Numerical Integration of Quantum Systems

Richard M. G. Boyne
CID: 01057503

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Abstract

1 Introduction

Quantum systems are described (either partially or fully) by its wave function, a complex mathematical description which determines the probability of the system being in a certain state [1]. These wave functions are often intricate, hence solving for certain situations frequently has no analytic solutions so numerical analysis is required. A common example is the solving the probability P, of a particle with wave function $\psi(\mathbf{r}, t)$ residing within a region of space R. This is given by [1]:

$$P = \int_R |\psi(\mathbf{r}, t)|^2 d\mathbf{r} \tag{1}$$

where t is time and $\mathbf{r}$ is position. The aim of this project was to solve the above expression numerically for an arbitrary wave function in one dimension at a fixed time. To find the optimal method multiple numerical integration algorithms were implemented and reviewed, these fall under the categories of Newton Coats and Monte Carlo methods.

2 Numerical Methods

For the purpose of this project a single particle is modelled as a wave packet in one dimensional free space. At some fixed point in time it has a wave function [2]:

$$\psi(z) = \pi^{-\frac{1}{4}} e^{ia(z)} e^{-\frac{z^2}{2}} \tag{2}$$

where z is the spacial position in arbitrary units and $a(z)$ is some real valued phase function (which becomes irrelevant to probability in equation 1). This wave function was solved here for comparison, however all programs were written to accept any given one dimensional continuous function over a finite range.

i) Newton Coats

Newton Coats are the simplest of quadrature numerical integration methods. The integrand is divided into N bins of equal width $h = \frac{R}{N}$, each bin is integrated independently and added together giving the integral.

The Trapezoidal rule uses a linear approximation within bin to estimate each bin integral [1]:

$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{2}[f(x_i) + f(x_{i+1})] + \mathcal{O}(h^3 \frac{d^2 f}{dx^2}) \tag{3}$$

where f is the integrand, $\mathcal{O}$ indicates the truncation error order and x_i, x_{i+1} are the bins boundaries. To reduce the local error N must increase (reducing h); by halving each bin it is possible to use the previous estimate T_j to find T_{j+1} without needing to sample previous bin edges [1]:

$$T_j = \frac{1}{2}T_j + h \sum_{i=1}^{(n-1)/2} f(x_{2i-1}) \tag{4}$$

This is the Extended Trapezoidal Rule and has the advantage of being a Markov Chain [3], where each new estimate is calculated only from the previous one (prior points are irrelevant). Therefore the iteration time is constant with increasing N allowing for high number of iterations to be computed quickly.

Simpsons $\frac{1}{3}$ rule is similar but instead approximates a quadratic, requiring an extra sample point but giving a higher order truncation errors:

$$\int_{x_i}^{x_{i+1}} f(x)dx = \frac{h}{3}[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})] + \mathcal{O}(h^5 \frac{d^4 f}{dx^4}) \tag{5}$$

As before there is an Extended Simpsons Rule for the halving of bins that follows a Markov Chain. The S_J Extended Simpsons iteration can be formed from a weighted sum of two successive Trapezoidal iterations:

$$S_j = \frac{4}{3}T_{j+1} - \frac{1}{3}T_j \tag{6}$$

Only closed form quadrature methods are used here as both limits of the integrand are assumed to be well defined. Due to the summing of all bins the global errors in T_j,S_j are $\mathcal{O}h^2$,$\mathcal{O}h^4$ respectively.

ii) Monte Carlo

Monte Carlo integration utilizes random numbers to estimate the integrand mean value over the integration range. In the simplest one dimensional case sampling by N uniform random numbers x_i, the integral over range [a,b] is:

$$\int_a^b f(x)dx = R\langle f \rangle = \frac{R}{N}\sum_{i=1}^{N} f(x_i) \tag{7}$$

Here the uncertainty is well approximated by the standard error [3] in $\langle f \rangle$, hence goes as $N^{-\frac{1}{2}}$ and converges on the true value as $N \to \infty$. This is unchanged in higher dimensions hence is very advantageous for multidimensional integrals.

Importance sampling uses the same principle but with the sample random numbers x_i distributed over a probability density function $p(x)$ normalised on the range:

$$\int_a^b f(x)dx = \int_a^b q(x)p(x)dx = \frac{1}{N}\sum_{i=1}^{N} q(x_i) = \langle q \rangle \tag{8}$$

By choosing $p(x)$ such that random samples x_i populate the region where $f(x)$ is large gives faster convergence to the true, therefore reducing uncertainty (calculated by the standard error of $\langle q \rangle$). Using a uniform PDF

retrieves equation 7. The method of sampling a pdf used here are transformation[3] and Gibbs sampling[3] methods.

The optimal PDF would be $f(x)$ normalised on the integration range, however this requires the integral that is being found. Adaptive importance sampling implements a changing PDF that tends towards this. The Vegas algorithm[3] uses a step pdf with irregular widths. After some samples are taken each step changes width based on its fractional integral contribution γ whilst keeping number of steps n_s and step area A_s constant. This is often implemented by subdividing each step $n_s k\gamma + 1$ times then regrouping every k steps. After regrouping each step is then re-normalised to have area A_s, giving a pdf of a closer approximation to the optimal pdf.

3 Implementation & Validation

i) Newton Coats

Successive iterations of equations 4 and 6 were implemented until the relative error of two successive iterations I_j and I_{j-1} fall below a user specified value ϵ:

$$|\frac{I_j - I_{j-1}}{I_j}| < \epsilon \tag{9}$$

If a single iteration has value of zero here this termination condition is invalid and the method will break, hence an exception is raised to prevent ambiguity as to the cause.

Both these methods are absolutely convergent (i.e. each iteration will be closer to the true value than the last) therefore it is reasonable to use the numerator here as the uncertainty in the calculated value. To ensure this approximation provides the correct order of errors expected from equations 3, 5 a validation plot of the error magnitude is compared to the expected uncertainty orders in h.

Each method is wholly validated by three known integrals, specified in appendix B, each being compared to their true values. The zero exception is also tested by running a sample anti-symmetric function over a symmetric interval (with the use of 'try, except' in python this does not stop the program running) . This confirms the functionality of the code and allows checking the correctness after modifications.

ii) Importance Sampling

In Importance sampling the integrand is sampled, with the same condition (equation 9) being used every 1000 iterations with the additional requirement of several consecutive triggers to terminate. This prevents accidental termination due to the random nature allowing for consecutive close integral values before the required accuracy has been reached.

Sampling via Gibbs method was insufficient here as large number of samples were required to correctly distribute random numbers on the given pdf, hence causing a much slower convergence which often satisfied the termination condition far too early. Therefore transformation method alone is used here, however this adds the requirement of pdfs that have a known cumulative distribution function which is not always feasible.

Both a uniform and linear pdf were used for this method, with the linear pdf for the sample wave function

normalised on the range $[0, 2]$ as:

$$PDF = -0.48z + 0.98 \tag{10}$$

Vegas is implemented by creating a given number of class instances for each step in the pdf, which are updated every 100 samples per bin. To cope with fractional step division numbers (i.e. λ is rarely an integer) the division number is rounded with the remainder carried over to the next bin. This keeps the impact of rounding local in the pdf, hence keeping to the intention of high division numbers in regions of high integral.

Unlike the previous methods termination requires the error calculated from total variance of iteration integrals to be less than the supplied accuracy rather than the relative error from two successive iterations. This is to prevent accidental termination due to the random nature of the integral estimates, similar to importance sampling however the previous method to cope is insufficient here due to a tendency to consistently over or underestimate (see the results section). This termination condition still uses the requirement of successive triggers.

Both Monte Carlo methods are validated with the same functions as Newton Coats (with pdfs for non-adaptive sampling given in B). Uncertainties are validated by comparison to previous Newton Coats results. To reduce burn in effects dominating the integral estimation the first 5 iterations are disregarded.

4 Results and Discussion

i) Newton Coats

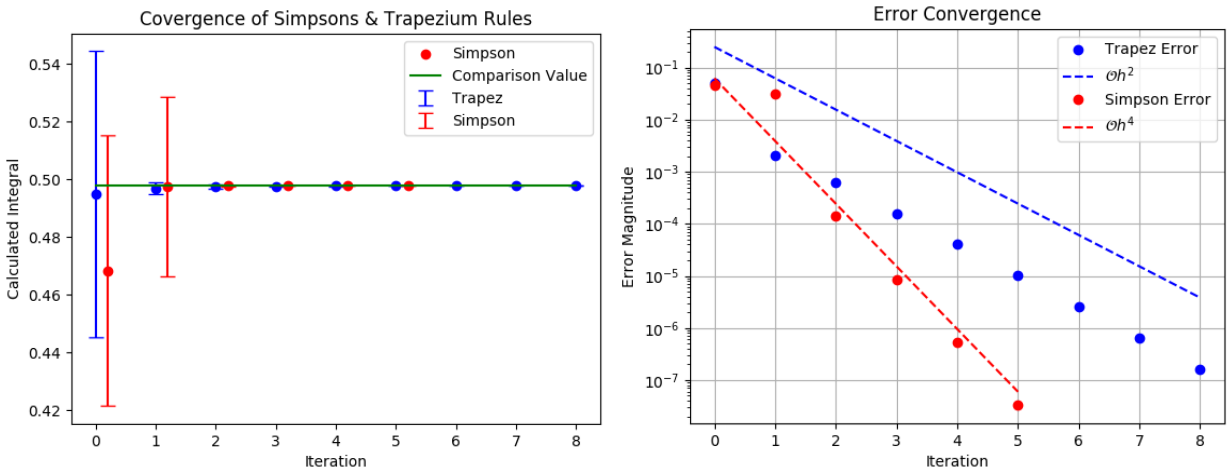

Figure 1: ***Left*** *shows the calculated integrals after successive iterations for both Newton Coats methods. The comparison value is the agreed solution of both methods and error bars are too small to be seen after the 3rd iteration. Trapezium and Simpsons terminate at* $0.4976611 \pm 1.6 \times 10^{-07}$ *&* $0.49766113 \pm 3.3 \times 10^{-08}$ *respectively.*
Right *shows the logarithmic errors after successive iterations with the expected orders of error for both methods also plotted. A few outliers are present, likely due to location of bin edges. The parallel gradients indicate calculated errors are sufficient.*

The results for the sample integral (equation 2) are shown above for a relative accuracy of 10^{-6}. Both agree

on the integral up to 6 decimal places, 0.4976611 with trapezium rule giving the larger error of 1.6×10^{-07}. The uncertainty in both methods are expected to be $\mathcal{O}h^2, h^4$ scaled with some constant determined by the integrates derivatives, it therefore makes sense that error plot lines are mismatched by a scalar factor. The parallel gradients show that the error calculations here are sufficient. The use of relative error in the uncertainty means that the termination condition here provides an answer that always has uncertainty less than the given relative accuracy.

Simpsons, Trapezium rules required 6,9 iterations respectively corresponding to 64,512 samples of the integrand. The degree of sample number reduction is shown to vary from the validation functions (appendix B) however for those functions Simpsons rule always requires less evaluations as expected from theory.

ii) Importance Sampling

Monte Carlo for both a uniform and linear pdf at a relative accuracies of 10^{-6} are shown in figure 2. As can be seen they provided general convergence however due to the random nature of Monte Carlo iterations can locally divergent. This can cause issues with termination, shown the linear pdf disagreeing with the previously found result (but only slightly). By interpreting the uncertainty as a standard deviation, (i.e. 68% of results should lie within) the uncertainty occasionally disagreeing with the known result is reasonable, particularly as approximately 30% of the data points seem to disagree in figure 2. This could possibly be avoided in the future by running the process several times with different random generator seeds and taking an average of the results.

Since this method uses variance as the error estimation, the result is often less certain than the supplied relative accuracy. This is non-ideal as one would have to give a higher ϵ to obtain the desired accuracy. An alternative to this would be to use the relative accuracy to gain an error estimation, however this almost always disagrees with the true results. This issue is a disadvantage of this implementation.

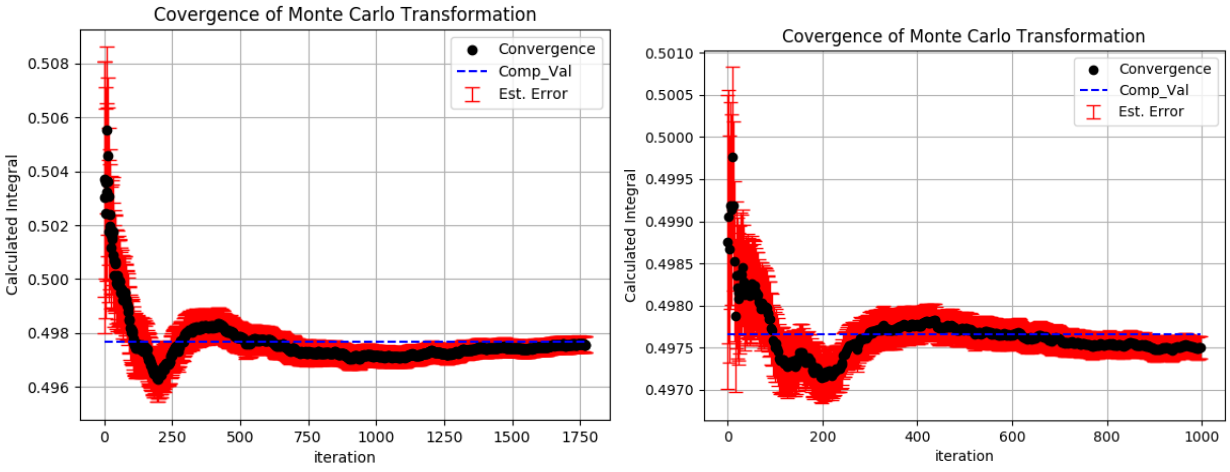

Figure 2: ***Left*** *shows calculated integrals and uncertainties for each iteration to* 10^{-6} *relative accuracy for uniform PDF. The Newton Coats results is plotted for comparison. Result after* 1.78×10^6 *iterations (2 min run time) is* 0.49757 ± 0.00029*, note the uncertainty is less than the relative uncertainty. The convergence is smooth but has a tendency to deviate in certain small regions, e.g. 600 to 1000 iterations* ***Right*** *is the same as the left but for the linear PDF (equation 10), Result after* 1.01×10^6 *iterations (1 min run time) is* 0.49749 ± 0.00013*, note the uncertainty is less than the relative uncertainty. Here the convergence is more jagged than for uniform PDF but reaches convergence faster with less uncertainty.*

The iterations required for different relative accuracies are shown in figure 3, note that 5/8 results agreed with previous results, agreeing with the standard deviation interpretation of errors. As expected the linear pdf gives more efficient convergence requiring around half the iterations for $\epsilon >= 10^{-4}$, due to sampling the function at a higher frequency in regions of greater importance. Comparison of the validation results (see appendix B) shows that in general this method is convergent for all the given functions though, as previously mentioned, occasionally disagrees with the know results.

This Monte Carlo method in these one dimensional instances is seen to be far less efficient than the Newton Coats integration, which were far faster, with less function evaluations and less uncertainty as well as being a far simpler in implementation. However if these problems were to be generalised to multiple dimensions, this Monte Carlo method would remain virtually unchanged (though the use of transformation method would have to be swapped for the slower but more general Gibbs sampling) where as Newton Coats would require much editing. Furthermore the Monte Carlo method would likely keep the same error magnitudes with increasing dimensions where as Newton Coats would increase, however in these cases Newton Coats are clearly better.

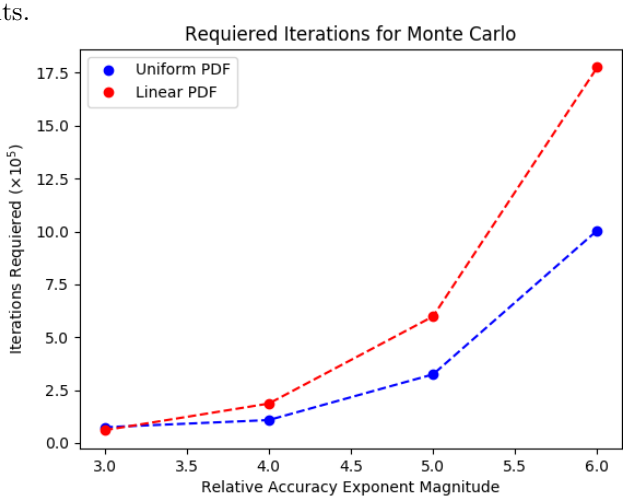

Figure 3: The number of iterations required for different relative accuracies. The linear PDF always provides faster convergence. in general the iterations required are increasing non-linearly making higher accuracies unreasonably long.

iii) Adaptive Importance Sampling

The Vegas algorithm provides reasonable results for relative accuracy of 10^{-4}, shown in figure 4. The adapting PDF is seen to give samples that follow the optimal pdf very well. Here the number of iterations required is 5×10^5, significantly more than transformation integration however the lack of required PDF and CDF makes this algorithm more favourable. Inspecting the difference of both Monte Carlo results from the true value, shows that Vegas is far closer on the 10^{-4} accuracy (0.12ϵ compared to 1.15ϵ), suggesting that iteration issues are likely due to terminating too late. The higher relative accuracy of 10^{-5} requires 16×10^6 iterations, further supporting this hypothesis. It makes sense that Vegas only has this issue as it uses the uncertainty from variance to determine termination. Alternative conditions such as using relative error gave even longer run times.

A possible cause of these termination and uncertainty issues could be due to non-optimal settings for other parameters, namely the number of step in the pdf and the number of divides. If these are improperly selected the pdf selected may vary significantly about the optimal pdf on a specific iteration, but balance out if several iterations samples are considered (as is done in figure 4). This may have the effect of causing iterations to vary more, leading to a higher variance and a much lower chance of meeting the relative accuracy termination condition, which would explain why neither provide decent termination conditions here. An improvement on this would require further investigation.

Validation results suggest the method is not generally stable as two of three validations functions disagree with the true values. Unlike previous disagreements these seems to be converging to incorrect values, whether this is the case for the sample wave function in question is hard to tell as higher relative accuracies are need to be sure (up to 10^{-5} relative accuracy it agrees). The exact cause if this instability is unclear, possibly

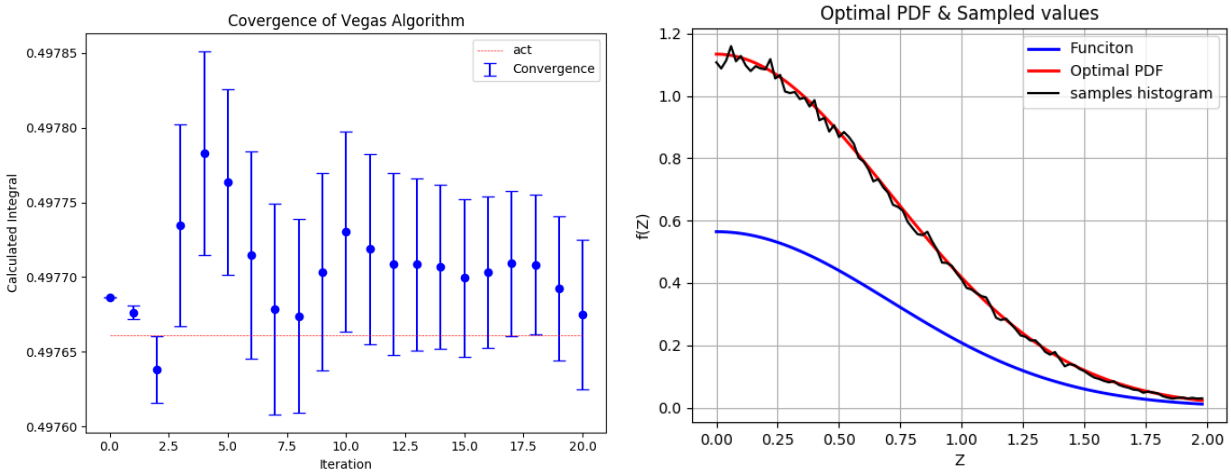

Figure 4: ***Left*** *shows Calculated integral and uncertainty for Vegas algorithms iterations to the relative accuracy of* 10^{-4}*. Final value after* 5×10^5 *iterations is* $0.497673 \pm 4.9 \times 10^{-5}$*, however difference from the Newton Coats value is* 1.2×10^{-6} *suggesting an overestimation of errors. The low uncertainty in early iterations is due to variance being low when only a few samples have been taken. Note several of the values disagree with the known values, similarly to transformation integration.*
Right *shows a histogram of the position values samples (black line) and the integrates optimal sampling PDF found by normalising the integrand over the range using the Newton Coats integral value. The integrand itself is also plotted for comparison. The histogram closely fitting indicates the algorithm works well at sampling optimally overall, however the samples at each iteration may vary from the optimal pdf significantly.*

due to the rounding method in the splitting of the sampling pdf, or an unnoticed bug in the code. Further investigation into this would be required. Due to this possible instability this method is not appropriate here, and Newton Coats methods are more preferable.

5 Conclusion

References

[1] H. D. Y. R. A. Freedman, *University Physics With Modern Physics*. Pearson Education, 14th ed., 2007. Pages: 1321–1327 (ISBN 10: 0-321-97361-5).

[2] Y. Uchida and P. Scot, "Project b2: Solving quantum systems numerically," 2017–18. Project debriefing.

[3] T. be Cited, "To be cited," To be Cited.

Appendices

A PDFs

The PDF used for importance sampling via transformation method for the sample wave function (equation 2) normalised on the range $[0, 2]$ is:

$$PDF = -0.48z + 0.98 \tag{11}$$

B Validation

For validation on all methods the following known integrals are used:

$$\int_0^{\pi/2} sin(z)dz = 1 \qquad \int_0^2 z^3/\pi = 4/\pi \qquad \int_0^2 \frac{e^{-0.5(z-1)^2}}{\sqrt{2\pi}} = 0.6827 \tag{12}$$

With the zero exception test run with a $sin(z)$ over the range $[-1, 1]$. For the Monte Carlo importance sampling (via transformation method), the following pdfs normalised on the above ranges were used, with associated CDFs also given:

PDF	CFD
$\frac{8z}{\pi}$	$\frac{\pi\sqrt{\frac{x}{4}}}{2}$
$\frac{3z^2}{8}$	$2\sqrt[3]{x}$
$z \quad for z \leqslant 1$	$\sqrt{2x} \quad for \quad x \leqslant 0.5$
$-z+2 \quad for \quad z > 1$	$\sqrt{2-2x} \quad for \quad x > 0.5$

Table 1: PDFs and CDFs for validations functions to be used in the Monte Carlo transformation integration method where $0 \leqslant x \leqslant 1$.

i) Newton Coats Validation Plots

ii) Monte Carlo Transformation Validation Plots

iii) Vegas Validation Plots