MA378 Chapter 3: Numerical Integration

§3.2 Simpson's Rule

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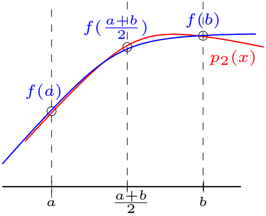


T. Simpson's Rule:
$\int_a^b f(x)dx \approx$
$\frac{b-a}{\mathbf{6}}\big(f(a) + 4f(\frac{a+b}{2}) + f(b)\big)$

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**[1]. which is based on integrating the quadratic interpolant to $f(x)$.

Simpson's Rule

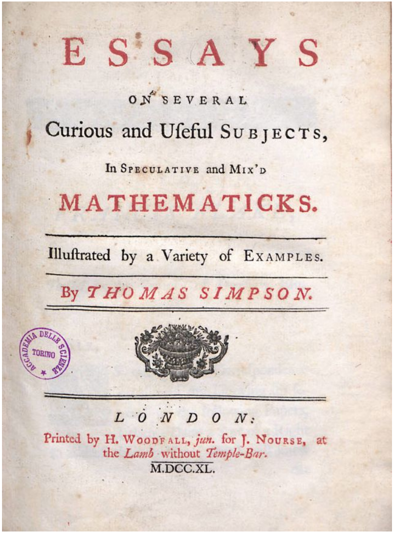
$$Q_2(f) = \frac{b-a}{6}\big(f(a) + 4f\big(\frac{a+b}{2}\big) + f(b)\big). \qquad (1)$$

[1] Thomas Simpson, 1710–1761. One of the most distinguished of a group of lecturers who taught in the London coffee-houses, 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.

2.1 Simpson's Rule



ESSAYS

ON SEVERAL

Curious and Uſeful SUBJECTS,

In SPECULATIVE and MIX'D

MATHEMATICKS.

Illuſtrated by a Variety of EXAMPLES.

By THOMAS SIMPSON.

LONDON:

Printed by H. WOODFALL, jun. for J. NOURSE, at the Lamb without Temple-Bar.

M.DCC.XL.

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

$a=0, \quad b=1$

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

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:

$g \equiv 1$ $\quad \int_0^1 g(x)\,dx = \int_0^1 1\,dx = 1.$ $\qquad Q_2(g) = q_0 + q_1 + q_2$

so $\quad q_0 + q_1 + q_2 = 1$

$g(x) = x$: $\quad \int_0^1 x\,dx = \frac{1}{2}x^2\Big|_0^1 = \frac{1}{2}$ $\qquad Q_2(g) = q_0(0) + q_1(\frac{1}{2}) + q_2(1)$

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

$g(x) = x^2$: $\quad \dots \quad \frac{1}{4}q_1 + q_2 = \frac{1}{3}$

2.2 Derivation

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) .

ie use $t : [0,1] \to [a,b]$

this gives

$$\int_a^b f(x)\,dx = \frac{(b-a)}{6}\left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right)$$

Example 2.1

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

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

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

$$= 0.70720195.$$

$$I(f) = \int_0^{\pi/4} f(x)dx = \frac{1}{\sqrt{2}} = 0.7071068.$$

Error is $\approx 9.516 \times 10^{-5}$ (Trapezium Rule: 0.0267).

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.

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.

2.4 Error estimates for the Trapezium Rule

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.

↳ mainly involves

calculating $\int_a^b \pi_2(x)\,dx = \int_a^b (x-a)(x-b)\,dx$.

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?

Since $f(x) = \cos(x)$, so $f''(x) = -\cos(x)$

so $M_2 = \max_{0 \leq x \leq \pi/4} |-\cos(x)| = 1$.

~~Thus~~ Then we can see that

$$\varepsilon_1 \leq 0.04037.$$

Compare with actual error: 0.0367.

Example 2.4

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

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

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

So Exact error is $\left| \frac{1}{3} - \frac{1}{2} \right| = \frac{1}{6}$.

Using $\mathcal{E}_1 \leq \frac{(b-a)^3}{12} M_2$, we get $\mathcal{E}_1 \leq \frac{1}{12} \cdot (2) = \frac{1}{6}$.

$\left(f(x) = x^2 \text{ so } f''(x) = 2 \right)$.

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}.

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 ...

$f(x) = x^3$ $\quad a=0, \quad b=1$

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

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

$$= \frac{1}{4}.$$

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

No Error!!

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 ...

Try $\int_{-1}^{1} x^3 \, dx$

$$\int_{-1}^{1} x^3 = \frac{1}{4} x^4 \Big|_{-1}^{1} = \frac{1}{4} - \frac{1}{4} = 0$$

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

$$= \frac{2}{6}(-1 + 0 + 1) = 0.$$

Still no error.

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

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

Finished here 1 March

(note: included Q_2 exact for all cubics).