Profiling and Benchmarking Software Engineering for Scientists

Efficiency is often a major concern when developing scientific software, and improving how long a program takes to run or how much memory it uses requires a detailed understanding of how the program works and the ability to compare the efficiency of two programs (or different versions of the same program). **Profiling** is the process of measuring how much time is spent in each section of a program during a particular execution. **Benchmarking** is the process of comparing the resources used by two different programs on the same input.

Profiling

A major challenge in program optimization is knowing where code can (and should) be improved. Before any time is spent improving a particular region of your program, you need to determine the proportion of time that was consumed by that code. This proportion will determine the maximum benefit that any optimization could provide. For example, if the total runtime for a program was 1 minute and a particular function ran for a total of 5 seconds, then the best possible optimization of that function (where the runtime of the function goes to zero) would produce a program that runs 1.09X faster. Understanding the balance between costs and benefits of different optimizations will help you identify and prioritize future improvements.

Python provides the dynamic analysis module cProfile for measuring the time spent running different functions. To profile a particular script, simply load the cProfile module in the execution command and the profile will be printed to standard out. You can control the order of the profile with the -s flag.

```
$ python -m cProfile -s tottime search.py 10000 1000 L
60244 function calls (60201 primitive calls) in 0.289 seconds
  Ordered by: internal time
                                      percall filename:lineno(function)
   ncalls tottime
                   percall
                             cumtime
    1000
             0.261
                      0.000
                               0.261
                                        0.000 search.py:4(linear_search)
   11000
             0.007
                      0.000
                               0.013
                                        0.000 random.py:173(randrange)
                                        0.001 {built-in method _imp.create_dynamic}
             0.006
                      0.001
                               0.006
   11000
             0.004
                               0.006
                                        0.000 random.py:223(_randbelow)
                      0.000
    11000
             0.003
                      0.000
                               0.016
                                        0.000 random.py:217(randint)
                      0.002
                                        0.016 search.py:29(<listcomp>)
             0.002
                               0.016
        1
                                        0.000 {method 'bit_length' of 'int' objects}
                               0.001
    11000
             0.001
                      0.000
        1
             0.001
                      0.001
                               0.289
                                        0.289 search.py:1(<module>)
```

The output summarises the total amount of work done in function calls and time, plus six columns for each function call:

ncalls: the number of calls,

tottime: the total time spent in the given function (and excluding time made in calls to sub-functions)

percall: the quotient of tottime divided by ncalls

cumtime: the cumulative time spent in this and all subfunctions (from invocation till exit).

percall: is the quotient of cumtime divided by primitive calls

filename: lineno(function): provides the respective data of each function

In the table above, the function call list is sorted by total time (-s tottime) and the functions that are higher in the list took more time and are good candidates for optimization.

It is important to understand that cProfile measures the performance of function calls. Since the time for all of the code in a function is summarized together, cProfile cannot identify subsets of functions are slow.

Benchmarking

The most basic way to test the resources used by a program is to use the GNU time program. This is not to be confused with time that is part of bash. While the bash time is useful for measuring how long a program rang, GNU time can also measure memory consumption.

It is very likely that your system has bash time, and it may also have GNU time. To tell the difference run time -V to get the version. If there is an error, then it is the bash version

GNU time

```
(swe4s) $ time -V
time (GNU Time) 1.8
Copyright (C) 2017 Free Software Foundation, Inc.
License GPLv3+: GNU GPL version 3 or later <a href="http://gnu.org/licenses/gpl.html">http://gnu.org/licenses/gpl.html</a>.
This is free software: you are free to change and redistribute it.
There is NO WARRANTY, to the extent permitted by law.
Written by David Keppel, David MacKenzie, and Assaf Gordo
```

bash time

```
(swe4s) $ time -V bash: -V: command not found
```

Even if the time -V gave an error, GNU time may still be on your system. Use the which command to check.

```
(swe4s) $ time -V
bash: -V: command not found
real
        0m0.002s
        0m0.001s
user
        0m0.001s
sys
(swe4s) $ which time
/home/jovyan/.conda/envs/swe4s/bin/time
(swe4s) $ /home/jovyan/.conda/envs/swe4s/bin/time -V
time (GNU Time) 1.8
Copyright (C) 2017 Free Software Foundation, Inc.
License GPLv3+: GNU GPL version 3 or later <a href="http://gnu.org/licenses/gpl.html">http://gnu.org/licenses/gpl.html</a>.
This is free software: you are free to change and redistribute it.
There is NO WARRANTY, to the extent permitted by law.
Written by David Keppel, David MacKenzie, and Assaf Gordon.
```

To install GNU time

```
(swe4s) $ conda install -c conda-forge time
```

The output of GNU time is highly configurable using the -f flag along with an output pattern. To get the total runtime and memory usage use -f '%e\t%M'. %e gives total elapsed time in seconds and %M gives the maximum memory usage in kilobytes.

When benchmarking a program, it is important to get the memory and time over a range of input sizes. These results will help you understand how your program will perform when considering larger problems.

```
(swe4s) $ for i in `seq 1 200000 1000000`; do time -f '%e\t%M' python grow.py $i; done 0.03 7080  
0.05 24440  
0.07 37784  
0.10 45692  
0.12 53628
```

GNU time is can only measure full program execution. To get a more detailed assessment of how long individual sections of code run, you must instrument your code with timers. Python provides the time module that makes it easy to store the time before the target block with t0 = time.time() and after the block with t1 = time.time(). The difference between t1 and t0 gives the elapsed time in seconds.

Suppose we are considering a program that uses binary search, which is faster than linear search but also requires the data to be sorted. To measure how much of the program is spent sorting and how much is spent searching we check the time before and after the two sections and compare the differences.

```
t0_sort = time.time()
D.sort()
t1_sort = time.time()

t0_search = time.time()
for q in Q:
    binary_search(q, D)
t1_search = time.time()

total_time = t1_search - t0_sort

print(total_time,(t1_sort-t0_sort)/(total_time),
    (t1_search-t0_search)/(total_time))
```

```
(swe4s) $ python search.py 10000 1000 B 0.0038118362426757812 0.4446459844883663 0.5550412809607206
```

The total time is 0.004 seconds with 44.5% of that time consumed by sort and 55.5% by search.