

University of Reading
School of Mathematics, Meteorology & Physics

**EFFICIENT EVALUATION OF HIGHLY
OSCILLATORY INTEGRALS**

Shaun Potticary

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This dissertation is submitted to the Department of Mathematics in partial fulfilment
of the requirements for the degree of Master of Science

Declaration

I confirm that this is my own work, and the use of all material from other sources has been properly and fully acknowledged.

Shaun Potticary

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1.) Introduction

Highly oscillatory integrals appear in many types of mathematical problems including wave scattering problems, quantum chemistry, electrodynamics and fluid dynamics and Fourier transforms. Although these integrals appear in many places, in this project we are going to concentrate on the wave scattering problem and the Fourier transforms. A Fourier transform is used when solving two dimensional partial differential equations, and in the evaluation of a complex Fourier series. In both cases the evaluation of the Fourier transform involves the evaluation of an integral that may be highly oscillatory, (commonly it is so). The question is how do we compute this? A Fourier transform is of the form

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)e^{-ikt} dt \quad (1.1)$$

The reason that the evaluation of these integrals is so important is because standard methods to evaluate complex integrals don't work well in the case that the integrand oscillates rapidly. This is why in this project specific techniques will be looked at for the problem and we will see how good at approximating (1.1) they are. Firstly the integrals that we are going to look at need to be defined. Two forms of highly oscillatory integrals are going to be looked at. The first one is a good place to start with our investigation.

Definition 1.1 - The general form our first integral that is dealt with in this project is:-

$$I[f] := \int_a^b f(x)e^{ikx} dx \quad (1.2)$$

where $f(x)$ is a smooth and slowly oscillating function. This integral is actually included in the second integral, but the techniques that we are going to use in this project actually are a lot simpler for this one. The form of $I[f]$ is a general form of a complex Fourier series and this is going to be our motivation of the first part of the project.

Definition 1.2 - The second integral that we are going to look at is:-

$$J[f] := \int_a^b f(x)e^{ikg(x)} dx \quad (1.2)$$

this is the general form of our oscillatory integrals and this is the integral that we will be mainly looking at, to be able to evaluate for functions $f(x)$ and $g(x)$. The two integrals both have the complex wave function with k being its wave number, so as k gets large then the wave frequency gets large too. The consequence of this is that in a small interval as the wave number gets large the number of waves in that interval would be more. This means the wavelength of one specific wave gets smaller and smaller, so numerical techniques would need to use a small step size to evaluate them accurately.

This project is going to investigate whether certain techniques for evaluating highly oscillatory integrals that are going to be looked at in this project work on the two integrals $I[f]$ and $J[f]$, and if they don't why not.

The techniques that are going to be covered in this project will be looked at in two parts. The first part of this project deals with the evaluation of $I[f]$. There are three different techniques that are going to be looked at for this integral. The first one is quadrature methods that are used for usual non oscillatory integrals, and we will see that when k gets large then these techniques give very poor results. In this section for quadrature methods we will look at four different types of quadrature methods and for each type of quadrature method we will look at the procedure that evaluates $I[f]$, the error of the procedure and the evaluation on one specific example.

The second method is an asymptotic method using integration by parts, this section will also look at the procedure and the error analysis. The last part of this section deals with the evaluation of an example, (the same as for the quadrature methods to keep consistency).

The third technique is covered in a paper by Arieh Iserles (1). It uses a method by Filon (1924) which is a quadrature type method, specifically designed to solve the oscillatory part of the integral exactly so that the numerical solution doesn't need small step sizes to solve the oscillatory part of it. This part of the project is the most important as in this part there are new types of methods for evaluating $I[f]$ that were only looked at again by Iserles in 2003 after a gap of nearly 80 years from Filon's original papers. On top of this the Filon type methods, we look at here have been changed from those in (1) by looking at less accurate quadrature methods, this is not dealt with by Arieh Iserles as he sees the Gaussian method to be better than any other method, but in order to focus on the difficulties associated with highly oscillatory integrals we will concentrate most of our attention on lower order quadrature methods

(namely the midpoint rule and the trapezium rule) so as to simplify the analysis. We do know that Gaussian quadrature gives better results in practice, though the analysis is too complicated to get good theoretical results beyond those already achieved in (1).

We should expect from this integral to get an $O(1/k)$ for the integral which is what the analytical solution would give, and so for any method to converge quickly we would expect the method to have a similar order.

For the second integral we will look at two types of methods. The first one is an asymptotic type method called method of stationary phase (MOSP) which is different for $g'(x)=0$ in $[a,b]$ than it is for $g'(x) \neq 0$ in $[a,b]$. The analysis for this part will not be in great detail, only the procedure is mainly shown in this section as it is this that is needed for the second part. The second method is a Filon type quadrature method used for the first integral but again it has the problem if $g'(x)=0$ in $[a,b]$ then a fix has to be used to get a solution. The quadrature method that is going to be used with Filon's work is the trapezoidal rule, as this is easier to work through the Gaussian method and should give good results. This project will therefore show a broad range of techniques that can be used on highly oscillatory integrals and how good or bad they are depending on factors including the wave number k and step sizes h . The project will deal with less accurate quadrature methods so as to simplify the analysis and give good error estimates that can be compared to the numerical results. For the second integral $J[f]$ we should expect to get two different types of orders for the integral depending on the derivative of $g(x)$. if $g'(x) \neq 0$ in $[a,b]$ the we should expect to get an order of $O(1/k)$ for the integral. If $g'(x)=0$ in $[a,b]$ at a point x_1 and $g''(x_1) \neq 0$ then the order of the integral will be $O(1/k^{1/2})$. This will all be dealt with in section 5)

Integral 1: Fourier Transforms

In this section we will deal with the first integral that we are interested in $I[f]$, as described in definition 1.1

2.) Quadrature Methods

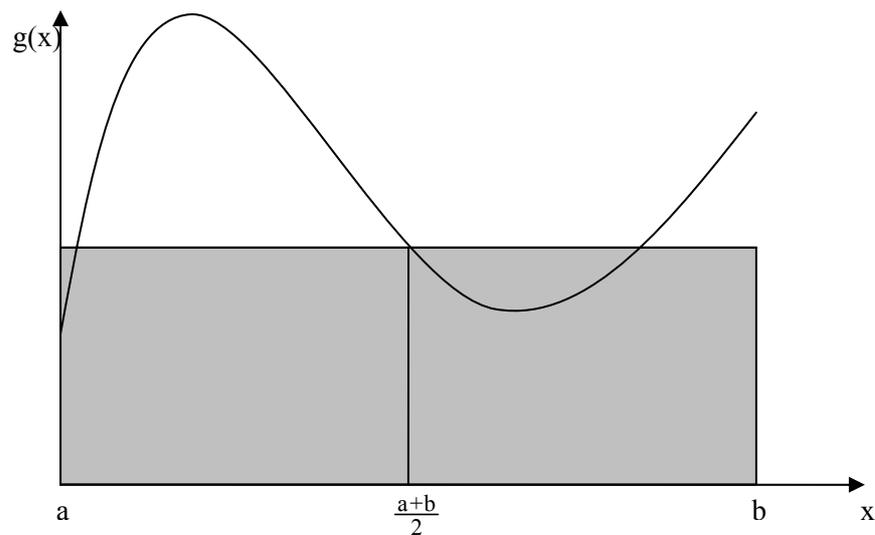
Midpoint Rule and the Composite Midpoint Rule

The Midpoint Rule is the easiest but also one of the least accurate of all the quadrature methods that we are going to look at in this project. The best way of looking at the Midpoint Rule is to see what the formula is on a general function $g(x)$, and then look at the error approximation for that. Once we have done this then we can look at the Midpoint Rule when our function is in fact our oscillatory integral $I[f]$. After we have looked at the Midpoint Rule we can look at what happens when we split up the interval $[a,b]$ into N separate intervals and then use the Midpoint Rule on each interval separately, this is called the Composite Midpoint Rule.

Definition 2.1 – The Midpoint Rule applied to a general function $g(x)$, between the limits $[a,b]$ is given below.

$$\int_a^b g(x)dx \approx (b-a)g\left(\frac{a+b}{2}\right) \quad (2.1)$$

The Midpoint Rule finds the midpoint of the interval $(\frac{a+b}{2})$ and calculates g at this point, and then this all has to be multiplied by the length of our interval, $(b-a)$. In fact the Midpoint Rule actually approximates the function $g(x)$ by a constant and then finds the area under the resulting rectangle. This means that our function $g(x)$ is a constant then it will solve the integral exactly. As a consequence the midpoint rule actually solves exactly for a polynomial of degree 1, which is because even though the midpoint rule doesn't approximate the line exactly, the integral is exact.

Figure 1- An example of the midpoint rule

The diagram above illustrates the Midpoint Rule for a general function $g(x)$, it is clear that when we have an oscillatory integral then the midpoint rule would be very bad at approximating $I[f]$.

The best way to look at how good or bad the midpoint rule can be is to look at the error analysis, and seeing what factors make the error grow or decrease and to see if when $g(x)$ is our oscillatory function we will expect to get different results.

Theorem 2.1 - The error term, when looking at the midpoint rule on a general function $g(x)$ is

$$\left(\frac{(b-a)^3}{24}\right) |g''(\xi)| \quad (2.2)$$

More so, when we are looking to apply the Midpoint Rule to our integral $I[f]$ the error term is defined by

$$\left(\frac{(b-a)^3}{24}\right) (k)^2 |f''(\xi)| \quad (2.3)$$

Proof

To work out the error we need to find $|I - I_m|$ where

$$I = \int_a^b g(x) dx \quad \text{The exact solution } I[f]$$

$$I_m = \int_a^b g\left(\frac{a+b}{2}\right) dx \quad \text{The midpoint method approximation to } g(x)$$

Now when we calculate $|I - I_m|$, and to make our calculation easier we can use Taylor series on $g(x)$, at the midpoint of the interval, so that the first term will cancel. The Taylor series of $g(x)$, will therefore be

$$g(x) = g\left(\frac{a+b}{2}\right) + \left(x - \left(\frac{a+b}{2}\right)\right)g'\left(\frac{a+b}{2}\right) + \left(x - \left(\frac{a+b}{2}\right)\right)^2 \frac{g''(\xi)}{2!} \quad (2.4)$$

Where g must satisfy $g \in C^2[a, b]$, so it is twice differentiable, and $\xi \in [a, b]$ then when we substitute this into $|e_m| := |I - I_m|$, (the error term) we get

$$|e_m| = \left| \int_a^b \left(x - \left(\frac{a+b}{2}\right)\right)g'\left(\frac{a+b}{2}\right)dx + \int_a^b \left(x - \left(\frac{a+b}{2}\right)\right)^2 \frac{g''(\xi)}{2!}dx \right| \quad (2.5)$$

Now the integrals above are easy to calculate because we only have one x term in each integral, and so we obtain

$$\begin{aligned} |e_m| &= \left| g'\left(\frac{a+b}{2}\right) \left[\frac{\left(x - \left(\frac{a+b}{2}\right)\right)^2}{2} \right]_a^b + \frac{g''(\xi)}{2} \left[\frac{\left(x - \left(\frac{a+b}{2}\right)\right)^3}{3} \right]_a^b \right| \\ &= \left| \frac{1}{2}g'\left(\frac{a+b}{2}\right) \left[\left(b - \left(\frac{a+b}{2}\right)\right)^2 - \left(a - \left(\frac{a+b}{2}\right)\right)^2 \right] + \frac{g''(\xi)}{6} \left[\left(b - \left(\frac{a+b}{2}\right)\right)^3 - \left(a - \left(\frac{a+b}{2}\right)\right)^3 \right] \right| \end{aligned}$$

The above equation does look complicated but in fact the first term cancels, and we are left with the second term only, which is of the form

$$e_m = |g''(\xi)| \frac{(b-a)^3}{24} \quad (2.6)$$

and this is our error term. As can be seen the error term is made up of two components, firstly we have $(b-a)$, which cannot be changed (and is automatically positive as b is greater than a , therefore the modulus sign can be omitted), and the second component is the second derivative of g . Now if we use the midpoint rule on $I[f]$, we need to replace our $g(x)$ with $f(x)e^{ikx}$ so the error term is the same except for $I[f]$ except that it includes the second derivative of $f(x)e^{ikx}$. This means the error term when the midpoint rule is applied to $I[f]$ is

$$e_m = \frac{(b-a)^3}{24} (ik)^2 | [f''(\xi) + 2ikf'(\xi) + f(\xi)(ik)^2] e^{ik\xi} | \quad (2.7)$$

Theorem 2.2 – the term $| [f''(\xi) + 2ikf'(\xi) + f(\xi)(ik)^2] e^{ik\xi} |$ can be simplified in the following way. Using modulus theory the this term can be split into two separate terms of the form

$$| [f''(\xi) + 2ikf'(\xi) + f(\xi)(ik)^2] e^{ik\xi} | \leq | [f''(\xi) + 2ikf'(\xi) + f(\xi)(ik)^2] | | e^{ik\xi} |$$

this term can be simplified to get one term, this is done by noticing that the modulus of the exponential term is equal to 1. The other term can also be simplified by splitting the term up using the triangular inequality giving us

$$|[f''(\xi) + 2ikf'(\xi) + f(\xi)(ik)^2]| \leq |f''(\xi)| + 2k|f'(\xi)| + k^2|f(\xi)|$$

now we need to notice that we can take k^2 out of the equation and the following term is true

$$|f''(\xi)| + 2k|f'(\xi)| + k^2|f(\xi)| \leq k^2[|f''(\xi)| + |f'(\xi)| + |f(\xi)|]$$

now we can combine many of the above terms into one constant leaving us with

$$k^2[|f''(\xi)| + |f'(\xi)| + |f(\xi)|] \leq Ck^2|f''(\tilde{\xi})|$$

for some $\tilde{\xi}$ in $[a,b]$, which from now on will be referred to as ξ . the term above can be added to (2.2) to form our error that was given in (2.3). So we notice that when k is large this error term is also going to be large. Throughout this thesis C denotes an absolute constant, whose value may vary from one line to the next.

The theorem above shows that the only way that this error term can be small, when k is large, is if $(b-a)$ is very small, but that isn't necessarily true. So the midpoint rule is a very poor approximation to $I[f]$ if k is large and $(b-a)$ is large. As we have the second derivative of $g(x)$ in our error term it is clear that if g was a first order polynomial the error would be zero, as was stated earlier.

The midpoint rule can be changed to get a better approximation, the way that this can be done is by using the Composite Midpoint Rule. The composite midpoint rule splits $[a,b]$ into N intervals, and applies the midpoint rule on each interval separately and sums them up.

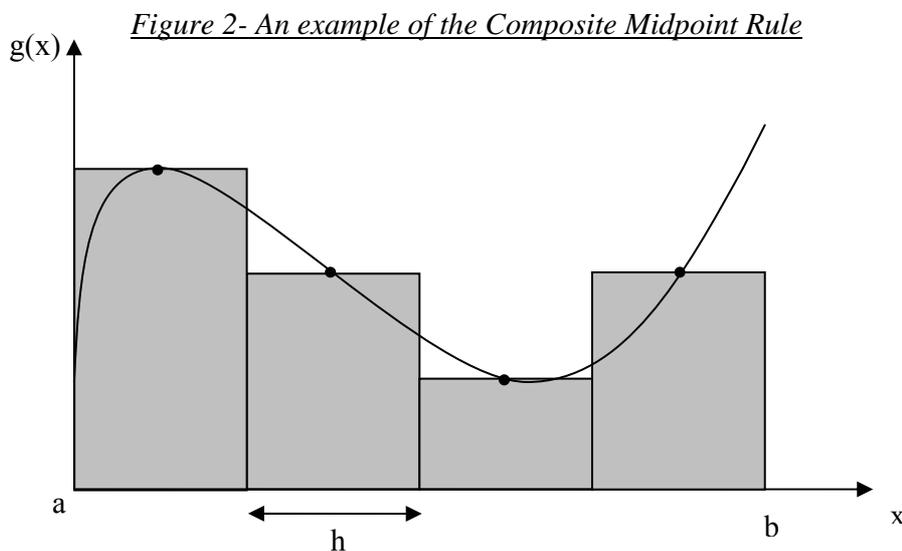
Definition 2.2- The Composite Midpoint Rule applied to a general function $g(x)$, between the limits $[a,b]$ is defined as

$$\int_a^b g(x)dx \approx \sum_{n=1}^N hg(a + (n - 1/2)h) \quad (2.8)$$

Where $h = \frac{b-a}{N}$, and N is the number of intervals that split up $[a,b]$. We use equal interval lengths because it is easier to calculate for the first three quadrature methods.

The way this quadrature method works is that it uses the midpoint in each interval and calculates g at that point and draws a line so that the interval is a rectangle, then calculates the area under that rectangle. The method does this under all the intervals

and adds them up to give an approximation to the true integral. The figure below shows an example of how the composite midpoint rule works. The function $g(x)$ is a general function and we have 4 intervals in $[a,b]$ for which the function is going to be approximated on. As can be seen the midpoint is shown and a horizontal line is drawn in each section. It is clear that the midpoint rule is not very good at approximating an integral when there are a small number of intervals but as the number of intervals N increases the approximation does get better. The reason that the composite midpoint rule is used in many cases is because it is easy to calculate and it is also easy to program.



The best way to see how good an approximation the Composite Midpoint Rule is would be to find out the approximate error.

Theorem 2.3 - The error term for the composite midpoint rule applied to a general function $g(x)$ is defined as

$$e_j \leq Ch^2|g''(\xi)| \quad (2.9)$$

and more so when we apply it to $I[f]$ we will have an error term

$$e_j \leq Ch^2(k)^2|f''(\xi)| \quad (2.10)$$

Where h is the step size of each section, $\xi \in [a,b]$ and C is an arbitrary constant, which will be determined..

Proof

The error of the composite midpoint rule applied to $g(x)$ is defined as $e_{cm} := |I - I_{cm}|$ where

$$I = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} g(x) dx \quad \text{The exact solution } I[f]$$

$$I_{cm} = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} g(a + (j-1/2)h) dx \quad \text{The composite midpoint approximation to } g(x)$$

we work through the error analysis in the same way as we did for the original Midpoint rule. We replace the $g(x)$ in I by a Taylor series applied at $a+(j-1/2)h$ to give

$$|e_{cm}| = \left| \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} (x - (a + (j-1/2)h)) g'(a + (j-1/2)h) dx + \int_{a+(j-1)h}^{a+jh} (x - (a + (j-1/2)h))^2 \frac{g''(\xi)}{2!} dx \right|$$

where once again $\xi \in [a, b]$. Now we can integrate, but noticing that the limits have changed from when we did this before, doesn't actually make a difference to the first term, this cancels as before leaving us only the second term and also noticing that

$(a + jh) - (a + (j-1)h) = h$ we get an error term

$$|e_{cm}| = \sum_{j=1}^N |g''(\xi)| \frac{h^3}{24} = \frac{Nh^3}{24} |g''(\xi)| = Ch^2 |g''(\xi)|$$

This is therefore the error as was given in (2.9) and the power of h has been decreased because we have summed up all of the intervals and $C=1/24$.

Definition 2.3 - Now we need a formula for the midpoint rule applied to $I[f]$, and this is produced by just replacing $g(x)$ by $f(x)e^{ikx}$ to give

$$\int_a^b f(x)e^{ikx} dx \approx \sum_{n=1}^N hf(a + (n-1/2)h)e^{ik(a+(n-1/2)h)} \quad (2.11)$$

As we saw for the original midpoint rule to get the error term when this is applied to $I[f]$ we need to replace $g(x)$ by $f(x)e^{ikx}$ and differentiate twice. We again use theorem 2.2 to simplify this term so the error term of the composite midpoint rule when applied to $I[f]$ is

$$e_j \leq Ch^2(k)^2 |f''(\xi)|$$

as defined in (2.10)

The theorem above shows us that now we can change how many intervals we have to get a better approximation. This method is a lot better than the original midpoint rule. This is of course obvious but the error does show us one very important aspect of the method, that it is again dependant on the second derivative of $g(x)$. This means that if the second derivative is large then so is the error. The method is therefore a fair approximation for most functions but when we look at the function that we are

interested in we see that the error term grows so our step size has to be very small for us to get a good result.

Lemma 2.1 - For our composite midpoint approximation to $I[f]$ it can be easier to write the error in the form of the greatest factors for which the error is dependant, this form is

$$e_j \leq C(hk)^2$$

So it is clear that if k is large like we are intending looking to solve for, then the error is going to grow at a rate of k squared. The only way to decrease the error is to make h very small. The second form for our error is the best to see what exactly we need to do to get a good result, (this of course is if all other terms are relatively small). In this case as k gets large we need to let h get small at the same rate and as the composite midpoint rule is a poor approximation on a non-oscillatory integral on an oscillatory integral it is even worse and h has to be very small for us to get a good approximation. We now need to be able to see some practical results of the composite midpoint rule, and to do this a program in Matlab has been created to find the error for a given function.

Example 2.1 - The function that we are going to look at is

$$\int_0^1 e^{(1+ik)x} dx \quad (2.12)$$

This is our integral $I[f]$, where here $f(x) = e^x$.

The program has been run to show how good the method is on a non oscillatory integral (when k is small), mildly oscillatory integral (when k is 10) and a highly oscillatory integral (when k is 100). The program calculates the approximate value, the exact value and the absolute error that is found. In the table below the program has been run with $k=1, 10$ and 100 for the number of step sizes being 4, 8, 16, 32, 64, and 128. We can approximately estimate the error that we should be seeing for our example. This is

$$e_j \leq C(hk)^2 \left| e^{(1+ik)\xi} \right|_{\xi \in [0,1]} \leq C(hk)^2$$

The third term is restricted and is included in the constant so we are looking at the error to be dependant on h and k . We should expect to get reasonable results when k is small, but not anything that will converge fast, and as k gets larger we should expect

to see that the results do get worse and it takes many intervals N to get the error even under 1.

Table 2.1

k	N	Error e_{cm}
1	4	8.598644053E-03
	8	2.148751918E-03
	16	5.374381485E-04
	32	1.343599540E-04
	64	3.35898850E-05
	128	8.3974712E-06
10	4	1.143894736E-01
	8	2.465250208E-02
	16	5.953557152E-03
	32	1.475782821E-03
	64	4.368165183E-04
	128	9.199263084E-05
100	4	1.704945960
	8	1.707292228
	16	1.690171991
	32	1.082230203E-02
	64	2.105996229E-03
	128	4.981234001E-04

The table above shows our results, it is clear that when k is small the midpoint needs about 16 intervals to get a really good result, but as k get bigger we see that the number of intervals needs to increase to get the same error. The next table shows about how many intervals, N , we need to get a 1% relative error. This is the error that we have divided by the exact solution

Table 2.2

k	1	10	20	40	80	160	320	640
N	9	64	129	258	516	1033	2066	4132

The table above gives a very interesting result, this is that as k doubles then the number that N has to increase by to get a 1% relative error is also double.

Trapezium rule and the Composite Trapezium Rule

The next quadrature method that we are going to look at is the Trapezium Rule. We would expect the Trapezium Rule to be better than the Midpoint Rule as it uses more points to get an approximation, but depending on the function it is applied on, the Trapezium Rule is pretty much the same as the Midpoint Rule. The Trapezium Rule calculates the function at the two endpoints and calculates the area under the trapezium formed.

Definition 2.4- The Trapezium rule when applied to a general function $g(x)$ between the limits $[a,b]$, is

$$\int_a^b g(x) \approx \left(\frac{1}{2}f(a) + \frac{1}{2}f(b)\right)(b-a) \quad (2.13)$$

The formula above is one way to look at the Trapezium Rule, but another way to look at it is that we wish to draw a line between $f(a)$ and $f(b)$, and then integrate under that line. The reason we wish to do this is because the error analysis is easier when looking at the Trapezium Rule in this way so from now on in this project the Trapezium Rule will be dealt with in the form of Definition 2.5.

Definition 2.5- The trapezium rule when applied to $g(x)$ in $[a,b]$ can be written as

$$\int_a^b g(x) \approx \int_a^b (cx + d)dx \quad (2.14)$$

where $c = \frac{g(b) - g(a)}{b-a}$ and $d = \frac{bg(a) - ag(b)}{b-a}$

Proof

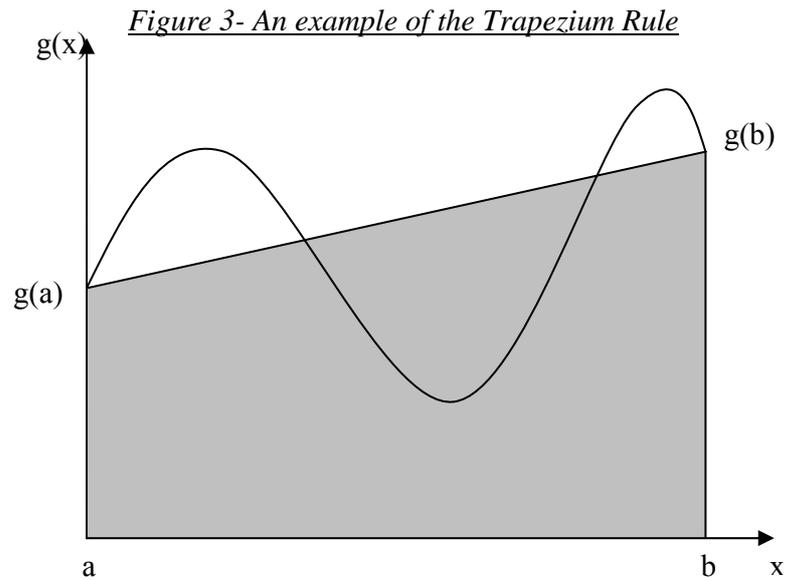
We wish to create a line that at $x=a$ is $g(a)$ and at $x=b$ is $g(b)$, so therefore we need to create two simultaneous equations of the form

$$1) \quad ca + d = g(a)$$

$$2) \quad cb + d = g(b)$$

Solving these equations for c and d gives us our formula.

The diagram below is a good example of how the trapezium rule works on a general function $g(x)$



The best way to see how good at approximating $g(x)$ the Trapezium Rule is to look at the error analysis.

Theorem 2.4- The error term for the Trapezium Rule when applied to a general $g(x)$ in $[a,b]$ is

$$e_t \leq \frac{(b-a)^3}{12} |g''(\xi)| \quad (2.15)$$

and when applied to $I[f]$ the error term becomes

$$e_m = \frac{(b-a)^3}{12} (k)^2 |f''(\xi)| \quad (2.16)$$

Proof

To work out the error we need to find $|e_t| = |I - I_t|$ where

$$I = \int_a^b g(x) dx \quad \text{The exact solution } I[f]$$

$$I_t = \int_a^b (cx + d) dx \quad \text{The trapezium approximation to } g(x), c \text{ and } d \text{ are as defined earlier}$$

so our error term is of the form

$$|e_t| = \left| \int_a^b [g(x) - cx - d] dx \right| \quad (2.17)$$

To get this term into a better form and to be able to find out the leading order of the error we need to use Theorem 2.5

Theorem 2.5 - From “Burden & Faires- Numerical analysis” p111 (2).

Suppose x_0, x_1, \dots, x_n are distinct numbers in $[a, b]$. Then for each x in $[a, b]$, a number ξ in (a, b) exists with

$$f(x) = P(x) + \frac{f^{(n+1)}(\xi)}{(n+1)!} (x - x_0)(x - x_1) \dots (x - x_n) \quad (2.18)$$

where $P(x)$ is a polynomial of degree n , which is the polynomial that interpolates f at the points x_0, x_1, \dots, x_n .

We can use this theorem in our error analysis, letting $P(x) = cx + d$ and $n=1$, and setting $x_0=a, x_1=b$ be the points in (2.18). then

$$g(x) - cx - d = \frac{g''(\xi)}{2} (x - a)(x - b) \quad (2.19)$$

and we can substitute this into (2.13) to give us our new error estimate

$$e_t = \left| \int_a^b \left[\frac{g''(\xi)}{2} (x - a)(x - b) \right] dx \right|$$

Now we can once again just integrate the expression above and input the limits to give us our error term.

$$\begin{aligned} e_t &= \left| \frac{g''(\xi)}{2} \int_a^b (x^2 - (a+b)x + ab) dx \right| = \left| \frac{g''(\xi)}{2} \left[\frac{x^3}{3} - \frac{(a+b)x^2}{2} + abx \right]_a^b \right| \\ &= \left| \frac{g''(\xi)}{2} \left(\frac{b^3}{3} - \frac{(a+b)b^2}{2} + ab^2 - \frac{a^3}{3} + \frac{(a+b)a^2}{2} - a^2b \right) \right| = \left| \frac{g''(\xi)}{12} \right| (a-b)^3 \end{aligned}$$

The error term is very similar to the error term that we have for the Midpoint Rule, except that the error term is over 12 not 24. The error term for the Trapezium Rule when applied to $I[f]$ is just the formula above with the usual change using Theorem 2.2 and so the error term is of the form

$$e_m = \frac{(b-a)^3}{12} (k)^2 |f''(\xi)|$$

as defined in (2.16)

The theorem above does make it seem that the error term for the Trapezium Rule is better than for the Midpoint rule but it is very misleading. The best way to look at the error is by the leading term order and the leading term order is k^2 , which both of the methods have. The Midpoint Rule or the Trapezium rule can be a better approximation as the ξ can be anywhere in $[a, b]$ so the $g''(\xi)$ term can be different for the Midpoint Rule and the Trapezium Rule. The Composite Trapezium Rule is constructed by the Trapezium Rule in the same way as the Composite Midpoint Rule

is constructed from the Midpoint rule. We can have two ways that we can construct the Composite Trapezium Rule and in Definition 2.6 these two ways have been stated.

Definition 2.6 - The composite trapezium rule is defined as below when applied to a general function $g(x)$ in $[a,b]$.

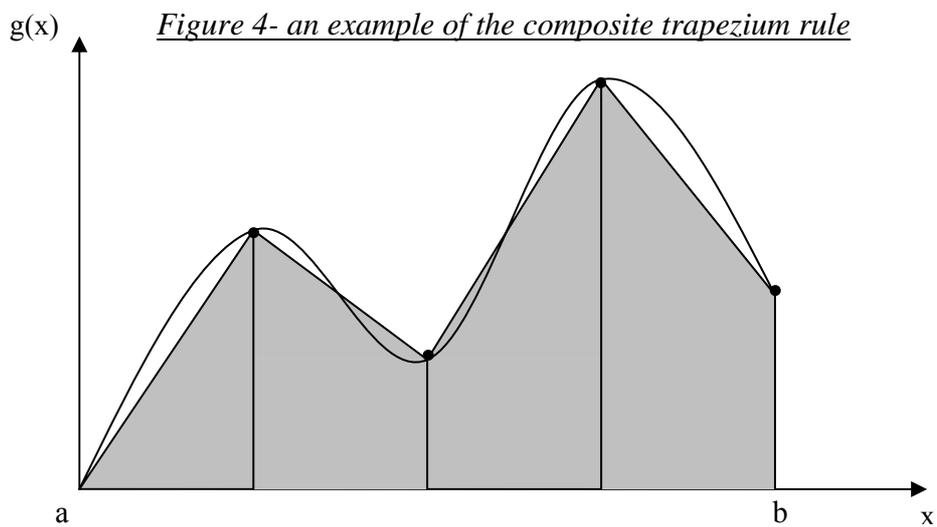
$$\int_a^b g(x)dx \approx \left(\sum_{n=1}^{N-1} hg(a + nh)\right) + \frac{1}{2}hg(a) + \frac{1}{2}hg(b) \quad (2.20),$$

and more so, when using the $(cx + d)$ notation the Composite Trapezium Rule is defined as

$$\int_a^b g(x)dx \approx \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} (cx + d)dx \quad (2.21)$$

$$\text{where } c = \frac{g(a + jh) - g(a + (j-1)h)}{h} \text{ and } d = \frac{(a + jh)g(a + (j-1)h) - (a + (j-1)h)g(a + jh)}{h}$$

The information above shows that once again we have two ways that we can create the Trapezium Rule. The first one is the most common way that it is written and this is why it has been added to this project, but we will concentrate on the second way more because it makes the error analysis a lot easier. The figure below shows an example of the Composite Trapezium Rule once again with four segments it is clear here that a better approximation is created.



Once again the best way of seeing how good the Composite Trapezium Rule is at evaluating the integral of $g(x)$ is by looking at the error formula.

Theorem 2.6 - The error formula for the Composite Trapezium Rule when applied to a general function $g(x)$ on $[a,b]$ is defined as

$$e_{ct} \leq \frac{h^2}{12} |g''(\xi)| \quad \xi \in [a,b] \quad (2.22)$$

and so the error for the Composite Trapezium Rule when applied to $I[f]$ is

$$e_{ct} = \frac{h^2}{12} (k)^2 |f''(\xi)| \quad (2.23)$$

Proof

In the same way as we found the error for the trapezium rule is applied here. We wish to find $|I - I_{ct}|$ where

$$I = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} g(x) dx \quad \text{the exact solution } I[f]$$

$$I_{ct} = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} (cx + d) dx \quad \text{the composite trapezium approximation to } g(x), c, d \text{ are as defined earlier}$$

Using Theorem 2.5 we can once again use (2.18) to give us

$$|e_{ct}| = \left| \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} \left[\frac{g''(\xi_j)}{2} (x - (a + (j-1)h))(x - (a + jh)) \right] dx \right| \quad (2.24)$$

if we integrate like we did before and then we get

$$\begin{aligned} e_t &= \left| \sum_{j=1}^N \frac{g''(\xi_j)}{2} \int_{a+(j-1)h}^{a+jh} (x^2 - \overbrace{(2a+h)x}^e + \overbrace{(a^2 + ah(2j-1) + h^2(j^2 - j))}^f) dx \right| = \frac{g''(\xi_j)}{2} \left[\frac{x^3}{3} - \frac{ex^2}{2} + fx \right]_{a+(j-1)h}^{a+jh} \\ &= \sum_{j=1}^N \frac{g''(\xi_j)}{12} (h)^3 = \frac{g''(\xi)}{12} |h^2| \end{aligned}$$

and if we use the Composite Trapezium Rule on $I[f]$ we will get

$$|e_k| = \frac{h^2}{12} (k)^2 |f''(\xi)|$$

by using theorem 2.2 to cancel terms down and is the same as (2.23)

The theorem above shows that the Composite Trapezium Rule has an error term very similar to the Composite Midpoint Rule. This means that once again either method could be better as when we look at the leading term order they are both of the form

$$e \leq C(hk)^2$$

and the rest of the error term is added to the arbitrary constant C , which will be different for both methods. The best way therefore is to look at some results.

Example 2.2 - Once again a program has been created for the composite trapezium rule, which finds the exact and the approximate solutions and finds the absolute error. The table below shows the results that have been found. It uses the example 2.1 on with the trapezium rule and then as we can compare results. We should expect to get a similar results to the midpoint rule when k is small but when k is large we shouldn't see much of a difference.

Table 2.3

k	N	Error e_{ct}
1	4	1.711979518E-02
	8	4.299504195E-03
	16	1.074876302E-03
	32	2.681907966E-04
	64	6.717976998E-05
	128	1.679494250E-05
10	4	2.110555658E-01
	8	4.835119869E-02
	16	1.184954854E-02
	32	2.947998577E-03
	64	7.361079223E-04
	128	1.839713650E-05
100	4	1.17143669276
	8	1.70964180098
	16	1.70846609499
	32	1.898876961E-02
	64	4.083283495E-03
	128	9.886440664E-04

The table below is once again how many intervals we need to get a 1% relative error and we can see that just like with the composite midpoint rule that as k doubles, we have to double N .

Table 2.4

k	1	10	20	40	80	160	320	640
N	12	91	180	365	730	1460	2921	5842

The Simpson's Rule and the Composite Simpson's Rule

The Simpson's rule is the third quadrature rule that we are going to look at in this project. This method is a better approximation than the last two methods because it uses more points to evaluate the solution. In fact the Simpson's rule uses the three nodes unlike the trapezium rule. And with those three nodes we have two endpoints, like the trapezium rule and a midpoint like the midpoint rule. We could say then the Simpson's rule is a combination of the last two methods. The Simpson's rule actually obtains a quadratic in each section so it will be able to fit the data a lot better.

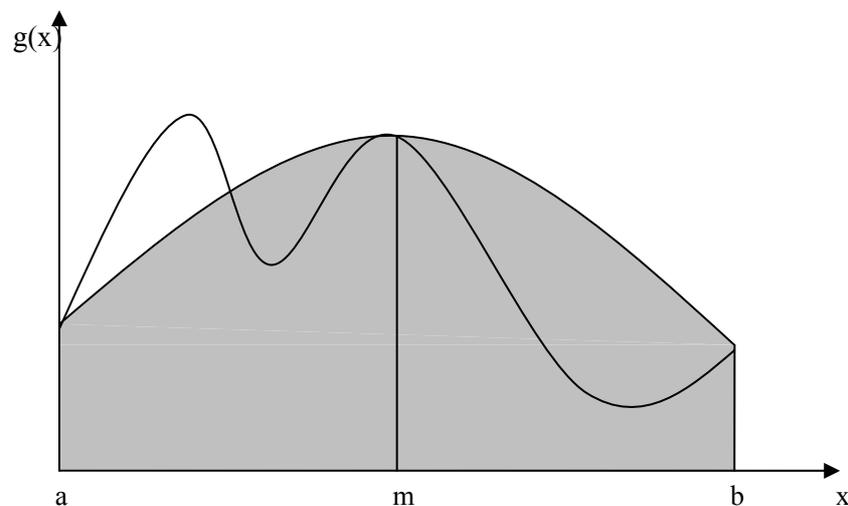
Definition 2.7 - The Simpson's rule when applied to a general function $g(x)$ in $[a,b]$ is defined as

$$\int_a^b g(x)dx \approx \frac{h}{3}(f(a) + 4f(m) + f(b)) \quad (2.26)$$

where here a and b are the end points of $[a,b]$ and m is the midpoint of the interval we are looking at. h here is $\frac{(b-a)}{2}$, half of the interval and m can be defined as

$m=(a + h)$. The reason that the form of the Simpson's rule has been defined as above and not as a polynomial is because when looking at it in this form the error term is easier to find. The diagram below shows the Simpson's rule for a general function $g(x)$ on $[a,b]$. It is clear that the Simpson's rule approximates the function by a quadratic.

Figure 5- An example of the Simpson's rule



From the diagram it is clear that the Simpson's rule is a lot better than the last two methods that we have looked at but the best way to look at this is to look at the error analysis

Theorem 2.7 - The error of the Simpson's rule when applied to a general function $g(x)$ in $[a,b]$ is

$$e_s \leq Sh^5 |g''''(\xi)| \quad (2.27)$$

and more so when the Simpson's rule is applied to $I[f]$ we would expect an error of

$$e_s \leq Sh^5 (k)^4 |f''''(\xi)| \quad (2.28)$$

Proof

The error term for the Simpson's rule is $|e_s| = |I - I_s|$ where

$$I = \int_a^b g(x) dx \quad \text{The exact solution } I[f]$$

$$I_t = \int_a^b \frac{(f(a) + 4f(m) + f(b))}{3} dx \quad \text{The Simpson's rule approximation to } g(x)$$

The error term actually comes from finding definition 2.7. In finding definition 2.7 we also find the error term. We can start by using Taylor series on $g(x)$ at the midpoint of $[a,b]$, which we will call x_1 .

$$g(x) = g(x_1) + g'(x_1)(x - x_1) + \frac{g''(x_1)}{2}(x - x_1)^2 + \frac{g^{(3)}(x_1)}{6}(x - x_1)^3 + \frac{g^{(4)}(\xi)}{24}(x - x_1)^4$$

now as we are wishing to find the integral of $g(x)$ we can integrate the above term and obtain

$$\int_a^b g(x) dx = [g(x_1)(x - x_1) + g'(x_1)(x - x_1)^2 + \frac{g^{(2)}(x_1)}{2}(x - x_1)^3 + \frac{g^{(3)}(x_1)}{6}(x - x_1)^4]_a^b + [\frac{g^{(4)}(\xi)}{24}(x - x_1)^5]_a^b$$

When we insert the limits into the above formula then some of the terms cancel, in fact when the power of $(x-x_1)$ is even then they cancel and when it is odd we obtain 2 times that power of h , so we will then obtain the equation

$$\int_a^b g(x) dx = 2hg(x_1) + \frac{h^3}{3}g''(x_1) + \frac{g^{(4)}(\xi)}{60}h^5 \quad (2.29)$$

we need to now to find a way of changing the second term into a more favorable form. To do this we need to use another theorem that has already been used.

Theorem 2.8- from Burden & Faires- Numerical analysis (2) p175.

If x_n is in $[a,b]$ then

$$f''(x_n) = \frac{1}{h^2} [f(x_n - h) - 2f(x_n) + f(x_n + h)] - \frac{h^2}{12} f'''(\xi) \quad (2.30)$$

where $x_n - h < \xi < x_n + h$

We can now just let $x_n = x_1$ and so $x_1 - h = a$ and $x_1 + h = b$. When we add this to (2.26) we get

$$\int_a^b g(x) dx = 2hg(x_1) + \frac{h}{3} [g(a) - 2g(x_1) + g(b)] - \frac{h^5}{36} g''''(\xi_1) + \frac{g''''(\xi_2)}{60} h^5$$

now the above formula is our definition of the Simpson's rule plus an error term. The problem is that the error term is in two pieces and to get this into one piece we need to use the following lemma

Lemma 2.2 - If $f^{(4)}$ is continuous on $[a, b]$ then the intermediate mean value theorem states that

$$f^{(4)}(\xi) = \frac{1}{2} [f^{(4)}(\xi_1) + f^{(4)}(\xi_2)]$$

so when substituting this in and taking the modulus of the error term we obtain the expression

$$e_s = \left| \frac{g^{(4)}(\xi)}{90} \right| h^5,$$

which is (2.27) with $S = \frac{1}{90}$. The error term for the Simpson's rule applied to $I[f]$ follows on in the same way as it has before and so we will have an error of

$$e_s = \frac{Ch^5(k)^4 |f^{(4)}(\xi)|}{90}$$

to get this we need to follow a similar line as we did for theorem 2.2, this though is not going to be proved but follows in a very similar fashion.

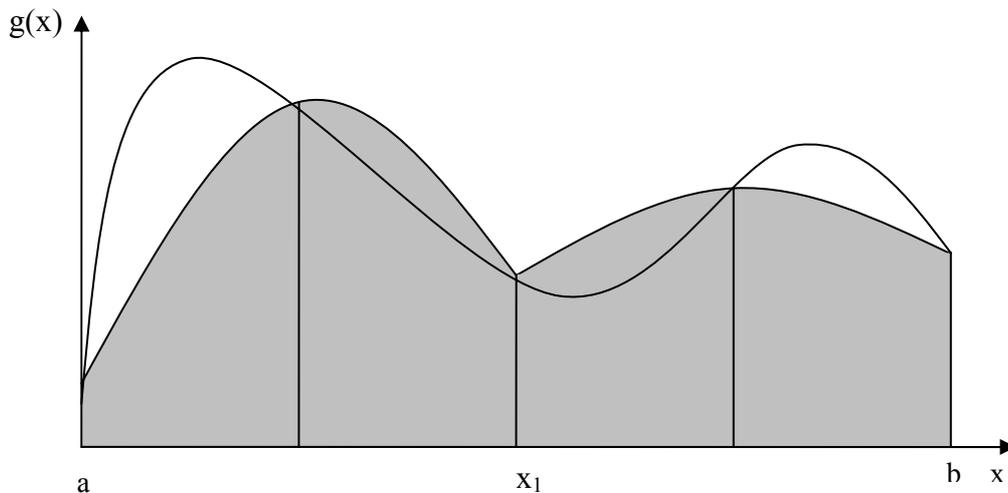
The above theorem shows that the Simpson's rule is a better approximation than the last two quadrature methods we have looked at in terms of the error when not looking at $I[f]$. When we do look at this method in respect to $I[f]$, the approximation to the error isn't actually any better than for the last two and if k is large it is worse as k^4 grows more than k^2 . Now we need to see what happens when we split the interval $[a, b]$ up to make the composite Simpson's rule.

Definition 2.8 - The composite Simpson's rule when applied to a general function $g(x)$ is of the form

$$\int_a^b g(x)dx \approx \frac{h}{3} [g(a) + g(b) + 2 \sum_{n=1}^{N/2-1} g(x_{2n}) + 4 \sum_{n=1}^{N/2} g(x_{2n-1})] \quad (2.31)$$

Where $x_n = a + nh$ and h is the size of each interval with equal length.. The best way to demonstrate this method is to look at the diagram below, as you can see in each interval there is a quadratic, though this is only a small example. When the interval length shortens the Simpson's rule becomes very exact and it is clear that this interval is halved then we would obtain a very good approximation. The diagram is therefore our formula with two sections. This is because unlike with the trapezium rule (which can only fit linear functions exactly) the Simpson's rule fits a quadratic exactly, so if we wanted to find the integral of a quadratic then it would give the correct answer. All this means that as an interval gets smaller then it is more likely to be able to fit a function before the trapezium rule or the midpoint rule.

Figure 6- An example of the composite Simpson's rule



Now we need to look at the error formula.

Theorem 2.9 - The error formula of the Simpson's Rule when applied to a general function $g(x)$ on $[a,b]$ is

$$e_{cs} \leq Fh^4 |g''''(\xi)| \quad \xi \in [a,b] \quad (2.32)$$

with F as an arbitrary constant. And more so when the Simpson's rule is applied to $I[f]$ we get an error term of

$$e_{cs} \leq Fh^4 (k)^4 |f^{(4)}(\xi)| \quad \xi \in [a,b] \quad (2.33)$$

Proof

If we follow through the proof of theorem 2.8, except we use a sum term and change of the limits we will obtain a very similar term as we did before and as we found that the error term of the method goes down by a power of h as we are summing all the terms this happens again and so we get the above terms.

So the power of h has grown to a quartic, which means that as h gets small, (ie. Less than one) the error gets very small, but on the other hand we have a fourth derivative of g in our error estimate, so if this is large then our error will increase.

Definition 2.9 - The Simpson's rule when applied to our first integral $I[f]$ on $[a,b]$ is defined as

$$\int_a^b f(x)e^{ikx} dx = \frac{h}{3} [f(a)e^{ika} + f(b)e^{ikb} + 2 \sum_{n=1}^{N-1} f(x_{2n})e^{ikx_n} + 4 \sum_{n=1}^N f(x_{2n-1})e^{ikx_{2n-1}}] \quad (2.34)$$

This formula is a bit more complex to program than the last two methods, but it isn't too complicated. Once again the best way to see the error is below and we have the same ration of (hk) as for the first two methods.

$$e_{cs} \leq F(hk)^4 \quad (2.35)$$

So the error estimate for the Simpson's rule applied to $I[f]$ is the same as for the Midpoint rule for large k, and if k is very, very large then h has to decrease dramatically to get a good result. The best way to look at how the Simpson's rule works in consideration to the Midpoint rule and the Trapezium rule is by looking at the ratio (hk) . If $(hk) < 1$ the Simpson's rule will be better at approximating the integral, but if $(hk) > 1$ then the Simpson's rule is worse, and h will have to be decreased to get a good result.

Example 2.3 -A program has been created again in Matlab for the Simpson's rule applied to example 2.1 with the same constraints as were used for the midpoint rule and the Trapezium Rule.

Table 2.5

k	N	Error e_1
1	4	1.433047207E-04
	8	8.957255308E-06
	16	5.598312319E-07
	32	3.498946311E-08
	64	2.186841795E-09
	128	1.366777543E-10
10	4	2.27130831E-01
	8	6.03838457E-03
	16	3.24500874E-04
	32	1.95783613E-05
	64	1.21307483E-06
	128	7.56535225E-08
100	4	1.70805212514
	8	1.70807325495
	16	1.70807460153
	32	5.57513418E-01
	64	8.85481914E-04
	128	4.29118644E-05

If we compare the results that we have already got we can see that for a small k the Simpson's rule is by far the best at getting the smallest error. The results show that when k is equal to 1 then the error for the Simpson's rule is very good for only four intervals, but on the other hand when k is 100 the Simpson's rule is not very effective until we have 64 intervals, this is because of the (hk) ratio and we need h to be sufficiently small to get a good ratio.

Table 2.6

k	1	10	20	40	80	160	320	640
N	2	14	30	62	124	248	496	994

The table above is once again that as k doubles, then N has to also double to get a 1% relative error. This is the result because when looking at the error terms for all

three methods used so far, the error term has the same ratio for h and k, therefore we get this result.

Gaussian Quadrature

The Gaussian quadrature method is the best quadrature method that we are going to look at; it gives $2N$ parameters to choose the weights and the nodes. For this method the nodes are not defined as $(a+nh)$ or $(a+(n-1/2)*h)$ but as the zeros of the Legendre Polynomials. The problem with the Legendre polynomials is that there is not an analytical formula for them, just an iterative formula. This makes it difficult to compute the solution, fortunately there is an program in matlab that will find the zero's for a specific N , which is used to evaluate our solution. The reason that the Legendre polynomials are used is because this is the optimal positions for the nodes. This has been proved before and will not be dealt with in this project, (we are going to take this for granted).

Definition 2.10 - The Gaussian quadrature method when applied to a general function $g(x)$ on $[a,b]$ is defined as

$$\int_a^b g(x)dx = \frac{b-a}{2} \int_{-1}^1 g\left(\frac{b-a}{2}x + \frac{b+a}{2}\right)dx = \frac{b-a}{2} \sum_{i=0}^N b_i g\left(\frac{b-a}{2}x_i + \frac{b+a}{2}\right) \quad (2.36)$$

where b_i are weights defined by

$$b_i = \int_a^b \prod_{\substack{j=1 \\ j \neq i}}^N \frac{x - x_j}{x_i - x_j} dx \quad (2.37)$$

and x_i denote the zero's of the Legendre polynomials which are of the form,

$$P_n(x) = \frac{d^n}{dx^n} \frac{(x^2 - 1)^n}{(2^n n!)} \quad (2.38)$$

Gaussian quadrature is designed to solve in the interval $[-1,1]$, so we have had to change the interval for our integral and so this makes our calculation even more complex.

Gaussian quadrature is designed to minimize any error that can occur for a general N , so as N gets large then the Gaussian method will get a lot better than the last three methods. As we have already spoken about, the nodes are not equally spaced like we have seen before but are placed in an optimal positions for different N s. The weights

are also optimal, this means that they have the greatest degrees of freedom, $2N$, to fit a polynomial to the function $g(x)$ and will fit a polynomial of degree $2N-1$ to $g(x)$ in each interval. Once again this has been proved before and won't be proved in this project. In all sources that I have read the Gaussian quadrature method is very highly rated and it is meant to be the best quadrature method, but this is for a general $g(x)$, not for our oscillatory integral and so we need to find an error estimate for this method.

Theorem 2.10 - The error estimate that was found from the Mathworld (7) website is

$$e_N \leq G \frac{1}{(2N)!} |g^{(2N)}(\xi)| \quad (2.39)$$

where $\xi \in [a,b]$ and G is an arbitrary constant. The error is no longer dependant on a power of h but on a factorial of N , the number of intervals. This means that when N is large the error will be very small, but once again we have a derivative of g in our error formula, and this time it is not an exact derivative but as N gets large the number of derivatives on g also gets large. So if the $(2N)$ 'th derivative of g is large then the error will also be large. Now we need to apply the Gaussian quadrature to $I[f]$ which is

$$\int_a^b g(x)dx = \frac{b-a}{2} \sum_{i=0}^N b_i f\left(\frac{b-a}{2}x_i + \frac{b+a}{2}\right) e^{ik\left(\frac{b-a}{2}x_i + \frac{b+a}{2}\right)} \quad (2.40)$$

Once again the error estimate for the Gaussian quadrature when applied to $I[f]$ is going to grow, as the $(2N)$ 'th derivative of $I[f]$ is going to be very large for large N , which is going to be larger than $N!$. This means that though Gaussian quadrature is the best quadrature method, when it is applied to $I[f]$ the error grows. There is once again a program created in matlab for the gauss method. The results are listed below for the example used for all the methods before. We should expect to get an error term of the form

$$e_m \leq G \frac{k^{2N}}{(2N)!} \quad (2.41)$$

This produced on the basis of Theorem 2.2, that the $(2N)$ 'th derivative is going to have leading term order of k^{2N} and the rest of the terms are all incorporated in the arbitrary constant G .

Example 2.4 - The example 2.1 is now going to be applied with Gaussian quadrature. The results below are the outcome of this example and to show the full effects of

Gaussian quadrature a few extra N s have been added. These are added to show that Gaussian quadrature is good when N is small, when k is small.

Table 2.7

k	N	Error e_1
1	1	1.373954840E-01
	4	1.483580528E-08
	8	1.110223024E-15
	16	0
	32	error calculated as zero
	64	after this
	128	
10	1	1.998667775780
	4	5.148383499E-02
	8	2.144931312E-07
	16	2.355138688E-16
	32	0
	64	error calculated as zero
	128	after this
100	1	1.65839419221
	4	3.73285228E-01
	8	7.13048250E-01
	16	3.75242466E-01
	32	1.996499003E-04
	64	1.824388152E-15
	128	1.396314475E-15

The table above shows that Gaussian quadrature is a lot better than any of the quadrature we have looked at, so if we are going to look at a medium oscillatory integral, then Gaussian quadrature would be alright at evaluating it, but we do need to look at different methods to see if we can get a better result. Table 2.8 is the table that shows how many intervals needed for specific values of k to get a 1% relative error.

Though not as clear as for the past few quadrature method the number of intervals N does roughly need to double when k doubles. This means that for all of the quadrature methods this property is observed. We can also notice that even though the values of N are small in the table below as k gets very large they will always double, making the number of intervals grow to very large numbers.

Table 2.8

k	1	10	20	40	80	160	320	640
N	2	6	9	15	27	49	93	177

It is clear from all the methods that we have looked at for simple quadrature methods, none of them are very good at evaluating our integral $I[f]$. the reason that this happens is because the error function for all quadrature methods include derivatives of the functions that are being solved for. When the function is highly oscillatory the derivative is very large, (in our case a power of k) and this make the error term grow too large. The only way that we can get good results is by decreasing h so that the powers of k are counteracted and the error decreases. The problem is that as k is going to be very large our step sizes have to be very small, and this is going to give us a lot of problems computationally. If h has to be very small the programs will take up a lot of memory and computational time. The programs above can actually solve for large k , but for practical problems k is going to be very large, larger than we have calculated for, and quadrature methods are not going to be good enough for us in this project.

3) Asymptotic Methods

In this section we will look at an asymptotic method called Integration by parts. It creates a finite term sum, found by integrating $I[f]$ by parts N times.

Definition 3.1 - The Integration by Parts approximation to $I[f]$ in $[a,b]$ is defined by

$$\int_a^b f(x)e^{ikx} dx = \sum_{n=1}^N \frac{(-1)^{n-1}}{(ik)^n} \left[(f^{(n-1)}(x)e^{ikx}) \right]_a^b + \frac{(-1)^N}{(ik)^{N+1}} \int_a^b f^{(N)}(x)e^{ikx} dx \quad (3.1)$$

Proof

Firstly we integrate $I[f]$ by parts to obtain

$$\begin{aligned} \int_a^b f(x)e^{ikx} dx &= \left[\frac{f(x)e^{ikx}}{ik} \right]_a^b - \frac{1}{ik} \int_a^b f'(x)e^{ikx} dx \\ &= \frac{1}{ik} \left[f(x)e^{ikx} \right]_a^b - \frac{1}{(ik)^2} \left[f'(x)e^{ikx} \right]_a^b + \dots \end{aligned}$$

If we integrate again by parts it is clear that there is a pattern that occurs and the solution is

$$\int_a^b f(x)e^{ikx} dx = \sum_{n=1}^N \frac{(-1)^{n-1}}{(ik)^n} \left[(f^{(n-1)}(x)e^{ikx}) \right]_a^b + \frac{(-1)^N}{(ik)^{N+1}} \int_a^b f^{(N)}(x)e^{ikx} dx$$

It is clear to see that the leading term order of this approximation is of $O(1/k)$, so as $k \rightarrow \infty$ then the error decreases. The error in this case is the remainder term defined below. This error goes to zero as k gets large, so as k gets large the approximation gets better. We can see that after about a few terms in the series the error would be very small as the inverse of a power of k , will be very small, and therefore negligible. Looking at the error it is clear that a remainder term can be created to see how good the error is.

Theorem 3.1 -The remainder term can be created as follows:-

$$R[f] = \frac{1}{(ik)^{N+1}} \int_a^b f^{(N)}(\xi)e^{ik\xi} dx \quad a < \xi < b \quad (3.2)$$

so the error term has the inverse of a power of k as its leading term so if k is large the error term is only very small.

This method is a good method as it gets a better approximation as k gets large, which as we saw the quadrature methods do not do this. Unfortunately with the asymptotic method when k is small we would obtain a very poor result, and especially when $k < 1$ then we would expect our error to increase when k gets smaller. The numerical results that we should expect to get would be that as k gets large our error should become less as N increases, but on the other hand as k gets small our error would grow. The next thing that needs to be solved is the way that we can program the integration by parts method. The problem we have here is that we have to be able to calculate derivatives and this can be very difficult to do. If we have a polynomial as our $f(x)$, the derivative is easy to calculate and it would be easy to produce a program for this. The same can be said for any sine, cosine and exponential functions. In short the derivatives that are in this method can be calculated by series that we determine.

Example 3.1 - We can now look at our example 2.1 with the integration by parts method, and see how good at approximating it the asymptotic method is. Once again we are going to use the same k 's and step sizes as before so that a good comparison can be made. An extra few N 's in our table are added to show that for a very small number of intervals we get a very good result. We should find that for $k=1$ our answer is not going to give an answer anywhere near the exact one as can be seen by our error term that it is always going to be $O(1)$ and will never home in on the answer. Other than for this we would not expect to get a good answer for $k < 1$, but as k gets large it will be a very fast approximation.

The second table is once again a table to show how many intervals are needed to get a 1% relative error. With this method once k get large a 1% error is obtained with just one approximation. When looking at the result we see that when $k=1$ we don't indeed have any good results, but when $k = 10$ we get better results as N gets large and we soon get an error small enough to be equal to zero when using 18d.p. We should expect that as k gets larger we will get even better results, but if k is less than 1 we would get worse results. The Asymptotic Method is a very good method when we are looking at $I[f]$, if k is large, but our results are clouded by one fact. In our example the derivative was calculated exactly because it never changed, but if we had to approximate the derivative then we would expect to get worse results depending on how good an approximation we use.

Table 3.1

k	N	Error e_1
1	1	1.65101002708
	2	1.65101002708
	4	1.65101002708
	8	1.65101002708
	16	1.65101002708
	32	1.65101002708
	64	1.65101002708
	128	1.65101002708
10	1	3.580851422E-02
	2	3.580851422E-03
	4	3.580851422E-05
	8	3.580851406E-09
	16	6.206335383E-17
	32	The error is calculated as 0 after this
	64	
	128	
100	1	1.923703353E-04
	2	1.923703353E-06
	4	1.923703321E-10
	8	0
	16	The error is calculated as 0 after this
	32	
	64	
	128	

Table 3.2

k	10	20	40	80	160	320	640
N	3	2	1	<1	<1	<1	<1

4) Filon Type Methods

In the paper ‘On the numerical quadrature of highly-oscillating integrals I: Fourier transforms 2003’ (1), Arieh Iserles looks at work first used by Filon in 1924, this work has largely been ignored for 75 years, but his work is seen as the best option for solving certain highly oscillatory integrals. His work used a quadrature formula for the $f(x)$ term and incorporates the oscillatory part of the integral to be part of the weights b_i so that this part doesn’t need to be approximated but is worked out exactly. As we use a quadrature formula for $f(x)$, we can use any one of the formula’s that have already been looked at. In his paper Iserles actually only looks at using Gaussian quadrature to evaluate $f(x)$, but in this project not only is Gaussian quadrature looked at but also a Midpoint and a Trapezium approximation is looked at to approximate $f(x)$. It is very interesting to see what happens when a lesser accurate method and it will also be very interesting to see how much better Filon type methods are on a different quadrature methods.

The Filon-Midpoint Rule

Firstly we will look at the midpoint rule and see how much of a better approximation we get when we use Filon quadrature with it.

Definition 4.1 - The Filon-Midpoint rule when applied to $I[x]$ in $[a,b]$ is defined as

$$\begin{aligned} \int_a^b f(x)e^{ikx} dx &= \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} f(x)e^{ikx} dx \approx \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} f(a+(j-1/2)h)e^{ikx} dx \\ &= \sum_{j=1}^N f(a+(j-1/2)h) \int_{a+(j-1)h}^{a+jh} e^{ikx} dx. \end{aligned} \quad (4.1)$$

So as can be seen $f(x)$ has been approximated by the midpoint rule, but e^{ikx} is still in its original form and must be integrated between each interval. With this method we do not have any degree of x multiplying e^{ikx} as the midpoint rule approximates $f(x)$ by a constant. This means that the integration part is easy for this particular method because e^{ikx} can just be integrated and the limits can be inputted. So the approximation is of the form

$$\sum_{j=1}^N f(a + (j-1/2)h) \left[\frac{e^{ikx}}{ik} \right]_{a+(j-1)h}^{a+jh} = \sum_{j=1}^N f(a + (j-1/2)h) \left(\left[\frac{e^{ik(a+jh)}}{ik} \right] - \left[\frac{e^{ik(a+(j-1)h)}}{ik} \right] \right) \quad (4.2)$$

For the result above we should expect to get a better result than we had for the normal midpoint rule. From what Arieh Iserles has written in his paper we should expect to get a very good result whether k is large or small, and it should be a combination of the asymptotic methods and the quadrature methods, which had problems when k was large or small.

Theorem 4.1 - The error term of the Filon-Midpoint rule when applied to $I[f]$ in $[a,b]$ is

$$e_{fm} \leq Ch^2k \quad (4.3)$$

Proof

The best way to look at the error is to try and find an approximation to it in terms of h and k . The best way to do this is to look at $|e_{fm}| = |I - I_{fm}|$ where

$$I = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} f(x) e^{ikx} dx \quad , \text{ which is the exact solution}$$

$$I_{fm} = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} f(a + (j-1/2)h) e^{ikx} dx \quad \text{which our Midpoint - Filon approximation}$$

if we do subtract these then we obtain the expression

$$|e_{fm}| = \left| \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} [f(x) - f(a + (j-1/2)h)] e^{ikx} dx \right| \quad (4.4)$$

we can now use Taylor series on $f(x)$ at the point $x = a + (j-1/2)h$, to give us

$$f(x) = f(a + (j-1/2)h) + (x - (a + (j-1/2)h)) f'(\xi)$$

So when we substitute this into our equation the first term cancels to give,

$$|e_{fm}| = \left| \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} [(x - (a + (j-1/2)h)) f'(\xi)] e^{ikx} dx \right| \quad (4.5)$$

The form above can easily be changed into a much easier form by using the transform $\tilde{x} = x - (a + (j-1/2)h)$ this then leaves us with one term for our x , multiplying the oscillatory part of our equation, the reason this is done is because we need to integrate by parts and the form below is the best way to do this,

$$|e_{fm}| = \left| \sum_{j=1}^N \int_{-h/2}^{h/2} [\tilde{x} f'(\xi)] e^{ik(\tilde{x} + a + (j-1/2)h)} dx \right| \quad (4.6)$$

We are lucky that the transform gives us a very good form, we have a constant power of e which we can take out

Looking at the first part of our integral as this is going to give the leading order term for the error. We can integrate this term by parts giving

$$\begin{aligned} |e_{fm}| &= \left| \sum_{j=1}^N f'(\xi) e^{a+(j-1/2)h} \left[\frac{x e^{ikx}}{ik} \right]_{-h/2}^{h/2} - \frac{1}{(ik)} \int_{-h/2}^{h/2} e^{ikx} dx \right| = \\ &= \left| \sum_{j=1}^N e^{a+(j-1/2)h} \left[\frac{(h/2) e^{ik(h/2)}}{ik} + \frac{(h/2) e^{-ik(h/2)}}{ik} - \frac{1}{(ik)^2} (e^{ik(h/2)} - e^{-ik(h/2)}) \right] \right| \end{aligned}$$

Now the above formula has two terms that can give leading terms. But this is misleading, because we can use Taylor series on the equation above when we change its form into

$$|e_{fm}| = \left| \sum_{j=1}^N \frac{f'(\xi) e^{a+(j-1/2)h}}{2ik} e^{-ik\frac{h}{2}} \left[h(e^{ikh} + 1) - \frac{2}{ik} (e^{ikh} - 1) \right] \right| \quad (4.7)$$

this form was created by taking $e^{-ikh/2}$ out of the equation and now we can use Taylor series on e^{ikh} to give

$$|e_{fm}| = \left| \sum_{j=0}^N \frac{f'(\xi) e^{a+(j-1/2)h}}{2ik} e^{-ik\frac{h}{2}} \left[h \left(2 + ikh + \frac{(ikh)^2}{2} + \frac{(ikh)^3}{6} + \dots \right) - \frac{2}{ik} \left(ikh + \frac{(ikh)^2}{2} + \frac{(ikh)^3}{6} + \dots \right) \right] \right|$$

now some of these terms cancel and leaves us with the first two terms left which are both of the same order, which gives

$$|e_{fm}| = \left| \sum_{j=0}^N \frac{f'(\xi) e^{a+(j-1/2)h}}{2ik} e^{-ik\frac{h}{2}} \left[h \left(\frac{(ikh)^2}{2} \right) - \frac{2}{ik} \left(\frac{(ikh)^3}{6} \right) \right] \right| \quad (4.8)$$

so we are left with two terms that can now be gathered together, along with the terms outside the bracket gives

$$|e_{fm}| = \left| \sum_{j=1}^N f'(\xi) e^{a+(j-1/2)h} e^{-ik\frac{h}{2}} \left(\frac{kh^3}{6} \right) \right| = |f'(\xi)| e^{a+(j-1)h} \frac{kh^2}{6} \quad (4.9)$$

so as we have the sum of the above term we lost a power of h , so we have an overall error term of order $O(kh^2)$. So when comparing the Filon-midpoint rule to the composite midpoint rule we see that we actually get better results by $O(1/k)$ with the Filon-Midpoint rule. This is a better approximation than for the composite midpoint rule, and the best way to see this is by looking at the practical results in the table below. With this result we can then program in the scheme to give us an estimate to the true solution.

Example 4.1 - We once again we will use the program on example 2.1 we have looked at for all our methods, where $f(x)=e^x$. We can then compare this method to see if it is any better than for the other methods.

Table 4.1

k	N	Error e_1
1	1	1.517042665E-01
	2	3.833265725E-02
	4	9.606426383E-03
	8	2.403026322E-03
	16	6.008447781E-04
	32	1.502166984E-04
	64	3.755451848E-05
	128	9.388651111E-06
10	1	8.947847961E-02
	2	1.449200059E-01
	4	2.090240306E-02
	8	4.792239803E-03
	16	1.174630106E-03
	32	2.922420913E-04
	64	7.297279522E-05
	128	1.823772724E-05
100	1	1.670305201E-02
	2	1.698160124E-02
	4	1.705566316E-02
	8	1.707445736E-02
	16	1.707917336E-02
	32	1.898678196E-04
	64	4.082912685E-05
	128	9.885567983E-06

Table 4.2

k	1	10	20	40	80	160	320	640
N	9	28	40	57	82	117	168	246

The tables above show us that in fact using the Filon methods for the midpoint rule we do get average results but not anywhere near as good as we have already got the only way we can see if this method is any good is by seeing what results we get when k is very large e.g. 10000. When we have k is 10000 and N being 100 for this method we get $6.8085749E-06$ error, whereas for Gaussian integration we get $1.5120047e-02$ error, and finally for the integration by parts method we get $5.5878500e-20$. So it is clear here that the asymptotic method is by far the best method. There is also a very good property that this method has, when looking at table 4.2, (the table that shows how many intervals needed for a 1% relative error for specific k s) when k doubles the value of N does not double, which was the property we found for all quadrature methods. This is because when looking at our error term when k doubles we would expect the N term to increase at a rate of $(C\sqrt{k})$ not (Ck) , where C is an arbitrary constant. This means that when k is very large and then is doubled, with all the quadrature methods we will find that N will also double, meaning that h will have to be very small to get a good result, but when looking at the Filon-Midpoint method the number of intervals needed will be less than double, and will therefore give a much better result than any quadrature method. This means that the Filon-Midpoint method is by far the best quadrature based method we have looked at so far on this basis.

Filon-Trapezoidal rule

If instead of using the midpoint approximation we use the trapezium rule for the Filon type method we can see if this makes a better approximation. To do this we need to find the trapezium rule approximation to $f(x)$ in terms of $(cx + d)$, not in the terms that we produced earlier. The reason we need to do this is because when using the Filon method we need to calculate moments

$$b_n = \int_a^b x^n e^{ikx} dx \quad (4.10)$$

where for the trapezium rule $n=1$.

Definition 4.2-The Filon- Trapezoidal approximation to $I[f]$ is defined by

$$\int_a^b f(x)e^{ikx} dx = \sum_{j=1}^N \frac{q(f(p) - pf(q))}{(q-p)} \left(\frac{e^{ikq}}{ik} - \frac{e^{ikp}}{ik} \right) + \sum_{j=1}^N \left(\frac{f(q) - f(p)}{q-p} \right) \left(\left(\frac{qe^{ikq}}{ik} - \frac{pe^{ikp}}{ik} \right) + \left(\frac{e^{ikq}}{(ik)^2} - \frac{e^{ikp}}{(ik)^2} \right) \right) dx$$

where $q = a + jh$ and $p = a + (j-1)h$

Proof

The trapezium rule works so that when we look in each interval we need to approximate $f(x) = cx + d$

$$I = \int_a^b f(x)e^{ikx} dx = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} f(x)e^{ikx} dx \approx \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} (cx + d)e^{ikx} dx$$

so to work this out we need to form simultaneous equations, which uses the information for the trapezium rule. These simultaneous equations are that if $q = a + jh$ and $p = a + (j-1)h$ then we get

$$1) cp + d = f(p)$$

$$2) cq + d = f(q)$$

if we work through these equations we obtain that

$$c = \frac{f(q) - f(p)}{q - p} \quad \text{and} \quad d = \frac{q(f(p) - pf(q))}{q - p}$$

and inserting this into our formula we obtain

$$I = \int_a^b f(x)e^{ikx} dx = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} f(x)e^{ikx} dx \approx \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} \left(\frac{f(q) - f(p)}{q - p} x + \frac{q(f(p) - pf(q))}{q - p} \right) e^{ikx} dx$$

Now we have two integrals to work out, one which is just like the midpoint rule one which can be integrated directly, and one which we have to use integration by parts to find it, so there for we get the result

$$\int_a^b f(x) dx = \sum_{j=1}^N \frac{q(f(p) - pf(q))}{(q-p)} \left(\left[\frac{e^{ikq}}{ik} \right] - \left[\frac{e^{ikp}}{ik} \right] \right) + \sum_{j=1}^N \left(\frac{f(q) - f(p)}{q-p} \right) \left(\left[\frac{qe^{ikq}}{ik} \right] - \left[\frac{pe^{ikp}}{ik} \right] + \left(\left[\frac{e^{ikq}}{(ik)^2} \right] - \left[\frac{e^{ikp}}{(ik)^2} \right] \right) \right) dx$$

Where p and q are as defined earlier.

Theorem 4.2 - The leading order error term for the Filon-Trapezoidal method is $O(h^2)$

Proof

To find the error we need to approximate $|e_{ft}| = |I - I_{ft}|$ here

$$I = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} f(x)e^{ikx} dx \quad \text{The exact solution } I[f]$$

$$I_{ft} = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} (cx + d)e^{ikx} dx \quad \text{The composite Filon - trapezoidal approximation to } I[f], c, d \text{ are as defined earlier}$$

We can use Theorem 2.5 to find the term $f(x) - cx - d$ to get

$$|e_{ft}| = \left| \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} (f(x) - cx - d)e^{ikx} dx \right| = \left| \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} \frac{f''(\xi)}{2} (x-a)(x-b)e^{ikx} dx \right|$$

In the same way that we saw this kind of term when looking at just the composite trapezium rule. So we need to integrate the above term, but firstly we need to gather like terms

$$|e_{ft}| = \left| \sum_{j=1}^N \frac{f''(\xi)}{2} \left[\int_{a+(j-1)h}^{a+jh} x^2 e^{ikx} dx - (a+b) \int_{a+(j-1)h}^{a+jh} x e^{ikx} dx + ab \int_{a+(j-1)h}^{a+jh} e^{ikx} dx \right] \right| \quad (4.11)$$

Now we have three moments to work out and the best way to do this is to do one at a time, with the easiest first, with $p = a + (j-1)h$ and $q = a + jh$, as we had them before when working through the trapezium rule.

$$1) \quad \int_p^q e^{ikx} dx = \frac{1}{ik} [e^{ikq} - e^{ikp}]$$

$$2) \quad \int_p^q x e^{ikx} dx = \left[\frac{x e^{ikx}}{ik} \right]_p^q - \frac{1}{ik} \int_p^q e^{ikx} dx = \frac{1}{ik} [q e^{ikq} - p e^{ikp} - \frac{1}{ik} (e^{ikq} - e^{ikp})]$$

3)

$$\int_p^q x^2 e^{ikx} dx = \left[\frac{x^2 e^{ikx}}{ik} \right]_p^q - \frac{2}{ik} \int_p^q x e^{ikx} dx = \frac{1}{ik} [q^2 e^{ikq} - p^2 e^{ikp} - \frac{2}{ik} [q e^{ikq} - p e^{ikp} - \frac{1}{ik} [e^{ikq} - e^{ikp}]]]$$

now when all these results is substituted into (4.11) we get

$$|e_{ft}| = \left| \sum_{j=1}^N \frac{f''(\xi)}{2} \left[\frac{q^2 e^{ikq}}{ik} - \frac{p^2 e^{ikp}}{ik} - \frac{2q e^{ikq}}{(ik)^2} + \frac{2p e^{ikp}}{(ik)^2} + \frac{2e^{ikq}}{(ik)^3} - \frac{2e^{ikp}}{(ik)^3} - \frac{pq e^{ikq}}{ik} - \frac{q^2 e^{ikq}}{ik} + \frac{p^2 e^{ikp}}{ik} \right. \right. \\ \left. \left. + \frac{pq e^{ikp}}{ik} + \frac{p e^{ikq}}{(ik)^2} + \frac{q e^{ikq}}{(ik)^2} - \frac{p e^{ikp}}{(ik)^2} - \frac{q e^{ikp}}{(ik)^2} - \frac{pq e^{ikq}}{ik} - \frac{pq e^{ikp}}{ik} \right] \right|$$

the term above does look very complicated but many terms do cancel and so we are able to obtain an easier form

$$|e_{ft}| = \left| \sum_{j=1}^N \frac{f''(\xi_j)}{2} \left[-\frac{qe^{ikq}}{(ik)^2} + \frac{pe^{ikp}}{(ik)^2} + \frac{pe^{ikq}}{(ik)^2} - \frac{qe^{ikp}}{(ik)^2} + \frac{2e^{ikq}}{(ik)^3} - \frac{2e^{ikp}}{(ik)^3} \right] \right|$$

the form above is not in the form that we would like it to be in. We would wish to have the expression above in terms of h and k, but at the moment it is only in the form of k, p and q, so we wish to get the above expression in terms of (q - p) which is equal to h. To do this we can bring out e^{ikp} to the front to give

$$|e_{ft}| = \left| \sum_{j=1}^N \frac{f''(\xi_j)e^{ikp}}{2(ik)^3} [(2 - hik)e^{ikh} - (2 + hik)] \right|$$

this term can now be made into terms of h by using Taylor series on $e^{ik(q-p)}$

$$|e_{ft}| = \left| \sum_{j=1}^N \frac{f''(\xi_j)e^{ikp}}{2(ik)^3} [(2 - hik) \left[1 + (ik)(h) + \frac{(ik)^2(h)^2}{2} + \dots \right] - (2 + hik)] \right|$$

no most of the above terms cancel leaving us with the error term of the form

$$|e_{ft}| = \left| \sum_{j=1}^N \frac{f''(\xi_j)e^{ikp}h^3}{12} \left[1 + \frac{ikh^4}{2} + \frac{(ik)^2h^5}{6} + \dots \right] \right|$$

So when we sum all of these terms we get a leading term order of h^2 . This means that when comparing the Filon-Trapezoidal method with the composite trapezium rule we see that the error term of $1/k^2$ less when using the Filon type method. This means that we should expect to get good results when using this method whether k is large or small.

Example 4.2 –A program has been created that applies example 2.1 for the Filon-Trapezoidal Method. The constraints that have been used before in all of the previous example are kept the same and we should hopefully see that as k gets large there is no bad results as this method should be independent of k. Table 4.3 is just the error incurred when applying the method for different ks and Ns. Table 4.4 is a table which represents how many intervals needed to get a 1% relative error for different ks.

Table 4.3

k	N	Error e_1
1	1	1.373716326E-01
	2	3.439271561E-02
	4	8.598958573E-03
	8	2.149751827E-03
	16	5.374381471E-04
	32	1.343595397E-04
	64	3.358988498E-05
	128	8.397471248E-06
10	1	8.561886880E-03
	2	1.450586786E-02
	4	2.089185991E-03
	8	4.787185384E-04
	16	1.173221697E-04
	32	2.918810328E-05
	64	7.288197229E-06
	128	1.821498663E-06
100	1	1.668654671E-04
	2	1.698124962E-04
	4	1.705581701E-04
	8	1.707451102E-04
	16	1.707918773E-04
	32	1.898675801E-06
	64	4.082873898E-07
	128	9.885451887E-08

Table 4.4

k	1	10	20	40	80	160	320	640
N	9	28	9	10	7	5	3	3

The results above show that by using the trapezium rule as our quadrature base in the Filon type method we get by far better result than when using the midpoint. The Filon type method can also be used with the Simpson's rule as well, but as we know that the general pattern will give us a better approximation than the last two but not as good as with the Gaussian method. As has already been stated Arieh Iserles only works on the Gaussian in his paper and the first two that are in this paper will not give as good an error as Iserles puts in his paper but are a lot easier to calculate. The next section is what Iserles worked on in his paper and his method is followed through here.

Filon - Gauss Method

Definition 4.3 - The form for Filon-Gauss method is below, where the l_n are Lagrangian interpolating polynomials, and x_n are nodes determined by the zero's of Legendre polynomials.

$$f(x) = \tilde{f}(x) = \sum_{n=1}^N l_n(x/h) f(x_n h)$$

where

$$l_j(x) = \prod_{\substack{i=1 \\ i \neq k}}^N \frac{x - x_i}{x_k - x_i} = \begin{cases} 1 & x = x_k \\ 0 & x \neq x_k \end{cases} \quad j=1,2,\dots,N$$

This now can be put all together to get our approximation that we are looking for

$$\begin{aligned} \int_a^b f(x) e^{ikx} dx &\approx \int_a^b \sum_{n=1}^N l_n(x/h) f(x_n h) e^{ikx} dx \\ &\Rightarrow \sum_{n=1}^N \left[\int_a^b l_n(x/h) e^{ikx} dx \right] f(x_n h) \end{aligned}$$

Now the part of the method that is the most important is the weights, as we need to be able to work these out exactly. The way we do this is that we see that there is a pattern of the integrals that we need to be able to solve for, they are of the form

$$b_n = \int_a^b x^n e^{ikx} dx$$

These integrals are called moments as we have seen then before, the way that these are worked out is by using asymptotic methods to get the leading term order of the integrals. If we integrate our form by parts then we obtain the formula

$$b_n = \int_a^b x^n e^{ikx} dx = \frac{[b^n e^{ikb} - a^n e^{ika}]}{ik} - \frac{1}{ik} \int_a^b nx^{n-1} e^{ikx} dx$$

Theorem 4.3 - The error term for the Filon-Gauss method when applied to $I[f]$ is when

(hk) << 1	error = $O(h^{N+1})$
(hk) = $O(1)$	error = $O(h^{N+1})$
(hk) >> 1	error = $O\left(\frac{h^{N+1}}{k}\right)$ If endpoints a and b are not included in the nodes x_0, x_1, \dots, x_N
	error = $O\left(\frac{h^{N+1}}{k^2}\right)$ If end points a and b are included in the nodes x_0, x_1, \dots, x_N

This is the result that Arieh Iserles gives in his paper. This is definitely the best result that we have obtained for our integral. It has very good advantages, these are that it uses a combination of quadrature and asymptotic methods, so that when we need to find out our integrals we obtain moments that are easier to solve than when we just used asymptotic methods, and we also get an inverse power of k as our leading order, therefore unlike with normal quadrature our results get better when k is large, which is the aim of this project. The problem with this method is that the analysis is very complicated and even though the results look good, we need change the nodes to incorporate the endpoints to get a very good result for an average h.

The Filon type methods do give good results for all different values of h and we never get any really, really bad results but for the midpoint type method we only get average results as it has a error of order $O(h^2k)$, and this error can get large for a large k. The method does though seem to give good results for large k compared to the other quadrature methods we have looked at which is good. The Filon-Trapezoidal Method has an error which is independent of k, so it has an error like the normal trapezium rule when applied to a general function $g(x)$, which we know is not very good but for our oscillatory integral the error term is very good. The analysis is also easy to follow through and is a lot easier to program than the gauss method. The last method we looked at was the gauss method, and just like with normal Gaussian quadrature the analysis is very complicated and not easy to find, and the only way that an error estimate is added in this project is because it is given in Iserles's paper.

Integral 2: Irregular oscillators

In this section we are going to look at the second integral that we are interested in . This integral was defined as $J[f]$ in definition 1.2.

5) Method of Stationary Phase

The method of stationary phase is very similar to the asymptotic method discussed in Chapter 3. The method has two variations, when $g'(x)=0$ anywhere in $[a,b]$ the integration by parts method breaks down and a solution needs to be inserted to get a result. We will look at the simple type first when $g'(x) \neq 0$ in $[a,b]$. The way we work this out is the same as we did before by using integration by parts. The method depends on dividing and multiplying the whole integral by $g'(x)$, this means that integration by parts can now proceed as before where we split the integral in the following way

Definition 5.1 – The form of the integration by parts method when applied to $J[f]$ when there are no stationary points is

$$I[x] = \int_a^b f(x) \frac{g'(x)}{g'(x)} e^{ikg(x)} dx = \int_a^b u v' dx$$

$$u = \frac{f(x)}{g'(x)}$$

$$v = e^{ikg(x)}$$

$$du = \left(\left(\frac{f(x)}{g'(x)} \right)' \right) dx$$

$$dv = g'(x) e^{ikg(x)} dx$$

$$= \left[\left[\frac{f(x) e^{ikg(x)}}{g'(x) ik} \right]_a^b - \frac{1}{ik} \int_a^b \left(\frac{f(x)}{g'(x)} \right)' e^{ikg(x)} dx \right]$$

this now can be carried on like before and it is clear to see that once again we get a pattern which means that we can find out the general integral which we need to find. It is

$$\int_a^b f(x) e^{ikx} dx = \sum_{n=1}^N \frac{1}{(ik)^n} \left[\left(\frac{f(x)}{g'(x)} \right)^{(n-1)} e^{ikg(x)} \right]_a^b + \frac{1}{(ik)^{N+1}} \int_a^b \left(\frac{f(x)}{g'(x)} \right)^{(N)} e^{ikx} dx$$

This again is just like our integration by parts problem above and it has its advantages and disadvantages. We can see that once again we have a leading order term of $1/k$ and our remainder term is of the form

$$R[f] = \frac{1}{(ik)^{N+1}} \int_a^b \left(\frac{f(\xi)}{g'(\xi)}\right)^{(N)} e^{ikx} dx \quad a < \xi < b$$

Now we have the problem when there is a stationary point in our interval i.e. if $g'(x)=0$ in $[a,b]$. What we do is separate the interval in to pieces, we will have the small area around the stationary point taken out and use the integration by parts method on the bits without the stationary point, and then work on the bits that do.

Theorem 5.1 - If we have a stationary point at say the point $x=a$ and no where else in our interval then the leading term is of order $O((1/k)^{1/2})$

Proof

The procedure follows the following steps

$$\int_a^b f(x)e^{ikg(x)} dx = \int_a^{a+\varepsilon} f(x)e^{ikg(x)} dx + \int_{a+\varepsilon}^b f(x)e^{ikg(x)}$$

this is the split interval, we can see that the area around the stationary point is now isolated by a small parameter ε and the second interval can be solved as before, using the integration by parts method

The second interval is solved in the following way

$$\int_{a+\varepsilon}^b f(x)e^{ikx} dx = \sum_{n=1}^N \frac{1}{(ik)^n} \left[\left(\frac{f(x)}{g'(x)} \right)^{(n-1)} e^{ikg(x)} \right]_{a+\varepsilon}^b + \frac{1}{(ik)^{N+1}} \int_{a+\varepsilon}^b \left(\frac{f(x)}{g'(x)} \right)^{(N)} e^{ikx} dx$$

It is clear that there is no irregular points in this integral (unlike if a was included) and we obtain an inverse of k leading order term with a remainder term like before.

The second integral that we need to work out is different, what we need to do is to remove the irregular point, we do this by using Taylor series on $g(x)$ and $f(x)$.

$$\begin{aligned} \int_a^{a+\varepsilon} f(x)e^{ikg(x)} dx &\approx f(a) \int_a^{a+\varepsilon} e^{ik[g(a) + \frac{(x-a)^2}{2!}g''(a) + \dots]} dx \\ &= f(a)e^{ikg(a)} \int_a^{a+\varepsilon} e^{ik[\frac{(x-a)^2}{2}]g''(a)} dx \end{aligned}$$

Now the integral above can be evaluated by using a substitution and so we get an expression of order $O(1/k^{1/2})$, so this is the order of the integral as we stated in the section 1). There are different types of evaluations that can be found using Method of Stationary Phase, these are going to be quickly dealt with here.

In theorem 5.1 there was only one stationary point that appeared in the evaluation, but what if we had W stationary point in $[a,b]$.

Theorem 5.2 – If there are points x_1, x_2, \dots, x_W for which $g'(x_i)=0$ but $g''(x_i) \neq 0$ for $i=1,2,\dots,W$ then the leading term of the error is $O(1/k^{1/2})$

Proof

If we have W stationary points then we can use theorem 5.1 to split every stationary points up like we did for just the one stationary points. This means that we will have W equations of the form

$$\int_{x_i}^{x_i+\varepsilon} f(x)e^{ikg(x)} dx \approx f(x_i) \int_{x_i}^{x_i+\varepsilon} e^{ik[g(x_i)+\frac{(x-x_i)^2}{2!}g''(x_i)+\dots]} dx$$

$$= f(x_i)e^{ikg(x_i)} \int_{x_i}^{x_i+\varepsilon} e^{ik[\frac{(x-x_i)^2}{2}]g''(x_i)} dx \quad i=1,2,\dots,W$$

which each equation will give leading term order of $O(1/k^{1/2})$, and so proved.

Theorem 5.3 – If we have 1 point x_1 , for which $g'(x_1)=0, g''(x_1)=0, \dots, g^{(p)}(x_1)=0$ but $g^{(p+1)}(x_1) \neq 0$, then the leading term of the error will be of the form $(1/k^{1/p})$

Proof

When looking at theorem 5.1 we can use Taylor series of $g(x)$ at the point x_1 , and all the terms with the first p derivatives will disappear to give us a term of the form

$$\int_{x_1}^{x_1+\varepsilon} f(x)e^{ikg(x)} dx \approx f(x_1) \int_{x_1}^{x_1+\varepsilon} e^{ik[g(x_1)+\frac{(x-x_1)^p}{p!}g^{(p)}(x_1)+\dots]} dx$$

$$= f(x_1)e^{ikg(x_1)} \int_{x_1}^{x_1+\varepsilon} e^{ik[\frac{(x-x_1)^p}{p!}]g^{(p)}(x_1)} dx$$

Now a substitution can be made in the same way as was used for theorem 5.1 and so we get leading term of $O(1/k^{1/p})$.

Theorem 5.4 – If we have W stationary points like theorem 5.1, then the point say x_i that has the most derivatives equaling zero say p derivatives, then the leading term behavior will be $O(1/k^{1/p})$.

6) Filon Type Methods

Filon-Trapezoidal Method

When using Filon type methods on our integral $J[f]$ we have to be careful with the $g(x)$ term in the exponential. If $g'(x) \neq 0$ in $[a,b]$ then an easy approximation can be found by using a combination of the Filon method and the Integration by parts method. On the other hand if $g'(x)=0$ at least once in $[a,b]$ then we would have to use method of stationary phase instead. The Filon-Trapezoidal method for $J[f]$ follows the same line as we did before up to where we need to integrate terms.

Definition 6.1 - The Filon-Trapezoidal approximation to $J[f]$ on $[a,b]$ is defined as

$$J = \int_a^b f(x)e^{ikg(x)} dx = \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} f(x)e^{ikg(x)} dx \approx \sum_{j=1}^N \int_{a+(j-1)h}^{a+jh} (cx + d)e^{ikg(x)} dx \quad (6.1)$$

where c and d are defined as

$$c = \frac{f(q) - f(p)}{q - p} \quad \text{and} \quad d = \frac{q(f(p) - pf(q))}{q - p}$$

with $q = a + jh$ and $p = a + (j-1)h$.

The above definition is the same Filon-Trapezoidal approximations as we used for the first integral, but we now have the problem that we have two integrals to find that we do not necessarily know how to work them out. We therefore have three cases in which we need to work through now

Case 1 - Integrals $\int_a^b xe^{ikg(x)} dx$ and $\int_a^b e^{ikg(x)} dx$ are known

In this case then we can follow the procedure that was looked at for the first integral. If we know these integrals then we can just insert them into (6.1). and we will get an expression very similar to what was found in chapter 4. There are unfortunately only a very few functions that the above integral is exact. The good examples of these are $1/2(x-1/2)^2$ which uses error formulae to work out the moments, and another is $\log_e(1+x)$ which can be worked out exactly. This can be seen in source 4) on pages 6 and 9. As there are only a few of these g 's that can be worked out exactly we need to find another way of finding these integrals.

Case 2 - Integrals $\int_a^b x e^{ikg(x)} dx$ and $\int_a^b e^{ikg(x)} dx$ are not known, but $g'(x) \neq 0$ in $[a,b]$.

In this case we need to use the integration by parts method on these integrals. We can

use Definition 5.1. For the integral $\int_a^b e^{ikg(x)} dx$ the method is

$$\int_a^b e^{ikg(x)} dx = \int_a^b \frac{g'(x)}{g'(x)} e^{ikg(x)} dx = \left[\frac{e^{ikg(x)}}{ikg'(x)} \right]_a^b - \frac{1}{ik} \int_a^b \left(\frac{1}{g'(x)} \right)' e^{ikg(x)} dx$$

we can follow this through for as many terms as we wish to get a good approximation.

We get a sum term of the form

$$\int_a^b e^{ikg(x)} dx = \sum_{n=1}^N \frac{1}{(ik)^n} \left[\left(\frac{1}{g'(x)} \right)^{(n)} e^{ikg(x)} \right]_a^b + \frac{1}{(ik)^N} \int_a^b \left(\frac{1}{g'(x)} \right)^{(N)} e^{ikg(x)} dx$$

for the integral $\int_a^b x e^{ikg(x)} dx$ we need to follow through a similar approximation

$$\int_a^b x e^{ikg(x)} dx = \int_a^b \frac{x'g(x)}{g'(x)} e^{ikg(x)} dx = \left[\frac{x e^{ikg(x)}}{ikg'(x)} \right]_a^b - \frac{1}{ik} \int_a^b \left(\frac{x}{g'(x)} \right)' e^{ikg(x)} dx$$

once again we get a sum term depending on how many approximations we wish to have and this is of the form

$$\int_a^b x e^{ikg(x)} dx = \sum_{n=1}^N \left[\frac{1}{(ik)^n} \left[\left(\frac{x}{g'(x)} \right)^{(n-1)} e^{ikg(x)} \right]_a^b + \frac{1}{(ik)^N} \int_a^b \left(\frac{x}{g'(x)} \right)^{(N)} e^{ikg(x)} dx \right]$$

Now we can put all of these terms together and substitute them into (6.1)

$$\sum_{j=1}^N \sum_{n=1}^N \left[\frac{c}{(ik)^n} \left(\frac{x}{g'(x)} \right)^{(n-1)} e^{ikg(x)} \right]_a^b + \frac{d}{(ik)^n} \left[\left(\frac{1}{g'(x)} \right)^{(n-1)} e^{ikg(x)} \right]_a^b$$

the above term does look complicated but it is just a combination of the integration by parts method used in chapter 5 and the Filon-Trapezoidal method used in chapter 4.

the above formula could have many problems. Even though we do not have an stationary points in $[a,b]$ we could in theory have a function g which has a derivative very small but not zero, and this means that the above term would blow up and our error term would increase so much that we would not be able to get a good result.

This is the very big problem with this method and this has to be taken into account if errors were to grow.

Case 3 - Integrals $\int_a^b x e^{ikg(x)} dx$ and $\int_a^b e^{ikg(x)} dx$ are not known, and $g'(x) = 0$ in $[a, b]$.

In this case the method of stationary phase must be used to approximate the moments. In this case we would have to take into account all of the possible outcomes of the method of stationary phase method (theorems 5.1, 5.2, 5.3 and 5.4). Each different case would affect the leading term behavior of this method and in the same way that definition 6.1 was created by the integration by parts method, a procedure would be created in the same mould. Unfortunately the method of stationary phase was not defined as the integration by parts method was and much work would need to be put into this method, so only a brief overview can be added here. It is clear that depending on which case we have from section 5) will have a big affect on the final answer and the leading term behavior will affect the final approximation.

Conclusion

In this project many different types of methods have been looked at on the two integrals that we are interested in. For the first integral $I[f]$ we have looked at 3 different types of methods, Quadrature methods, Asymptotic methods and Filon type methods. Out of these three methods the Asymptotic method was by far the best when k is large, giving brilliant results, but when k is small the method gives very poor results. The quadrature methods gives very poor results for k large, and the best of these methods, the Gaussian quadrature method gets very good results for small k but as k gets large the error grows so that we would have to decrease h so much that it becomes very expensive to calculate the approximation. The third and final type of method we looked at was the Filon type methods. These methods do decrease the error whether k is large or small. The two methods that were looked at in detail the midpoint and trapezoidal type methods do decrease the error compared to the quadrature methods and when k is very large they do give very good results. Also with these methods the analysis is very easy to follow through and the error terms are easy to find. When comparing the error terms of the same quadrature and the Filon quadrature we do get very good results with the Filon type methods. The Midpoint Rule compared with the Filon midpoint rule gives $1/k$ better results, so that when k is very large there is going to be a big difference in the results. The trapezoidal method for the Filon quadrature was $1/k^2$ better than for the normal trapezium quadrature, and this means that when k is only relatively large we would expect to get very good results, which we saw in practice. On top of this the methods are very easy to program and don't use too much memory to approximate $I[f]$ to get a good accurate result. In all when looking at $I[f]$ all the quadrature method do when k is large is increase the error. The asymptotic method is by far the best approximation but the result are misleading and if a difficult derivative of $f(x)$ is involved then the approximation would not be as good. The best method though, when looking at all values of k and the ease of finding an approximation is the Filon type methods. The Gauss type method though is not easy to follow through, the approximation does give very good results in theory but the analysis and the programming are very complicated as is the integration of the moments. The other two methods though are very useful, they give good results and also are very good for analysis and programming.

The second integral that we looked at $J[f]$ we looked at two different types of methods, but not in any great detail. We did find that when we get a $g(x)$ instead of x we get very difficult analysis, with a lot of integration that needs to be approximated by asymptotic methods. Unfortunately this was not completed and only a brief overview was seen with this method, but as with the first integral $I[f]$, the Filon-trapezoidal method was a very good compared with the other method that were looked at, we should expect to get similar results on $J[f]$.

7) Bibliography and Literature Review

1) On the Numerical Quadrature of Highly-Oscillating Integral I: Fourier transforms - Arieh Iserles - IMA Journal of Numerical Analysis 2004 p365-391

This is a paper that was published by the Cambridge Professor Arieh Iserles in 2003. It deals with the integral $I[f]$ when $k = \omega$, so that the paper is based on Fourier transforms. The first part of the paper deals with Gaussian Quadrature, in this section it is stated that Gaussian quadrature is the best possible Quadrature method available and follows the procedure that the Gaussian Quadrature method is too expensive to find a suitable approximation to $I[f]$. Though this is true, Gaussian quadrature does give good results for an averagely big k but no where near as good as the Filon-Gauss method described here in this paper. The next part of the Paper deals with the Filon-Gauss method, it gives the error estimates that are given in Theorem 4.3, these error estimates are very good and if they are accurate then this is by far the best result that has been seen for oscillatory integrals. The problem is that when in the paper he works through his error estimate proof it is very complicated and is very hard to follow, this means that not only is the analysis hard, nut also the procedure of the method is hard too. The last part of the paper deals with other types of methods that can be used also. These methods are Zamfirescu's Method, Levin's Method and lastly a revisit of lie group Methods.

2) Numerical Analysis - Richard L. Burden and J. Douglas Faires- 6th edition 1997 Brooks/Cole publishing company

This is a book, and the pages that I dealt with were mainly were p188-205 and p222-228.

The first set of pages deal with the first three quadrature methods in this paper, the Midpoint rule, Trapezium rule and the Simpson's rule. The book firstly looks at all of the General methods and errors in chapter 2.2, and in 2.3 the book goes on to composite rules. All of the error estimates that are included in this paper are derived from these chapters and also other parts of the book have been used to prove these error estimates. The second set of pages deal with Gaussian quadrature, the pages state the Gaussian quadrature method and how it works but doesn't work through any error estimates.

3) Advanced Mathematical Methods for scientists and engineers - C.M. Bender & S.A. Orszag 1978 - p252-261 and p276-280

This source is where the asymptotic type methods in this project were found. The first set of pages deal with the integration by parts method found in chapter 3. the second set of pages deal with the Method of Stationary Phase found in chapter 5.

4) On the numerical quadrature of highly-oscillating integrals II: Irregular Oscillators - Arieh Iserles – IMA journal of Numerical Analysis 25 (2005) p25-44.

This is the second paper that Arieh Iserles follows through the numerical quadrature of highly oscillating integrals. The first part of the paper is a recap of the first paper 1) giving the error term only in terms of ω and not of h as well. This is good though as it shows that if h is large then the method does still get a good result if k is also large. The paper then moves on to the second integral $J[f]$ with respect to Gaussian quadrature, (which is not dealt with in this project, but the basis of the Filon-Trapezoidal method is to see if it has easier analysis.) He begins this part of his paper by giving us his error estimate to be $O(k^{-\beta})$ where $\beta > \alpha_i$. The next part of the paper deals with a geometric model which is his way of finding the solution of the moments he works through this by setting up a geometric sum model to solve the moments. The formula he gives is

$$\int_a^b x^m e^{ikg(x)} dx = \sum_{j=1}^N v_j(k) d_j^m k^{-\alpha_j}$$

where v_j are periodic functions and the d_j are nodes and the α_j are to be determined depending on $J[f]$. The next part of the paper he works through the proof of the error. This part does get very complicated and gets very complex. He then works through an example of $g(x) = 1/2(x-1/2)^2$. This part of the paper is very good as it shows how the value of β is derived by using error functions to solve the moments. The next part of the paper deals with $g'(x) = 0$ in $[0,1]$ and uses method of stationary phase to give the error estimate of $(k^{1/s})$. This in fact has been worked through this paper in section 5 and the error estimate is the same. The rest of the paper is Iserles working through what he sees as the loose ends of the method, this is good but very complicated to

follow through and most of it could be skipped through, but Iserles shows here that he does look through all types of scenarios.

5) Efficient quadrature of highly oscillatory integrals using derivatives - Arieh Iserles – Proceedings of the Royal Society A (2005)

This is the third paper Iserles published on highly oscillating integrals. This paper deals with asymptotic method applied with Filon's ideas. The paper begins by looking at $J[f]$ when there are no stationary points and working through the integration by parts method that is in section 5) of this thesis. The notation of the paper is very good in this section defining

$$\sigma_0 = f(x)$$

$$\sigma_{k+1} = \frac{d}{dx} \frac{\sigma_k[f](x)}{g'(x)}$$

This notation goes very well with the method and his makes the whole method very easy to understand. He then uses the integration by parts method with Filon quadrature and gives an error estimate to be $O(k^{-s-1})$ as $k \rightarrow \infty$ where s is the number of terms in the integration by parts method used. The paper then goes on to prove this theorem. The next section deals with stationary points in $(0,1)$ and defines the Method of stationary phase method . The paper then uses this method on Filon quadrature giving an error estimate to be $O(k^{-s-1/(r+1)})$ where s is the number of terms in the method of stationary phase method and r is the number of derivatives the stationary point is equal to zero for, see theorem 5.3.

6) On quadrature methods for highly oscillatory integrals and their implementation- A Iserles & S.P Norsett – BIT Numerical Mathematics 44: p 755-772 (2004)

In this paper Iserles uses Hermitian interpolation instead of Gaussian on Filon type methods. Unfortunately most of this was not covered in this thesis but a reference must be made to it.

7) Mathworld Website - <http://mathworld.wolfram.com/>

This was used for the Gaussian quadrature error estimate.