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

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

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

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

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 $0 \le x \le 1$.

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

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, $|e^{-x^2}| \le 1$. Also, the derivative $\frac{d}{dx}(4x^4-12x^2+3) = 16x^3-24x = 16x\big(x^2-\frac{3}{2}\big)$ is negative for all $0 < x \le 1$. Consequently, as x runs from 0 to 1, the factor $(4x^4-12x^2+3)$ decreases from $(4x^4-12x^2+3)\big|_{x=0} = 3$ and to $(4x^4-12x^2+3)\big|_{x=1} = -5$. So, on the domain of integration, $\big|4x^4-12x^2+3\big| \le 5$. All together,

$$0 \le x \le 1 \implies |e^{-x^2}| \le 1,\ \big|4x^4-12x^2+3\big| \le 5 \implies \big|\tfrac{d^4}{dx^4}e^{-x^2}\big| \le 4\times 5\times 1 = 20$$

and we may set $M = 20$. The error introduced by the n step Simpson's Rule is at most $\frac{M}{180}\frac{(b-a)^5}{n^4} \le \frac{20}{180}\frac{(1-0)^5}{n^4} = \frac{1}{9n^4}$. This error is at most 10^{-6} if

$$\tfrac{1}{9n^4} \le 10^{-6} \iff n^4 \ge \tfrac{1}{9}10^6 \iff n \ge \sqrt[4]{\tfrac{1}{9}10^6} = 18.3$$

So 20 steps of the Simpson's Rule will do the job.

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 $\frac{\pi}{6} \le x \le \frac{\pi}{2}$.

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

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.