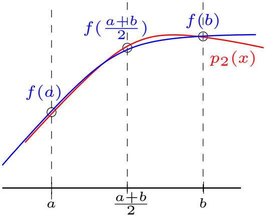
MA378 Chapter 3: Numerical Integration

§3.2 Simpson's Rule

Dr Niall Madden

February 2024



T. Simpson's Rule:
$\int_a^b f(x)dx \approx$
$\frac{b-a}{\mathbf{6}}\big(f(a) + 4f(\frac{a+b}{2}) + f(b)\big)$

H. Simpson's Rule:
"*If something is hard to do, it is not worth doing*".

2.1 Simpson's Rule

Following on from the Trapezium Rule, we'll consider the **3-point Newton-Cotes scheme** which is based on integrating the quadratic interpolant to $f(x)$.

Simpson's Rule

$$Q_2(f) = \frac{b-a}{6}\big(f(a) + 4f\big(\frac{a+b}{2}\big) + f(b)\big). \tag{1}$$

So this is

$$Q_2(f) = q_0 f_0 + q_1 f_1 + q_2 f_2$$

with $x_0 = a \qquad x_1 = \frac{a+b}{2} \qquad x_2 = b$

$q_0 = 1/6 \qquad q_1 = 2/3 \qquad q_2 = 1/6$

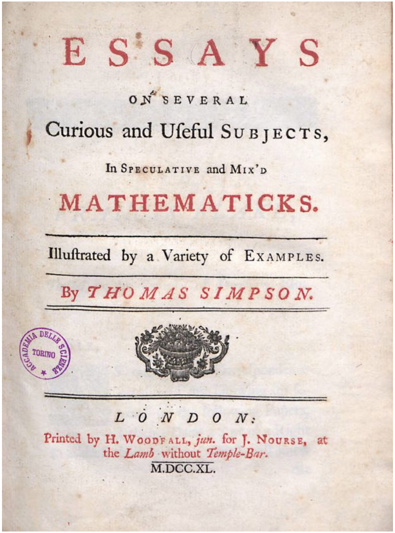
The rule is named after **Thomas Simpson**, 1710–1761.

He was one of the most distinguished of a group of a lecturers who taught in the London coffee-houses and pubs, which he did to supplement his earnings as a weaver.

Hutton (famous text-book writer) said of him

> *It has been said that Mr Simpson frequented low company, with whom he used to guzzle porter and gin: but it must be observed that the misconduct of his family put it out of his power to keep the company of gentlemen, as well as to procure better liquor.*

The method was known well before Simpson's time: it had been used by Cavalieri (a student of Galileo) in 1639, James Gregory, Johannes Kepler, and others.



Simpson does seem to have been a colourful character... He eventually appointed head of mathematics at the Royal Military Academy at Woolwich, and had a major impact on the introduction of calculus to the curriculum. His text-books were quite famous (and controversial) at the time.

He's most famous for "Simpson's Rule", which he did not invent: he learned it from Newton. But Newton got credited with the modern form of the Newton-Raphson method, which was devised by Simpson.

2.2 Derivation

$x_0 = 0, \quad x_1 = \frac{1}{2} \quad x_2 = 1$

To show how to derive Simpson's Rule, we'll use the **Method of Undetermined Coefficients** again.

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

First restrict our attention to approximating $\int_0^1 g(x)dx$. This method should be exact for all constant, linear and quadratic polynomials. Taking

$$g(x) \equiv 1, \qquad g(x) = x \quad \text{and} \qquad g(x) = x^2,$$

we get the set of equations:

$g(x) \equiv 1$ $\quad Q(g) = q_0 + q_1 + q_2 \quad \int_0^1 g(x)dx = 1$

$\Rightarrow q_0 + q_1 + q_2 = 1$

$g(x) = x$ $\quad Q(g) = q_0(0) + q_1(\frac{1}{2}) + q_2(1) \quad \int_0^1 g(x)dx = \frac{1}{2}$

$\Rightarrow \frac{1}{2}q_1 + q_2 = \frac{1}{2}$.

$g(x) = x^2$ $\quad Q(g) = q_0(0) + q_1(\frac{1}{4}) + q_2(1) \Rightarrow \frac{1}{4}q_1 + q_2 = \frac{1}{3}$

 That is $q_0 = 1/6$, $q_1 = \frac{2}{3}$, $q_2 = 1/6$.

This is easily solved giving

$$\int_0^1 g(x)dx \approx \frac{1}{6}g(0) + \frac{2}{3}g(1/2) + \frac{1}{6}g(1). \qquad (2)$$

To extend this to the interval $[a, b]$, we again use a change of variables to get the general Simpson's Rule (1) .

This gives $x_0 = a$ $\quad x_1 = \frac{a+b}{2}$ $\quad x_2 = b$.

$q_0 = \frac{b-a}{6}$ $\quad q_1 = \frac{2}{3}(b-a)$ $\quad q_2 = \frac{b-a}{6}$.

Finished here Wed 21/02/2024

Example 2.1

Use Simpson's rule to estimate $\int_0^{\pi/4} \cos(x)dx$, and calculate the (exact) error $|\int_a^b f(x)dx - Q_2(f)|$.

$$Q_2(f) = \frac{b-a}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$$

$$= \left(\frac{\pi}{4}\right)\left(\frac{1}{6}\right)\left(\cos(0) + 4\cos\left(\frac{\pi}{8}\right) + \cos\left(\pi/4\right)\right)$$

$$= \cdots = 0.70720195.$$

We can verify that $\left|\int_a^b f(x)\,dx - Q_2(f)\right| = 9.5166 \times 10^{-5}$

For Trap Rule Error $\approx 3.67 \times 10^{-2}$.

2.3 Newton-Cotes methods

Recall...

Newton-Cotes quadrature

The **Newton-Cotes** quadrature rule for $\int_a^b f(x)dx$ is

$$Q_n(f) := q_0 f(x_0) + q_1 f(x_1) + q_2 f(x_2) + \cdots + q_n f(x_n).$$

- The quadrature points are the equally spaced points $a = x_0 < x_1 < \cdots < x_n = b$.
- The quadrature weights, q_0, q_1, ..., q_n, are chosen so that

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

where p_n is the polynomial of degree n that interpolates f at the x_i.

We'll now derive error estimates for general Newton-Cotes methods, and look at the specific cases of the Trapezium and Simpson's rules. $M_{n+1} = \max_{a \le x \le b} |f^{(n+1)}(x)|$

Theorem 2.2

Let $M_{n+1} := \max_{a \le x \le b} |f^{(n+1)}(x)|$, *and* $\pi_{n+1}(x)$ *be the usual nodal polynomial. Define*

$$\mathcal{E}_n := \Big| \int_a^b f(x)dx - Q_n(f) \Big|.$$

Then

$$\mathcal{E}_n \le \frac{M_{n+1}}{(n+1)!} \int_a^b |\pi_{n+1}(x)| dx,$$

The proof just comes directly Cauchy's Theorem.

Theorem 2.3

For the **Trapezium Rule**, Q_1,

$$\mathcal{E}_1 \leq \frac{(b-a)^3}{12} M_2. \tag{3}$$

The proof is an exercise.

The key step is computing

$$\int_a^b (x - x_0)(x - x_1)\, dx$$

This result will be important at the end of Section 3.3.

2.4 Error estimates for the Trapezium Rule

Example

Use (3) to get an upper bound on the error for the estimate of $\int_0^{\pi/4} \cos(x)dx$ using the Trapezium rule. How does this compare with the actual error?

Here $f(x) = \cos(x)$ so $f''(x) = -\cos(x)$

Then $M_2 = \max\limits_{0 \leq x \leq \pi/4} \cos(x) = \cos(0) = 1$

So $\mathcal{E}_1 \leq \dfrac{(\pi/4)^3}{12}(1) \approx 0.04037$

Note : Actual Error is 0.0367.

2.4 Error estimates for the Trapezium Rule

Example 2.4

If use the Trapezium Rule to estimate the integral of x^2 on the interval $[0, 1]$ we get

$$\int_0^1 x^2 dx = \frac{1}{3} \qquad \text{and} \qquad Q_1(x^2) = \frac{1}{2}(0+1) = \frac{1}{2}.$$

So the error is $1/6$, exactly as the theory predicts.

2.5 Error estimates for Simpson's rule

One can also use our theorem to show that for Simpson's Rule

$$\mathcal{E}_2 \leq \frac{(b-a)^4}{196} M_3, \tag{4}$$

but don't bother because, although correct, it is not *sharp* (that is, it is pessimistic).

Example

If we use (4) to get an upper bound on the error for the estimate of $\int_0^{\pi/4} \cos(x)dx$ using **Simpson's** rule, we would get an estimate of 1.387×10^{-3}. The actual error is 9.5166×10^{-5}.

2.5 Error estimates for Simpson's rule

Example 2.5

We expect Simpson's Rule to give *exactly* the right answer for integrals of constant, linear and quadratic functions. If we take $f(x) = x^3$, $a = 0$ and $b = 1$, then formula above suggests that (approx) $\mathcal{E}_2 \leq 0.03$. But ...

From the theory, we would expect

$$\mathcal{E}_2 \leq \frac{(1)^4}{196} 6 = \frac{3}{98}.$$

However, $\int_0^1 x^3\,dx = \frac{1}{4} x^4 \Big|_0^1 = \frac{1}{4}$.

$$Q_2(x^3) = \frac{1-0}{6}\left(f(0) + 4 f(1/2) + f(1)\right)$$

$$= \frac{1}{6}\left(0 + \frac{1}{2} + 1\right) = \frac{1}{6} \times \frac{3}{2} = \frac{1}{4}.$$

So Error is 0!

2.5 Error estimates for Simpson's rule

This is not the only problem for which we would get an exactly correct answer if we use Simpson's Rule.

It is possible to prove (but we won't) that the error in Simpson's is zero if $f^{(iv)} \equiv 0$.

However, we'll study a more general approach that will help us develop other surprisingly accurate methods. That is the subject of Section 3.3: "Precision".

ie if f is any cubic polynomial.

2.6 Exercises

Exercise 2.1

Deduce the 4-point Newton-Cotes Rule for estimating the integral $\int_0^1 f(x)dx$:

$$Q_3(f) = q_0 f(x_0) + q_1 f(x_1) + q_2 f(x_2) + q_3 f(x_3).$$

Extend the rule to estimate the integral of functions over $[a, b]$.

Exercise 2.2

Prove the error bound given for the Trapezium rule. That is, show that

$$|\int_a^b f(x)dx - Q_1(f)| := \mathcal{E}_1 \leq \frac{(b-a)^3}{12} M_2.$$