Simple Numerical Integrators – Determining Step Size

In a typical application, one is required to evaluate a given integral $\int_a^b f(x)\,dx$ to some specified accuracy. For example, if you are manufacturer and your machinery can only cut materials to an accuracy of $\frac{1}{10}^{\rm th}$ of a millimeter, there is no point in making design specifications more accurate than $\frac{1}{10}^{\rm th}$ of a millimeter.

The choice of n, the number of steps, required to achieve the specified accuracy is based on the facts that

a) If $|f''(x)| \le M$ for all x in the domain of integration, then

the total error introduced by the Midpoint Rule is bounded by $\frac{M}{24}\frac{(b-a)^3}{n^2}$

b) If $|f''(x)| \le M$ for all x in the domain of integration, then

the total error introduced by the Trapezoidal Rule is bounded by $\frac{M}{12}\frac{(b-a)^3}{n^2}$

c) If $|f^{(4)}(x)| \le M$ for all x in the domain of integration, then

the total error introduced by Simpson's Rule is bounded by $\frac{M}{180}\frac{(b-a)^5}{n^4}$

For example, if the integral in question is $\int_0^1 \sin x\,dx$, then $a=0$, $b=1$ and $f(x)=\sin x$. In this, rather trivial, case $f''(x) = -\sin x$ and $f^{(4)}(x) = \sin x$. As $\sin x$ never has magnitude greater than one, one may choose $M=1$ in applying each of the facts a), b) and c). But this is not the only allowed M. It is perfectly legitimate, though silly, to use $M=2$. Furthermore, $\sin x$ increases as x runs from 0 to $\frac{\pi}{2} > 1$. Consequently, the largest value of $\sin x$ on the interval $0 \le x \le 1$ is $\sin 1$. Thus it it also correct to use $M = \sin 1$. The moral here is that there are many legal values of M. The smaller the (legal) value of M you use, the better the bound on the error given in facts a), b) and c).

Example 1 Suppose, for example, that we wish to use the Midpoint Rule to evaluate $\int_0^1 e^{-x^2}\,dx$ to within an accuracy of 10^{-6}. (In fact this integral cannot be evaluated exactly, so one must use numerical methods.) The first two derivatives of the integrand are

$$\frac{d}{dx}e^{-x^2} = -2xe^{-x^2} \quad \text{and} \quad \frac{d^2}{dx^2}e^{-x^2} = \frac{d}{dx}\big(-2xe^{-x^2}\big) = -2e^{-x^2} + 4x^2e^{-x^2} = 2(2x^2-1)e^{-x^2}$$

As x runs from 0 to 1, the factor $2x^2-1$ increases from $2x^2-1\Big|_{x=0} = -1$ to $2x^2-1\big|_{x=1} = 1$. So, on the domain of integration, $|2x^2-1| \le 1$. As x runs from 0 to 1, the factor e^{-x^2} decreases from $e^{-x^2}\Big|_{x=0} = 1$ to $e^{-x^2}\big|_{x=1} = e^{-1}$. So, on the domain of integration, $|e^{-x^2}| \le 1$. All together,

$$0 \le x \le 1 \Longrightarrow |2x^2-1| \le 1,\ e^{-x^2} \le 1 \Longrightarrow \big|2(2x^2-1)e^{-x^2}\big| \le 2\times 1\times 1 = 2$$

so that $|f''(x)| \le 2$ for all $0 \le x \le 1$ and we are allowed to take $M=2$. We now know that the error introduced by the n step Midpoint Rule is at most $\frac{M}{24}\frac{(b-a)^3}{n^2} \le \frac{2}{24}\frac{(1-0)^3}{n^2} = \frac{1}{12n^2}$. This error is at most 10^{-6} if

$$\frac{1}{12n^2} \le 10^{-6} \iff n^2 \ge \frac{1}{12}10^6 \iff n \ge \sqrt{\frac{1}{12}10^6} = 288.7$$

So 289 steps of the Midpoint Rule will do the job.

Example 2 Suppose now that we wish to use Simpson's Rule to evaluate $\int_0^1 e^{-x^2}\,dx$ to within an accuracy of 10^{-6}. To determine the number of steps required, we must determine how big $\frac{d^4}{dx^4}e^{-x^2}$ can get when $0 \le x \le 1$.

$$\begin{aligned} \tfrac{d^3}{dx^3}e^{-x^2} &= \tfrac{d}{dx}\big(2(2x^2-1)e^{-x^2}\big) = 8xe^{-x^2} - 4x(2x^2-1)e^{-x^2} = 4(-2x^3+3x)e^{-x^2} \\ \tfrac{d^4}{dx^4}e^{-x^2} &= \tfrac{d}{dx}\big(4(-2x^3+3x)e^{-x^2}\big) = 4(-6x^2+3)e^{-x^2} - 8x(-2x^3+3x)e^{-x^2} \\ &= 4(4x^4-12x^2+3)e^{-x^2} \end{aligned}$$

We now have to find an M such that $g(x) = 4(4x^4-12x^2+3)e^{-x^2}$ obeys $|g(x)| \le M$ for all $0 \le x \le 1$. Here are three different methods for finding such an M.

Method 1: The first method is to find the largest and small value that $g(x)$ takes on the interval $0 \le x \le 1$ by checking the values of $g(x)$ at its critical points and at the end points of the interval of interest. I warn you that, while this method gives the smallest possible value of M, it involves a lot more work than the other methods. It is **not recommended**. Since

$$g'(x) = 4(16x^3-24x)e^{-x^2} - 8x(4x^4-12x^2+3)e^{-x^2} = -8x(4x^4-20x^2+15)e^{-x^2}$$

the critical points of $g(x)$ are $x = 0$ and

$$x^2 = \tfrac{20\pm\sqrt{400-4\times4\times15}}{8} = \tfrac{20\pm\sqrt{160}}{8} = \tfrac{5\pm\sqrt{10}}{2} = 4.081139, 0.918861 \Longrightarrow x = \pm2.020183, \pm0.958572$$

Since

$$g(0) = 12,\ \ g(0.958572) = -7.419481,\ \ g(1) = -20e^{-1} = -7.357589$$

we know that $g(x)$ only takes values between -7.419481 and 12, so we may choose $M = 12$.

Method 2: Consider the three factors 4, $4x^4-12x^2+3$, and e^{-x^2} of $g(x)$ separately. For $0 \le x \le 1$, $e^{-x^2} \le e^{-0} = 1$ and

$$\big|4x^4-12x^2+3\big| \le 4x^4+12x^2+3 \le 4+12+3 = 19$$

Hence

$$0 \le x \le 1 \Longrightarrow |g(x)| \le 4\big|4x^4-12x^2+3\big|e^{-x^2} \le 4\times19\times1 = 76$$

So we may choose $M = 76$.

Method 3: Again consider the three factors 4, $4x^4-12x^2+3$ and e^{-x^2} of $g(x)$ separately. But this time, consider the positive terms of $4x^4-12x^2+3$ and the negative terms of $4x^4-12x^2+3$ separately. For $0 \le x \le 1$,

$$3 \le 4x^4+3 \le 7 \text{ and } -12 \le -12x^2 \le 0$$

Adding these two inequalities together gives

$$-9 \le 4x^4-12x^2+3 \le 7$$

Consequently, the maximum value of $|4x^4-12x^2+3|$ for $0 \le x \le 1$ is no more than 9 and

$$\big|g(x)\big| \le 4\times9\times1 = 36$$

We have now found three different possible values of M – all are allowed. In general, the error introduced by the n step Simpson's Rule is at most $\frac{M}{180}\frac{(b-a)^5}{n^4}$. In this example, $a = 0$ and $b = 1$ so that this error is at most 10^{-6} if

$$\tfrac{M}{180n^4} \le 10^{-6} \iff n^4 \ge \tfrac{M}{180}10^6 \iff n \ge \sqrt[4]{\tfrac{M}{180}10^6} = \begin{cases} 16.1 & \text{if } M = 12 \\ 21.1 & \text{if } M = 36 \\ 25.5 & \text{if } M = 76 \end{cases}$$

So if we take $M = 12$, we conclude that 18 steps of the Simpson's Rule will do the job. If we take $M = 36$, we conclude that 22 steps will do the job and if we take $M = 76$, we conclude that 26 steps will do the job. This is a typical case. Method 1 gives a slightly smaller of n than the much simpler procedures of Methods 2 and 3. But usually this gain in n is not worth the extra effort required to apply Method 1.

Example 3 Let $I = \int_{\pi/6}^{\pi/2} \ln(\sin x)\,dx$. How large should n be in order that the approximation $I \approx T_n$ be accurate to within 10^{-4}?

Solution. Let $f(x) = \ln(\sin x)$. First, we have to find an M such that $|f''(x)| \le M$ for all $\frac{\pi}{6} \le x \le \frac{\pi}{2}$.

$$f(x) = \ln(\sin x) \Longrightarrow f'(x) = \tfrac{\cos x}{\sin x} = \cot x \Longrightarrow f''(x) = -\csc^2 x = -\tfrac{1}{\sin^2 x}$$

As x runs from $\frac{\pi}{6}$ to $\frac{\pi}{2}$, $\sin x$ increases from $\sin\frac{\pi}{6} = \frac{1}{2}$ to $\sin\frac{\pi}{2} = 1$. So the largest value of $|f''(x)| = \frac{1}{\sin^2(x)}$ on the interval $\frac{\pi}{6} \le x \le \frac{\pi}{2}$ occurs at $x = \frac{\pi}{6}$, where the denominator is the smallest, and is $\frac{1}{\sin^2\frac{\pi}{6}} = \frac{1}{(1/2)^2} = 4$. Thus $|f''(x)| \le 4$ for all $\frac{\pi}{6} \le x \le \frac{\pi}{2}$ and we may choose $M = 4$.

We wish to find n so that

$$\tfrac{M(b-a)^3}{12n^2} \le 10^{-4}$$

In this case $M = 4$, $a = \frac{\pi}{6}$ and $b = \frac{\pi}{2}$ so

$$\tfrac{4(\pi/2-\pi/6)^3}{12n^2} \le 10^{-4} \iff n^2 \ge \tfrac{4(\pi/3)^3}{12}10^4 = \tfrac{\pi^3}{3^4}10^4 \iff n \ge \tfrac{\pi^{3/2}}{3^2}10^2 = 61.87$$

So any $n \ge 62$ will do the job.