A Thesis Title

Author Name

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I, Author Name, confirm that the work presented in this thesis is my own. Where information has been derived from other sources, I confirm that this has been indicated in the work.

Abstract

My research is about stuff.

It begins with a study of some stuff, and then some other stuff and things.

There is a 300-word limit on your abstract.

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Acknowledgements

Acknowledge all the things!

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Chapter 1

Introduction

Some stuff about things.[1] Some more things.

Inline citation: Anne Author. Example Journal Paper Title. *Journal of Classic Examples*, 1(1):e1001745+, January 1970

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Etiam lobortis facilisis sem. Nullam nec mi et neque pharetra sollicitudin. Praesent imperdiet mi nec ante. Donec ullamcorper, felis non sodales commodo, lectus velit ultrices augue, a dignissim nibh lectus placerat pede. Vivamus nunc nunc, molestie ut, ultricies vel, semper in, velit. Ut porttitor. Praesent in sapien. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Duis fringilla tristique neque. Sed interdum libero ut metus. Pellentesque placerat. Nam rutrum augue a leo. Morbi sed elit sit amet ante lobortis sollicitudin. Praesent blandit blandit mauris. Praesent lectus tellus, aliquet aliquam, luctus a, egestas a, turpis. Mauris lacinia lorem sit amet ipsum. Nunc quis urna dictum turpis accumsan semper.

Chapter 2

Contur Overview

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Etiam lobortis facilisis sem. Nullam nec mi et neque pharetra sollicitudin. Praesent imperdiet mi nec ante. Donec ullamcorper, felis non sodales commodo, lectus velit ultrices augue, a dignissim nibh lectus placerat pede. Vivamus nunc nunc, molestie ut, ultricies vel, semper in, velit. Ut porttitor. Praesent in sapien. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Duis fringilla tristique neque. Sed interdum libero ut metus. Pellentesque placerat. Nam rutrum augue a leo. Morbi sed elit sit amet ante lobortis sollicitudin. Praesent blandit blandit mauris. Praesent lectus tellus, aliquet aliquam, luctus a, egestas a, turpis. Mauris lacinia lorem sit amet ipsum. Nunc quis urna dictum turpis accumsan semper.

Chapter 3

Profiling Contur

An important part of the task of optimising contur is to first perform a profile of the code. This section will outline the steps taken to produce a profile of contur and how the results were used. We will start by introducing cProfile, which is the Python profiler which was used to carry out the profile. Then we will discuss Snakeviz and gprof2dot, these are the two tools which we used to visualize the profiling results produced by cProfile. Finally we will conclude the section by performing an initial profile of the contur package before any code optimization was attempted. This initial profile will serve as our benchmark to measure the effectiveness of our later attempts to improve the run time performance of contur.

3.1 Profiling with cProfile

3.1.1 Why cProfile?

Let us first begin by considering some of the features we ideally require from our chosen profiler. At a minimum a profiler must obviously be able to time how long it takes our code to run. This basic requirement is essential to be able to determine if our attempted improvements to the code do in fact actually improve run performance. In addition to just providing the total run time of contur we will also require our profiler to provide a split of the runtime among the functions/sub-functions which compose contur. A split of the run time like this will highlight parts of the code that consume disproportionately large amounts of CPU or are repetitively called, suggesting optimisation improvements can be made.

cProfile is a module within the Python standard library which meets these requirements. Our main motivations for using cProfile are as follows:

- Provides a full profile of program with output include total run time, time taken at each individual step, and number of calls to individual functions;
- Easy to save the output of the profile in prof files which can then be read by tools built to visualize profiling results;
- Performing the profile with cProfile is quick and easy and requires minimal new code;

3.1.2 Using cProfile

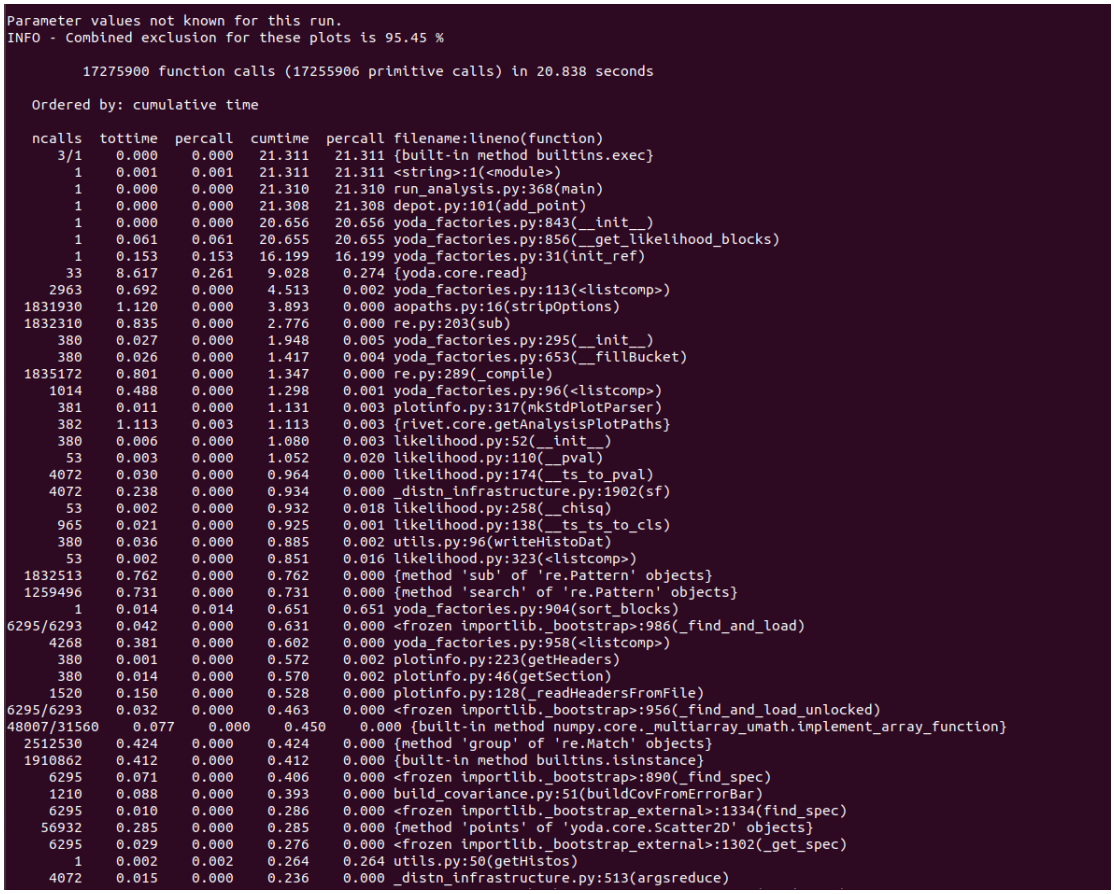
The last version of contur which exists in the main contur repository before any optimisation changes were attempted can be found at commit 49a67e03. In this section we will walk through the steps required to profile this version of contur running on a single yoda file. The steps required to perform the profile on a contur grid run are the same, so the in the next section we will just provide the results for a grid run of this version of contur.

The simplest way of performing a profile with cProfile is via cProfile's run method. To profile contur using the run method we just pass contur's main function to the run method. We can make this adjustment to contur's code by updating the main run script here as follows

```
import cProfile


if __name__ == "__main__":
        cls_args = get_args(sys.argv[1:],'analysis')
        cProfile.run("main(cl_args)", sort=cumtime) #perform profile
```

After updating the run script as above we can now run contur as normal to get the below terminal output from the profile



```
Parameter values not known for this run.
INFO - Combined exclusion for these plots is 95.45 %

         17275900 function calls (17255906 primitive calls) in 20.838 seconds

   Ordered by: cumulative time

   ncalls  tottime  percall  cumtime  percall filename:lineno(function)
      3/1    0.000    0.000   21.311   21.311 {built-in method builtins.exec}
        1    0.001    0.001   21.311   21.311 <string>:1(<module>)
        1    0.000    0.000   21.310   21.310 run_analysis.py:368(main)
        1    0.000    0.000   21.308   21.308 depot.py:101(add_point)
        1    0.000    0.000   20.656   20.656 yoda_factories.py:843(__init__)
        1    0.061    0.061   20.655   20.655 yoda_factories.py:856(__get_likelihood_blocks)
        1    0.153    0.153   16.199   16.199 yoda_factories.py:31(init_ref)
       33    8.617    0.261    9.028    0.274 {yoda.core.read}
     2963    0.692    0.000    4.513    0.002 yoda_factories.py:113(<listcomp>)
  1831930    1.120    0.000    3.893    0.000 aopaths.py:16(stripOptions)
  1832310    0.835    0.000    2.776    0.000 re.py:203(sub)
      380    0.027    0.000    1.948    0.005 yoda_factories.py:295(__init__)
      380    0.026    0.000    1.417    0.004 yoda_factories.py:653(__fillBucket)
  1835172    0.801    0.000    1.347    0.000 re.py:289(_compile)
     1014    0.488    0.000    1.298    0.001 yoda_factories.py:96(<listcomp>)
      381    0.011    0.000    1.131    0.003 plotinfo.py:317(mkStdPlotParser)
      382    1.113    0.003    1.113    0.003 {rivet.core.getAnalysisPlotPaths}
      380    0.006    0.000    1.080    0.003 likelihood.py:52(__init__)
       53    0.003    0.000    1.052    0.020 likelihood.py:110(__pval)
     4072    0.030    0.000    0.964    0.000 likelihood.py:174(__ts_to_pval)
     4072    0.238    0.000    0.934    0.000 _distn_infrastructure.py:1902(sf)
       53    0.002    0.000    0.932    0.018 likelihood.py:258(__chisq)
      965    0.021    0.000    0.925    0.001 likelihood.py:138(__ts_ts_to_cls)
      380    0.036    0.000    0.885    0.002 utils.py:96(writeHistoDat)
       53    0.002    0.000    0.851    0.016 likelihood.py:323(<listcomp>)
  1832513    0.762    0.000    0.762    0.000 {method 'sub' of 're.Pattern' objects}
  1259496    0.731    0.000    0.731    0.000 {method 'search' of 're.Pattern' objects}
        1    0.014    0.014    0.651    0.651 yoda_factories.py:904(sort_blocks)
6295/6293    0.042    0.000    0.631    0.000 <frozen importlib._bootstrap>:986(_find_and_load)
     4268    0.381    0.000    0.602    0.000 yoda_factories.py:958(<listcomp>)
      380    0.001    0.000    0.572    0.002 plotinfo.py:223(getHeaders)
      380    0.014    0.000    0.570    0.002 plotinfo.py:46(getSection)
     1520    0.150    0.000    0.528    0.000 plotinfo.py:128(_readHeadersFromFile)
6295/6293    0.032    0.000    0.463    0.000 <frozen importlib._bootstrap>:956(_find_and_load_unlocked)
48007/31560    0.077    0.000    0.450    0.000 {built-in method numpy.core._multiarray_umath.implement_array_function}
  2512530    0.424    0.000    0.424    0.000 {method 'group' of 're.Match' objects}
  1910862    0.412    0.000    0.412    0.000 {built-in method builtins.isinstance}
     6295    0.071    0.000    0.406    0.000 <frozen importlib._bootstrap>:890(_find_spec)
     1210    0.088    0.000    0.393    0.000 build_covariance.py:51(buildCovFromErrorBar)
     6295    0.010    0.000    0.286    0.000 <frozen importlib._bootstrap_external>:1334(find_spec)
    56932    0.285    0.000    0.285    0.000 {method 'points' of 'yoda.core.Scatter2D' objects}
     6295    0.029    0.000    0.276    0.000 <frozen importlib._bootstrap_external>:1302(_get_spec)
        1    0.002    0.002    0.264    0.264 utils.py:50(getHistos)
     4072    0.015    0.000    0.236    0.000 _distn_infrastructure.py:513(argsreduce)
```

Figure 3.1: Output of cProfile run method

From figure 3.1 above we can summarise the main output from the single yoda file contur run:

- From line one of the profiling results we can see that the run had c.a. 17 million function calls and took c.a. 20 seconds to run;
- The next line tells us that we are ordering the profiling results by cumulative time (cumtime column). The cumulative time for a function is the time spent to run a function and all other functions called within the function (so the cumtime for the main function will be the total run time of the program as all other functions are called within main);
- From line three on we have the profiling information for the functions and sub-functions which compose the contur run. The main columns which stand out here are 'ncalls' which gives the number of calls made to the function,

'tottime' which gives the total time spent in the function excluding calls to sub functions and finally 'cumtime' which as already explained gives the run time for each function including all the calls to sub functions.;

The above profiling is already useful, it gives us things like the run time and the break down of the run time between the components of contur. However the printed results in the current form are not very readable, a detailed knowledge of the functions that compose contur would be needed to take any advantage of the run time broken down by components in its current form. Additionally we don't just want to print result to the terminal and work from there, we would preferable save the profiling results to some file format so our results are reusable across time.

To meet both these objectives for the profiling we from here on we will print the data from our profile into '.prof' files which can then be read by tools which help visualise the profiling results. We do this by introducing the Profile class of cProfile and using this to perform our profiles from here on in as opposed to using the run method, the updated code to perform the profiling with the Profile class is given below.

```
import cProfile, pstats, io

if __name__ == "__main__":
        cls_args = get_args(sys.argv[1:],'analysis')

        pr = cProfile.Profile()
        pr.enable()

        main(cl_args)

        pr.disable()
        pr.dump_stats('outfile.prof'')
```

3.2 Visualizing Profiling Results

To visualise our profiling results we will use two open source tools Snakeviz and gprof2dot. As what follows will show, we can use both of these tools in a complementary way, as opposed to a simple choose of one or the other, to help make best of use of the profiling data we produce with cProfile.

3.2.1 Snakeviz

Snakeviz is a browser based graphical viewer for the output of Python's cProfile profiler module. Snakeviz can easily be pip installed with the following terminal command

```
$ pip install snakeviz
```

once installed we can invoke snakeviz to visualise an arbitrary .prof file as follows

```
$ snakeviz profile_file.prof
```

After invoking snakeviz as outlined above the web browser interface for the tool will open and the user can explore the profiling results. Snakeviz allows user interaction to adjust how results are rendered, the two main plotting options available in Snakeviz are icicle plots and sunburst plots. From here on we will use Snakeviz's icicle plot to explore profiling results, additionally due to the constraints of the static form this document is written in we will just examine static snapshots of the overall display in Snakeviz's viewer. These static snapshots of the Snakeviz viewer are sufficient to summarise profiling results, using Snakeviz's viewers ability to adjust rendering though can be useful to get a feel and understanding for new profiling results, the interested reader is recommended to play around with Snakeviz's viewer functionality further.

Below in figure 3.2 we show a snapshot of an icicle plot from a profile of our initial starting contur code on a single yoda file. From the figure we can seen that the icicle plot is showing the same information as figure 3.1 in just a more visually appealing way, with the addition that in the icicle plot we can see the ordering of the calls to the components of code that compose a contur run. This ordering is very

useful additional information, for example from the ordering it jumps out at us that the call to yoda.core to read the yoda passed to contur takes a large proportion of the run time for a single contur run. From this we can already understand that a lot of the run time for a single contur run comes from just reading in data.

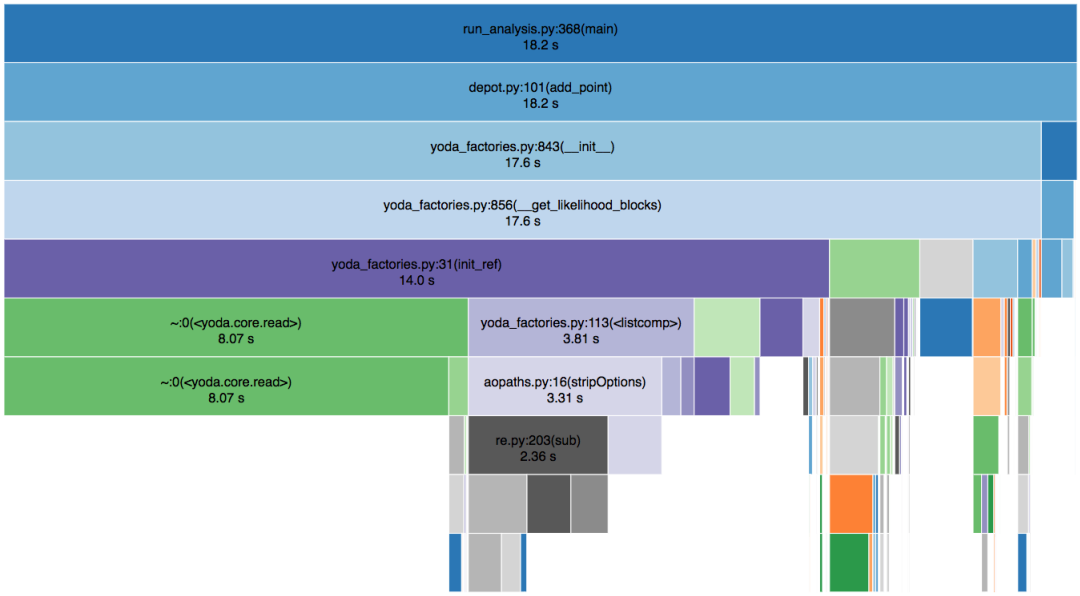


Figure 3.2: Contur single yoda run starting point - Example snakeviz icicle plot

3.2.2 gprof2dot

gprof2dot is a python script that converts the output of the cProfile to dot plots. These dot plots can be used to complement the information we get from the icicle plots. The icicle plots and the user interface offered by snakeviz offer a means to see the absolute run of our code and how this absolute run time breaks down among the components of the program. The dot plot complement complements this information by providing a rendering which makes the flow of the code (i.e. the progression of the code from the call to main through the components that compose the program) more easily visible and additionally showing the relative weight run time wise of the components of the code. This visualisation can be useful to both quickly spot bottlenecks in the code and also just to get a better understand of how a large code base works.

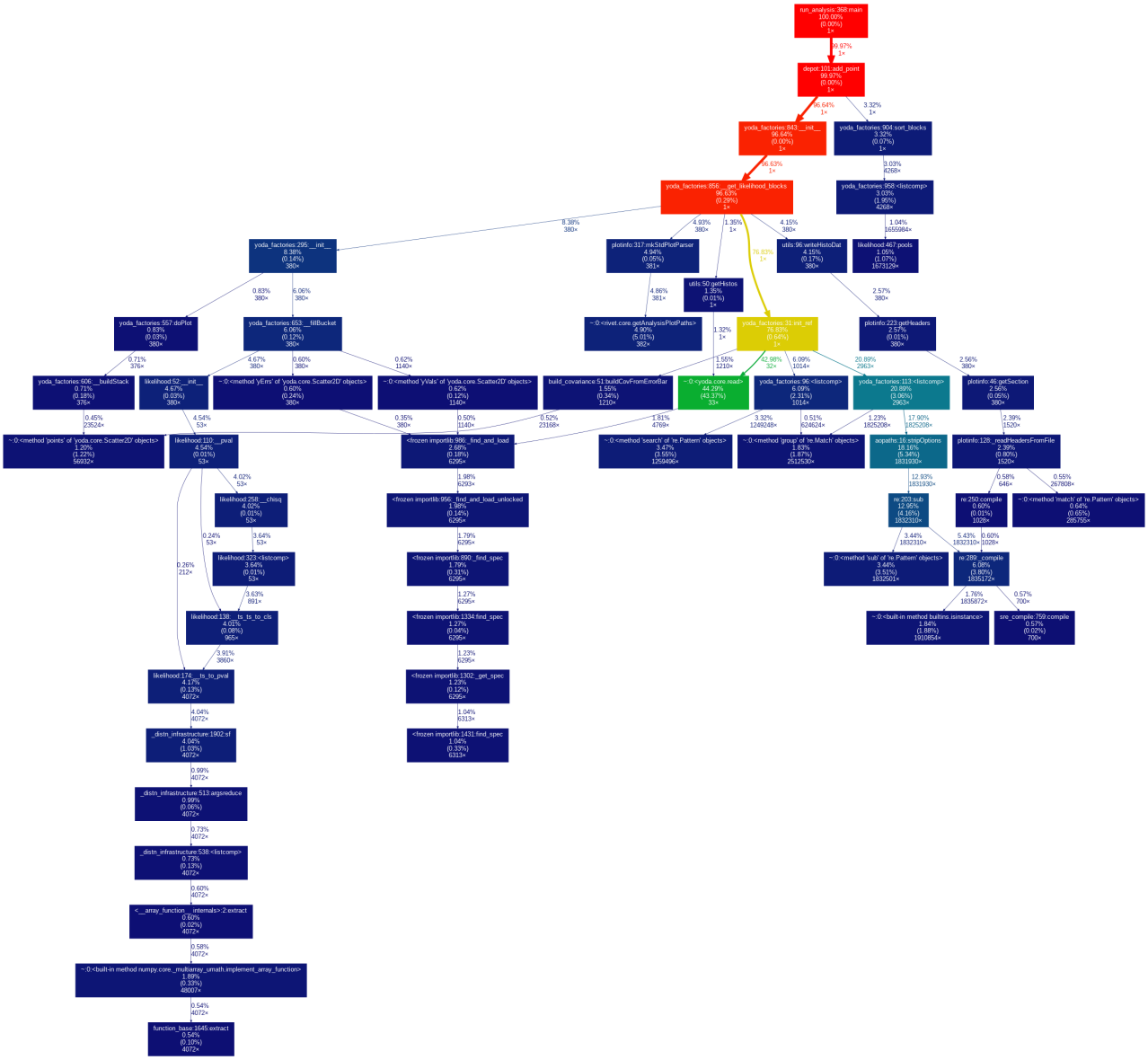


Figure 3.3: Contur single yoda run starting point - Example gprof2dot

We can see example of the dot plots produced by gprof2dot in figure 3.3 above. This plot is visualising the same single yoda contur run as in figure 3.2, so is a good way of demonstrating the complementary nature of the icicle plot and the dot plots for visualising our profiling results. Following the coloring scheme in the dot plot (red to yellow to green) the observation we previously made using the icicle plot about the weight of data reading in the run time can be seen in the dot plot where we can see c.a. 42% of run time is spent reading yoda files.

3.3 Initial Profile Results

In the previous section while introducing the visualisation tools we gave the initial profiling results resulting from running contur on a single yoda file (see figure 3.2 and 3.3) before any optimisation of the code was attempted. As previously discussed, in practical settings contur is generally run on a grid of yoda files as opposed to a single yoda file, so along with our initial single yoda run profile we will also perform an initial profile of contur on a test grid. The grid we use to perform this profile is a 10×10 grid, so composed of 100 yoda files in total, we will use this reference grid through out to profile contur's grid run.

In figure 3.4 below we see the icicle plot for the grid run, from this we can see that for the grid of 100 yoda files we have a run time of around 1100 seconds or close to 20 minutes.

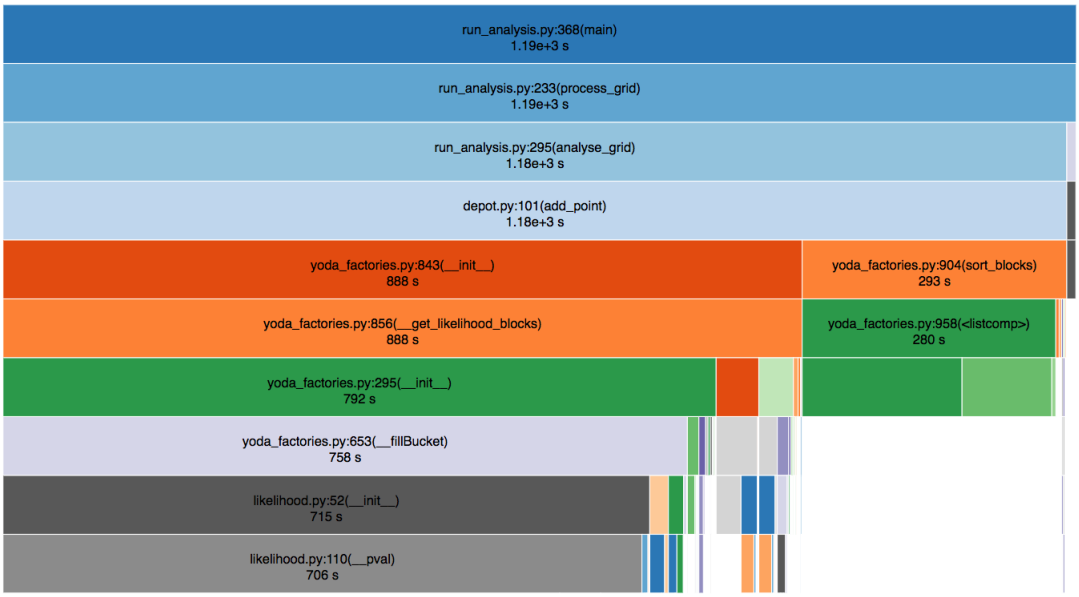


Figure 3.4: Contur grid run - icicle plot

We can also see from the plot that the main contribution to the run time seems to be coming from two blocks of the code. This is best seen in the dot plot figure 3.5 below where we can see that the sort blocks method contributes c.a. 25% of the run and the ts to pval method which contributes c.a. 49%, so both of these methods in combination are close to three quarters of the run time for the contur grid run.

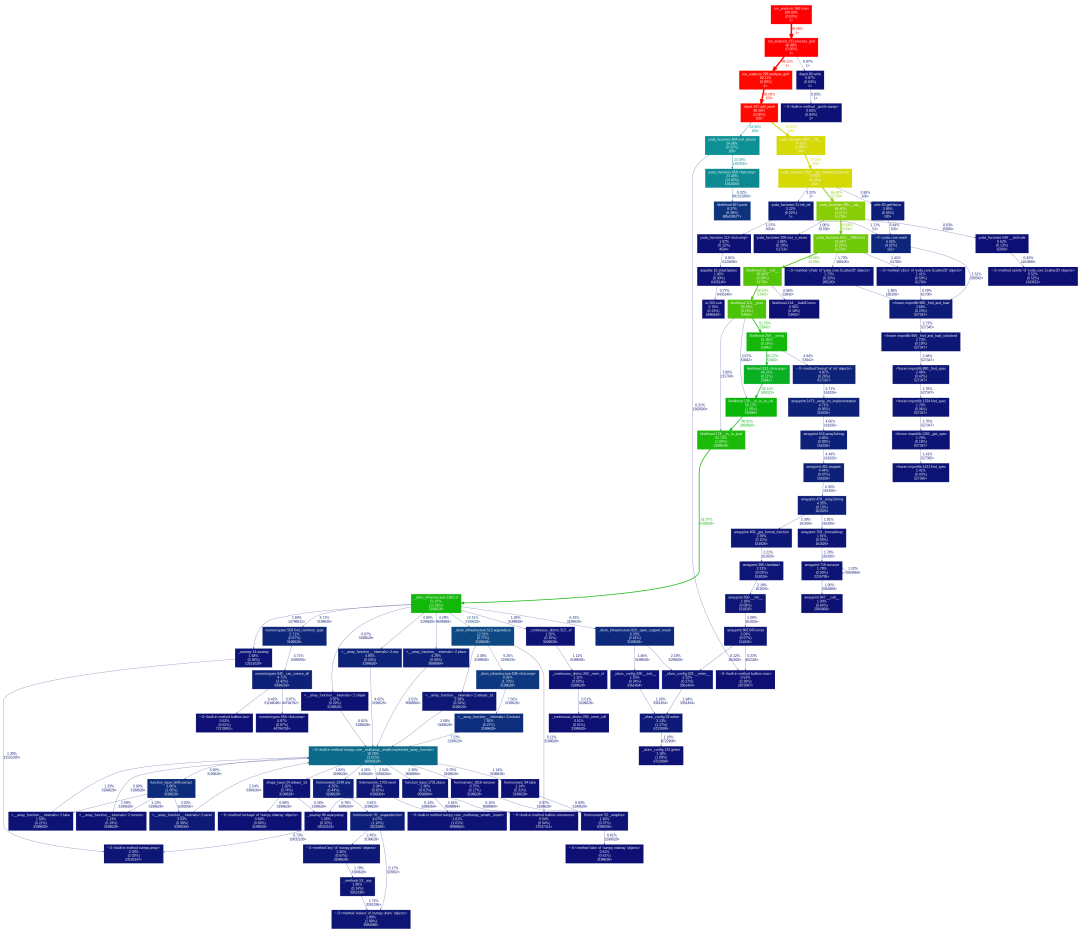


Figure 3.5: Contur grid run - dot plot

Chapter 4

Testing Contur

Before attempting to update contur code to improve it's run time performance we need to give some consideration into how we can ensure that we don't break some of contur's existing functionality via our changes. Our changes for optimisation should complete the same tasks as the code we are updating and return the same outputs. In this chapter we will outline how we attempt to ensure the optimisation changes don't break existing contur functionality via improving existing testing within contur.

4.1 Contur Existing Tests

Prior to work carried out in this thesis contur had a limited set of tests implemented within python's pytest framework. In the contur repository these tests can be found in the test folder. Within the tests folder there are two separate scripts to run tests, `test_batch_submit.py` and `test_executables.py`. These tests effectively test that functionality within contur runs without error, however the tests don't have any visibility on the output of the contur run (except if the run throws an error before completion) or perform any form of unit testing. The main one of these scripts of relevance for the additional tests we will add in subsequent sections is `test_executables.py` which checks that contur runs on a single yoda file and on grid runs without errors. To carry out these tests pytest does a single yoda and grid contur run[1]. These runs are of relevance to us because we can use their outputs to create regression tests as we will outline in the next section.

[1]The tests folder contains a single yoda file and a 4×4 grid for the grid run

4.2 Regression Testing

The simplest test we can put in place to try and mitigate the risk that changes to code don't break contur in some way is to try and ensure that these changes don't alter the final output of the contur run. This can be achieved by introducing regression testing into contur's suite of tests. Regression tests will consist of comparing the output of our contur run with the updated code (labeled the target) against the output of contur before we made the change (labeled the base). The regression test is passed if our target output is equal to base output[2].

Implementing these regression tests within the pytest framework will allow us to carry out these comparison of new results against old results automatically just by running pytest. Thus the regression tests we implement in contur will be of wider use to other contur developers to help ensure updates to contur code do not unintentionally alter the output of contur. Before outlining in greater detail how went about implementing the regression tests it is useful to first give greater clarity on the file format of the results output by contur.

4.2.1 Contur Run Output Format

Single yoda file contur runs and grid runs output their results in their formats. A single yoda file contur run outputs a text file with the results printed on the text file. A example of such an output is shown in figure 4.1 below. For regression testing purposes we can simple compare that base and target text files are the same excluding the first three lines of the text file which give the location where contur is running to produce the text file[3]

[2]The target output in this case can be said to regress to base, hence the name regression testing.

[3]This can be seen 4.1, if we included these first three lines in our comparison then the single yoda file regression test would always fail whenever contur is run from a different location which is not something we want to happen.

```
Run Information
Contur is running in /Users/jonbutterworth/gitstuff/contur-dev/tests
on analysis objects in ['sources/testPoint.yoda']
Using search analyses
Excluding Higgs to WW measurements
Excluding secret b-veto measurements
Excluding ATLAS WZ SM measurement
Building all available data correlations, combining bins where possible
Building default background model from data, ignoring (optional) SM theory predictions

Sampled at:
CZdL1x1: 1.062202380952381
CZdL3x3: -1.062202380952381
CZuL1x1: 1.062202380952381
CZuL3x3: -1.062202380952381
CZuR1x1: 1.062202380952381
CZuR3x3: -1.062202380952381
cotH: 4.5
mZp: 3578.9473684210525
Combined exclusion for these plots is 100.00 %

pools
ATLAS_13_METJET
0.39844652
/ATLAS_2016_I1458270/d05-x01-y01
ATLAS_13_EEJET
0.03740851
/ATLAS_2019_I1718132/d59-x01-y01
ATLAS_13_MMJET
0.08701654
```

Figure 4.1: Example output from single yoda file contur run - txt file

The grid run returns a .map file which contains a pickled .....

4.2.2 Implementing Regression Tests

4.2.3 Including Theory Runs

4.3 Unit Testing

4.3.1 Likelihood Class

4.3.2 YodaFactories Class

4.3.3 Functions

Chapter 5

Optimising Contur

5.1 Single Yoda Run

5.2 Grid Run

For research purposes, contur users will in general be spending most of their time running contur on a grid as opposed to single yoda files. So focusing our optimisation efforts on the grid run is likely to produce more practical benefits for users. In addition we have two other motivations for focusing our efforts on optimising the grid run:

- There is more scope for achieving meaningful improvements in run time with the grid run. This viewpoint comes from observing from figure 3.2 that the single yoda run time only takes around 20 seconds, while from figure 3.4 we can see that the run time for smallish grid[1] takes up to 20 minutes. Thus decreasing runtime for the single yoda by 50% will only save us 10 seconds in absolute terms, while the equivalent decrease for the grid run would save us 10 minutes[2];

- There is more scope for the grid run runtime to increase with changing research needs. The runtime for the grid run is highly dependent on the size of the grid

[1] The grid we are profiling contur on is 10×10, so contains 100 yoda files, for research purposes it is common to run such a 10×10 grid across three different energy buckets (7,10 and 13 TeV), which each bucket having 100 yoda files for a total of 300 yoda files. So the 20 minutes we profiled for a single 10×10 would likely be close to an hour if run across the three energy buckets

[2] Or 30 minutes for the case where the grid has three energy buckets and 300 yoda files.

used, as the grid grows in size so will the runtime. There is a practical limit how big a grid can be for contur resulting from this increasing runtime, in effect once a grid is so large it is too slow to run contur on it. Optimisation to the grid run that not only improve runtime on the current standard size grids but also reduce the speed that runtime increases with increasing runtime could have very practical benefits like making contur runs feasible on large grids where previously the run time was too slow;

For the above reasons the main focus of the optimisation from here on in will be on the grid run. From the dot plot in figure 3.5 arising from the data produced from our initial grid profile we can see that grid runtime arises from two branches in the code flow, the first arising from the sort blocks method[3], which takes c.a. 25% of runtime and the second being the likelihood calculation[4] which takes most of the remainder of the runtime. Our initial efforts will focus on making optimisation improvements for these two parts for the program.

5.2.1 Sort Blocks

5.2.1.1 Background

Before discussing the sort blocks method in detail it is first necessary to give some background into the flow of a contur grid run and where the sort blocks method sits within that flow. A grid run in contur is effectively just a group of single yoda runs performed within a loop with some slight differences[5][6]. So we can focus in on the operations contur performs on each yoda file it is passed in the grid.

The yoda factories class in contur coordinates the run on each yoda file. When passed a yoda file yoda factories collects the data in the yoda file[7] and the background

[3] See dark green box in dot plot

[4] sequence of boxes in the dot plot starting as yellow and morphing to green

[5] The most notable difference being in a single yoda contur run a large part of run time is spent reading in yoda files from Rivet with the background data. In the grid run this data reading is done for the first yoda file in the grid, but it is not necessary to repeat it for each new yoda file in the grid because the data read in for the first yoda file can be reused.

[6] The Depot class handles coordinating the contur run across the grid, the add point method in the Depot class used to run contur on individual yoda files in the grid

[7] The yoda file passed to yoda factories contains the signal events for the beyond standard model we are using contur to test

experimental data needed to test against is also collected from Rivet[8]. The yoda file is composed of analysis objects, each analysis object is a histogram (is this correct? namely what I see as analysis object in the code is just another name for histogram) for which a confidence level can be calculated. The yoda factories class loops through these analysis objects, for each analysis object an instance of contur's likelihood class is created, the likelihood class compute the confidence level for the analysis object and stores it as its CLS attribute. The yoda factory performs this whole loop upon instantiation[9] and stores a list of likelihood object[10] in its likelihood block attribute.

Yoda factories's sort blocks method is called after instantiation of a yoda factories object, so after all of the above calculations are carried out. Each likelihood object in yoda factories has collected has a pools attribute which gives the pool to which the analysis object used to create the likelihood object belongs. The sort blocks method simply buckets the likelihood objects by pool[11], and then for each pool it takes the likelihood object with the largest confidence level and discards the rest (Jon - please shout if this understanding is not correct).

5.2.1.2 Changes made

The profiling results in the dot plot in figure 3.2 are precise enough that we can pin point the major slow point in the sort blocks method to be the list comprehension in line 958 of yoda factories[12]. This list comprehension sits within a loop and the whole blocks of code looks as follows

```
for p in pools:
  if not p == omitted_pools:
    for item in like_blocks:
      if item.CLs == max([x.CLs for x in like_blocks if x.pools == p]) \
```

[8] When running with theory option standard model simulated results will also be collected from Rivet

[9] This statement is true for our starting version of contur, as will be shown in 5.2.2, updates we will make for the likelihood optimisation will alter this flow

[10] Each likelihood object in this list will have the confidence level for the analysis object it refers to stored in its CLS attribute

[11] So collects all the likelihood objects with the same pool into a single bucket

[12] This can also be easily picked up in the icicle plot when using Snakeviz's graphical viewer

In the above block of code the list comprehension in the last line is used to find the likelihood block in the pool with the largest confidence. The list comprehension on its own is not what makes the list comprehension is placed within a nested for loop, which loops over pools and then within each pool iterate we have another loop over likelihood blocks. So in each yoda file the number of times we perform this list comprehension is the number of pools multiplied by the number of likelihood objects, and this is only for a single yoda file, across the whole grid we are doing this 100 times. Figure 5.1 below shows that for our 10×10 grid we are calling this list comprehension over a million times. So although each comprehension on its own takes less than .002 seconds this multiplied by a million still gives us a run time of over 200 seconds.

ncalls	tottime	percall	cumtime	percall	filename:lineno(function)
1392600	176.5	0.0001268	280.1	0.0002012	yoda_factories.py:958(<listcomp>)

Figure 5.1: List comprehension in sort blocks - Run time info

The optimisation change adopted here was to move the calculation of the max confidence level for each pool performed by the list comprehension outside of the nested for loop, thus reducing dramatically the number of times the calculation is performed. In its place we now only perform the calculation once per yoda file[13] and store the results in a dictionary whose key is the pool and value is the max confidence level for the pool. This dictionary is then used in place of the list comprehension in the above for loop. So within the nested for loop we have replaced a call to a list comprehension with a run time per call of 10^{-4} with a dictionary with a runtime per call[14] of 10^{-7}, so the 10^6 calls made in the loop will take 10^2 seconds with our old implementation but only 10^{-1} seconds with the new implementation.

5.2.1.3 Impact of changes

Below we see the impact of the optimisation on the run time for the sort blocks method. In figure 5.2 we can see that prior to optimisation the run time of the list

[13] So in our 10×10 grid we go from perform the calculation over 1 million times to exactly 100 times, once for each yoda file in the grid

[14] See https://towardsdatascience.com/faster-lookups-in-python-1d7503e9cd38

comprehension is in line with our expectations from the previous section with a run time of 280 seconds, order 10^2 as expected and total run time[15] for sort blocks is 293 seconds While in figure **??** we see that we have a post optimisation run time of 7 seconds for the whole of the sort blocks method. This run time would support the hypothesis that the run time for calling the dictionary in place of the list comprehension is of order 10^{-1} seconds and additional would suggest that the optimisation change made the calculation of the maximum confidence level for each pool slightly faster too, as prior to optimisation sort blocks had 13 seconds of run time outside of the list comprehension, now after optimisation total run time is just 7 seconds.

Figure 5.2: Sort blocks grid run time - Before optimisation

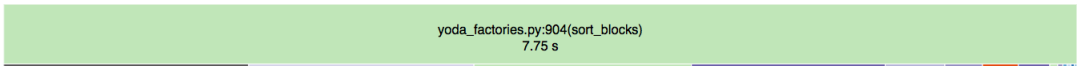


Figure 5.3: Sort blocks grid run time - After optimisation

5.2.2 Likelihood Calculation

5.2.2.1 Background

In the outline of the background for the sort blocks method in section 5.2.1 we touched on when the likelihood class comes into the flow of a contur run, namely how the yoda factory loops through all the analysis objects in the passed yoda file, instantiating a likelihood object for each analysis object which computes a confidence level. We however ignored the details of how these confidence levels are computed. We can see from the icicle plot in figure 3.4 that a material proportion of contur's run time is spent within the likelihood class[16].

[15] Remember the list comprehension is only part of the sort blocks method, not the whole of it so we will have additional run time from other parts of the method

[16] From the icicle plot we can see that out of a run time of around 1100 seconds we spend 715 seconds in the likelihood class calculations

Before outlining the steps taken to reduce the likelihood run time it is worth briefly outlining in greater detail the steps within the likelihood class to compute the confidence level for each analysis object. Upon instantiation the likelihood class computes two chi-square test statistics, a background and target test statistic (greater detail needs to be added here). These test statistics are then converted into p-values by assuming the test statistics are normally distributed and computing their survival function value[17]. We use the sf method of the norm class found in scipy.stats to compute the p-values. Once a background and target p-values are computed they can be combined to calculate the confidence level for the analysis object.

Drilling down into the initial grid run profile results for the likelihood class we can see in figure 5.4 that the ts to pval method is where most of the run time is coming from in the likelihood object. This method computes p-values to test statistic and really just calls scipy.stats.norm.sf under the hood, so from here on we can focus our efforts on the scipy.stats.norm.sf method.

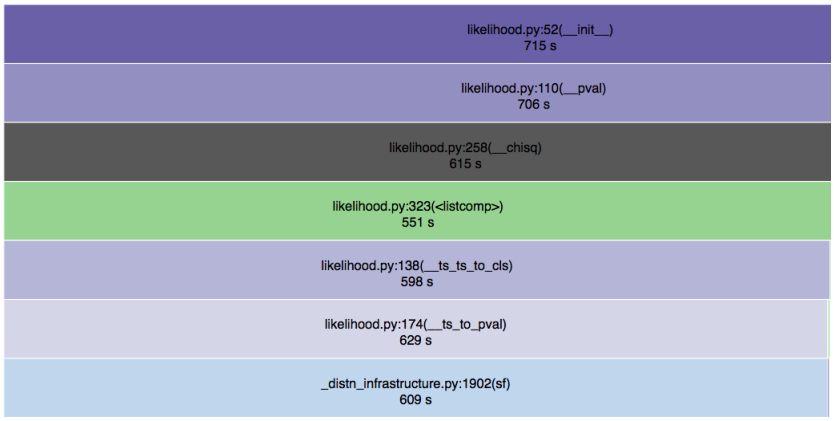


Figure 5.4: Likelihood object - Initial profile

From figure 5.5 below it becomes apparent that the large run time we observe from calling the survival function results from the large number of calls we make to the function. Each call to the survival function takes c.a. 0.0002 seconds, but we make over 3 million calls resulting in a total run of over 600 seconds.

[17]Defined by 1-cdf, so the area of the distribution to the right of the test statistic

ncalls	tottime	percall	cumtime	percall	filename:lineno(function)
3199628	19.69	6.153e-06	628.7	0.0001965	likelihood.py:174(__ts_to_pval)

Figure 5.5: Likelihood object - ts to pval details

5.2.2.2 Scipy Survival Method

From the previous section it should be clear that the survival function and reducing the number of times we call it is key to reducing the run time in the likelihood object. It is thus helpful to first understand better where the calls to the survival function arise when a likelihood class is instantiated. Within a likelihood object we get calls to the scipy survival function via the following routes:

1. Every time the ts to pval method is called we have one call to survival function. Upon instantiation this method is called twice explicitly, giving us two calls to survival function ;

2. The ts ts to cls method calls ts to pval twice internally, so every time this method is called we have two calls to the survival function. The method is called once upon instantiation giving us two more calls to the survival function.;

3. The chisq method which computes the chi square test statistics will only call the survival function when an inverse for the covariance matrix of the analysis object cannot be computed[18]. When the method calls the survival function the number of times it makes the calls is twice the number of buckets in the analysis object. So this is a minimum of 2 calls but potentially much more than 2 ;

From the above we see that each analysis object will have at least 4 calls to the survival function[19], so across a whole yoda file the number of calls to the survival function will be at least 4 multiplied by the number of analysis objects in the yoda

[18] In the code the survival function will only be called when the condition ”self.covBuilt and sb nuisance is not None” is false

[19] In practise it will be a lot more than this becuase of the chisq calls

file[20]. Finally we have 100 yoda files in our grid, which need to be summed across to give the total number of calls we make to the survival function in our grid run.

To reduce the number of calls to the survival function we will adopt two approaches. The first is simple to check if we are making any unnecessary calls to the survival function anywhere that can easily be got rid of, this approach is simple but will not likely give high returns. The second approach is to take greater advantage of numpy's array functionality to see if via collecting test statistics into numpy arrays and passing these arrays of test statistics to the survival function, reducing the overall number of calls[21].

For the second approach to be effective we would require the run time for the survival function if passed a numpy array of length n to be significantly less than the run if we just made n separate calls to the survival function. We would expect this to be the case as the Scipy functions are built to enable fast array based computation on numpy arrays. Figure 5.6 below shows the result of the profile we performed to test the performance of calling the survival function n times within a loop or passing an array of length n once. The x axis gives the value of n on the a log scale while the y axis gives the run time for the loop (orange line) and the array (blue line) on a log scale. So from the plot we can see that our starting profile with n between 10^6-10^7 should give a run time between 10^2-10^3 seconds which is in line with the c.a. 600 seconds we actually observe.

[20]For perspective here, the 10×10 grid we profiled on had c.a. 60,000 likelihood objects created across 100 yoda files suggesting on average each yoda file had 600 valid analysis objects

[21]So for example if we had four test statistics we wanted to pass to the survival function we would collect the test statistics into a single array and pass the array once to the survival function as opposed to four individual calls to the survival function

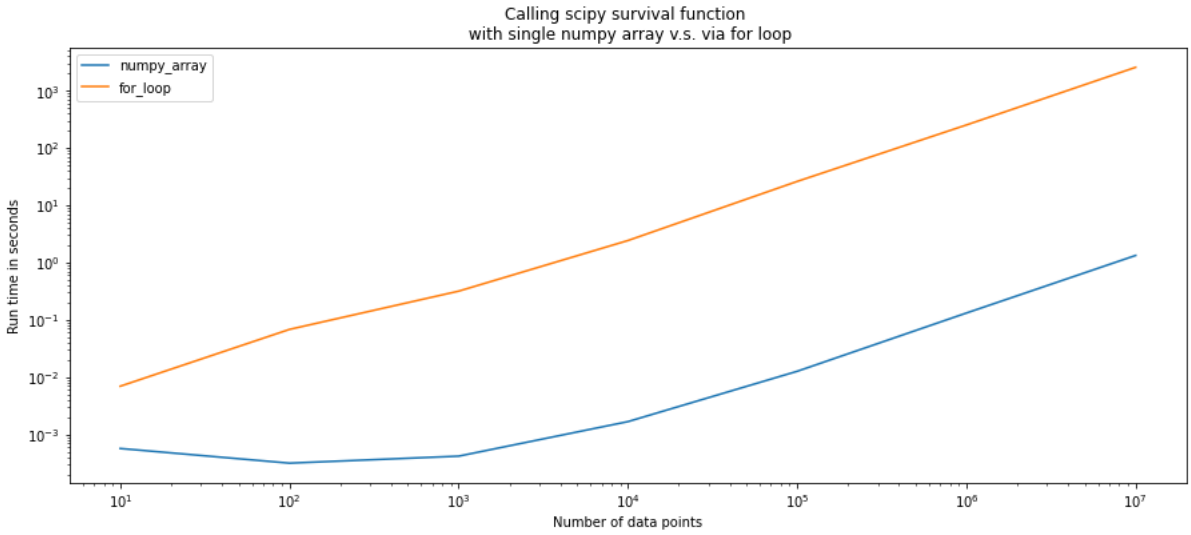


Figure 5.6: Scipy Survival Function - Loop vs Array

5.2.2.3 Changes made

The optimisation changes to the likelihood calculation were made via multiple commits to the contur repository over the space of a couple weeks, they can be grouped into three groups of changes:

1. Within likelihood objects making use of numpy arrays to reduce the number of calls to the survival function;
2. Within likelihood objects reducing unnecessary calls to the survival function;
3. Making use of numpy arrays to reduce the number of calls to the survival function across likelihood objects;

Of the above changes the first two are least disruptive in terms of their impact in overall flow of a contur run as they only make changes within the likelihood class. While the third change is more substantial as it alters the flow of a contur run between yoda factories and the likelihood class.

The first change[22] involves passing a tuple of background and signal test statistics to the ts to pval method and to the ts ts to cls methods, as opposed to passing the test statistics as separate calls. This reduces the calls to the survival function for

[22]The change can be found in commit 0b807895

these values from 4 to 2. In addition within the chisq method we also now pass a tuple of test statics as opposed to making separate calls to the survival function. This ensures that whenever the chisq method makes on a call to the survival function it only makes 1 call, so after all these changes, for analysis object we get at least 2 calls to the survival function and at most 3.

The second change[23] made is motivated from the observation that the ts ts to cls method has a call to ts to pval within it, so it computes the p value within the call. This is unnecessary as we have already computed the p value. The change introduce the pval to cls method which directly takes a p value and computes a confidence level from it. Negating the need to make another call to the survival function, so after this change we now have a minimum of 1 call to the survival function and a maximum of 2 in each analysis object.

From here on in let us simplify and assume that we have exactly 2 calls to the survival function for each analysis object and for each yoda file we have m analysis objects. So in a grid with n yoda files after the above changes we have $2 \times n \times m$ calls to the survival function. So on our 100 yoda file grid assuming $m = 600$ this will still give us 120,000 calls to the survival function. Additionally we can see with an expanding grid size this number of calls will grow, for example with 1,000 yoda files the number of calls to the survival function will be above 1 million again. So the current configuration is not robust against future increases in grid size which may be used by contur. The final set of optimisation changes we will make will resolve this issue by getting rid of the run time dependence on m.

To achieve this, let us first remind ourselves how the the current set up works. Upon instantiation of the yoda factories class we loop through all analysis objects instantiating a likelihood object for each and doing the full likelihood calculation (i.e. computing the confidence level) upon instantiation of the class. So at the end of this process we have a yoda factory object with a likelihood blocks attribute that contains all the likelihood objects. This process can be split into steps that allow us eliminate dependence on the number of analysis objects. This can be done by

[23]The change can be found in commit 15ef923d

instead of using the survival function within the likelihood object, we can instead just collect test statistics in the likelihood object which can then be collected into a numpy array in yoda factories composed of test statistics from all the likelihood objects, this array can then be passed once the survival function.

Implementing this change in practise is spread across two commits[24].

For the first commit we introduce the likelihood blocks ts to cls function, which takes a list of likelihood blocks and computes a confidence level for each likelihood block in the list. In terms of the flow of contur, with this change we alter the likelihood object so it no longer calculates the confidence level upon instantiation, so when we instantiate yoda factories we now have a list of likelihood objects in the likelihood blocks attribute with just test statistics not confidence level, we pass this list to the new function which does the confidence level calculation. After this change we will $n + (n \times m)$ calls to the survival function.

For the second commit we introduce the likelihood blocks find dominant ts function. This function finds the chi square test statistic in an analysis object that gives the largest confidence when the covariance matrix does not have a valid inverse. Thus it moves the calls to the survival function that take place within the chisqr method into a single call in yoda factories. After this change the number of calls to the survival function will be $2n$ so we have removed the dependence on m of the number of calls.

5.2.2.4 Impact of changes

The impact of the optimisation on the run time for the likelihood class and the associated new functions can be seen in figure 5.7 below. From the figure we can see that impact of the optimisation on the run time for the confidence level calculation has been substantial, from a starting run time of c.a. 600 seconds the optimisation has reduced the total run time to just below 20 seconds.

[24]The first commit 299b03a8 introduces the likelihood blocks ts to cls function, while the second commit 2769e1c2 introduces the likelihood blocks find dominant ts function

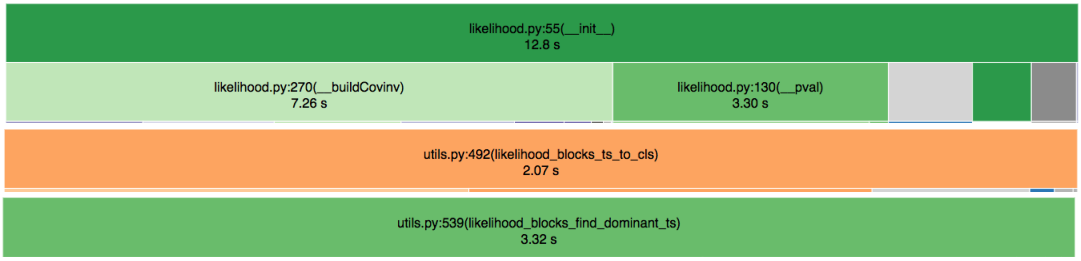


Figure 5.7: Likelihood object and new functions - Profile after optimisation

Chapter 6

General Conclusions

Appendix A

An Appendix About Stuff

(stuff)

Appendix B

Another Appendix About Things

(things)

Appendix C

Colophon

This is a description of the tools you used to make your thesis. It helps people make future documents, reminds you, and looks good.

(example) This document was set in the Times Roman typeface using LaTeX and BibTeX, composed with a text editor.

Bibliography

[1] Anne Author. Example Journal Paper Title. *Journal of Classic Examples*, 1(1):e1001745+, January 1970.