§3 Numerical Integration

§3.2 Simpson's Rule

MA378/531 – Numerical Analysis II ("NA2")

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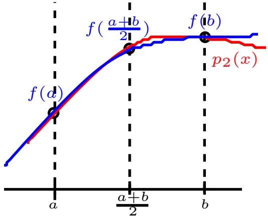

T. Simpson's Rule:
$\int_a^b f(x)dx \approx$
$\frac{b-a}{4}\Big(f(a) + 4f(\frac{a+b}{2}) + f(b)\Big)$

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

$x_0 = a, \quad x_1 = \frac{a+b}{2}, \quad x_2 = b$

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 $f(x)$.

$h = \frac{b-a}{2}$.

Simpson's Rule

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

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[1] Thomas Simpson, 1710–1761. One of the most distinguished of a group of itinerant 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.

To show how to derive it, we'll use the ***Method of Undetermined Coefficients*** again. Rule: $q_0 f(a) + q_1 f(\frac{a+b}{2}) + q_2 f(b)$

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:

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

$g(x) = x$ $\quad Q_2(x) = \frac{1}{2} q_1 + q_2 = \int_0^1 x\,dx = \frac{1}{2}$

$g(x) = x^2$ $\quad Q(x^2) = \frac{1}{4} q_1 + q_2 = \int_0^1 x^2\,dx = \frac{1}{3}$.

This is easily solved giving

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

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

Example

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

$$Q_2(f) = \frac{b-a}{6}\left(f(0) + 4f(\pi/8) + f(\pi/4)\right)$$

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

$$= 0.70720195.$$

Also, $I(f) = \int_0^{\pi/4} \cos(x)\,dx = 0.70710678.$

Error: $|I(f) - Q_2(f)| = 9.5166 \times 10^{-5}.$

(Compare with Trap Error 0.0367)

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

Let $M_{n+1} := \max_{a \leq x \leq b} |f^{(n+1)}(x)|$, *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

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

The proof just comes directly Cauchy's Theorem.

Theorem

*For the **Trapezium Rule**, Q_1,*

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

The proof is an exercise. involves computing $\int_a^b (x-a)(x-b)dx$

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?

Answer:

$$\mathcal{E}_1 \leq \frac{(\pi/4)^3}{12} = 0.0403\,7,$$

Because $f(x) = \cos(x)$ so $f''(x) = -\cos(x)$, so $M_2 = |-\cos(0)| = 1$

Compare with actual error: 0.0367. So this is pretty sharp.

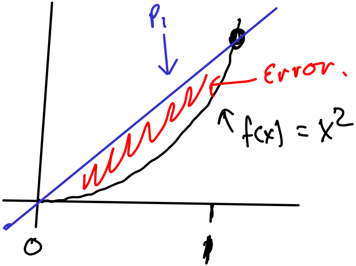
Error estimates for the Trapezium Rule

Example

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.



$f(x) = x^2, \quad f'(x) = 2x,$

$f''(x) = 2.$ So

$M_2 = \max_{0 \le x \le 1} 2 = 2.$

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

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

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

Example

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. How does this compare with the actual error?

Here $M_3 = \max_{0 \leq x \leq \pi/4} |f'''(x)| = \max_{0 \leq x \leq \pi/4} |\sin(x)| = \sin(\pi/4)$

Then $\mathcal{E}_2 \leq \frac{(b-a)^4}{194} M_3 = 1.387 \times 10^{-3}$.

Actual Error: 9.5166×10^{-5}

Example

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 ...

$I(f) = \int_0^1 x^3\,dx = \frac{1}{4} x^4 \Big|_0^1 = \frac{1}{4}.$ (true answer)

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

$= \frac{1}{6}\left(\frac{1}{2} + 1\right) = \frac{1}{6} \times \frac{3}{2} = \frac{1}{4}$ "My approximation"

No Error — why??

Example

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Another Example: Estimate $\int_{-1}^{1} x^3\,dx$.

$$\int_{-1}^{1} x^3\,dx = \frac{1}{4}x^4 \Big|_{-1}^{1} = \frac{1}{4}(1)^4 - \frac{1}{4}(-1)^4 = 0.$$

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

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

So: interval does not matter!!