Chapter 2

Numerical Integration – also called quadrature

The goal of numerical integration is to approximate

$$\int_a^b f(x)dx$$

numerically.
This is useful for 'difficult' integrals like

$$\frac{sin(x)}{x}; \quad sin(x^2); \quad \sqrt{1+x^4}$$

Or worse still for multiple-dimensional integrals where "multi" could be 2 or 20 or 10^6 etc.

2.1 A basic principle

If we cannot do $\int_a^b f(x)dx$, we approximate $f(x)$ with a function we can integrate.
(usually by a polynomial ie $f(x) = ax + bx^2 + cx^3 + ...$) When we integrate a function we calculate the area below the curve.

DRAWINGS

2.2 Trapezoidal Rule

Approximate the function between 'a' and 'b' by a line segment ie

$$f(x) = cx$$

DRAWING
area under line segment $= \frac{1}{2}$ area of a trapezoidal

$$\begin{aligned} \text{area of a trapezoidal} &= \text{base * height} \\ &= \text{h* [f(a)+f(b)]} \quad \text{DRAWING} \\ \tfrac{1}{2}\text{ area of a trapezoidal} &= \tfrac{h}{2}[f(a)+f(b)] \end{aligned}$$

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(a)+f(b)]$$

Which gives us the **Trapezoidal Rule**.

$$\int_a^b f(x)dx \approx \frac{b-a}{2}[f(a)+f(b)]$$

What did we miss?
DRAWING

2.2.1 Extending the Trapezoidal Rule

Before we took one giant step across the interval we now break this into 'n' small steps of size h, where

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

Then we apply the trapezoidal rule at each step
DRAWING

$f(x)$ approximated by a series of polynomials - one for each step.
Apply trapezoidal rule to each segment and add

$$\begin{aligned} T &= \text{trap. area} \\ &= \tfrac{1}{2}h(y_0+y_1)+\tfrac{1}{2}h(y_1+y_2)+\tfrac{1}{2}h(y_2+y_3)+...+\tfrac{1}{2}h(y_{n-1}+y_n) \\ &= h(\tfrac{1}{2}y_0+y_1+y_2+y_3+...+y_{n-1}+\tfrac{1}{2}y_n) \end{aligned}$$

but we have

$$y_0 = f(a); \quad y_1 = f(x_1); \quad y_2 = f(x_2); \quad ... \quad y_n = f(b)$$

And we now have the extend trapezoidal rule

$$= h(\frac{1}{2}f(a)+f(x_1)+f(x_2)+f(x_3)+...+f(x_{n-1})+\frac{1}{2}f(b))$$

EXAMPLE

2.2.2 Error estimates

In any subinterval, say $[x_{k-1}, x_k]$
$\int_{x_{k-1}}^{x_k} f(x)dx$ approximate by trapezoidal rule
ie

$$\int_{x_{k-1}}^{x_k} f(x)dx \approx T_k = \frac{h}{2}[f(x_{k-1})+f(x_k)]$$

Q: whats the size of the error on this interval?

$$\int_{x_{k-1}}^{x_k} f(x)dx = T_k + err(x)$$

$f(x)$ was approximated by a polynomial $\sim f(x) \to x+a$. We can write $f(x)$ as a Taylor expansion about a nearby pt. $x_{k-\frac{1}{2}}$ let $x \in [x_{k-1}, x_k]$

$$\begin{aligned} f(x) &= f(x_{k-\frac{1}{2}}) + (x - x_{k-\frac{1}{2}})f'(x_{k-\frac{1}{2}}) \\ &\quad + \tfrac{(x-x_{k-\frac{1}{2}})}{2!}f''(x_{k-\frac{1}{2}}) + ... \end{aligned}$$

and if $x = x_k$

$$(x_k - x_{k-1}) = h \quad \to (x_k - x_{k-\frac{1}{2}}) = \frac{h}{2}$$

The approximating polynomial is of degree 1 $\sim \; x+a$
it accurately represents $f(x)$ up to the first derivative but not beyond:

$$\frac{d^2(x+a)}{dx^2} = 0 \Rightarrow \quad \text{cannot know } f''(x)$$

$$f(x) \approx f(x_{k-\frac{1}{2}}) + (x - x_{k-\frac{1}{2}})f'(x_{k-\frac{1}{2}})$$

and the error starts at the next term

$$error = \frac{(x - x_{k-\frac{1}{2}})^2}{2!}f''(x_{k-\frac{1}{2}})$$

We cannot know $f''(x)$ so say $M_k = max\{f''(x)|x \in [x_{k-1}, x_k]\}$ and write

$$error = \frac{(x - x_{k-\frac{1}{2}})^2}{2!}M_k$$

So, trapezoidal rule fails to integrate a term $= \frac{(x-x_{k-\frac{1}{2}})^2}{2!}M_k$
Do the integration and compare results from trapezoid and true integration

$$\int_{x_{k-1}}^{x_k} \frac{(x - x_{k-\frac{1}{2}})^2}{2!}M_k dx = \left.\frac{(x - x_{k-\frac{1}{2}})^3}{3.2!}\right|_{x_{k-1}}^{x_k} M_k$$

$$= \left[\frac{(x_k - x_{k-\frac{1}{2}})^3}{3.2!} - \frac{(x_{k-1} - x_{k-\frac{1}{2}})^3}{3.2!}\right] M_k$$

$$= \left[\frac{(\frac{h}{2})^3}{3.2!} + \frac{(\frac{h}{2})^3}{3.2!}\right] M_k = \frac{h^3}{3.4.2!}M_k$$

Now we integrate the error by applying the trapezoidal rule:

$$\int_{x_{k-1}}^{x_k} \frac{(x-x_{k-\frac{1}{2}})^2}{2!} M_k dx \rightarrow$$
$$M_k \frac{h}{2}\left[\frac{(x_k-x_{k-\frac{1}{2}})^2}{2!} + \frac{(x_{k-1}-x_{k-\frac{1}{2}})^2}{2!}\right]$$
$$= M_k \frac{h}{2}\left[\frac{\frac{h}{2})^2}{2!} + \frac{\frac{h}{2})^2}{2!}\right]$$
$$= M_k \frac{h^3}{4.2!}$$

Therefore the error made by applying Trapezoidal Rule over the interval $[x_{k-1}, x_k]$ is

$$= \text{Error from Trap Rule} - \text{True Error}$$
$$= \left[\frac{h^3}{4.2!} - \frac{h^3}{3.4.2!}\right] M_k = \frac{h^3}{12} M_k$$

Now, for N subintervals the total error is = no of steps × error at each step

$$= N * \frac{h^3}{12} M_k$$

$$= N \times \frac{1}{12}\frac{(b-a)^3}{N^3} M_k$$
$$= \frac{1}{12}\frac{(b-a)^3}{N^2} f''$$

The error formula tells us that if we double N (number of steps) the error decreases by a factor of 4 ie N^2

Useful to know.

Sometimes you're given a target accuracy and a range.

You decide the stepsize h, using the error formula.

EXAMPLE

2.3 Simpson's Rule

Consider

$$\int_a^b f(x)dx$$

approximate $f(x)$ with polynomial of degree two

$$Ax^2 + Bx + C$$

ie a parabola.

Any 3 noncollinear point in the place can be fitted with a parabola.

Thus Simpson's Rule: approximate curves with parabolas

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From this we get the area of the shaded region

$$A_p = \frac{h}{3}(y_0 + 4y_1 + y_2)$$

Eg. applying this formula from $x = a$ to $x = b$ we get

$$\int_a^b f(x)dx \approx \frac{h}{3}(f(a) + 4f(\frac{a+b}{2}) + f(b))$$

2.3.1 Deriving A_p

Simplifying the previous plot

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vspace1 in Area under $y = Ax^2 + Bx + C$ for $x = -h$ to h is

$$\begin{aligned} A_p &= \int_{-h}^{h}(Ax^2 + Bx + C)dx \\ &= \frac{Ax^3}{3} + fracBx^2 2 + Cx\Big]_{-h}^{h} \\ &= \frac{2Ah^3}{3} + 2Ch \\ &= \frac{h}{3}(2Ah^2 + 6C) \end{aligned}$$

We also know the curve passes through 3 points

$$(-h, y_0); \quad (0, y_1); \quad (h, y_2)$$

$$y_0 = Ah^2 - Bh + c; \quad y_1 = C; \quad y_2 = Ah^2 + Bh + C$$

$$\begin{aligned} C &= y_1 \\ Ah^2 - Bh &= y_0 - y_1 \\ Ah^2 + Bh &= y_2 - y_1 \\ 2Ah^2 &= y_0 + y_2 - 2y_1 \end{aligned}$$

expressing A_p in terms of y_0, y_1, y_2

$$A_p = \frac{h}{3}(2Ah^2 + 6C) = \frac{h}{3}((y_0 + y_2 - 2y_1) + 6y_1)$$

$$A_p = \frac{h}{3}((y_0 + 4y_1 + y_2)$$

And we now have **Simpson's rule**.

$$\int_{x-h}^{x+h} f(x)dx \approx \frac{h}{3}(f(x-h) + 4f(x) + f(x+h))$$

Note: the area calculated, for each subinterval is of width $2h$.

2.3.2 Extended Simpson's Rule

We extend the formula for n subintervals.
DRAWING
n must be even to have each subinterval of width $2h$.

Calculate each area and sum
Let S denote ans from Simpson's rule

$$\begin{aligned} S = \; & \tfrac{h}{3}(y_0 + 4y_1 + y_2) + \tfrac{h}{3}(y_2 + 4y_3 + y_4) + ... + \\ & \tfrac{h}{3}(y_{n-2} + 4y_{n-1} + y_n) \end{aligned}$$

From this we get the **Extended Simpson's Rule**

$$S = \frac{h}{3}(y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + ... + 4y_{n-1} + y_n)$$

EXAMPLES

2.3.3 Error of the Simpson's Rule

degree	Exact	Simpson Rule
		$\frac{h}{3}(f(a) + 4f(\frac{a+b}{2}) + f(b))$
0	$\int_0^1 1dx = 1$	$\frac{0.5}{3}(1 + 4(1) + 1) = 1$
1	$\int_0^1 xdx = 0.5$	$\frac{0.5}{3}(0 + 4(0.5) + 1) = 0.5$
2	$\int_0^1 x^2dx = \frac{1}{3}$	$\frac{0.5}{3}(0^2 + 4(0.5)^2 + 1^2) = \frac{1}{3}$
3	$\int_0^1 x^3dx = \frac{1}{4}$	$\frac{0.5}{3}(0^3 + 4(0.5)^3 + 1^3) = \frac{1}{4}$
4	$\int_0^1 x^4dx = \frac{1}{5}$	$\frac{0.5}{3}(0^4 + 4(0.5)^4 + 1^4) = \frac{5}{24}$

We get an exact answer for any $f(x)$ up to degree 3 ie up to x^3.
From the Taylor expansion a la Trapezoid rule

$$error - \frac{(x - x_k)^4}{4!} f^{(4)}(x)$$

at $x \in [x_{k-1}, x_{k+1}]$.
DRAWING

We now proceed as in a similar fashion to the the Trapezoidal case, to find the error. We integrate the error term over subintervals of size $2h$

$$error = \frac{(x - x_k)^4}{4!} f^{(4)}(x),$$

$$M_k = max\{f(x) | x \in [x_{k-1}, x_{k+1}]\}$$

$$\begin{aligned}
\int_{x_{k-1}}^{x_{k+1}} \frac{(x-x_k)^4}{4!}dx &= \frac{(x-x_k)^5}{5.4!}\Big|_{x_{k-1}}^{x_{k+1}} M_k \\
&= \left[\frac{(x_{k+1}-x_k)^5}{5.4!} - \frac{(x_{k-1}-x_k)^5}{5.4!}\right] M_k \\
&= \left[\frac{h^5}{5.4!} + \frac{h^5}{5.4!}\right] M_k \\
&= \frac{2h^5}{5.4!} M_k
\end{aligned}$$

and by Simpson's Rule

$$\begin{aligned}
\int_{x_{k-1}}^{x_{k+1}} \frac{(x-x_k)^4}{4!}dx &\to M_k \frac{h}{3}\left[\frac{(x_{k-1}-x_k)^4}{4!}\right. \\
&\quad \left. +4\frac{(x_k-x_k)^4}{4!} + \frac{(x_{k+1}-x_k)^4}{4!}\right] M_k \\
&= \frac{h}{3}\left[\frac{h^4}{4!} + 0 + \frac{h^4}{4!}\right] M_k \\
&= \frac{2h^5}{3.4!} M_k
\end{aligned}$$

So the **error for the Simpson rule** is

$$\frac{2h^5}{3.4!}M_k - \frac{2h^5}{5.4!}M_k = \frac{h^5}{90}M_k$$

For a length $2h$. For 1 step of size h error $= \frac{h^5}{90}M_k$.
Therefore the error for the extended rule for N steps is

$$= N \times \frac{h^5}{180} M_k$$

$$= N \times \frac{(b-a)^5}{N^5}\frac{1}{180}M_k$$

$$= \frac{(b-a)^5}{N^4}\frac{1}{180}M_k$$

Therefore if f double N the error decreases by a factor $2^4 = 16$.
This shows that Simpson' rule is considerably more accurate than Trapezoidal.
EXAMPLE

2.4 Polynomials of low degree

If $f(x)$ is a polynomial of degree less than 4
$\Rightarrow$ fourth derivative=0
$\Rightarrow$ Simpson's error=$\frac{(b-a)^5}{N^4}\frac{f^{(4)}(x)}{180}$
$\frac{(b-a)^5}{N^4}\frac{0(x)}{180} = 0$
Therefore no error in the Simpson's approx of $\int_a^b f(X)dx$
ie if $f(x)$ is constant $\sim$ a;
linear $\sim$ x;
quadratic $\sim$ x^2;
cubic $\sim$ x^3.
Simpson's rule give an exact answer for $\int_a^b f(X)dx$ whether the # subdivisions.
EXAMPLE

2.5 Summary

2.5.1 Trapezoidal Rule

The Trapezoidal Rule

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(a) + f(b)]$$

and the extended rule

$$\begin{aligned}
\int_a^b f(x)dx \approx\ & h[\tfrac{1}{2}f(a) + f(x_1) + f(x_2) + f(x_3) + \\
& ... + f(x_{n-1}) + \tfrac{1}{2}f(b)]
\end{aligned}$$

The error $= \frac{h^3}{12}M_k$ or in other words:
the error is $O(h^3)$

2.5.2 Simpson's Rule

Simpson's Rule

$$\int_a^b f(x)dx \approx \frac{h}{3}[f(a) + 4f(\frac{a+b}{2}) + f(b)]$$

and the extended rule

$$\begin{aligned}\int_a^b f(x)dx \approx\ & \tfrac{h}{3}[f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) \\ & + 2f(x_4) + ... + 4f(x_{n-1}) + f(x_n)]\end{aligned}$$

and the error in each step is $O(h^5)$
ie error $= \frac{h^5}{180} M_k$