

Chapter 1

Introduction

Most real mathematical problems do not have analytical solutions. However, they do have real solutions. In order to obtain these solutions we must use other methods such as graphical representations, or numerical analysis. Numerical analysis is the mathematical method that uses numerical approximations to obtain numerical answers to the problem. Numerical analysis also considers the accuracy of an approximation, and when the approximation is good enough. Numerical answers are useful because we use numbers to build our world, not with the exact analytical solution, such as $\frac{e^\pi}{\sqrt{27}}$

The ever-increasing advances in computer technology has enabled many in science and engineering to apply numerical methods to simulate physical phenomena. Numerical methods are often divided into elementary ones such as finding the root of an equation, integrating a function or solving a linear system of equations to intensive ones like the finite element method. Intensive methods are often needed for the solution of practical problems and they often require the systematic application of a range of elementary methods, often thousands or millions of times over. In the development of numerical methods, simplifications need to be made to progress towards a solution: for example general functions may need to be approximated by polynomials and computers cannot generally represent numbers exactly anyway. As a result, numerical methods do not usually give the exact answer to a given problem, or they can only tend towards a solution getting closer and closer with each iteration. Numerical methods are generally only useful when they are implemented on computer using a **computer programming language**.

The study of the behavior of numerical methods is called numerical analysis. This is a mathematical subject that considers the modeling of the error in the processing of numerical methods and the subsequent re-design of methods.

Numerical analysis involves the study of methods of computing numerical data. In many problems this implies producing a sequence of approximations; thus the questions involve the rate of convergence, the accuracy (or even validity) of the answer, and the completeness of the response. (With many problems it is difficult to decide from a program's termination whether other solutions exist.) Since many problems across mathematics can be reduced to linear algebra, this too is studied numerically; here there are significant problems with the amount of time necessary to process the initial data. Numerical solutions to differential equations require the determination not of a few numbers but of an entire function; in particular, convergence must be judged by some global criterion. Other topics include numerical simulation, optimization, and graphical analysis, and the development of robust working code.

Numerical linear algebra topics: Solutions of linear systems $AX = B$, eigenvalues and eigenvectors,

tors, matrix factorizations. Calculus topics: numerical differentiation and integration, interpolation, solutions of nonlinear equations $f(x) = 0$. Statistical topics: polynomial approximation, curve fitting.

Further information on the elementary methods can be found in books on numerical methods or books on numerical analysis. Dedicated text books can be found on each of the intensive methods. Details of available books can be accessed through www.science-books.net.

Need help understanding numerical methods?

1. What is the use of numerical methods in real life application?
2. Need a brief explanation of numerical methods
3. Fixed Point Iteration, Linear Interpolation and Newton-Raphson Method, what are the differences to their uses?

Best Answer

1. um, everywhere? From a cash machine, to calculating how much chemicals to put to produce laundry detergent, to construction of buildings and bridges.
2. The ever-increasing advances in computer technology has enabled many in science and engineering to apply numerical methods to simulate physical phenomena. Numerical methods are often divided into elementary ones such as finding the root of an equation, integrating a function or solving a linear system of equations to intensive ones like the finite element method. Intensive methods are often needed for the solution of practical problems and they often require the systematic application of a range of elementary methods, often thousands or millions of times over. In the development of numerical methods, simplifications need to be made to progress towards a solution: for example general functions may need to be approximated by polynomials and computers cannot generally represent numbers exactly anyway. As a result, numerical methods do not usually give the exact answer to a given problem, or they can only tend towards a solution getting closer and closer with each iteration. Numerical methods are generally only useful when they are implemented on computer using a computer programming language.
3. Visit these sites: <http://math.fullerton.edu/mathews/n2003/FixedPointMod.html>
<http://en.wikipedia.org/wiki/Linear-interpolation>
<http://mathworld.wolfram.com/Newton'sMethod.html>

Other answers

2. Numerical Methods refers to procedures to find approximate solutions when exact solutions cannot be found in a straightforward manner.
3. Linear interpolation assumes that if two points on a graph are given, any point in between them can be found by connecting the original two points by a straight line.

Newton Raphson is a method to find approximate solutions to an equation through an iterative process where each calculated value is used as the starting point for the next calculated value. NRM requires that you can evaluate the first derivative of that equation.

1.1 What is Numerical Analysis?

- It is a way to do highly complicated mathematics problems on a computer.
- it is also known as a technique widely used by scientists and engineers to solve their problems.

1.2 Two issues of Numerical Analysis:

- How to compute? This corresponds to algorithmic aspects;
- How accurate is it? That corresponds to error analysis aspects.

1.3 Advantages and Disadvantages of Numerical Analysis:

Although numerical solutions are just an approximation, an estimate of an exact solution (numerical values are "near" solutions or often referred to as inexact solutions) due to

- 1.) truncation errors,
- 2.) round off errors,
- 3.) chop off errors,

Other than the truncation errors involved in numerical methods, numerical algorithms are computationally involved, calling for powerful computing abilities and machines. The schemes are usually multi steps and multi terms.

However, numerical techniques are widely applied in solving real world problem.

1.3.1 Hard or impossible classical solutions

It can obtain numerical answers of the problems that have very hard analytical techniques or sometimes impossible to solve (no "exact or classical" solution).

Example 1.3.1 Finding the classical solution to an integral

$$\int e^{x^2} dx$$

is quite very hard if not impossible.

Example 1.3.2 Solving a simple looking first order ordinary differential equation

$$\frac{dy}{dx} = x^2 + y^2$$

analytically is not easy at all.

1.3.2 Tabulated data

Usually we only have tabulated data when faced with complex real world models, and do not have an explicitly defined function.

Example 1.3.3 To compute the area under the curve defined by the table below

x	1	3	5	7
$f(x)$	-3	5	21	45

will be analytically impossible since we do not know the explicit definition of $f(x)$ that was used to generate the table above. To compute

$$\int_1^7 f(x)dx$$

will not be possible.

The table above was actually generated by $f(x) = x^2 - 4$ which we did not know prior, and too hard to interpolate.

1.4 Important Notes:

- 1.) Numerical analysis solution is always numerical.
- 2.) Results from numerical analysis is an approximation.

1.5 Numerical Errors

When we get into the real world from an ideal world and finite to infinite, errors arise.

1.5.1 Sources of Errors:

- 1.) Mathematical problems involving quantities of infinite precision.
- 2.) Numerical methods bridge the precision gap by putting errors under firm control.
- 3.) Computer can only handle quantities of finite precision.

1.5.2 Types of Errors:

1.5.2.1 Truncation error

Truncation error is a consequence of doing only a finite number of steps in a calculation that would require an infinite number of steps to do exactly. A simple example of a calculation that will be affected by truncation error is the evaluation of an infinite sum using the NSum function. The computer certainly isn't going to compute values for all of the terms in an infinite sum. The terms that are left out lead to truncation error.

Truncation Error: The essence of any numerical method is that it is approximate-this usually occurs because of truncation, e.g., $\cos x \cong 1 - \frac{x^2}{2}$ or terminating an infinite sequence of operations after a finite number have been performed.

It is not possible by numerical techniques alone to get an accurate estimate of the size of the

truncation error in a result. It is possible for any purely numerical algorithm, including the algorithms used by numerical functions in Mathematica, to produce incorrect results, and to do so without warning. The only way to be certain that results from functions like NIntegrate and NDSolve are correct is to do some independent analysis, possibly including detailed investigation of the algorithm that was used to do the calculation. Such investigations are an important part of the field of numerical analysis.

For example, after using Taylor expansion

$$\begin{aligned} e^x &= 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots \\ \cos x &= 1 - \frac{x^2}{2!} + \frac{x^4}{4!} - \frac{x^6}{6!} + \frac{x^8}{8!} - \dots \\ \sin x &= x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \frac{x^9}{9!} + \dots \end{aligned}$$

You could realize that there are many terms you have truncated off in the expansion, that's why ...

1.5.2.2 Round off errors

Numbers can be stored only up to a fixed finite number of digits: Additional digits may be rounded or chopped. Rounding error is sometimes characterized by ξ_{machine} , the largest (positive) number that the machine (computer) cannot distinguish between 1 and $1 + \xi_{\text{machine}}$.

Roundoff error, or representation error, is the error associated with the fact that the computer keeps only a finite number of digits in calculations with inexact numbers. Since it is not possible (except in special cases) to represent all of the digits in numbers like $1/3$ or π or $\sqrt{2}$, computers store only the first few digits in numerical approximations of these numbers. In typical situations, the computer will store only the first 16 decimal digits or the first 53 binary digits. The remaining digits are discarded. The discarded digits lead to errors in the result. One of the more conspicuous symptoms of roundoff error is the appearance of tiny non-zero numbers in results that would otherwise be zero.

Although the ability to reduce the effects of roundoff error by raising the precision of a calculation is certainly very useful, it is far from a universal solution to all problems with numerical error.

- 1.) 1.8625 to three decimal places, it becomes 1.863
- 2.) 1.8625 to two decimal places, it becomes 1.86
- 3.) 1.8625 to one decimal place, it become 1.9

1.5.2.3 Human Errors

Such as Computing tools/machines, Mathematical equation/model, propagated error.

Chapter 2

Numerical Techniques of Integration

There are two main reasons for you to need to do numerical integration: analytical integration may be impossible or infeasible, or you may wish to integrate tabulated data rather than known functions. In this section we outline the main approaches to numerical integration. Which is preferable depends in part on the results required, and in part on the function or data to be integrated.

This will be useful when we cannot find an elementary antiderivative for $f(x)$ or if the function is defined using data obtained from some experiment.

Numerical integration is the numerical approximation of the integral of a function. For a function of one variable, it amounts to finding the area under the graph of the function. That is finding I where

$$I = \int_a^b f(x) \, dx$$

Methods generally replace the integral by a weighted sum of n weights and n function evaluations, so that

$$I = \sum_{i=1}^n W_i f(x_i) \, dx$$

For a function of two variables it is equivalent to finding an approximation to the volume under the surface. Numerical integration is often also referred to as quadrature or sometimes cubature for functions of two or more variables. Returning to the one variable case, numerical integration involves finding the approximation to an integral of a function $f(x)$ through its evaluation at a set of discrete points. There are two distinct approaches to this. Firstly methods like the trapezium rule or Simpson's rule determine the integral through evaluating $f(x)$ at regularly spaced points. These are generally referred to as Newton-Cotes formulae.

Alternative methods termed Gaussian Quadrature methods have arisen that select irregularly-placed evaluation points, chosen to determine the integral as accurately as possible with a given set of points.

Gaussian Quadrature methods are important as they often lead to very efficient methods. In numerical integration the efficiency of the method relates to the accuracy obtained with respect to the number of evaluations of the function $f(x)$. In intensive methods such as the boundary element method integrations may need to be performed millions of times so the efficiency of the methods needs to be considered sometimes.

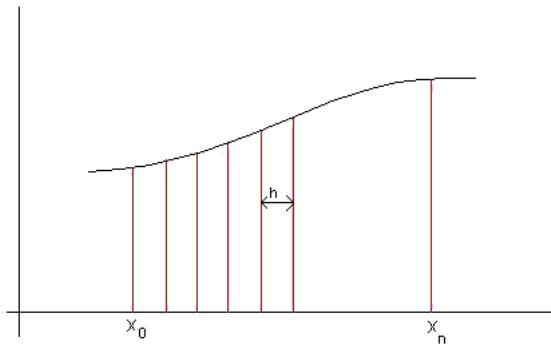
2.1 Manual Method

If you were to perform the integration by hand, one approach is to superimpose a grid on a graph of the function to be integrated, and simply count the squares, counting only those covered by 50% or more of the function. Provided the grid is sufficiently fine, a reasonably accurate estimate may be obtained.

2.2 Trapezoidal/Trapezium rule

2.2.1 Composite Trapezoidal Rule

To derive the rule, we use the following figure



We divide $[a, b]$ into n equal subintervals, each a Trapezium with width $h = \frac{(b - a)}{n}$

$$I = \int_a^b f(x)dx = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \dots + \int_{x_i}^{x_{i+1}} f(x)dx + \dots + \int_{x_{n-1}}^{x_n} f(x)dx.$$

Applying the trapezium equation, we get compute the total areas of all the n trapeziums

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_1)] + \frac{h}{2} [f(x_1) + f(x_2)] + \dots + \frac{h}{2} [f(x_{n-2}) + f(x_{n-1})] + \frac{h}{2} [f(x_{n-1}) + f(x_n)] \\ I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \end{aligned} \quad (2.1)$$

2.2.2 Trapezoidal Rule Truncation Error

$$\begin{aligned} E_{trunc} &= -\frac{h^3}{12} [f''(c_1) + f''(c_2) + \dots + f''(c_n)] \\ |E_{trunc}| &\leq \frac{M(b-a)^3}{12n^2} = \frac{M(b-a)h^2}{12} \end{aligned} \quad (2.2)$$

such that the second derivative f'' is continuous on $[a, b]$ and that

$$|f''(\xi)| < M \quad \forall \xi \in [a, b] \quad (2.3)$$

and

$$h = \frac{b-a}{n}$$

Example 2.2.1 Approximate the integral

$$I = \int_0^1 x^2 dx$$

using the composite Trapezoidal rule with step length $h = 0.2$

Solution

Since

$$\begin{aligned} I &= \int_0^1 f(x)dx = \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &= \frac{h}{2} [f(0) + f(1) + 2 \{f(0.2) + f(0.4) + f(0.6) + f(0.8)\}] \\ &= \frac{0.2}{2} [(0)^2 + (1)^2 + 2 \{(0.2)^2 + (0.4)^2 + (0.6)^2 + (0.8)^2\}] \\ &= 0.3400 \end{aligned}$$

Analytical solution is

$$\int_0^1 x^2 dx = \left[\frac{x^3}{3} \right]_0^1 = \frac{1}{3}$$

Absolute error committed is

$$\left| 0.340 - \frac{1}{3} \right| \simeq 0.00667$$

We have noted that the error obtained is much smaller than that obtained with the pure Trapezoidal rule in the previous example. In fact the smaller the error, i.e the better the approximation.

The truncation error is

$$|E_{trunc}| \leq \frac{M(b-a)^3}{12n^2} = \frac{2(1)^3}{(12)^5} = 0.00667$$

Since

$$f''(x) = 2, |f''(x)| < 2 \text{ on } [0, 1]$$

Example 2.2.2 Approximate the integral

$$I = \int_{-2}^2 e^{-\frac{x^2}{2}} dx$$

by the composite Trapezoidal rule with $h = 1.0$, the exact value of the integral I to 4 decimal places is 2.3925.

Since $h = 1.0$, then,

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &= \frac{(1.0)}{2} \left[e^{-\frac{(-2)^2}{2}} + e^{-\frac{(2)^2}{2}} + 2 \left\{ e^{-\frac{(-1)^2}{2}} + e^{-\frac{(0)^2}{2}} + e^{-\frac{(1)^2}{2}} \right\} \right] \\ &= 0.5 [0.13534 + 0.13534 + 2 \{0.60653 + 1.00000 + 0.60653\}] \\ &= 2.3484 \end{aligned}$$

with absolute error of $|2.3925 - 2.3484| = 0.0441$.

Example 2.2.3 Numerically estimate

$$\int_1^2 \frac{1}{x+1} dx$$

using

1.) Trapezium rule

$$\frac{h}{2}[f_0 + f_1] = \frac{1}{2} \left[\frac{1}{2} + \frac{1}{3} \right] = 0.416$$

2.) Composite Trapezium rule with $h = 0.2$

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &\simeq \frac{h}{2} [f(1.0) + f(2.0) + 2 \{f(1.2) + f(1.4) + f(1.6) + f(1.8)\}] \\ &\simeq \frac{(0.2)}{2} \left[\frac{1}{1+1} + \frac{1}{1+2} + 2 \left\{ \frac{1}{1+1.2} + \frac{1}{1+1.4} + \frac{1}{1+1.6} + \frac{1}{1+1.8} \right\} \right] \\ &\simeq \frac{0.2}{2} \left[\frac{1}{2} + \frac{1}{3} + 2 \left\{ \frac{1}{2.2} + \frac{1}{2.4} + \frac{1}{2.6} + \frac{1}{2.8} \right\} \right] \\ &\simeq 0.4059 \end{aligned}$$

Example 2.2.4 Evaluate

$$\int_0^3 (2x + 3) dx$$

by the Trapezium rule with four intervals (5 ordinates).

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &\simeq \frac{h}{2} [f(0) + f(3.0) + 2 \{f(0.75) + f(1.5) + f(2.25)\}] \\ &\simeq \frac{0.75}{2} [3 + 9 + 2 \{4.5 + 6 + 7.5\}] \\ &\simeq 18.0000 \end{aligned}$$

The classical (analytical, exact) solution is given by

$$\int_0^3 (2x + 3) dx = x^2 + 3x \Big|_0^3 = 18$$

To have the absolute error as

$$|18 - 18| = 0.0000$$

The truncation error is

$$|E_{trunc}| \leq \frac{M(b-a)^3}{12n^2} = \frac{(0)(3)^3}{(12)4^2} = 0.0000$$

Since

$$f''(x) = 0, |f''(x)| < 0 \text{ for } [0, 3]$$

Example 2.2.5 Evaluating $\int_1^3 \sin x dx$ by the Trapezium rule with 100 points, it gives the answer as 1.5302437923

But can you think of a way of programming this easily??

Example 2.2.6 Estimate $\int_0^3 \sin x^2 dx$ by the Trapezium algorithm

n	Sum of areas of Trapezoids
4	0.43358
8	0.70404
16	0.75723
32	0.76954
64	0.77256
128	0.77331
256	0.77350
512	0.77355
1024	0.77356
2048	0.77356

0.77356 appears to be a reasonable estimate of our integral.

Example 2.2.7 Using the Trapezoidal scheme, approximate $\int_0^1 \sqrt{2x+1} dx$ with $h = 0.25$.

x	0	0.25	0.5	0.75	1
$\sqrt{2x+1}$	1	1.22	1.41	1.58	1.73

$$\begin{aligned} A &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &= \frac{h}{2} [f(0) + f(1) + 2 \{f(0.25) + f(0.5) + f(0.75)\}] + E_{trunc} \\ &\approx \frac{1}{2}(0.25) [1 + 1.73 + 2 \{1.22 + 1.41 + 1.58\}] \\ &= 1.39 \end{aligned}$$

Analytically (the classical or exact value) is

$$\int_0^1 (2x+1)^{\frac{1}{2}} dx = \left[\frac{1}{3} (2x+1)^{\frac{3}{2}} \right]_0^1 = 1.3987$$

The error committed by the Trapezoidal rule is 0.0087

1.) Repeat the problem with $h = 0.2$

2.) Repeat the problem with $h = 0.1$

Exercise 2.2.1 Compute the approximate value of $\int_0^1 (x^2 + 1)^{-1} dx$ by using the Trapezoidal rule with ten subintervals. Then compare with the actual value of the integral. Determine the truncation error bound and compare with the actual error.

Exercise 2.2.2 If the Trapezoidal rule is used to compute $\int_2^5 \sin x dx$ with $h = 0.01$, obtain an upper bound error.

Exercise 2.2.3 How large must n be if the Trapezoidal rule is to estimate $\int_0^2 \exp\{-x^2\} dx$ with an error not exceeding 10^{-6} ?

Example 2.2.8 Numerically approximate

$$\int_0^2 [2 + \cos(2\sqrt{x})] dx$$

by using the Trapezoidal algorithm with

$$1.) n = 4 \Rightarrow h = \frac{1}{2}$$

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &\approx \frac{1}{2}(0.5) \left[(2 + \cos(2\sqrt{0})) + (2 + \cos(2\sqrt{2})) + \right. \\ &\quad \left. 2 \left\{ (2 + \cos(2\sqrt{0.5})) + (2 + \cos(2\sqrt{1})) + (2 + \cos(2\sqrt{1.5})) \right\} \right] \\ &\approx \frac{1}{2}(0.5) \left[3 + 2 + \cos(2\sqrt{2}) + 2 [(2 + \cos \sqrt{2}) + (2 + \cos 2) + (2 + \cos \sqrt{6})] \right] \\ &\approx 3.4971 \end{aligned}$$

$$2.) n = 8 \Rightarrow h = \frac{1}{4}$$

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &= \frac{1}{8} \left[(2 + \cos(2\sqrt{0})) + (2 + \cos(2\sqrt{2})) + \right. \\ &\quad \left. 2 \left\{ (2 + \cos(2\sqrt{0.25})) + (2 + \cos(2\sqrt{0.5})) + (2 + \cos(2\sqrt{0.75})) + (2 + \cos(2\sqrt{1})) + \right. \right. \\ &\quad \left. \left. (2 + \cos(2\sqrt{1.25})) + (2 + \cos(2\sqrt{1.5})) + (2 + \cos(2\sqrt{1.75})) \right\} \right] \\ &\approx 3.4693 \end{aligned}$$

3.) Compute the analytical value of the definite integral.

4.) Considering your results in part 3.) above, state any two reasons on how to reduce the errors in numerical integration.

Increasing the number of subintervals

Avoiding round off errors by computing final solution at once

Note 2.2.1 For trigonometric functions, the calculator is to be set in radians.

Exercise 2.2.4 Consider the integral $\int_0^1 \sin\left(\frac{x^2}{2}\pi\right) dx$. Suppose that we wish to integrate numerically with error $< 10^{-5}$. What interval width h is needed if the Trapezoidal rule is to be used?

Example 2.2.9 How large should we take n in order to guarantee that the Trapezoidal rule used in approximation of the integral $\int_0^2 \frac{1}{x+1} dx$ is accurate to within 0.0001.

Solution : Using the Truncation error of Trapezoidal, (2.2) on page (p. 7). Since $f(x) = \frac{1}{x+1} \Rightarrow f''(x) = \frac{2}{(1+x)^3}$ on $[0, 2] \Rightarrow M = 2$. Therefore,

$$|E_{trunc}| \leq \frac{M(b-a)^3}{12n^2} = \frac{2(2)^3}{12n^2} = 0.0001 \Rightarrow n = 115.47 = 115$$

■

Exercise 2.2.5 Approximate $\int_1^3 \frac{1}{x} dx$ by the Trapezoidal rule with an error of utmost 0.1.

Example 2.2.10 Find the area under the curve using trapezoidal rule formula which passes through the following points:

x	0	0.5	1	1.5
y	5	6	9	11

Solution : Using Trapezoidal Rule Formula,

$$\begin{aligned} \text{Area} &= \frac{h}{2} \left[y_0 + y_n + 2(y_1 + y_2 + y_3 + \dots + y_{n-1}) \right] \\ &= \frac{0.5}{2} \left[5 + 11 + 2(6 + 9) \right] \\ &= 11.5 \end{aligned}$$

Therefore, the area under the curve is 11.5 sq units. ■

Example 2.2.11 Using Trapezoidal Rule Formula find the area under the curve $y = x^2$ between $x = 0$ and $x = 4$ using the step size of 1.

Solution :

$$\begin{aligned} \text{Area} &= \frac{h}{2} \left[y_0 + y_n + 2(y_1 + y_2 + y_3 + \dots + y_{n-1}) \right] \\ &= \frac{1}{2} \left[0 + 16 + 2(1 + 4 + 9) \right] \\ &= 22 \end{aligned}$$

Therefore, the area under the curve is 22 sq units. ■

Example 2.2.12 Find the area under the curve using the trapezoidal rule formula which passes through the following points:

x	0	0.5	1	1.5
y	4	7	10	15

Solution : The area under the curve is 13.25 sq units. ■

2.3 Simpson's Rule

Note 2.3.1 We can obtain the Simpson's rule by various ways. One of the most popular ways is from Lagrange's quadratic interpolation polynomial. The Simpson's rule approximates the area under the curve $y = f(x)$ from x_0 to x_2 by the area under a parabolic curve.

Interpolating $f(x)$ by a Lagrange polynomial of degree 2 i.e. $P_2(x)$ then

$$f(x) = P_2(x) + E_{trunc}(x)$$

So

$$\int_{x_0}^{x_2} f(x)dx = \int_{x_0}^{x_2} P_2(x)dx + \int_{x_0}^{x_2} E_{trunc}(x)dx \quad (2.4)$$

Results

Summing up all the three cases, equation (2.4) becomes

$$\begin{aligned} \int_{x_0}^{x_2} P_2(x)dx &= \frac{h}{3}[f_0 + 4f_1 + f_2] + E_{trunc}(x) \quad \text{Thus} \\ \int_{x_0}^{x_2} P_2(x)dx &= \frac{h}{3}[f_0 + 4f_1 + f_2] \end{aligned} \quad (2.5)$$

Relation equation (2.5) is the Simpson's rule for approximating the integral. The integral for the error in equation (2.4), becomes

$$\int_{x_0}^{x_2} E_{trunc}(x)dx = \int_{x_0}^{x_2} \frac{(x - x_0)(x - x_1)(x - x_2)}{3!} f^{(4)}(c(x))dx$$

This can be shown (with difficulty!, for $n = 2$) to be

$$-\frac{Mh^5}{90} = -\frac{1}{90}M \left(\frac{b-a}{2}\right)^5$$

That the fourth derivative f^4 is continuous on $[a, b]$ and that $|f^4(x)| < M$ for all x in $[a, b]$.

Example 2.3.1

Use Simpson's rule ($n = 2$) to approximate the integral $I = \int_0^1 x^2 dx$.

Solution Since

$$I = \int_0^1 f(x)dx \simeq \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]$$

But

$$x_0 = 0, \quad x_1 = \frac{1}{2}, \quad x_2 = 1, \quad h = \frac{(1-0)}{2} = \frac{1}{2}.$$

Therefore

$$I \simeq \frac{1}{6} \left[f(0) + 4f\left(\frac{1}{2}\right) + f(1) \right] = \frac{1}{6} \left[0^2 + 4 \left(\frac{1}{2}\right)^2 + 1^2 \right] = \frac{1}{3} = 0.3\bar{3}$$

But the exact value of the integral is $\frac{1}{3} = 0.33\bar{3}$. It should not surprise you that the Simpson" rule has generated the exact value of the integral. In fact the general result is that for $f(x)$ a polynomial of degree two or less, the Simpson" rule will always generate the exact value of the integral. This will later be stated as a theorem.

2.3.1 Composite Simpson's 1/3 Rule

The composite Simpson's 1/3 rule is commonly referred to as the Simpson's rule.

Definition 2.3.1 *Simpson's 1/3 rule:* The Simpson's algorithm for a definite integral $\int_a^b f(x)dx$ is given by

$$\int_a^b f(x) dx \approx \frac{h}{3} \left[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + 4f(x_5) + 2f(x_6) + \dots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n) \right] \quad (2.6)$$

$$\int_a^b f(x) dx = \frac{h}{3} \left[f(x_0) + 2 \sum_{j=1}^{n/2-1} f(x_{2j}) + 4 \sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] \quad (2.7)$$

Remark 2.3.1 Simpson's 1/3 rule: After first and last points, others take on coefficients (4, 2) repeatedly till second last point.

Alternatively, the expansion of (2.7) gives or factorisation of (2.6):

$$A = \frac{h}{3} \left[f(x_0) + f(x_n) + 2 \left\{ f(x_2) + f(x_4) + \dots + f(x_{2n-2}) \right\} + 4 \left\{ f(x_1) + f(x_3) + \dots + f(x_{2n-1}) \right\} \right] + E_T \quad (2.8)$$

Remark 2.3.2 *Simpson's 1/3 rule* requires an **even** number of subintervals.

Remark 2.3.3 Simpson's 1/3 rule: After first and last points, others take on coefficients (4, 2, 4, 2, ...) repeatedly till second last point.

2.3.2 Simpson's Rule Truncation Error

The truncation error in Simpson's rule is given by

$$E_{trunc} = -\frac{h^5}{90} [f^{(4)}(c_1) + f^{(4)}(c_2) + \dots + f^{(4)}(c_n)] = -\frac{h^5}{90} f^{(4)}(c_2) \times n = -\frac{(b-a)h^4}{180} f^{(4)}(\xi)$$

where $a \leq \xi \leq b$. Therefore

$$E_{trunc} = \frac{(b-a)h^4}{180} f^{(4)}(\xi), \quad \xi \in [a, b] \quad (2.9)$$

Alternatively, the truncation error is given by

$$E_{trunc} = \frac{(b-a)^5}{180n^4} f^{(4)}(\xi), \quad \xi \in [a, b]$$

since

$$h = \frac{b-a}{n}$$

Example 2.3.2 Use S_2 to approximate $\int_0^1 x^3 dx$. Estimate a bound for the error in S_2 .

Solution : Since $[0,1]$ is divided into two subintervals S_2 , each subinterval has length $\Delta x = \frac{1-0}{2} = \frac{1}{2}$. The endpoints of these subintervals are $\left\{0, \frac{1}{2}, 1\right\}$. If we set $f(x) = x^3$, then

$$S_2 = \frac{1}{3} \cdot \frac{1}{2} \left[f(0) + 4f\left(\frac{1}{2}\right) + f(1) \right] = \frac{1}{6} \left(0 + 4 \cdot \frac{1}{8} + 1 \right) = \frac{1}{4}.$$

Since $f^{(4)}(x) = 0$ and consequently we see that

$$E_{trunc} \leq \frac{(b-a)h^4}{180}(0) = 0$$

This bound indicates that the value obtained through Simpson's rule is exact. A quick check will verify that, in fact, $\int_0^1 x^3 dx = \frac{1}{4}$. ■

Example 2.3.3 Evaluate the integral $\int_0^2 \sqrt{1+e^x} dx$ using Simpson's rule by taking $n = 4$.

Solution :

$$h = \frac{b-a}{n} = \frac{2-0}{4} = 0.5$$

So the 4 subintervals are $[0, 0.5]$, $[0.5, 1]$, $[1, 1.5]$, and $[1.5, 2]$.

By Simpson's rule formula,

$$\begin{aligned} & \int_0^2 \sqrt{1+e^x} dx \\ & \approx \frac{0.5}{3} \left[f(0) + 4f(0.5) + 2f(1) + 4f(1.5) + f(2) \right] \\ & = \frac{0.5}{3} \left(1.414213562 + 6.509957014 + 3.85656937 + \right. \\ & \quad \left. + 9.36520288 + 2.896386731 \right) \\ & = 4.0070549278 \end{aligned}$$
■

Remark 2.3.4 The composite Simpson's rule is commonly referred to as the Simpson's rule.

Example 2.3.4 Use the Simpson's method to compute the integral

$$I = \int_{-2}^2 e^{-\frac{x^2}{2}} dx$$

Using step size $h = 1.0$. Recall the exact value of I to 4 decimal places is 2.3925.

Using the Simpson's rule with $h = 1.0 \Rightarrow n = 4$, an even number of subintervals, using Equation (2.8), we have,

$$\begin{aligned} I &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\ I &\simeq \frac{1.0}{3} \left[e^{-\frac{(-2)^2}{2}} + e^{-\frac{(2)^2}{2}} + 2 \left\{ e^{-\frac{(0)^2}{2}} \right\} + 4 \left\{ e^{-\frac{(-1)^2}{2}} + e^{-\frac{(1)^2}{2}} \right\} \right] \\ I &\simeq 2.3743 \end{aligned}$$

The absolute error committed is $|2.3925 - 2.3743| = 0.0182$. We note that the error is much smaller than that obtained when using Trapezoidal rule in the Example 2.2.2 on page (p. 8) though same step size is used.

Note 2.3.2 Simpson's rule (2.8) only work for even number of subintervals.

Example 2.3.5 Determine the definite integral $\int_1^2 \frac{1}{x} dx$ using Simpson with $n = 6$.

$$\begin{aligned} \int_1^2 \frac{1}{x} dx &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\ &\approx \frac{1}{18} \left[1 + \frac{1}{2} + 2 \left\{ \frac{3}{4} + \frac{3}{5} \right\} + 4 \left\{ \frac{6}{7} + \frac{2}{3} + \frac{6}{11} \right\} \right] \\ &\approx \frac{14411}{20790} \approx 0.6931697 \end{aligned}$$

Example 2.3.6 Estimate $\int_2^3 \frac{dx}{x+1}$ using Simpson's rule with $n = 4$.

$$\begin{aligned} \int_2^3 \frac{dx}{x+1} &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\ &\approx \frac{0.25}{3} [f(2) + f(3) + 2 \{f(2.5)\} + 4 \{f(2.25) + f(2.75)\}] \\ &\approx \frac{0.25}{3} \left[\frac{1}{3} + \frac{1}{4} + 2 \left\{ \frac{1}{3.5} \right\} + 4 \left\{ \frac{1}{3.25} + \frac{1}{3.75} \right\} \right] \\ &\approx 0.2876831 \end{aligned}$$

1.) Compute its exact value and hence the error committed

$$\begin{aligned} \int_2^3 \frac{dx}{x+1} &= \ln(x+1)|_2^3 = 0.287682 \\ \Rightarrow \text{Absolute error} &= |0.287682 - 0.2876831| \approx 0.00036 \end{aligned}$$

2.) Repeat the problem above using $h = 0.1$.

3.) Comment on the effect of h on the numerical solutions.

4.) Repeat the problem using the Trapezoidal rule. Which of the two techniques is more accurate?

Note 2.3.3 For $f(x)$ a trigonometric function, we use (Your calculator should be in) Radians.

Example 2.3.7 It is required to obtain $\int_0^2 e^{x^2} dx$ exact to 4 decimal places. What should h be for Simpson's rule.

Since the error term is $-\frac{(b-a)}{180} h^4 f^{(4)}(\xi)$, with $f(x) = e^{x^2}$, then

$$\begin{aligned}f'(x) &= 2xe^{x^2} \\f''(x) &= 2(e^{x^2} + 2xe^{x^2}) = 2e^{x^2}(1 + 2x^2) = e^{x^2}(2 + 4x^2) \\f'''(x) &= 2xe^{x^2}(2 + 4x^2) + 8xe^{x^2} \\&= e^{x^2}(4x + 8x^3 + 8x) \\&= e^{x^2}(12x + 8x^3) \\f^{(iv)}(x) &= 8e^{x^2}(2x^4 + 5x^2 + 1) \\&< 424e^4\end{aligned}$$

So

$$-\frac{(b-a)}{180} h^4 f^{(4)}(\xi) = \frac{2h^4}{180} (424e^4) < (0.5)10^{-4}$$

to have $h < 0.057$, say choose $h = 0.05$.

Exercise 2.3.1 Compute an approximate value of $\int_0^1 (x^2+1)^{-1} dx$ using Composite Simpson's rule with

$$1.) \quad h = 0.1 \qquad \qquad 2.) \quad h = 0.5$$

Compare with the actual value of the integral in each case. Next, determine the truncation error bound and compare with the actual error.

Exercise 2.3.2 If the Simpson's rule is used to compute $\int_2^5 \sin x dx$ with $h = 0.75$, obtain an upper bound on the error.

Exercise 2.3.3 Establish the composite Simpson's rule over $(n-1)$ even subintervals

$$\int_a^b f(x) dx = \frac{h}{3} [(f(a) + f(b)) + 4 \sum_{i=1}^{\frac{(n-1)}{2}} f(a + (2i-1)h) + 2 \sum_{i=1}^{\frac{(n-3)}{2}} f(a + 2ih)] + E_{trunc}$$

where, $h = \frac{(b-a)}{(n-1)}$ and $E_{trunc} = -\frac{(b-a)}{180} h^4 f^{(4)}(\xi)$ for some $\xi \in [a, b]$.

Exercise 2.3.4 Consider the integral $\int_0^1 \sin\left(\frac{\pi x^2}{2}\right) dx$. Suppose that we wish to integrate numerically with error $< 10^{-5}$. What interval width h is needed if the Simpson's rule is to be used?

Exercise 2.3.5 Compute $\int_0^2 (x^3 + 1) dx$ by using $h = \frac{1}{4}$ and compare with the exact value of the integral.

Example 2.3.8

- 1.) Solve the integral $\int_0^2 [2 + \cos(2\sqrt{x})] dx$ in Example 2.2.8 on page (p. 11) using the Simpson's algorithm with $n = 4$.

$$\begin{aligned}
 I &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\
 &\approx \frac{1}{6} \left[(2 + \cos(2\sqrt{0})) + (2 + \cos(2\sqrt{2})) + 2 \left\{ (2 + \cos(2\sqrt{1})) \right\} \right. \\
 &\quad \left. + 4 \left\{ (2 + \cos(2\sqrt{0.5})) + (2 + \cos(2\sqrt{1.5})) \right\} \right] \\
 &\approx \frac{1}{6} \left[3 + 2 + \cos(2\sqrt{2}) + 2 \{(2 + \cos 2)\} + 4 \{(2 + \cos \sqrt{2}) + (2 + \cos \sqrt{6})\} \right] \\
 &\approx \frac{1}{6} \left[5 + \cos(2\sqrt{2}) + 2 \{(2 + \cos 2)\} + 4 \{(2 + \cos \sqrt{2}) + (2 + \cos \sqrt{6})\} \right] \\
 &\approx 3.46008250981 \\
 &\approx 3.46008
 \end{aligned}$$

- 2.) Show that using the Simpson's scheme with $n = 8$, the integral is $I \approx 3.46000$.

$$\begin{aligned}
 I &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\
 &\approx \frac{1}{12} \left[(2 + \cos(2\sqrt{0})) + (2 + \cos(2\sqrt{2})) \right. \\
 &\quad \left. + 2 \left\{ (2 + \cos(2\sqrt{0.5})) + (2 + \cos(2\sqrt{1})) + (2 + \cos(2\sqrt{1.5})) \right\} \right. \\
 &\quad \left. + 4 \left\{ (2 + \cos(2\sqrt{0.25})) + (2 + \cos(2\sqrt{0.75})) + (2 + \cos(2\sqrt{1.25})) + (2 + \cos(2\sqrt{1.75})) \right\} \right] \\
 &\approx 3.460002979 \\
 &\approx 3.46000
 \end{aligned}$$

- 3.) The classical value is given by

$$\int_0^2 [2 + \cos(2\sqrt{x})] dx = 2x + (0.5) \cos(2\sqrt{x}) + \sqrt{x} \sin(2\sqrt{x}) \Big|_0^2 = 3.46000$$

- 4.) What is the effect of the size of n , the number of subintervals? The more the subintervals, the more accurate the numerical approximations.
- 5.) Which of the two numerical schemes is more superior? The Simpson's rule is more accurate compared to the Trapezoidal method that estimated the definite integral to
- (a) $I = 3.4971$ for $n = 4$, and
 - (b) $I = 3.4693$ for $n = 8$

as computed in Example 2.2.8 on page (p. 11).

Example 2.3.9 Evaluate $\int_0^4 (1 + x^2) dx$ with $n = 4$, using

1.) Classical techniques

$$\int_0^4 (1 + x^2) dx = x + \frac{x^3}{3} \Big|_0^4 = \frac{76}{3} \approx 25.3333$$

2.) Simpson's scheme formula for even number of subintervals, Equation (2.8)

$$\begin{aligned} I &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\ &\approx \frac{1}{3} \left[f(0) + f(4) + 2 \{f(2) + f(4)\} + 4 \{f(1) + f(3)\} \right] \\ &\approx \frac{1}{3} \left[1 + 17 + 2 \{5\} + 4 \{2 + 10\} \right] \\ &\approx \frac{76}{3} \\ &\approx 25.3333 \end{aligned}$$

Having used the correct formula, the Simpson's approximation is very close, if not equal to the analytical, exact solutions in part 1.) above.

3.) Trapezoidal method

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &\approx \frac{1}{2} \left[f(0) + f(4) + 2 \{f(1) + f(2) + f(3)\} \right] \\ &\approx \frac{1}{2} \left[1 + 17 + 2 \{2 + 5 + 10\} \right] \\ &\approx \frac{52}{2} \\ &\approx 26.0000 \end{aligned}$$

Remark 2.3.5 The inferior Trapezoidal algorithm 3.) generate a less accurate solution compared to Simpson rule formula in 2.) which is a superior method.

Example 2.3.10 Evaluate the integral $\int_1^2 e^{x^3} dx$ using Simpson's rule by taking $n = 4$.

Solution :

$$h = \frac{b-a}{n} = \frac{2-1}{4} = 0.25$$

So the 4 subintervals are $[1, 1.25]$, $[1.25, 1.5]$, $[1.5, 1.75]$, and $[1.75, 2]$.

By Simpson's rule formula,

$$\begin{aligned} & \int_1^2 f(x) dx \\ & \approx \frac{0.25}{3} [f(1) + 4f(1.25) + 2f(1.5) + 4f(1.75) + f(2)] \\ & = \frac{0.25}{3} (2.71828182845905 + 28.2027463392796 \\ & \quad + 58.4485675624699 + 850.36813958881 \\ & \quad + 2980.95798704173) \\ & = 326.724643530062 \end{aligned}$$

■

Example 2.3.11 Evaluate the integral $\int_0^2 \sin \sqrt{x} dx$ using Simpson's rule by taking $n = 8$.

Solution :

$$h = \frac{b-a}{n} = \frac{2-0}{8} = 0.25$$

So the 8 sub-intervals are $[0, 0.25]$, $[0.25, 0.5]$, $[0.5, 0.75]$, $[0.75, 1]$, $[1, 1.25]$, $[1.25, 1.5]$, $[1.5, 1.75]$, and $[1.75, 2]$.

By Simpson's rule formula,

$$\begin{aligned} & \int_0^2 f(x) dx \\ & \approx \frac{0.25}{3} [f(0) + 4f(0.25) + 2f(0.5) + 4f(0.75) + 2f(1) + 4f(1.25) + 2f(1.5) + 4f(1.75) + f(2)] \\ & = \frac{0.25}{3} (0 + 1.91770215441681 + 1.29927387816012 \\ & \quad + 3.04703992566516 + 1.68294196961579 \\ & \quad + 3.59696858641514 + 1.88143866748289 \\ & \quad + 3.87769904361669 + 0.987765945992735) \\ & = 1.52423584761378 \end{aligned}$$

■

Example 2.3.12 Using Trapezoidal rule compute the integral $\int_0^1 e^{x^2} dx$, where the table for the values of $y = e^{x^2}$ is given below:

x	0.0	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
y	1.00000	1.01005	1.04081	1.09417	1.17351	1.28402	1.43332	1.63231	1.89648	2.2479	2.71828

Solution : Here, $h = 0.1$, $n = 10$,

$$\frac{y_0 + y_{10}}{2} = \frac{1.0 + 2.71828}{2} = 1.85914,$$

and

$$\sum_{i=1}^9 y_i = 12.81257.$$

such that the area by Trapezoidal's rule is given by

$$A = \frac{h}{2} [y_0 + y_{10} + 2 \{y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7 + y_8 + y_9\}]$$

$$A = h \left[\frac{y_0 + y_{10}}{2} + \{y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7 + y_8 + y_9\} \right]$$

Thus,

$$\int_0^1 e^{x^2} dx = 0.1 \times [1.85914 + 12.81257] = 1.467171$$

■

Example 2.3.13 Using the table for the values of $y = e^{x^2}$ as is given in Example 2.3.12, compute the integral $\int_0^1 e^{x^2} dx$, by Simpson's rule.

Solution : Here, $h = 0.1$, $n = 10$, thus we have an even number of subintervals. Further,

$$y_0 + y_{10} = 1.0 + 2.71828 = 3.71828,$$

$$\sum_{i=1, i-odd}^9 y_i = y_1 + y_3 + y_5 + y_7 + y_9 = 7.26845,$$

$$\sum_{i=2, i-even}^8 y_i = y_2 + y_4 + y_6 + y_8 = 5.54412.$$

such that the area by Simpson's rule is given by

$$A = \frac{h}{3} [y_0 + y_{10} + 2 \{y_2 + y_4 + y_6 + y_8\} + 4 \{y_1 + y_3 + y_5 + y_7 + y_9\}]$$

Thus,

$$\int_0^1 e^{x^2} dx = \frac{0.1}{3} \times [3.71828 + 2 \times 5.54412 + 4 \times 7.268361] = 1.46267733$$

■

Example 2.3.14 Compute the integral $\int_{0.05}^1 f(x)dx$, where the table for the values of $y = f(x)$ is given below:

x	0.05	0.1	0.15	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9	1.0
y	0.0785	0.1564	0.2334	0.3090	0.4540	0.5878	0.7071	0.8090	0.8910	0.9511	0.9877	1.0000

Solution : Note that here the points are not given to be equidistant, so as such we can not use any of the above two formulae. However, we notice that the tabular points 0.05, 0.10, 0.15 and 0.20 are equidistant and so are the tabular points 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9 and 1.0. Now we can divide the interval in two subinterval: [0.05, 0.2] and [0.2, 1.0]; thus,

$$\int_{0.05}^1 f(x)dx = \int_{0.05}^{0.2} f(x)dx + \int_{0.2}^1 f(x)dx.$$

The integrals then can be evaluated in each interval. We observe that the second set has odd number of points (even subintervals). Thus, the first integral is evaluated by using Trapezoidal rule and the second one by Simpson's rule (of course, one could have used Trapezoidal rule in both the subintervals).

For the first integral $h = 0.05$ and for the second one $h = 0.1$. Thus, first part by Trapezoidal scheme,

$$\int_{0.05}^{0.2} f(x)dx = \frac{0.05}{2} \times [0.0785 + 0.3090 + 2(0.1564 + 0.2334)] = 0.0291775,$$

and, second part by Simpson's rule,

$$\begin{aligned} \int_{0.2}^{1.0} f(x)dx &= \frac{0.1}{3} \times [(0.3090 + 1.0000) + 2 \times (0.5878 + 0.8090 + 0.9511) \\ &\quad + 4 \times (0.4540 + 0.7071 + 0.8910 + 0.9877)] \\ &= 0.6054667, \end{aligned}$$

which gives,

$$\int_{0.05}^1 f(x)dx = 0.0291775 + 0.6054667 = 0.6346442$$

It may be mentioned here that in the above integral, $f(x) = \sin\left(\frac{\pi}{2}x\right)$ and that the value of the integral is 0.6346526. It will be interesting for the reader to compute the two integrals using Trapezoidal rule and compare the values. ■

2.4 Mid-Point Rule

If f is continuous on $[a, b]$ and $f(x) \geq 0 \forall x \in (a, b)$, we partition $[a, b]$ into n subintervals of equal lengths.

Definition 2.4.1 If m_i is the midpoint of the i^{th} interval then

$$\int_a^b f(x)dx = \sum_{i=1}^n (\Delta x_i) f(m_i) \quad (2.10)$$

Example 2.4.1 Approximate the integral

$$\int_1^3 \sqrt{\sin^4(x) + 7} dx$$

with

$$n = 4$$

using the midpoint rule.

Solution : The midpoint rule (also known as the midpoint approximation) uses the midpoint of a subinterval for computing the height of the approximating rectangle:

$$\int_a^b f(x) dx \approx \Delta x \left[f\left(\frac{x_0+x_1}{2}\right) + f\left(\frac{x_1+x_2}{2}\right) + f\left(\frac{x_2+x_3}{2}\right) + \dots + f\left(\frac{x_{n-2}+x_{n-1}}{2}\right) + f\left(\frac{x_{n-1}+x_n}{2}\right) \right]$$

where

$$\Delta x = \frac{b-a}{n}$$

We have that

$$\begin{aligned} f(x) &= \sqrt{\sin^4(x) + 7} \\ a &= 1 \\ b &= 3 \end{aligned}$$

and

$$n = 4$$

Therefore,

$$\Delta x = \frac{3-1}{4} = \frac{1}{2}$$

Divide the interval

$$[1, 3]$$

into

$$n = 4$$

subintervals of the length

$$\Delta x = \frac{1}{2}$$

with the following endpoints:

$$a = 1$$

$$\begin{array}{c} \frac{3}{2} \\ \frac{2}{2} \\ 2 \\ \frac{5}{2} \\ 3 = b \end{array}$$

Now, just evaluate the function at the midpoints of the subintervals.

$$f\left(\frac{x_0 + x_1}{2}\right) = f\left(\frac{1 + \frac{3}{2}}{2}\right) = f\left(\frac{5}{4}\right) = \sqrt{\sin^4\left(\frac{5}{4}\right) + 7} \approx 2.794821922941848$$

$$f\left(\frac{x_1 + x_2}{2}\right) = f\left(\frac{\frac{3}{2} + 2}{2}\right) = f\left(\frac{7}{4}\right) = \sqrt{\sin^4\left(\frac{7}{4}\right) + 7} \approx 2.817350905627184$$

$$f\left(\frac{x_2 + x_3}{2}\right) = f\left(\frac{2 + \frac{5}{2}}{2}\right) = f\left(\frac{9}{4}\right) = \sqrt{\sin^4\left(\frac{9}{4}\right) + 7} \approx 2.714130913751178$$

$$f\left(\frac{x_3 + x_4}{2}\right) = f\left(\frac{\frac{5}{2} + 3}{2}\right) = f\left(\frac{11}{4}\right) = \sqrt{\sin^4\left(\frac{11}{4}\right) + 7} \approx 2.649758163512828$$

Finally, just sum up the above values and multiply by

$$\Delta x = \frac{1}{2} :$$

$$\begin{aligned} & \frac{1}{2} \left[2.794821922941848 + 2.817350905627184 + 2.714130913751178 + 2.649758163512828 \right] \\ &= 5.488030952916519 \end{aligned}$$

Therefore

$$\int_1^3 \sqrt{\sin^4(x) + 7} dx \approx 5.488030952916519$$

■

Example 2.4.2 Find the integral using the midpoint rule $\int_1^2 \frac{1}{x} dx$ with $n = 10$

The step width is given by $\Delta x_i = \frac{2 - 1}{10} = \frac{1}{10}$ such that $f(x) = \frac{1}{x} \Rightarrow f(m_i) = \frac{1}{m_i}$

$$\begin{aligned} \int_1^2 \frac{1}{x} dx &= \Delta x \sum_{i=1}^n f(m_i) \\ &= \frac{1}{10} [f(1.05) + f(1.15) + f(1.25) + f(1.35) + \dots + f(1.75) + f(1.85) + f(1.95)] \\ &= \frac{1}{10} \left[\frac{1}{1.05} + \frac{1}{1.15} + \frac{1}{1.25} + \frac{1}{1.35} + \frac{1}{1.45} + \frac{1}{1.55} + \frac{1}{1.65} + \frac{1}{1.75} + \frac{1}{1.85} + \frac{1}{1.95} \right] \\ &= 0.69284 \end{aligned}$$

Note 2.4.1 The Mid-point algorithm is the Riemann sum at mid point, not the upper (right end) Riemann and not the lower (left end) Riemann sum.

2.4.1 Mid-Point Truncation Error

If

$$|f''(\xi)| < M, \forall \xi \in [a, b]$$

then the truncation error in the Mid-point scheme is given by

$$E_{trunc} = \frac{M(b-a)^3}{24n^2} \quad (2.11)$$

Example 2.4.3 The exact solution for $\int_0^1 \cos x dx = \sin 1 \approx 0.8414709848$. For different step length $h = \Delta x$, show the Mid-Point rule results below:

h	$I_{Midpoint}(h)$	Absolute Error
0.500000	0.85030065	8.8×10^{-3}
0.250000	0.84366632	2.2×10^{-3}
0.125000	0.84201907	5.5×10^{-4}
0.062500	0.84160796	1.4×10^{-4}
0.031250	0.84150523	3.4×10^{-5}
0.015625	0.84147954	8.6×10^{-6}
0.007813	0.84147312	2.1×10^{-6}
0.003906	0.84147152	5.3×10^{-7}
0.001953	0.84147112	1.3×10^{-7}
0.000977	0.84147102	3.3×10^{-8}

Example 2.4.4 Use the midpoint rule to estimate $\int_0^1 x^2 dx$ using four subintervals. Compare the result with the actual value of this integral.

Solution : Each subinterval has length $\Delta x = \frac{1-0}{4} = \frac{1}{4}$. Therefore, the subintervals consist of

$$\left[0, \frac{1}{4}\right], \left[\frac{1}{4}, \frac{1}{2}\right], \left[\frac{1}{2}, \frac{3}{4}\right], \text{ and } \left[\frac{3}{4}, 1\right].$$

The midpoints of these subintervals are $\left\{\frac{1}{8}, \frac{3}{8}, \frac{5}{8}, \frac{7}{8}\right\}$. Thus,

$$\begin{aligned} M_4 &= \frac{1}{4} \cdot f\left(\frac{1}{8}\right) + \frac{1}{4} \cdot f\left(\frac{3}{8}\right) + \frac{1}{4} \cdot f\left(\frac{5}{8}\right) + \frac{1}{4} \cdot f\left(\frac{7}{8}\right) \\ &= \frac{1}{4} \cdot \frac{1}{64} + \frac{1}{4} \cdot \frac{9}{64} + \frac{1}{4} \cdot \frac{25}{64} + \frac{1}{4} \cdot \frac{49}{64} \\ &= \frac{21}{64} = 0.328125. \end{aligned}$$

Since

$$\int_0^1 x^2 dx = \frac{1}{3},$$

the absolute error in this approximation is:

$$\left|\frac{1}{3} - \frac{21}{64}\right| = \frac{1}{192} \approx 0.0052,$$

and we see that the midpoint rule produces an estimate that is somewhat close to the actual value of the definite integral. ■

Example 2.4.5 Use the midpoint rule with $n = 2$ to estimate $\int_1^2 \frac{1}{x} dx$.

Solution : $\frac{24}{35}$ ■

Example 2.4.6 Approximate the integral

$$\int_0^1 \sqrt{2x+1} dx$$

with

$$n = 4$$

using the midpoint rule.

Solution : The midpoint rule (also known as the midpoint approximation) uses the midpoint of a subinterval for computing the height of the approximating rectangle:

$$\int_a^b f(x) dx \approx \Delta x \left[f\left(\frac{x_0+x_1}{2}\right) + f\left(\frac{x_1+x_2}{2}\right) + f\left(\frac{x_2+x_3}{2}\right) + \dots + f\left(\frac{x_{n-2}+x_{n-1}}{2}\right) + f\left(\frac{x_{n-1}+x_n}{2}\right) \right]$$

where

$$\Delta x = \frac{b-a}{n}$$

We have that

$$f(x) = \sqrt{2x+1}, a = 0, b = 1, n = 4$$

Therefore,

$$\Delta x = \frac{1-0}{4} = 0.25$$

Divide the interval $[0, 1]$ into $n = 4$ subintervals of the length $\Delta x = \frac{1}{4}$ with the following endpoints:

$$a = 0, 0.25, 0.5, 0.75, 1 = b$$

Now, find the function at the midpoints of the subintervals.

$$\begin{aligned} f\left(\frac{x_0+x_1}{2}\right) &= f\left(\frac{0+0.25}{2}\right) = f(0.125) = \sqrt{20.125+1} = 1.11803398874989 \\ f\left(\frac{x_1+x_2}{2}\right) &= f\left(\frac{0.25+0.5}{2}\right) = f(0.375) = \sqrt{20.375+1} = 1.32287565553230 \\ f\left(\frac{x_2+x_3}{2}\right) &= f\left(\frac{0.5+0.75}{2}\right) = f(0.625) = \sqrt{20.625+1} = 1.500000000000000 \\ f\left(\frac{x_3+x_4}{2}\right) &= f\left(\frac{0.75+1}{2}\right) = f(0.875) = \sqrt{20.875+1} = 1.65831239517770 \end{aligned}$$

Finally, just sum up the above values and multiply by $\Delta x = \frac{1}{4} = 0.25$

$$\begin{aligned} &0.25(1.11803398874989 + 1.32287565553230 + 1.500000000000000 + 1.65831239517770) \\ &= 1.39980550986497 \end{aligned}$$

Therefore,

$$\int_0^1 \sqrt{2x+1} dx \approx 1.399805509864973$$

■

2.5 Comparison of the Numerical Integration Techniques

2.5.1 Truncation Errors Comparisons

- 1.) Error bound for midpoint rule

$$E_M \leq \frac{M(b-a)^3}{24n^2}$$

where M is the maximum value of $|f''(x)|$ over $[a, b]$.

- 2.) Error bound for trapezoidal rule

$$E_T \leq \frac{M(b-a)^3}{12n^2}$$

where M is the maximum value of $|f''(x)|$ over $[a, b]$.

- 3.) Error bound for Simpson's rule

$$E_S \leq \frac{M(b-a)^5}{180n^4}$$

where M is the maximum value of $|f^{(4)}(x)|$ over $[a, b]$.

Example 2.5.1 Determine the Midpoint rule truncation error in approximating $\int_0^\pi \sin x \, dx$

Solution :

1.) The integral $\int_0^\pi \sin x \, dx$ has $b - a = \pi$.

2.) The second derivative of the integrand satisfies

$$\left| \frac{d^2}{dx^2} \sin x \right| = |-\sin x| \leq 1$$

So we take $M = 1$.

3.) So the error, E_M , introduced when n steps are used is bounded by

$$\begin{aligned} |E_M(n)| &\leq \frac{M}{24} \frac{(b-a)^3}{n^2} \\ &= \frac{\pi^3}{24} \frac{1}{n^2} \\ &\approx 1.29 \frac{1}{n^2} \end{aligned}$$

■

Example 2.5.2 What value of n should be used to guarantee that an estimate of $\int_0^1 e^{x^2} dx$ is accurate to within 0.01 if we use the midpoint rule?

Solution : We begin by determining the value of M , the maximum value of $|f''(x)|$ over $[0, 1]$ for $f(x) = e^{x^2}$. Since $f'(x) = 2xe^{x^2}$, we have

$$f''(x) = 2e^{x^2} + 4x^2e^{x^2}.$$

Thus,

$$|f''(x)| = 2e^{x^2}(1 + 2x^2) \leq 2 \cdot e \cdot 3 = 6e.$$

From the error-bound Equation, we have the error in M_n

$$E_M \leq \frac{M(b-a)^3}{24n^2} \leq \frac{6e(1-0)^3}{24n^2} = \frac{6e}{24n^2}.$$

Now we solve the following inequality for n (accurate to within 0.01):

$$\frac{6e}{24n^2} \leq 0.01$$

Thus,

$$n \geq \sqrt{\frac{600e}{24}} \approx 8.24.$$

Since n must be an integer satisfying this inequality, a choice of $n = 9$ would guarantee that

$$\left| \int_0^1 e^{x^2} dx - M_n \right| < 0.01.$$

■

Example 2.5.3 Use Equation (truncation error) to find an upper bound for the error in using M_4 (Midpoint rule with 4 steps) to estimate $\int_0^1 x^2 dx$.

Solution : $f''(x) = 2$, so $M = 2$ such that

$$E_M = \frac{1}{192}$$

■

Example 2.5.4 Estimate a bound for the error in Simpson's rule in approximating $\int_0^1 x^3 dx$ with $n = 2$.

Solution : Since $f^{(4)}(x) = 0$ and consequently $M = 0$, we see that

$$E_S \leq \frac{0(1)^5}{180 \cdot 2^4} = 0.$$

This bound indicates that the value obtained through Simpson's rule is exact. ■

Exercise 2.5.1 Let $f(x) = -\frac{1}{12}x^4 + \frac{7}{6}x^3 - 3x^2$.

- 1.) Find a reasonable value M such that $|f''(x)| \leq M$ for all $1 \leq x \leq 6$.
- 2.) Find a reasonable value M such that $|f^{(4)}(x)| \leq M$ for all $1 \leq x \leq 6$.

Exercise 2.5.2 Let $f(x) = x \sin x + 2 \cos x$. Find a reasonable value M such that $|f''(x)| \leq M$ for all $-3 \leq x \leq 2$.

Exercise 2.5.3 Consider the quantity

$$A = \int_{-\pi}^{\pi} \cos x \, dx.$$

Find the upper bound on the error using Simpson's rule with $n = 4$ to approximate A .

Exercise 2.5.4 Give a function $f(x)$ such that:

- $f''(x) \leq 3$ for every x in $[0, 1]$, and
- the error using the trapezoidal rule approximating $\int_0^1 f(x) \, dx$ with $n = 2$ intervals is exactly $\frac{1}{16}$.

Exercise 2.5.5 True or False: for fixed positive constants M, n, a , and b , with $b > a$,

$$\frac{M(b-a)^3}{24n^2} \leq \frac{M(b-a)^3}{12n^2}$$

Exercise 2.5.6 True or False: for a function $f(x)$ and fixed constants n, a , and b , with $b > a$, the n -interval midpoint approximation of $\int_a^b f(x) \, dx$ is more accurate than the n -interval trapezoidal approximation.

2.5.2 Numerical Solutions Comparison

Example 2.5.5 Estimate $\int_0^1 \frac{4}{1+x^2} dx$ using the midpoint rule with $n = 8$ subintervals.

Solution :

- 1.) First we set up all the x -values that we will need. Note that $a = 0$, $b = 1$, $\Delta x = \frac{1}{8}$ and

$$x_0 = 0 \quad x_1 = \frac{1}{8} \quad x_2 = \frac{2}{8} \quad \dots \quad x_7 = \frac{7}{8} \quad x_8 = \frac{8}{8} = 1$$

Consequently, the midpoints \bar{x}

$$\bar{x}_1 = \frac{1}{16} \quad \bar{x}_2 = \frac{3}{16} \quad \bar{x}_3 = \frac{5}{16} \quad \dots \quad \bar{x}_8 = \frac{15}{16}$$

- 2.) We apply the midpoint rule to the integrand $f(x) = \frac{4}{1+x^2}$

$$\begin{aligned} \int_0^1 \frac{4}{1+x^2} dx &\approx \left[\overbrace{\frac{4}{1+\bar{x}_1^2}}^{f(\bar{x}_1)} + \overbrace{\frac{4}{1+\bar{x}_2^2}}^{f(\bar{x}_2)} + \dots + \overbrace{\frac{4}{1+\bar{x}_7^2}}^{f(\bar{x}_{n-1})} + \overbrace{\frac{4}{1+\bar{x}_8^2}}^{f(\bar{x}_n)} \right] \Delta x \\ &= \left[\frac{4}{1+\frac{1}{16^2}} + \frac{4}{1+\frac{3^2}{16^2}} + \frac{4}{1+\frac{5^2}{16^2}} + \frac{4}{1+\frac{7^2}{16^2}} + \frac{4}{1+\frac{9^2}{16^2}} \right. \\ &\quad \left. + \frac{4}{1+\frac{11^2}{16^2}} + \frac{4}{1+\frac{13^2}{16^2}} + \frac{4}{1+\frac{15^2}{16^2}} \right] \frac{1}{8} \\ &= [3.98444 + 3.86415 + 3.64413 + 3.35738 + 3.03858 + \\ &\quad 2.71618 + 2.40941 + 2.12890] \frac{1}{8} \\ &= 3.1429 \end{aligned}$$

where we have rounded to four decimal places

- 3.) In this case we can compute the integral exactly (which is one of the reasons it was chosen as an example):

$$\int_0^1 \frac{4}{1+x^2} dx = 4 \arctan x \Big|_0^1 = \pi$$

- 4.) So the absolute error in the approximation generated by eight steps of the midpoint rule is

$$|3.1429 - \pi| = 0.0013$$

- 5.) The relative error is then

$$\frac{|approximate - exact|}{exact} = \frac{|3.1429 - \pi|}{\pi} = 0.0004$$

That is the error is 0.0004 times the actual value of the integral.

- 6.) We can write this as a percentage error by multiplying it by 100

$$\text{percentage error} = 100 \times \frac{|approximate - exact|}{exact} = 0.04\%$$

That is, the error is about 0.04% of the exact value.



Example 2.5.6 Approximate $\int_0^\pi \sin x \, dx$ applying the midpoint rule with $n = 8$ subintervals to the above integral.

Solution :

- 1.) We again start by setting up all the x -values that we will need. So $a = 0, b = \pi, \Delta x = \frac{\pi}{8}$ and

$$x_0 = 0 \quad x_1 = \frac{\pi}{8} \quad x_2 = \frac{2\pi}{8} \quad \dots \quad x_7 = \frac{7\pi}{8} \quad x_8 = \frac{8\pi}{8} = \pi$$

Consequently,

$$\bar{x}_1 = \frac{\pi}{16} \quad \bar{x}_2 = \frac{3\pi}{16} \quad \dots \quad \bar{x}_7 = \frac{13\pi}{16} \quad \bar{x}_8 = \frac{15\pi}{16}$$

- 2.) Applying the mid point rule with the integrand $f(x) = \sin x$

$$\begin{aligned} \int_0^\pi \sin x \, dx &\approx \left[\sin(\bar{x}_1) + \sin(\bar{x}_2) + \dots + \sin(\bar{x}_8) \right] \Delta x \\ &= \left[\sin\left(\frac{\pi}{16}\right) + \sin\left(\frac{3\pi}{16}\right) + \sin\left(\frac{5\pi}{16}\right) + \sin\left(\frac{7\pi}{16}\right) + \sin\left(\frac{9\pi}{16}\right) + \right. \\ &\quad \left. \sin\left(\frac{11\pi}{16}\right) + \sin\left(\frac{13\pi}{16}\right) + \sin\left(\frac{15\pi}{16}\right) \right] \frac{\pi}{8} \\ &= \left[0.1951 + 0.5556 + 0.8315 + 0.9808 + 0.9808 + \right. \\ &\quad \left. 0.8315 + 0.5556 + 0.1951 \right] \times 0.3927 \\ &= 5.1260 \times 0.3927 = 2.013 \end{aligned}$$

- 3.) The exact value is given by

$$\int_0^\pi \sin x \, dx = [-\cos x]_0^\pi = -\cos \pi + \cos 0 = 2.$$

- 4.) So with eight subintervals (steps) of the midpoint rule we achieved

$$\text{absolute error} = |2.013 - 2| = 0.013$$

$$\text{relative error} = \frac{|2.013 - 2|}{2} = 0.0065$$

$$\text{percentage error} = 100 \times \frac{|2.013 - 2|}{2} = 0.65\%$$

With little work we have managed to estimate the integral to within 1% of its true value. ■

Example 2.5.7 Estimate $\int_0^1 \frac{4}{1+x^2} dx$ using the Trapezoidal rule with $n = 8$ subintervals.

Solution :

$$\begin{aligned}\int_0^1 \frac{4}{1+x^2} dx &\approx \left[\overbrace{\frac{4}{1+x_0^2}}^{f(x_0)} + 2 \cdot \overbrace{\frac{4}{1+x_1^2}}^{f(x_1)} + \cdots + 2 \cdot \overbrace{\frac{4}{1+x_7^2}}^{f(x_{n-1})} + \overbrace{\frac{4}{1+x_8^2}}^{f(x_n)} \right] \frac{\Delta x}{2} \\ &= \left[\frac{4}{1+0^2} + 2 \cdot \frac{4}{1+\frac{1}{8^2}} + 2 \cdot \frac{4}{1+\frac{2^2}{8^2}} + 2 \cdot \frac{4}{1+\frac{3^2}{8^2}} \right. \\ &\quad \left. + 2 \cdot \frac{4}{1+\frac{4^2}{8^2}} + 2 \cdot \frac{4}{1+\frac{5^2}{8^2}} + 2 \cdot \frac{4}{1+\frac{6^2}{8^2}} + 2 \cdot \frac{4}{1+\frac{7^2}{8^2}} + \frac{4}{1+\frac{8^2}{8^2}} \right] \frac{1}{8(2)} \\ &= \left[4 + 2(3.939) + 2(3.765) + 2(3.507) \right. \\ &\quad \left. + 2(3.2) + 2(2.876) + 2(2.56) + 2(2.266) + 2 \right] \frac{1}{16} \\ &= 3.139\end{aligned}$$

The exact value of the integral is still π . So the error in the approximation generated by eight steps of the trapezoidal rule is

$$|3.139 - \pi| = 0.0026,$$

which is

$$100 \frac{|3.139 - \pi|}{\pi} \% = 0.08\%$$

of the exact answer. Notice that this is roughly twice the error that we achieved using the midpoint rule in Example 2.5.5 on page 31. ■

Example 2.5.8 Approximate $\int_0^\pi \sin x dx$ with the Trapezoidal rule with $n = 8$.

Solution :

$$\begin{aligned}\int_0^\pi \sin x dx &\approx \left[\sin(x_0) + 2 \cdot \sin(x_1) + \cdots + 2 \cdot \sin(x_7) + \sin(x_8) \right] \frac{\Delta x}{2} \\ &= \left[\sin 0 + 2 \cdot \sin \frac{\pi}{8} + 2 \cdot \sin \frac{2\pi}{8} + 2 \cdot \sin \frac{3\pi}{8} + 2 \cdot \sin \frac{4\pi}{8} + 2 \cdot \sin \frac{5\pi}{8} \right. \\ &\quad \left. + 2 \cdot \sin \frac{6\pi}{8} + 2 \cdot \sin \frac{7\pi}{8} + \sin \frac{8\pi}{8} \right] \frac{\pi}{16} \\ &= \left[0 + 2(0.3827) + 2(0.7071) + 2(0.9239) + 2(1.0000) + 2(0.9239) + \right. \\ &\quad \left. 2(0.7071) + 2(0.3827) + 0 \right] \times 0.1963 \\ &= 1.974\end{aligned}$$

The exact answer is $\int_0^\pi \sin x dx = -\cos x \Big|_0^\pi = 2$. So with eight steps of the trapezoidal rule we achieved $100 \frac{|1.974 - 2|}{2} \% = 1.3\%$ accuracy. Again this is approximately twice the error we achieved in Example 2.5.6 on page 32 using the midpoint rule. ■

Remark 2.5.1 These two examples suggest that the midpoint rule is more accurate than the trapezoidal rule. Indeed, this observation is born out by a rigorous analysis of the error.

Example 2.5.9 Estimate $\int_0^1 \frac{4}{1+x^2} dx$ using the Simpson's rule with $n = 8$ subintervals.

Solution :

$$\begin{aligned} & \int_0^1 \frac{4}{1+x^2} dx \\ & \approx \left[\frac{4}{1+0^2} + 4 \frac{4}{1+\frac{1}{8^2}} + 2 \frac{4}{1+\frac{2^2}{8^2}} + 4 \frac{4}{1+\frac{3^2}{8^2}} + 2 \frac{4}{1+\frac{4^2}{8^2}} \right. \\ & \quad \left. + 4 \frac{4}{1+\frac{5^2}{8^2}} + 2 \frac{4}{1+\frac{6^2}{8^2}} + 4 \frac{4}{1+\frac{7^2}{8^2}} + \frac{4}{1+\frac{8^2}{8^2}} \right] \frac{1}{8 \times 3} \\ & = \left[4 + 4 \times 3.938461538 + 2 \times 3.764705882 + 4 \times 3.506849315 + 2 \times 3.2 \right. \\ & \quad \left. + 4 \times 2.876404494 + 2 \times 2.56 + 4 \times 2.265486726 + 2 \right] \frac{1}{8 \times 3} \\ & = 3.14159250 \end{aligned}$$

With the absolute error as

$$|3.14159250 - \pi| = 1.5 \times 10^{-7}$$

It is striking that the absolute error approximating with Simpson's rule is so much smaller than the error from the midpoint and trapezoidal rules.

midpoint error	= 0.0013
trapezoid error	= 0.0026
Simpson error	= 0.00000015

See Example 2.5.5 and Example 2.5.7. ■

Example 2.5.10 Approximate $\int_0^\pi \sin x \, dx$ with the Simpson's rule with $n = 8$.

Solution :

$$\begin{aligned}
 & \int_0^\pi \sin x \, dx \\
 & \approx \left[\sin(x_0) + 4\sin(x_1) + 2\sin(x_2) + \dots + 4\sin(x_7) + \sin(x_8) \right] \frac{\Delta x}{3} \\
 & = \left[\sin(0) + 4\sin\left(\frac{\pi}{8}\right) + 2\sin\left(\frac{2\pi}{8}\right) + 4\sin\left(\frac{3\pi}{8}\right) + 2\sin\left(\frac{4\pi}{8}\right) \right. \\
 & \quad \left. + 4\sin\left(\frac{5\pi}{8}\right) + 2\sin\left(\frac{6\pi}{8}\right) + 4\sin\left(\frac{7\pi}{8}\right) + \sin\left(\frac{8\pi}{8}\right) \right] \frac{\pi}{8 \times 3} \\
 & = \left[0 + 4 \times 0.382683 + 2 \times 0.707107 + 4 \times 0.923880 + 2 \times 1.0 \right. \\
 & \quad \left. + 4 \times 0.923880 + 2 \times 0.707107 + 4 \times 0.382683 + 0 \right] \frac{\pi}{8 \times 3} \\
 & = 15.280932 \times 0.130900 \\
 & = 2.00027
 \end{aligned}$$

With only eight subintervals/steps of Simpson's rule we achieved

$$100 \left(\frac{2.00027 - 2}{2} \right) = 0.014\% \text{ accuracy.}$$

Again we contrast the error we achieved with the other two rules:

<i>midpoint error</i>	$= 0.013$
<i>trapezoid error</i>	$= 0.026$
<i>Simpson error</i>	$= 0.00027$

■

Remark 2.5.2 These last two examples suggest that the Simpson's rule is more accurate than the midpoint rule and the trapezoidal rule. Indeed, this observation is born out by a rigorous analysis of the error.

Note 2.5.1 Two obvious considerations when deciding whether or not a given algorithm is of any practical value are

- 1.) the amount of computational effort required to execute the algorithm
- 2.) the accuracy that this computational effort yields.

To get a first impression of the error behaviour of these methods, we apply them to a problem whose answer we know exactly:

$$\int_0^\pi \sin x \, dx = -\cos x \Big|_0^\pi = 2.$$

To be a little more precise, we would like to understand how the errors of the three methods change as we increase the effort we put in (as measured by the number of steps n). The following table lists the error in the approximate value for this number generated by our three rules applied with three different choices of n . It also lists the number of evaluations of f required to compute the approximation.

	Midpoint		Trapezoidal		Simpson's	
n	error	# evals	error	# evals	error	# evals
10	8.2×10^{-3}	10	1.6×10^{-2}	11	1.1×10^{-4}	11
100	8.2×10^{-5}	100	1.6×10^{-4}	101	1.1×10^{-8}	101
1000	8.2×10^{-7}	1000	1.6×10^{-6}	1001	1.1×10^{-12}	1001

Observe that

- 1.) Using 101 evaluations of f worth of Simpson's rule gives an error 75 times smaller than 1000 evaluations of f worth of the midpoint rule.
- 2.) The trapezoidal rule error with n steps is about twice the midpoint rule error with n steps.
- 3.) With the midpoint rule, increasing the number of steps by a factor of 10 appears to reduce the error by about a factor of $100 = 10^2 = n^2$.
- 4.) With the trapezoidal rule, increasing the number of steps by a factor of 10 appears to reduce the error by about a factor of $10^2 = n^2$.
- 5.) With Simpson's rule, increasing the number of steps by a factor of 10 appears to reduce the error by about a factor of $10^4 = n^4$.

Example 2.5.11 With the composite Trapezoidal Rule, approximate

$$I = \int_0^1 x^2 dx$$

using

1.) $h = 0.25$

2.) $h = 0.5$

Hence, Compare your solutions with the exact solution.

Solution :

1.) With $h = 0.25$

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] \\ \int_0^1 x^2 dx &= \frac{0.25}{2} [f(0) + f(1) + 2 \{f(0.25) + f(0.5) + f(0.75)\}] \\ &= \frac{0.5}{2} [0 + 1 + 2(0.25^2 + 0.5^2 + 0.75^2)] \\ &= \frac{2.75}{8} = 0.34375 \end{aligned}$$

2.) With $h = 0.5$

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] \\ \int_0^1 x^2 dx &= \frac{0.5}{2} [f(0) + f(1) + 2 \{f(0.5)\}] \\ &= \frac{0.5}{2} [0 + 1 + 2(0.5^2)] \\ &= \frac{1.5}{4} = 0.375 \end{aligned}$$

3.) exact solution

$$\begin{aligned} \int_0^1 x^2 dx &= \left[\frac{x^3}{3} \right]_0^1 \\ &= \frac{1}{3} - (0) \\ &= \frac{1}{3} \\ &= 0.3333 \end{aligned}$$

Errors.

When $h = 0.25$, the error is

$$|0.33333 - 0.34375| = 0.01042$$

With $h = 0.5$, the error is

$$|0.33333 - 0.375| = 0.04167$$



Example 2.5.12 Apply the Mid-point Rule to estimate

$$I = \int_0^1 x^2 dx$$

using

1.) $h = 0.25$

2.) $h = 0.5$

Hence, Compare your solutions with the exact solution.

Solution :

1.) For $h = 0.25$ Each subinterval has length $\Delta x = 0.25 = \frac{1}{4}$. Therefore, the subintervals consist of

$$\left[0, \frac{1}{4}\right], \left[\frac{1}{4}, \frac{1}{2}\right], \left[\frac{1}{2}, \frac{3}{4}\right], \text{ and } \left[\frac{3}{4}, 1\right].$$

The midpoints of these subintervals are $\left\{\frac{1}{8}, \frac{3}{8}, \frac{5}{8}, \frac{7}{8}\right\}$. Thus,

$$\begin{aligned} M_4 &= \frac{1}{4} \cdot f\left(\frac{1}{8}\right) + \frac{1}{4} \cdot f\left(\frac{3}{8}\right) + \frac{1}{4} \cdot f\left(\frac{5}{8}\right) + \frac{1}{4} \cdot f\left(\frac{7}{8}\right) \\ &= \frac{1}{4} \cdot \frac{1}{64} + \frac{1}{4} \cdot \frac{9}{64} + \frac{1}{4} \cdot \frac{25}{64} + \frac{1}{4} \cdot \frac{49}{64} \\ &= \frac{21}{64} = 0.328125. \end{aligned}$$

2.) For $h = 0.5 = \frac{1}{2}$. Therefore, the subintervals consist of

$$\left[0, \frac{1}{2}\right], \text{ and } \left[\frac{1}{2}, 1\right].$$

The midpoints of these subintervals are $\left\{\frac{1}{4}, \frac{3}{4}\right\}$. Thus,

$$\begin{aligned} M_2 &= \frac{1}{2} \cdot f\left(\frac{1}{4}\right) + \frac{1}{2} \cdot f\left(\frac{3}{4}\right) \\ &= \frac{1}{2} \cdot \frac{1}{16} + \frac{1}{2} \cdot \frac{9}{16} \\ &= \frac{10}{32} = 0.3125. \end{aligned}$$

3.) Absolute error: Since

$$\int_0^1 x^2 dx = \frac{1}{3},$$

the absolute error in this approximation is:

(a) For $h = 0.25$

$$\left| \frac{1}{3} - \frac{21}{64} \right| = \frac{1}{192} \approx 0.0052,$$

(b) For $h = 0.5$

$$\left| \frac{1}{3} - \frac{10}{32} \right| = \frac{1}{48} \approx 0.0208,$$

and we see that the midpoint rule produces an estimate that is somewhat close to the actual value of the definite integral than the Trapezoidal rule.

■

2.5.3 Steps Required to Accuracy

Example 2.5.13 How many steps n required for approximating

$$\int_0^1 e^{-x^2} dx$$

using the *midpoint rule* to within an accuracy of 10^{-6} .

Solution :

- 1.) The integral has $a = 0$ and $b = 1$.
- 2.) The first two derivatives of the integrand are

$$\begin{aligned}\frac{d}{dx} e^{-x^2} &= -2xe^{-x^2} && \text{and} \\ \frac{d^2}{dx^2} e^{-x^2} &= \frac{d}{dx}(-2xe^{-x^2}) = -2e^{-x^2} + 4x^2 e^{-x^2} = 2(2x^2 - 1)e^{-x^2}\end{aligned}$$

- 3.) As x runs from 0 to 1, $2x^2 - 1$ increases from -1 to 1, so that

$$0 \leq x \leq 1 \implies |2x^2 - 1| \leq 1, e^{-x^2} \leq 1 \implies |2(2x^2 - 1)e^{-x^2}| \leq 2$$

So we take $M = 2$.

- 4.) The error introduced by the n step midpoint rule is at most

$$\begin{aligned}E_M &\leq \frac{M}{24} \frac{(b-a)^3}{n^2} \\ &\leq \frac{2}{24} \frac{(1-0)^3}{n^2} = \frac{1}{12n^2}\end{aligned}$$

- 5.) We need this error to be smaller than 10^{-6} so

$$\begin{aligned}E_M &\leq \frac{1}{12n^2} \leq 10^{-6} && \text{and so} \\ 12n^2 &\geq 10^6 && \text{clean up} \\ n^2 &\geq \frac{10^6}{12} = 83333.3 && \text{square root both sides} \\ n &\geq 288.7\end{aligned}$$

So 289 steps of the midpoint rule will do the job.

- 6.) In fact $n = 289$ results in an error of about 3.7×10^{-7} .

That seems like far too much work, and the trapezoidal rule will have twice the error.



Example 2.5.14 How many steps n required for approximating

$$\int_0^1 e^{-x^2} dx$$

using the *Simpson's rule* to within an accuracy of 10^{-6} .

Solution :

- 1.) The integral has $a = 0$ and $b = 1$.
- 2.) The first four derivatives of the integrand are

$$\begin{aligned}\frac{d}{dx} e^{-x^2} &= -2xe^{-x^2} && \text{and} \\ \frac{d^2}{dx^2} e^{-x^2} &= \frac{d}{dx}(-2xe^{-x^2}) = -2e^{-x^2} + 4x^2 e^{-x^2} = 2(2x^2 - 1)e^{-x^2}\end{aligned}$$

such that the third and fourth derivatives are given by

$$\begin{aligned}\frac{d^3}{dx^3} e^{-x^2} &= \frac{d}{dx} \{2(2x^2 - 1)e^{-x^2}\} = 8xe^{-x^2} - 4x(2x^2 - 1)e^{-x^2} \\ &= 4(-2x^3 + 3x)e^{-x^2} \\ \frac{d^4}{dx^4} e^{-x^2} &= \frac{d}{dx} \{4(-2x^3 + 3x)e^{-x^2}\} \\ &= 4(-6x^2 + 3)e^{-x^2} - 8x(-2x^3 + 3x)e^{-x^2} \\ &= 4(4x^4 - 12x^2 + 3)e^{-x^2}\end{aligned}$$

- 3.) Now for any x , then $e^{-x^2} \leq 1$. Also, for $0 \leq x \leq 1$

$$\begin{aligned}0 &\leq x^2, x^4 \leq 1 && \text{so} \\ 3 &\leq 4x^4 + 3 \leq 7 && \text{and} \\ -12 &\leq -12x^2 \leq 0 && \text{adding these together gives} \\ -9 &\leq 4x^4 - 12x^2 + 3 \leq 7\end{aligned}$$

Consequently, $|4x^4 - 12x^2 + 3|$ is bounded by 9 and so

$$\left| \frac{d^4}{dx^4} e^{-x^2} \right| \leq 4 \times 9 = 36$$

So, take $M = 36$.

- 4.) The error introduced by the n step *Simpson's rule* is at most

$$\begin{aligned}E_S &\leq \frac{L}{180} \frac{(b-a)^5}{n^4} \\ &\leq \frac{36}{180} \frac{(1-0)^5}{n^4} = \frac{1}{5n^4}\end{aligned}$$

- 5.) In order for this error to be no more than 10^{-6} we require n to satisfy

$$\begin{aligned}E_S &\leq \frac{1}{5n^4} \leq 10^{-6} && \text{and so} \\ 5n^4 &\geq 10^6 \\ n^4 &\geq 200000 && \text{take fourth root} \\ n &\geq 21.15\end{aligned}$$

So 22 steps of *Simpson's rule* will do the job.

- 6.) Just $n = 22$ steps (as compared to midpoint $n = 289$ steps results in an error of about 3.7×10^{-7}) results in an error of about 3.5×10^{-8} .

That seems like far too less work, as compared to work required by Midpoint and the Trapezoidal rule. ■

2.6 Numerical Integration Chapter Examples

Exercise 2.6.1 Using $n = 4$ and all three rules to approximate the value of the following integral

$$\int_0^2 e^{x^2} dx$$

- | | |
|--------------------|-------------|
| 1.) Mid-Point rule | 14.48561253 |
| 2.) Trapezium rule | 20.64455905 |
| 3.) Simpson's rule | 17.35362645 |

Maple gives the exact solution as $\int_0^2 e^{x^2} dx = 16.45262776$. Therefore, the Simpson's technique is more superior followed by the Trapezoidal rule and then the Mid-point algorithm.

Exercise 2.6.2 Show that the error (absolute error) in the Trapezium rule to compute $\int_1^2 \frac{1}{x} dx$ is $\frac{2}{600} \simeq 0.0017$.

Example 2.6.1 Evaluate $\int_0^4 \left(1 + \frac{1}{1+x^2}\right)^{\frac{1}{2}} dx$ by Simpson rule with $n = 4$.

$$\frac{13.72624}{3} = 4.575412$$

Example 2.6.2 Use Trapezoidal rule and Simpson's rule with 2 subintervals to estimate the following integral $\int_0^4 x^3 dx$

- 1.) Trapezoidal rule

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &\approx \frac{2}{2} [f(0) + f(4) + 2 \{f(2)\}] \\ &\approx \frac{2}{2} [0^3 + 4^3 + 2 \{2^3\}] \\ &\approx 80.0000 \end{aligned}$$

- 2.) Simpson rule

$$\begin{aligned} I &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\ &\approx \frac{2}{3} [f(0) + f(4) + 4 \{f(2)\}] \\ &\approx \frac{2}{3} [0^3 + 4^3 + 4 \{2^3\}] \\ &\approx 64.0000 \end{aligned}$$

- 3.) Analytical (Exact or Classical)

$$\int_0^4 x^3 dx = \frac{x^4}{4} \Big|_0^4 = 64.0000$$

Example 2.6.3 Approximate $\int_0^4 x^2 dx$ with $n = 8$ subintervals using

1.) Trapezoidal rule

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &\approx \frac{0.5}{2} [f(0) + f(4) + 2 \{f(0.5) + f(1) + f(1.5) + f(2) + f(2.5) + f(3) + f(3.5)\}] \\ &\approx 21.5000 \end{aligned}$$

2.) Upper (right-end) Riemann sum

$$I = \bar{S}_n = \frac{1}{2} [0.5^2 + 1^2 + 1.5^2 + 2^2 + 2.5^2 + 3^2 + 3.5^2 + 4^2] = 25.5000$$

3.) Lower (left-end) Riemann sum

$$I = \underline{S}_n = \frac{1}{2} [0^2 + 0.5^2 + 1^2 + 1.5^2 + 2^2 + 2.5^2 + 3^2 + 3.5^2] = 17.5000$$

4.) Average of Riemann sum

$$\frac{\bar{S}_n + \underline{S}_n}{2} = \frac{25.5000 + 17.5000}{2} = 21.5000$$

Same as Trapezoidal rule!!!

5.) Mid-point Riemann sum

$$I = S_n = \frac{1}{2} [0.25^2 + 0.75^2 + 1.25^2 + 1.75^2 + 2.25^2 + 2.75^2 + 3.25^2 + 3.75^2] = 21.2500$$

Same as Midpoint rule!!!

6.) Analytical methods

$$\int_0^4 x^2 dx = \frac{x^3}{3} \Big|_0^4 = \frac{64}{3} \approx 21.3333$$

Remark 2.6.1

- The Trapezoid Rule is nothing more than the average of the left-hand and right-hand Riemann Sums. It provides a more accurate approximation of total change than either sum does alone.
- Simpson's Rule is a weighted average that results in an even more accurate approximation.
- The Mid-point rule is the Riemann sums at mid points (Not the average of the two Riemann sums, that would be Trapezoidal)

Example 2.6.4 Determine the smallest number of subintervals required to guarantee accuracy to within 0.002 in the approximation of $\int_0^1 e^{x^2} dx$ using Trapezoidal rule.

Solution : Using the Truncation error of Trapezoidal, (2.2) on page (p. 7). Since $f(x) = e^{x^2} \Rightarrow f''(x) = 4x^2 e^{x^2} + 2e^{x^2}$ on $[0, 1] \Rightarrow M = 6e$. Therefore,

$$|E_{trunc}| \leq \frac{M(b-a)^3}{12n^2} = \frac{6e(1-0)}{12n^2} = 0.002 \Rightarrow n = 36.86 = 37$$



Example 2.6.5 Given the tabulated function

t	-4	-2	0	2	4
$W(t)$	7	4	3	-1	2

Estimate

$$\int_{-2}^4 W(t)dt$$

using the Trapezoidal rule with 3 subintervals.

$$\begin{aligned} I &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &\approx \frac{2}{2} [W(-2) + W(4) + 2 \{W(0) + W(2)\}] \\ &\approx \frac{2}{2} [4 + 2 + 2 \{3 + (-1)\}] \\ &\approx 10.0000 \end{aligned}$$

Example 2.6.6 Write down the correct formula to use Simpson's rule and 4 subintervals for

$$\int_2^{10} f(x)dx$$

$$\begin{aligned} I &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\ &\approx \frac{2}{3} [f(2) + f(10) + 2 \{f(6) + f(8)\}] \end{aligned}$$

Exercise 2.6.3 Use the Riemann sum formula at mid point to compute the definite integral in Example 2.4.2 above. Compare both answers to the classical value of the definite integral.

Example 2.6.7 Estimate $\int_0^1 \cos(x^3 + x) dx$ using five ordinates (four intervals). The interval width, $h = 0.25$ using

1.) Trapezoidal rule

$$I = \frac{0.25}{2} [1.0000 - 0.41615 + 2 \{0.96493 + 0.81096 + 0.38843\}] = 0.6141$$

2.) Simpson's method

$$I = \frac{0.25}{3} [1.0000 - 0.41615 + 2 \{0.81096\} + 4 \{0.96493 + 0.38843\}] = 0.6349$$

Example 2.6.8 Apply the mid-point scheme to approximate $\int_0^1 \cos x dx$ using $h = 0.25$.

Solution :

$$\begin{aligned} \int_0^1 \cos x dx &= \Delta x \sum_{i=1}^n f(m_i) \\ &= (0.25) [f(0.125) + f(0.375) + f(0.625) + f(0.875)] \\ &= (0.25) [\cos(0.125) + \cos(0.375) + \cos(0.625) + \cos(0.875)] \\ &= (0.25) [0.992197667 + 0.930507621 + 0.810963119 + 0.640996858] \\ &= 0.8436663 \end{aligned}$$



Example 2.6.9 Given $\int_1^2 \frac{dx}{x}$. How large should n be to guarantee that the Trapezoidal Rule approximation of the integral is accurate to within 0.0001?

Since

$$|E_T| \leq \frac{2(2-1)^3}{12n^2} \leq 0.0001 = 10^{-4},$$

then

$$6n^2 \geq 10^4 \Leftrightarrow n > \frac{10^2}{\sqrt{6}} \approx 40.8 \Rightarrow n \geq 41.$$

Example 2.6.10 Estimate the number of subintervals required to guarantee accuracy of the integral $\int_1^2 \frac{1}{x} dx$ within 0.005 using the Trapezoidal rule approximation. $n \geq \sqrt{\frac{100}{3}} \approx 5.77 \geq 6$

Exercise 2.6.4 Determine the smallest value of n such that the Trapezoidal Rule approximation of the integral in Example 2.6.9, is accurate to within 0.000001?

Example 2.6.11 Determine the definite integral $\int_0^1 (2+x) dx$, with $n = 4$ using the

1.) Trapezoidal rule

x	0	0.25	0.5	0.75	1
$(x+2)$	2	2.25	2.5	2.75	3.0

$$\begin{aligned} A &= \frac{h}{2} [f(x_0) + f(x_n) + 2 \{f(x_1) + f(x_2) + \dots + f(x_{n-1})\}] + E_{trunc} \\ &= \frac{h}{2} [f(0) + f(1) + 2 \{f(0.25) + f(0.5) + f(0.75)\}] + E_{trunc} \\ &\approx \frac{1}{2}(0.25) [2 + 3.0 + 2 \{2.25 + 2.5 + 2.75\}] \\ &= 2.5000 \end{aligned}$$

2.) Simpson's method

x	x_0	x_1	x_2	x_3	x_4
$(x+2)$	0	0.25	0.5	0.75	1
	2	2.25	2.5	2.75	3.0

$$\begin{aligned} \int_0^1 (x+2) dx &= \frac{h}{3} [f(x_0) + f(x_n) + 2 \{f(x_2) + f(x_4) + \dots + f(x_{2n-2})\} + 4 \{f(x_1) + f(x_3) + \dots + f(x_{2n-1})\}] + E_T \\ &= \frac{h}{3} [f(0) + f(1) + 2 \{f(0.5)\} + 4 \{f(0.25) + f(0.75)\}] + E_T \\ &\approx \frac{0.25}{3} [2 + 3 + 2 \{2.5\} + 4 \{2.25 + 2.75\}] \\ &\approx 2.5 \approx 2.5000 \end{aligned}$$

3.) Mid-point algorithm

4.) Compare your results with the exact value of I . Which of the techniques is more superior?

The analytical technique,

$$I = \int_0^1 (x+2) dx = \frac{x}{2} + 2x \Big|_0^1 = \left[\left(\frac{1}{2} + 2 \right) - (0 + 0) \right] = 2.5$$

For this specific function, both numerical methods give a similar solution, both accurate