Computational Mathematics/Information Technology

Dr Oliver Kerr

2009–10

Introduction

In many problems we may want to find integrals like

$$\int_{x=a}^{x=b} f(x)\, dx$$

where we know or can calculate $f(x)$, but cannot do the integration explicitly.

What can we do?

Introduction

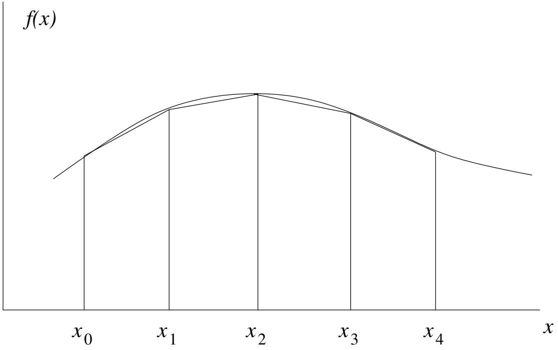
In many problems we may want to find integrals like

$$\int_{x=a}^{x=b} f(x)\, dx$$

where we know or can calculate $f(x)$, but cannot do the integration explicitly.

What can we do?
We have already seen one thing in the work sheets — integrate a spline.

Trapezium rule



The area under the first line segment is

$$\int_{x_0}^{x_1} f(x_0) + (x - x_0)\frac{(f(x_1) - f(x_0))}{(x_1 - x_0)}\,dx = \frac{f(x_0) + f(x_1)}{2}(x_1 - x_0)$$

Apply this to our integral

$$\int_{x=a}^{x=b} f(x)\, dx$$

Let us divide the interval into N intervals. There will be a gap of

$$h = (b - a)/N$$

between our xs. So

$$x_0 = a, \quad x_1 = a + h, \quad x_2 = a + 2h, \ \ldots, \quad x_N = a + Nh = b$$

Then our guess at the integral will be the **Trapezium rule**:

$$\int_{x=a}^{x=b} f(x)\,dx \approx \sum_{n=0}^{N-1} h(f(a+nh)+f(a+(n+1)h)/2$$

$$= \frac{h}{2}(f(a)+2f(a+h)+2f(a+2h)+\cdots+2f(b-h)+f(b))$$

How accurate is this?

Then our guess at the integral will be the **Trapezium rule**:

$$\int_{x=a}^{x=b} f(x)\, dx \approx \sum_{n=0}^{N-1} h(f(a+nh) + f(a+(n+1)h)/2$$

$$= \frac{h}{2}(f(a) + 2f(a+h) + 2f(a+2h) + \cdots + 2f(b-h) + f(b))$$

How accurate is this?

It will depend on N.

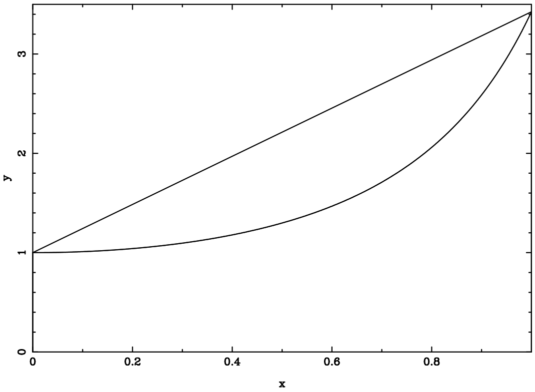
We will look at an example where we can do the integration. We will integrate

$$f(x) = \sec^2(x)$$

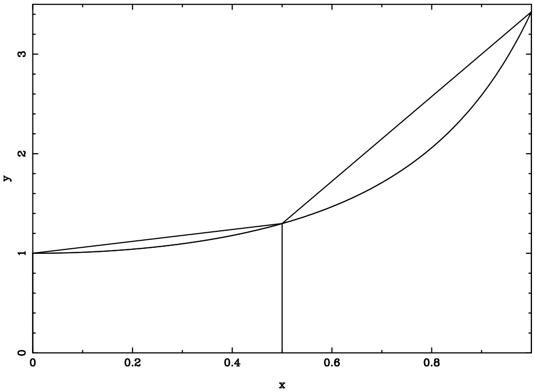
between $x = 0$ and $x = 1$

$$\int_0^1 \sec^2 x \, dx = \tan 1 \approx 1.557407725$$

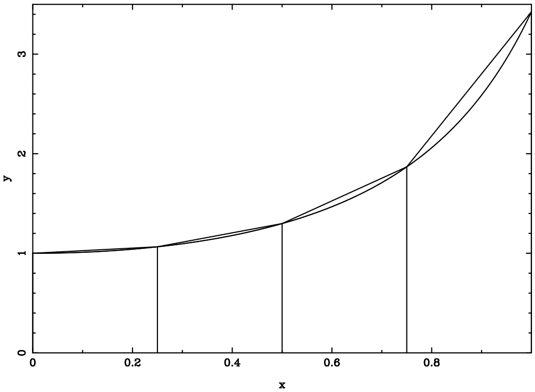
We will see what happens as we increase N



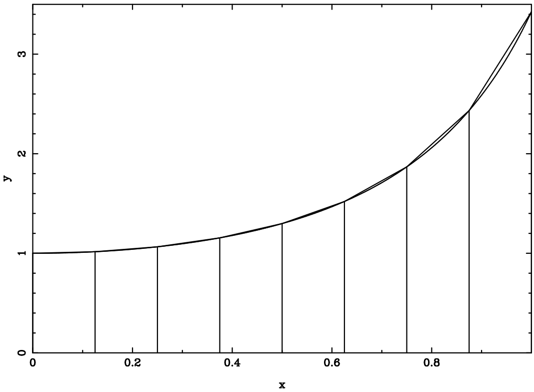
$N = 1$, Estimate= 2.21275949, Error= 0.655351758



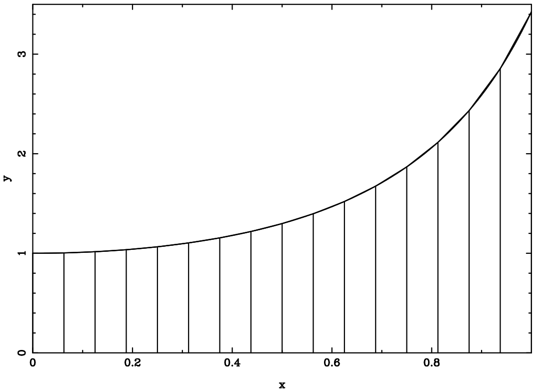
$N = 2$, Estimate$= 1.75560296$, Error$= 0.198195219$



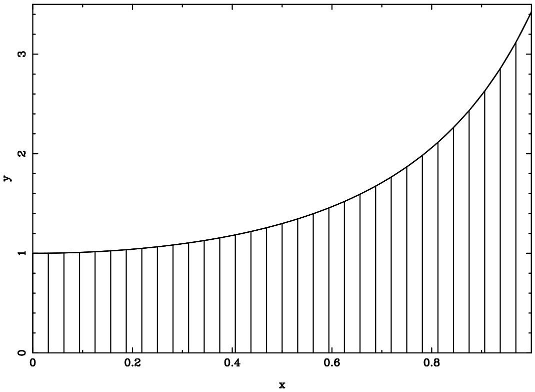
$N = 4, \quad \text{Estimate}= 1.61106944, \quad \text{Error}= 0.0536617041$



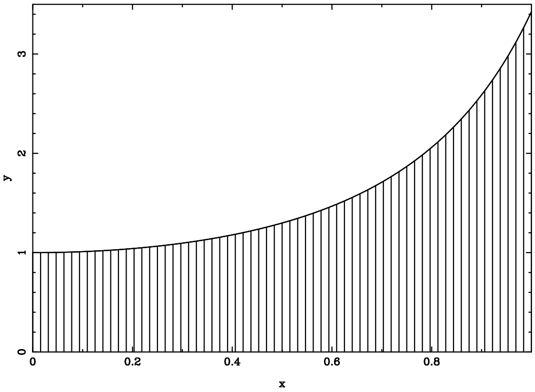
$N = 8, \quad \text{Estimate}= 1.57117105, \quad \text{Error}= 0.0137633085$



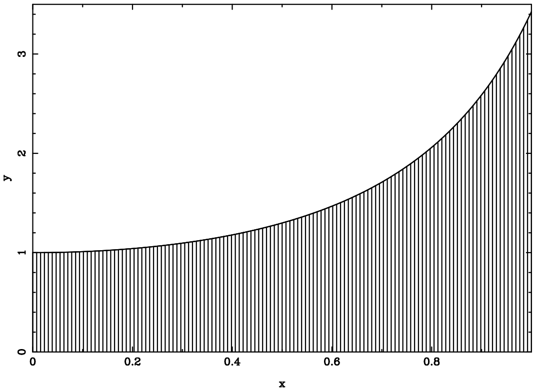
$N = 16$, Estimate$= 1.56087255$, Error$= 0.003464818$



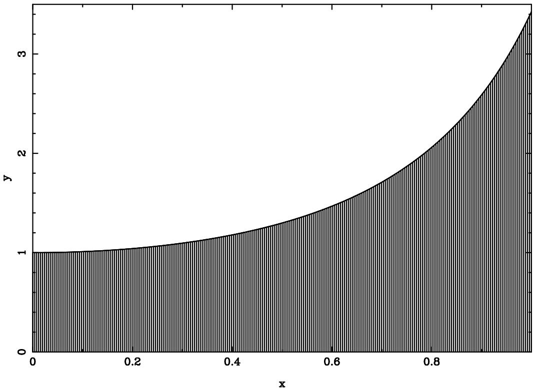
$N = 32$, Estimate= 1.55827546, Error= 0.000867724419



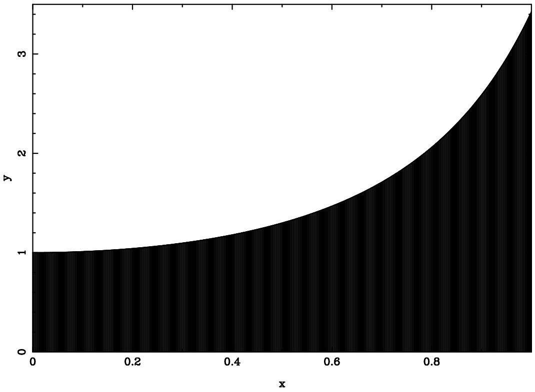
$N = 64$, Estimate= 1.55762482, Error= 0.000217080116



$N = 128$, Estimate$= 1.5574621$, Error$= 0.000054359436$



$N = 256$, Estimate$= 1.5574218$, Error$= 0.0000140666962$



$N = 512$, Estimate= 1.55741155, Error= 0.00000381469727

N	Estimate	Error
1	2.21275949	0.655351758
2	1.75560296	0.198195219
4	1.61106944	0.0536617041
8	1.57117105	0.0137633085
16	1.56087255	0.003464818
32	1.55827546	0.000867724419
64	1.55762482	0.000217080116
128	1.55746210	5.4359436E-05
256	1.55742180	1.40666962E-05
512	1.55741155	3.81469727E-06
1024	1.55740809	3.57627869E-07
2048	1.55740845	7.15255737E-07
4096	1.55740631	-1.43051147E-06
8192	1.55740643	-1.31130219E-06

The error is roughly reduced by a factor of 4 each time we double N.

Two questions:

1. Is this to be expected?
2. Can we do better?

To find the estimate of the error we look at the error in one segment from a to $a+h$.

We will use the result

$$f(a+x) = f(a) + xf'(a) + x^2 f''(a+\theta(x)x)/2$$

for some $0 < \theta(x) < 1$. This means the second derivative is evaluated somewhere between a and $a+x$.

If we integrate

$$f(a+x) = f(a) + xf'(a) + x^2 f''(a+\theta(x)x)/2$$

for x between 0 and h we get

$$\int_0^h f(a+x)\,dx = \int_0^h f(a) + xf'(a)\,dx + \int_0^h x^2 f''(a+\theta(x)x)/2\,dx$$

We need an estimate of $f'(a)$, but we just use our result again.

$$f(a+h) = f(a) + hf'(a) + h^2 f''(a+\theta(h)h)/2$$

so

$$f'(a) = \frac{f(a+h) - f(a)}{h} - hf''(a+\theta(h)h)/2$$

Hence

$$\int_0^h f(a) + xf'(a)\,dx = hf(a) + \frac{h^2}{2}f'(a)$$

$$= hf(a) + \frac{h^2}{2}\left(\frac{f(a+h)-f(a)}{h} - hf''(a+\theta(h)h)/2\right)$$

$$= h\frac{f(a)+f(a+h)}{2} - \frac{h^3}{4}f''(a+\theta(h)h)$$

We are left with

$$\int_0^h x^2 f''(a+\theta(x)x)/2\,dx$$

which is an integral we cannot do — but we can make an estimate.

If

$$\left|f''(x)\right| < M \quad \text{for all} \quad 0 \le x \le h$$

then

$$\left|\int_0^h x^2 f''(a+\theta(x)x)/2\,dx\right| \le \int_0^h x^2 \left|f''(a+\theta(x)x)/2\right|\,dx$$

$$< \int_0^h x^2 M/2\,dx = \frac{h^3}{6}M$$

Combining these results gives

$$\int_0^h f(a+x)\,dx = h\frac{f(a)+f(a+h)}{2} + (\text{various terms}) \times h^3$$

If we add N terms like this then the error will be the sum of N terms all proportional to h^3. But $h = (b-a)/N$ so

$$\int_{x=a}^{x=b} f(x)\,dx = \frac{h}{2}(f(a)+2f(a+h)+2f(a+2h)+\cdots+2f(b-h)+f(b))$$

$$+(\text{various terms}) \times h^2$$

Simpson's rule

How can we do better?

Simpson's rule

How can we do better?

Let

$$I_n = \frac{h}{2}(f(a) + 2f(a+h) + 2f(a+2h) + \cdots + 2f(b-h) + f(b)),$$

where $h = (b-a)/N$.

Then

$$\int_{x=a}^{x=b} f(x)\,dx = I_N + A/N^2 + \text{smaller terms}$$

Simpson's rule

How can we do better?

Let

$$I_n = \frac{h}{2}(f(a) + 2f(a+h) + 2f(a+2h) + \cdots + 2f(b-h) + f(b)),$$

where $h = (b-a)/N$.

Then

$$\int_{x=a}^{x=b} f(x)\,dx = I_N + A/N^2 + \text{smaller terms}$$

$$\int_{x=a}^{x=b} f(x)\,dx = I_{2N} + A/(2N)^2 + \text{smaller terms}$$

$$\int_{x=a}^{x=b} f(x)\,dx = I_N + A/N^2 + \text{smaller terms}$$

$$\int_{x=a}^{x=b} f(x)\,dx = I_{2N} + A/(2N)^2 + \text{smaller terms}$$

Take 4 times the bottom equation and subtract off the top one to get rid of the A terms:

$$3\int_{x=a}^{x=b} f(x)\,dx = 4I_{2N} - I_N + \text{smaller terms}$$

$$\int_{x=a}^{x=b} f(x)\, dx = I_N + A/N^2 + \text{smaller terms}$$

$$\int_{x=a}^{x=b} f(x)\, dx = I_{2N} + A/(2N)^2 + \text{smaller terms}$$

Take 4 times the bottom equation and subtract off the top one to get rid of the A terms:

$$3\int_{x=a}^{x=b} f(x)\, dx = 4I_{2N} - I_N + \text{smaller terms}$$

This should be more accurate as the $1/N^2$ error terms have gone.

We now have

$$3\int_{x=a}^{x=b} f(x)\,dx \approx 4I_{2N} - I_N$$

This can be written as

$$\int_{x=a}^{x=b} f(x)\,dx$$

$$= \frac{h}{3}\big(f(a)+4f(a+h)+2f(a+2h)+4f(a+3h)+2f(a+4h)+\cdots$$

$$\cdots+2f(b-2h)+4f(b-h)+f(b)\big)$$

This is Simpson's rule.

N	Estimate	Error
2	1.60321748	0.0458097458
4	1.56289148	0.00548374653
8	1.55787134	0.000463604927
16	1.55743992	3.21865082E-05
32	1.55740976	2.02655792E-06
64	1.55740821	4.76837158E-07
128	1.55740786	1.1920929E-07
256	1.55740786	1.1920929E-07
512	1.55740798	2.38418579E-07
1024	1.55740702	-7.15255737E-07