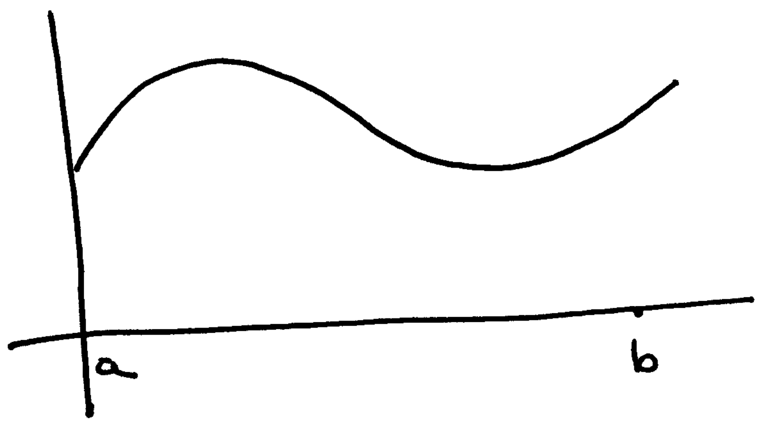
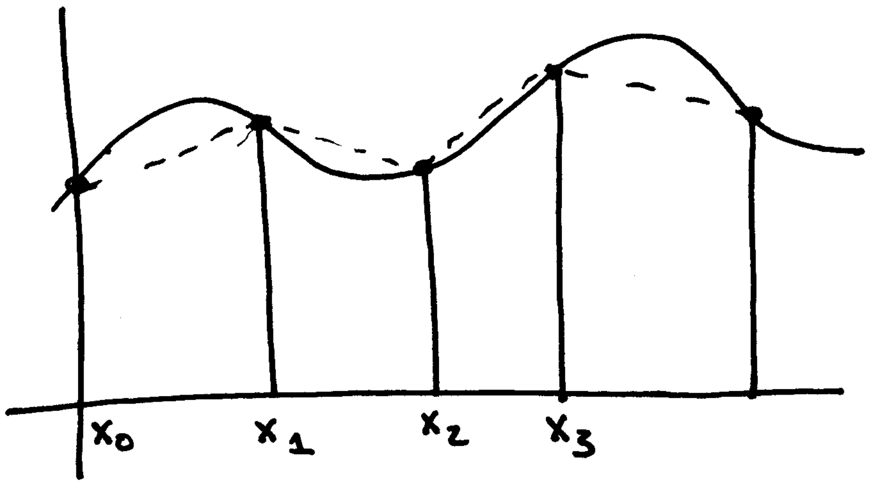
Numerical Integration

We now turn our attention to numerical integration. Our task is to compute a definite integral to a specified precision.



One way to do this, of course, is by computing Riemann sums. It suffices to say that this is terrible.

A much better rule is the trapezoid rule:



Observe

$$\text{Area of trapezoid } x_i, x_{i+1} = \underbrace{\left(\tfrac{1}{2}\left(f(x_{i+1})+f(x_i)\right)\right)}_{\text{average height}} \underbrace{\left(x_{i+1}-x_i\right)}_{\text{width}}$$

so

$$\int_a^b f(x)\,dx \approx \frac{1}{2}\sum_{i=0}^{n-1}(x_{i+1}-x_i)\left[f(x_{i+1})+f(x_i)\right].$$

with uniform spacing $h = x_{i+1} - x_i$, we can rewrite this

$$\frac{1}{2}\sum_{i=0}^{n-1} h\left[f(x_{i+1}) + f(x_i)\right]$$

$$= \frac{1}{2}\Big(hf(x_0) + hf(x_1) + hf(x_1) + \ldots\ldots + hf(x_{n-1}) + hf(x_{n-1}) + hf(x_n)\Big)$$

$$= h\Big(\frac{1}{2}(f(x_0) + f(x_n)) + \sum_{i=1}^{n-1} f(x_i)\Big).$$

We will do some examples with Mathematica soon. Right now we try to work out an error estimate:

Theorem. If f is C^2 on $[a,b]$ and the trapezoid rule with spacing h is used to compute the integral $\int_a^b f(x)\,dx$, then

$$\int_a^b f(x)\,dx - T(h) = -\frac{1}{12}(b-a)\,f''(\xi)\,h^2,$$

for some ξ in $[a,b]$.

(You saw this in 2200, but without proof. Now we are ready to prove it.)

Proof. Suppose $h=1$, $a=0$ and $b=1$. We have to show

$$\int_0^1 f(x)\,dx - \frac{1}{2}\left[f(0)+f(1)\right] = -\frac{1}{12}f''(\xi).$$

This is done by integrating the error formula for polynomial interpolation:

$$f(x)-p(x) = \frac{1}{2}f''(\xi)\ x(x-1).$$

and using the Mean Value Theorem for integrals: if $g(x) \geq 0$ on $[a,b]$ and $f(x)$ is continuous on (a,b), $\exists$ some ξ in (a,b) so

$$\int_a^b f(x)g(x)\,dx = f(\xi)\int_a^b g(x)\,dx.$$

Now we need to change variables.

Let

$$g(t) = f(a + t(b-a)), \quad x(t) = a + (b-a)t$$

then we know $dx = (b-a)\,dt$ and

$$\int_a^b f(x)\,dx = \int_0^1 f(x(t))\,(b-a)\,dt$$

$$= (b-a)\int_0^1 g(t)\,dt.$$

$$= (b-a)\left(\frac{1}{2}\big(g(0)+g(1)\big) - \frac{1}{12}\,g''(\xi)\right)$$

$$= \frac{b-a}{2}\left(f(a)+f(b) - \frac{1}{2}\,g''(\xi)\right).$$

Now

$$g(t) = f(x(t))$$

so

$$g'(t) = f'(x(t))\cdot x'(t)$$
$$= f'(x(t))\cdot(b-a)$$

and

$$g''(t) = f''(x(t))\cdot(b-a)^2$$

We then have

$$\int_a^b f(x)\,dx = \frac{b-a}{2}[f(a)+f(b)] - \frac{(b-a)^3}{12} f''(\xi).$$

Now suppose that $a = x_i$ and $b = x_{i+1}$. We then have $h = b-a$ so

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = h\left[\frac{f(a)+f(b)}{2}\right] - \frac{h^3}{12} f''(\xi).$$

Summing over $i = 0, \dots, n-1$, we get the error in the trapezoid role as

$$= -\frac{h^3}{12}\sum_{i=0}^{n-1} f''(\xi_i)$$

Now $h = \frac{b-a}{n}$, so we have

$$= -\frac{h^2}{12}(b-a)\underbrace{\left[\frac{1}{n}\sum_{i=0}^{n-1} f''(\xi_i)\right]}_{\text{average value of } f''(\xi_i)}$$

But the average of all these $f''(\xi_i)$ must surely be between

$$\min_{x \in [a,b]} f''(x) \leq \frac{1}{n} \sum f''(\xi_i) \leq \max_{x \in [a,b]} f''(x).$$

So there is some $\xi \in [a,b]$ so

$$f''(\xi) = \frac{1}{n} \sum_{i=0}^{n-1} f''(\xi_i)$$

as desired. $\square$.

Of course, the standard use for the error in trapezoid rule formula is to predict how many points we need to attain a given accuracy in integration.

Example. How many function evaluations are needed to compute

$$\int_0^1 \frac{\sin x}{x}\,dx \quad \text{to within } 10^{-5} \text{ error?}$$

We let

$$f(x) = \frac{\sin x}{x}$$

We need a bound on $f''(x)$. Computing

$$f'(x) = -\frac{1}{x^2}\sin x + \frac{\cos x}{x}$$

$$f''(x) = \frac{2}{x^3}\sin x - \frac{1}{x^2}\cos x - \frac{1}{x^2}\cos x - \frac{\sin x}{x}$$

$$= \frac{2\sin x - 2x\cos x - x^2 \sin x}{x^3}$$

makes one feel extremely unhappy.

Our salvation, as always, comes from the theory of Taylor series:

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!} + \cdots$$

so

$$f(x) = \frac{\sin x}{x} = 1 - \frac{x^2}{3!} + \frac{x^4}{5!} - \frac{x^6}{7!} + \cdots$$

$$f'(x) = -\frac{2x}{3!} + \frac{4x^3}{5!} - \frac{6x^5}{7!} + \cdots$$

$$f''(x) = -\frac{2}{3!} + \frac{12x^2}{5!} - \frac{30x^4}{7!} + \cdots$$

Now this is an alternating series, so

$$-\frac{2}{3!} \leq f''(x) \leq -\frac{2}{3!} + \frac{12x^2}{5!}$$

for any x. In particular

$$|f''(x)| \leq \frac{1}{3} - \frac{12}{5!} \leq \frac{1}{3} - \frac{\cancel{3}\cdot\cancel{4}}{2\cdot\cancel{3}\cdot\cancel{4}\cdot 5} \leq \frac{-1}{10} + \frac{1}{3} \leq \frac{-3}{30} + \frac{10}{30}$$

$$\leq \frac{7}{30} \leq \frac{1}{2}.$$

Thus we have

$$|\text{Error}| \leq \frac{1}{12} \cdot (b-a) h^2 |f''(\xi)|$$

$$\leq \frac{1}{12} 1 \cdot \frac{1}{n^2} \cdot \frac{1}{2}$$

$$\leq \frac{1}{24n^2}$$

If we want

$$\frac{1}{24n^2} < 10^{-5} = \frac{1}{10^5}$$

we get

$$10^5 < 24n^2$$

or

$$n > \sqrt{\frac{10^5}{24}} = 91.3.$$

Therefore 92 points should suffice.

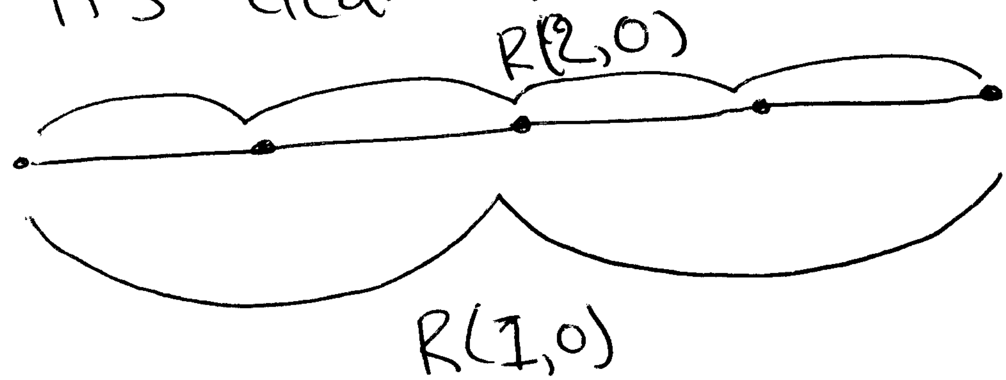
Now we will shortly ask the question: can we write down the error in the trapezoid rule as a power series and use Richardson extrapolation to start killing error terms?

(The answer is: heck, yes!)

But there are a few formalities to get out of the way. We suppose

$$R(n,0) := \text{result of trapezoid rule with } 2^n \text{ subintervals.}$$

Now it's clear that



half the function evaluations involved in computing $R(n+1,0)$ have already been done while computing $R(n,0)$.

Observe

$$R(n,0) = \frac{1}{2}R(n-1,0) + \left[R(n,0) - \frac{1}{2}R(n-1,0)\right].$$

Now consider

$$R(n,0) - \frac{1}{2}R(n-1,0).$$

If $h = (b-a)/2^n$, we have

$$R(n,0) = h\sum_{i=0}^{2^n-1} f(a+ih) + \frac{h}{2}[f(a)+f(b)]$$

$$\frac{1}{2}R(n-1,0) = \frac{(\cancel{2}h)}{\cancel{2}}\sum_{i=0}^{2^{n-1}-1} f(a+i(2h)) + \frac{1}{\cancel{2}}\frac{\cancel{2}h}{2}[f(a)+f(b)]$$

$$= \sum_{\substack{i=0 \\ i \text{ is odd}}}^{2^{n}-1} f(a+ih) = \sum_{k=1}^{2^{n-1}} f(a+(2k-1)h).$$

So we have

Theorem.

$$R(n,0) = \frac{1}{2} R(n-1,0) + h \sum_{k=1}^{2^{n-1}} f[a+(2k-1)h]$$

where $h = (b-a)/2^n$. $R(0,0) = \frac{1}{2}(b-a)[f(a)+f(b)]$.