def count_seqio(fastq_filename):
    count = 0
    for record in SeqIO.parse(fastq_filename, "fastq"):
        count += 1
    print "%i records in %s" % (count, fastq_filename)
    return count

import profile
profile.run("count_seqio('SRR014849.fastq')",
            sort="cumulative")
```

Example: Counting FASTQ with SeqIO.parse

```
94696 records in /Users/pjcock/repositories/examples/SRR014849.fastq
2557126 function calls (2462430 primitive calls) in 24.585 CPU seconds
```

Ordered by: cumulative time

ncalls	tottime	percall	cumtime	percall	filename:lineno(function)
1	0.000	0.000	24.585	24.585	profile:0(count_seqio(filename))
1	0.000	0.000	24.578	24.578	<string>:1(<module>)
1	0.595	0.595	24.578	24.578	count_fastq.py:6(count_seqio)
94697	0.863	0.000	23.983	0.000	__init__.py:446(parse)
94697	4.803	0.000	23.115	0.000	QualityIO.py:945(FastqPhredIterator)
94697	4.753	0.000	9.037	0.000	QualityIO.py:788(FastqGeneralIterator)
94696	2.734	0.000	6.247	0.000	SeqRecord.py:147(__init__)
473482/378786	2.168	0.000	2.839	0.000	:0(len)
378785	1.803	0.000	1.803	0.000	:0(readline)
378786	1.558	0.000	1.558	0.000	:0(isinstance)
378784	1.430	0.000	1.430	0.000	:0(rstrip)
94696	0.736	0.000	1.099	0.000	Seq.py:71(__init__)
94696	0.670	0.000	0.986	0.000	Seq.py:200(__len__)
94696	0.727	0.000	0.727	0.000	:0(min)
94696	0.702	0.000	0.702	0.000	:0(max)
94696	0.531	0.000	0.531	0.000	SeqRecord.py:67(__init__)
94696	0.498	0.000	0.498	0.000	:0(split)
1	0.007	0.007	0.007	0.007	:0(setprofile)
...					

Example: Counting FASTQ with SeqIO.parse

- Note these times are slower than with no profiling
- Overall time for SeqIO.parse was 23.983 seconds
- Of this 9.037 seconds was for FastqGeneralIterator
- Big overhead creating SeqRecord objects, 6.247 seconds
- We don't need the SeqRecord objects here...

See also <http://news.open-bio.org/news/2009/09/biopython-fast-fastq/>

Example: Counting FASTQ with FastqGeneralIterator

```
from Bio.SeqIO.QualityIO import FastqGeneralIterator

def count_low(fastq_filename):
    count = 0
    with open(fastq_filename) as handle:
        for values in FastqGeneralIterator(handle):
            count += 1
    print "%i records in %s" % (count, fastq_filename)
    return count

import profile
profile.run("count_seqio('SRR014849.fastq')",
            sort="cumulative")
```

Example: Counting FASTQ with FastqGeneralIterator

```
94696 records in /Users/pjcock/repositories/examples/SRR014849.fastq
    1136359 function calls in 9.415 CPU seconds
```

Ordered by: cumulative time

ncalls	tottime	percall	cumtime	percall	filename:lineno(function)
1	0.000	0.000	9.415	9.415	profile:0(count_low(filename))
1	0.000	0.000	9.415	9.415	<string>:1(<module>)
1	0.392	0.392	9.415	9.415	count_fastq.py:21(count_low)
94697	4.789	0.000	9.024	0.000	QualityIO.py:788(FastqGeneralIterator)
378785	1.728	0.000	1.728	0.000	:0(readline)
378784	1.451	0.000	1.451	0.000	:0(rstrip)
284087	1.055	0.000	1.055	0.000	:0(len)
1	0.000	0.000	0.000	0.000	:0(setprofile)
1	0.000	0.000	0.000	0.000	:0(open)
1	0.000	0.000	0.000	0.000	:0(__enter__)
0	0.000		0.000		profile:0(profiler)

Testing

- Write some tests *before* trying to optimise!

Only optimize if you need to

- ➊ Get it right
- ➋ Test really is right
- ➌ Profile if slow
- ➍ Optimize
- ➎ Repeat from 2

Fast and wrong is *NOT* useful!