First Year Report

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April 29, 2011

Abstract

Contents

1 Introduction

This PhD project is focused on the development of analysis techniques to be used in the extraction of polarisation observables in the N* program at CLAS. Within the last 7 months, much time has been spent on getting accustomed to various aspects of the physics research environment. Several new topics were explored; primarily Bayesian analysis (specifically Nested Sampling), object-oriented programming and baryon spectroscopy.

A toy nested sampling program in C was provided and explored in order to become familiar with the algorithm. The source code was then used to create a similar object-oriented program. This provided an opportunity to not only introduce the concept of object orientation (specifically C++), but also to check the functional capabilities against those of the original C program. Once the object-oriented program provided acceptable results, it was generalised in order to be applied to a variety of problems.

The generalised program was then used to extract simplified spin observables from simulated data. This provided the opportunity to fine-tune the program and find any problems with the program. At this point, it was discovered that the program had an exceedingly long run-time when a high number of iterations were used, despite optimisation efforts. The possibility of applying some of the programming techniques used in graphics processing units (GPUs) will be considered as a potential solution to the long run-time.

In addition to becoming accustomed to the computational skills, there has been some introduction to Jefferson Lab and the CLAS Collaboration. A collaboration meeting in Paris was attended and a probationary membership to the collaboration has been approved. Several training courses and exercises were done in preparation for shiftwork at Jefferson Lab's Experimental Hall B, including General Safety, Radiation Worker Safety and Oxygen Deficiency Hazard training.

2 Background

2.1 Baryon Spectroscopy and Spin Observables

In order to become accustomed with the correlations and behaviour of spin observables, a small standalone program was created. The aim of this macro was to generate dummy variables used to calculate the sixteen spin observables and output plots showing correlations between various observables.

Eight values were randomly generated from a Gaussian distribution over the surface of an 8-sphere. These values were then combined to create four normalised complex amplitudes, a_1 to a_4. Dummy values for these sixteen observables were calculated based on the expressions given in Table 1 below:

Table 1: Spin Observables in terms of Complex Amplitudes[4]

Observable	Type	Amplitude Combination
B	Single	$\|a_1\|^2 + \|a_2\|^2 - \|a_3\|^2 - \|a_4\|^2$
R		$\|a_1\|^2 - \|a_2\|^2 + \|a_3\|^2 - \|a_4\|^2$
T		$\|a_1\|^2 - \|a_2\|^2 - \|a_3\|^2 + \|a_4\|^2$
E	Beam-target	$2\Re(a_1 a_3^* + a_2 a_4^*)$
F		$2\Im(a_1 a_3^* - a_2 a_4^*)$
G		$2\Im(a_1 a_3^* + a_2 a_4^*)$
H		$-2\Re(a_1 a_3^* - a_2 a_4^*)$
C_x	Beam-recoil	$-2\Im(a_1 a_4^* - a_2 a_3^*)$
C_z		$2\Re(a_1 a_4^* + a_2 a_3^*)$
O_x		$2\Re(a_1 a_4^* - a_2 a_3^*)$
O_z		$2\Im(a_1 a_4^* + a_2 a_3^*)$
T_x	Target-recoil	$2\Re(a_1 a_2^* - a_3 a_4^*)$
T_z		$2\Im(a_1 a_2^* - a_3 a_4^*)$
L_x		$-2\Im(a_1 a_2^* + a_3 a_4^*)$
L_z		$2\Re(a_1 a_2^* + a_3 a_4^*)$

Histograms were generated such that each observable was plotted against each other observable in order to determine any correlations between them.

Plots showing circular patterns indicated that the two observables present in the histogram had a spherical correlation. These have been documented in papers such as [4]. A significant number of plots showed rectangular patterns. Pairs of observables that formed such a pattern were listed in order to find sets of three observables in which every possible pair constituted a rectangularly distributed histogram. Thirteen such triples were found, and when plotted in three dimensions, formed a tetrahedron.

The equations defining the thirteen tetrahedra are shown below.

The significance of these thirteen triples is still being explored.

2.2 CLAS at Jefferson Lab

The CEBAF Large Acceptance Spectrometer (CLAS) Collaboration is based in Hall B of Jefferson Lab.

2.3 Nested Sampling

Nested sampling is a modern model comparison technique based on the principles of Bayesian statistics. Most conventional analysis tools rely on the more widely known

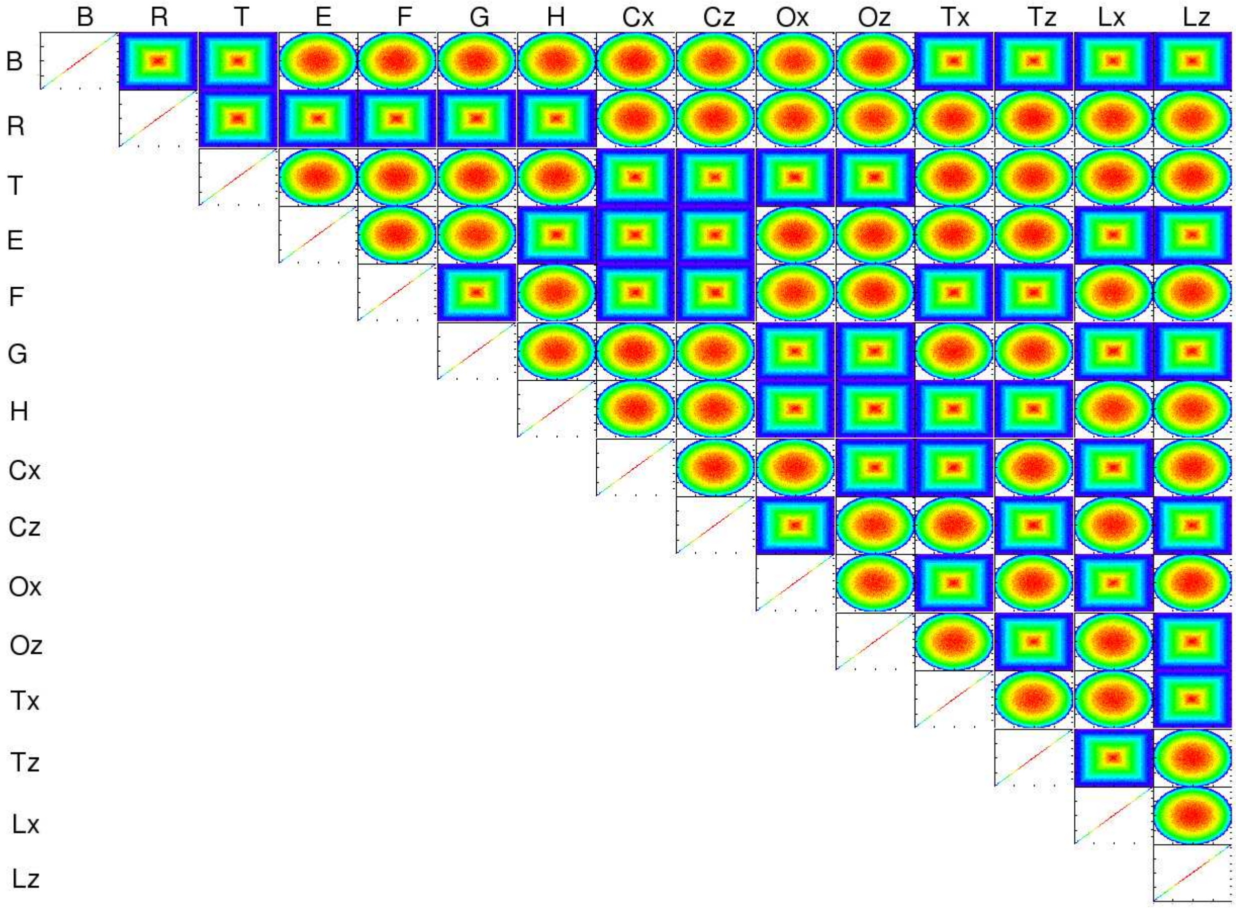


Figure 1: Observables were plotted against each other to show relationships between sets of observables.

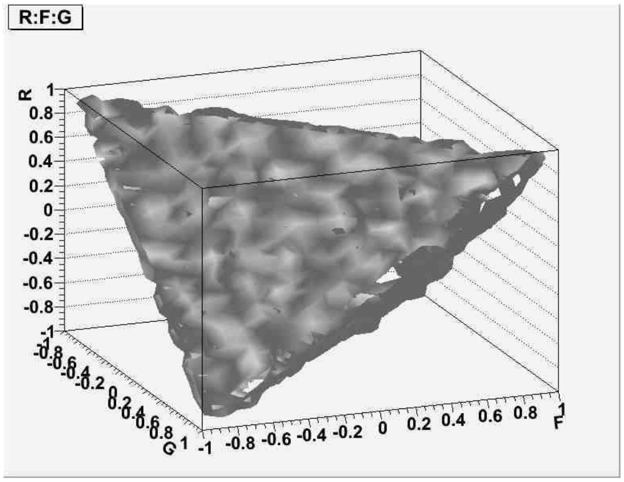
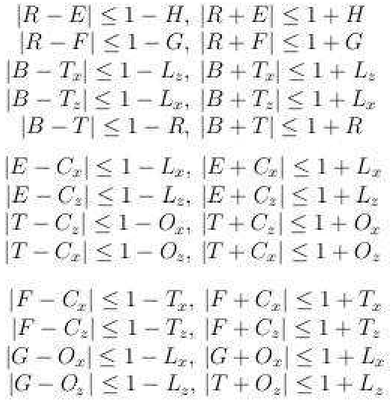


Figure 2: Tetrahedron resulting from plotting R, F and G in three dimensions.

frequentist approach. In this approach, data is collected, and values such as the mean and standard deviation are extracted. Any inferences are then based on the



$$
\begin{gathered}
|R-E| \leq 1-H,\ |R+E| \leq 1+H \\
|R-F| \leq 1-G,\ |R+F| \leq 1+G \\
|B-T_x| \leq 1-L_z,\ |B+T_x| \leq 1+L_z \\
|B-T_z| \leq 1-L_x,\ |B+T_z| \leq 1+L_x \\
|B-T| \leq 1-R,\ |B+T| \leq 1+R
\end{gathered}
$$

$$
\begin{gathered}
|E-C_x| \leq 1-L_x,\ |E+C_x| \leq 1+L_x \\
|E-C_z| \leq 1-L_z,\ |E+C_z| \leq 1+L_z \\
|T-C_z| \leq 1-O_x,\ |T+C_z| \leq 1+O_x \\
|T-C_x| \leq 1-O_z,\ |T+C_x| \leq 1+O_z
\end{gathered}
$$

$$
\begin{gathered}
|F-C_x| \leq 1-T_x,\ |F+C_x| \leq 1+T_x \\
|F-C_z| \leq 1-T_z,\ |F+C_z| \leq 1+T_z \\
|G-O_x| \leq 1-L_x,\ |G+O_x| \leq 1+L_x \\
|G-O_z| \leq 1-L_z,\ |T+O_z| \leq 1+L_z
\end{gathered}
$$

Figure 3: The thirteen tetrahedral correlations correspond to the following triples: $REH, RFG, BT_xL_z, BT_zL_x, BTR, EC_xL_x, EC_zL_z, TC_zO_x, TC_xO_z, FC_xT_x, FC_zT_z, GO_xL_x$ and GO_zL_z.

distribution of these statistics. As such, the results are only based on a probability, and are not themselves probability statements. The frequentist approach does not involve any knowledge or expectation of the results, and this is the key difference between frequentist and Bayesian statistics. [3]
Bayesian statistics involves making an estimation of the results prior to any calculations. This 'guess' is used to form a distribution with a easily determined mean and variance, known as the 'Prior'. Bayes' Theorem (Eqn 1) is then used to combine the prior distribution with the data and produce a posterior distribution, the statistics of which determine the resulting mean, variance, etc. [2]

$$prob(X|Y,I) = \frac{prob(Y|X,I) \times prob(X|I)}{prob(Y|I)} \tag{1}$$

where I denotes any background information, X and Y are propositions, and $prob(X|Y,I)$ denotes the probability of X given Y and I.

The idea of Bayesian statistics can be expressed in the form of a simple equation [1]:

$$Prior \times Likelihood \longrightarrow Evidence \times Posterior \tag{2}$$

where

$$Prior = \pi(\theta)d\theta \tag{3}$$

$$Likelihood = L(\theta) \tag{4}$$

$$Evidence = Z = \int LdX \tag{5}$$

$$Posterior = p(\theta)d\theta \tag{6}$$

and

$$dX = \pi(\theta)d\theta \tag{7}$$

The prior is a distribution, or set of points that act as an initial starting point, an estimation or expectation of the results. Each point has an associated likelihood determined by a likelihood function. This is usually dependent on the applicable data. If, for example, in an effort to determine the x-coordinate of an object, the prior would consist of a set of possible x-coordinates. The likelihood associated with each point describes how likely that point is the x-coordinate of the object.

The output of a Bayesian calculation contains two pieces. The evidence, Z, is useful in comparing model assumptions. Bayes factors, or ratios of evidence, are used to compare any two models at any time without the need to recalculate anything [1]. The posterior is the distribution of points that result from the calculation. These posterior points are determined primarily by the prior and likelihood.

Nested sampling is unique in that it extracts both parts of the Bayesian output. For a specific problem, a prior is determined, as well as a problem-specific likelihood function. Each point in the prior is assigned a likelihood value based on the likelihood function. The nested sampling algorithm then finds the point with the lowest likelihood, i.e. the 'worst' point. A weight is determined for this worst point. Two values are then calculated - the natural log of the evidence, $log(Z)$, and the *information* H, defined below [2].

$$H = \int log(\frac{dP}{dX})dP \tag{8}$$

where dP is the posterior. The values associated with the point - the point itself, its likelihood and its weight are all stored in the posterior. The worst object is then overwritten with a copy of a 'surviving' point (any point other than the worst). This copy is then slightly altered, usually by adding a small randomly generated number. The likelihood of this 'new' point is then calculated and compared to that of the 'worst' object. If it is found to be lower than the previously determined lowest likelihood, the new point is altered again. This process uses an MCMC to ensure that the resulting new point is only a slight change from a surviving point, and that its likelihood is at least higher than that of the overwritten 'worst' object.

This process is iterated through for either a predetermined number of iterates or until some termination condition is met.[1, 2]

The following diagram shows the process of nested sampling pictorially. In this example, an object is placed at x = 3. The prior consists of a set of x values distributed linearly on the interval (0,5). The likelihood of the object being found at a given x-position is defined by the function below.

$$L = 6x - x^2 - 2 \tag{9}$$

The distribution of the points after each iterate of the nested sampling algorithm is shown in each line of the diagram below.

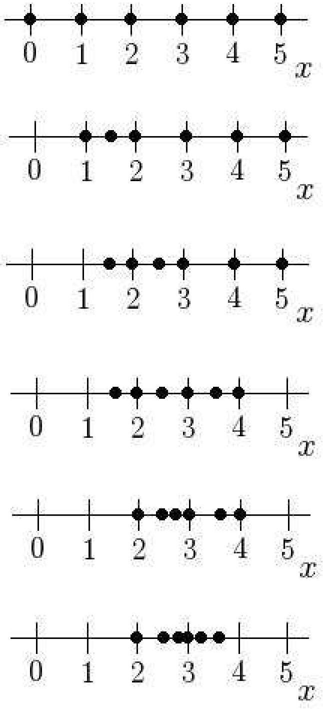


Figure 4: After each iterate, the values begin converging on 3 - the position of the object.

3 Nested Sampling

3.1 The Lighthouse Problem

In order to become accustomed with both programming and the concept of Nested Sampling, a toy problem from [2] was attempted:

"A lighthouse is somewhere off a piece of straight coastline at a position α along the shore and a distance β out at sea. It emits a series of short highly collimated flashes at random intervals and hence at random azimuths. These pulses are intercepted on the coast by photo-detectors that record only the fact that a flash has occurred, but not the angle from which it came. ***N*** *flashes have so far been recorded at positions x_k. Where is the lighthouse?"*[2]

The 64 values of x_k were previously generated with the lighthouse being positioned at (1,1) and were provided by [2].

Source code in C was provided and used to create an object-oriented program in C++. The results of both approaches were compared and found to be equivalent, which ensured the functionality of the C++ version of the program. The purpose of using object orientation was to ensure that the program was as generic as possible in order for it to be applied to other problems. Several methods, however, were

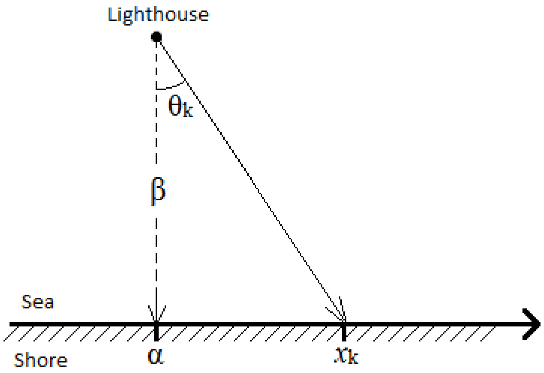


Figure 5: Diagram of Sivia's Lighthouse Problem [2]

problem-specific.

The prior was assumed to be uniform on x = (-2,2) and y = (0,2). That is, arrays of x and y coordinates were filled with values randomly generated on (0,1) and mapped to the intervals (-2,2) and (0,2) respectively. Each (x,y) point was then used to calculate a likelihood value that reflected the probability of the lighthouse being situated at those coordinates.

$$LogL = \sum log(\frac{(y/\pi)}{(D[k]-x)^2+y^2}) \tag{10}$$

where D is the array of flash positions x_k and the expression is summed from k = 0 to 63.

The nested sampling algorithm is then run using the calculated likelihood values. During each iteration, the Explore() function was called in order to overwrite the point with the lowest likelihood with an evolved copy of another point, as discussed in Section 2.2. In this problem, small random numbers were added to the x and y values and a new likelihood was calculated. If this new likelihood was less than that of the 'worst' object, it was rejected and the loop was run through again, with slightly larger random numbers added. This loop, a Markov Chain Monte Carlo algorithm, was iterated twenty times in order to obtain a slightly altered copy of a surviving point with a likelihood greater than that of the overwritten point.
The size of the prior (i.e. the number of samples used initially) and the number of iterates were altered in order to obtain an idea of the optimal set-up of the program. The results of these tests are shown below.

Once a sufficient set of initial values was found, the results of the object-oriented program were compared to those obtained from the original C program. The following plots show the comparison.

It was apparent from these plots that the two versions of the code were consistent with each other. This test was used to ensure that the object-oriented version was

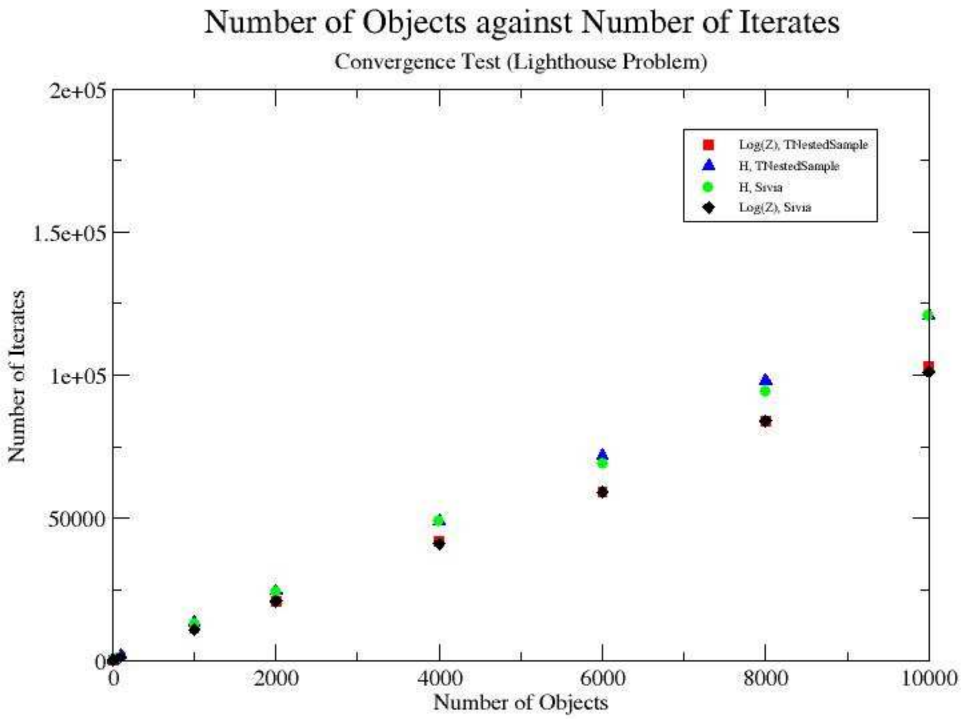


Figure 6: Graph denoting the relation between number of objects (points) and number of iterates. For each number of objects, the number of iterates at which the log of the evidence and the information were found not to change (i.e. the number of iterates required for them to converge) were plotted, respectively.

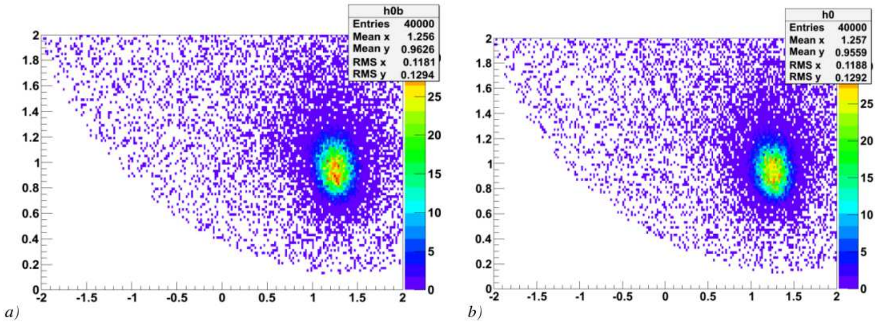


Figure 7: The results of running both versions of the code with the same initial values are shown above. a) The C code provided by Sivia; b) The object-oriented C++ code.

functional to at least the same degree as the C code provided. This was particularly useful in becoming familiar with programming in an object-oriented language.

3.2 Applications to Baryon Spectroscopy

Once a working version of the generic object-oriented nested sampling program was achieved, it was applied to a more physics-related problem. The first task in this physics application was to extract the value of one observable - the photon-beam asymmetry, B (defined in Table I). An event generator was used to generate dummy data, given a specific value for B. This data consisted of azimuthal angles and polarisation states.

In this case, each point in the prior was described by eight normalised values randomly generated from a Gaussian distributed over the surface of an 8-sphere, in a similar manner as described in Section 3. These values were then combined to form four complex transversity amplitudes, which were used to calculate a value of B based on the expression in Table I. The likelihood associated with each calculated value of B was determined by the equations below.

$$\tilde{A} = \frac{P_\gamma B \cos 2\phi + \delta L}{1 + P_\gamma B \cos 2\phi \delta L} \tag{11}$$

$$X = \frac{1}{2}(1 \pm \tilde{A}) \tag{12}$$

$$logL = \sum log(X) \tag{13}$$

where P_γ is the photon polarisation number, δL is the luminosity asymmetry and $logL$ is the natural logarithm of the likelihood. In Eqn. 6, $\tilde{A}$ was added or subtracted based on whether the associated polarisation perpendicular or parallel, respectively. These values were summed for all events - that is, all angles and polarisation states. These values were then used as usual in the nested sampling algorithm. The Explore() function added a small randomly generated number to each of the eight initial values. The small randomly generated number was determined by a Gaussian distribution of a set width. This width was altered after each iteration of the MCMC loop in the function. As per the Lighthouse example described in Section **Lighthouse**, a new likelihood value was calculated and compared to that of the 'worst' point in order to ensure that the new point was at least more likely than that which had been overwritten. The results of the program were compared to the value of B input into the event generator.

3.2.1 Evolved Prior

It was possible to add some complexity to the simple observable extraction program by using a more dynamic prior. In the initial run of the program, a posterior distribution would be generated. It was found that this posterior could be used to generate points in the prior, rather than randomly generating a set of points. This would allow the program to use fewer numbers of iterates.

4 Analysis Program

4.1 SCons

In the CLAS Collaboration at Jefferson Lab, a software construction tool called SCons[5] has become increasingly popular. It is a simple, relatively easy-to-use alternative to the more commonly used Makefile. The nested sampling program developed in this project was compiled using this SCons program. SCons is scripted using Python, and is thus fairly intuitive to code. The main file, required to be named 'sconstruct', imported any required Python scripts, listed the source code files to be compiled and any compiler flags required. Several Python scripts were imported in order to compile using ROOT libraries. This provided a straightforward alternative to the complicated standard, autoconf.

4.2 Structure and Coding

An object-oriented (specifically C++) approach to the program was taken in order to make the nested sampling algorithm as generic as possible. The program was comprised of two main classes, with a third acting as the user's front end (where various changes can be made). A combination of C++ and ROOT libraries were used.

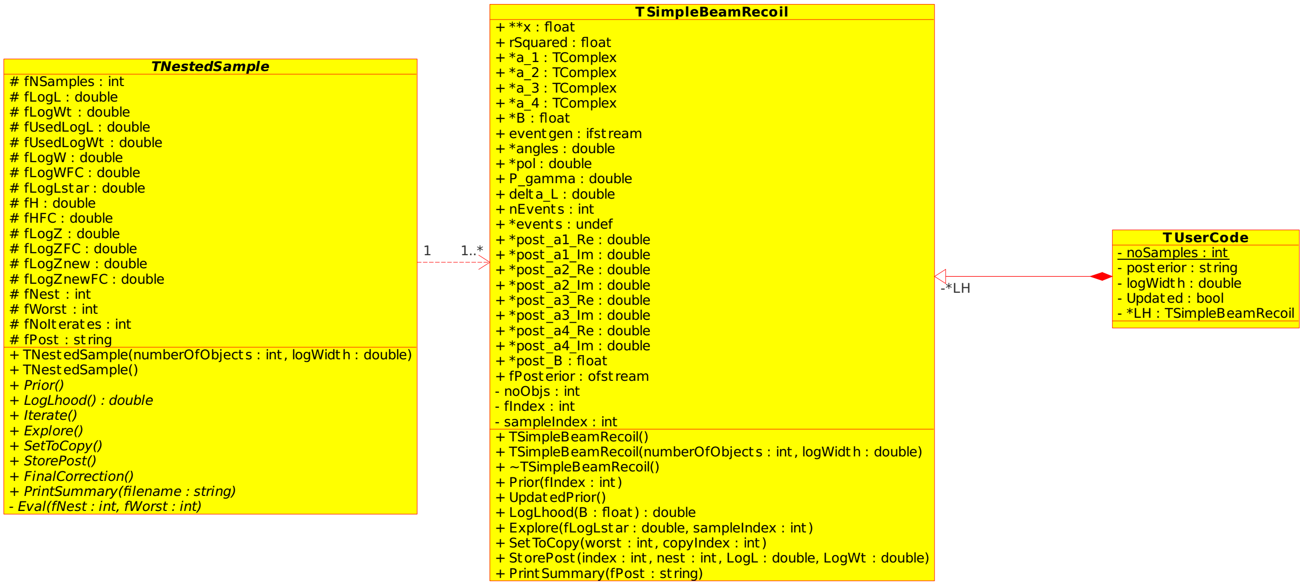


Figure 8: Class diagram showing methods, attributes and associations.

An abstract class, TNestedSample, was used for defining the generic methods - Iterate(), Eval() and FinalCorrection(). These methods are responsible for the iteration over the nested sampling algorithm, termination and the nested sampling algorithm itself. Other methods, such as Prior(), Explore() and PrintSummary(), must be defined for each derived class (i.e. for each application) as they are problem-specific.

The front end class, called TUserCode, determined which derived class would be used, called all required functions and set some initial values. In principle, one could have multiple derived classes (i.e. applications to different problems) in one directory, and the user would be able to specify in TUserCode which derived class to use. Each derived class would inherit the generic methods from the parent class. For example, both Sivia's Lighthouse problem and the application to simple B observable extraction used the same abstract parent class - they differed solely in the derived classes.
The nested sampling algorithm was contained in the Eval() method. This private method was called from within the Iterate() method, which determined the number of iterations required in order to ensure a sufficiently precise result. A termination condition was determined based on work by Skilling[1].

4.3 Output

The nested sampling program generated an output in several forms. Basic information about the running of the program was output to the screen, as shown in Figure 3. In addition to outputting to the screen, a ROOT tree (written to a .root file) was also created. This tree was used to store many types of information in the form of branches. The ROOT tree was used to examine the results visually.

During testing of the program, additional text files were output in order to ensure that various sections of the code were working as intended. In particular, the introduction of an evolved prior required several files to be created and examined in ROOT.

4.4 Performance Testing

Several performance tests were carried out on the program in order to determine its ability to extract the desired observables. All tests were done using data simulated by an event generator.

4.4.1 Event Generator

4.4.2 Timing Tests

5 Conclusions

6 Future Work

Despite promising results, there is still much work to be done in the development of this Nested Sampling analysis program. In the next twelve months, the program will be improved through a number of amendments. Initially, the nested sampling program was simple and basic. The level of complexity has been (and will continue to be) increased until it can be run on experimental data. The first step in this development is to handle all observables. Instead of simply extracting the B observable, all sixteen observables will be extracted. Calculations of statistical errors must also be included in the program.

Once this improvement has been implemented, it will be tested with data from experiment that has previously been studied. The results will be compared to those obtained from a maximum-likelihood analysis program in order to ensure an acceptable level of accuracy. Once a sufficient degree of accuracy has been shown (and any necessary tweaks and adjustments have been made), the program will be used to evaluate new experimental data.

One of the drawbacks of this nested sampling approach is the excessive run-time required to obtain good results. As discussed previously, this poses a significant problem. The amount of time required to run the program using a sufficient number of iterations is longer than desired, despite optimisations. The possibility of applying programming techniques used in graphics card programming and graphics processing unit (GPU) programming, in particular data parallelisation, will be strongly considered. If successful, this would dramatically reduce the amount of time required to run the program with a high number of iterations. The implications of this improvement could enable the program to handle exceptionally large data sets in just minutes, making it a desirable alternative to maximum likelihood methods.

In addition to improving the analysis program, some time will be spent at the Jefferson Lab in Newport News, Virginia. This time will be spent doing training and shifts in experimental hall B.

References

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