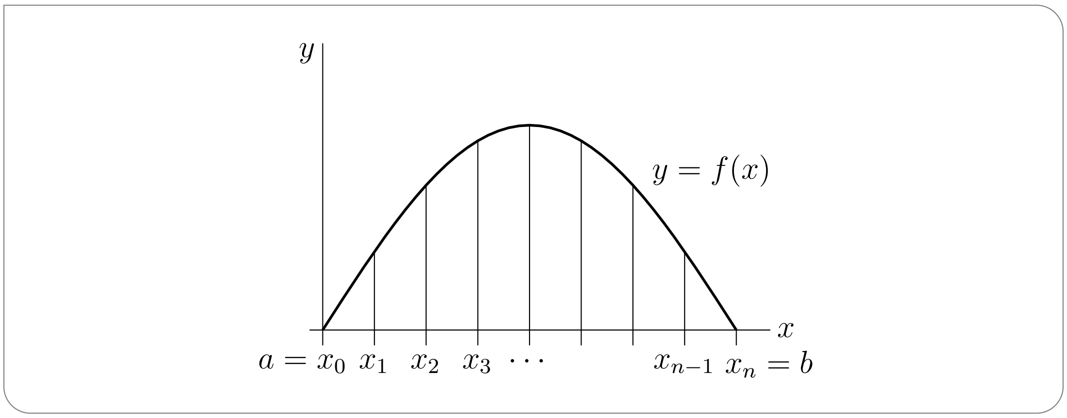
Numerical Integration

It is very common to encounter integrals that are too complicated to evaluate explicitly. We now study how to find (approximate) numerical values for integrals, without having to evaluate them algebraically.

Three Simple Numerical Integrators — Derivation

We start by deriving three simple algorithms for generating, numerically, approximate values for the definite integral $\int_a^b f(x)\,dx$. In each algorithm, we first select an integer $n > 0$, called the "number of steps". We then divide the interval of integration, $a \le x \le b$, into n equal subintervals, each of length $\Delta x = \frac{b-a}{n}$. The first subinterval runs from $x_0 = a$ to



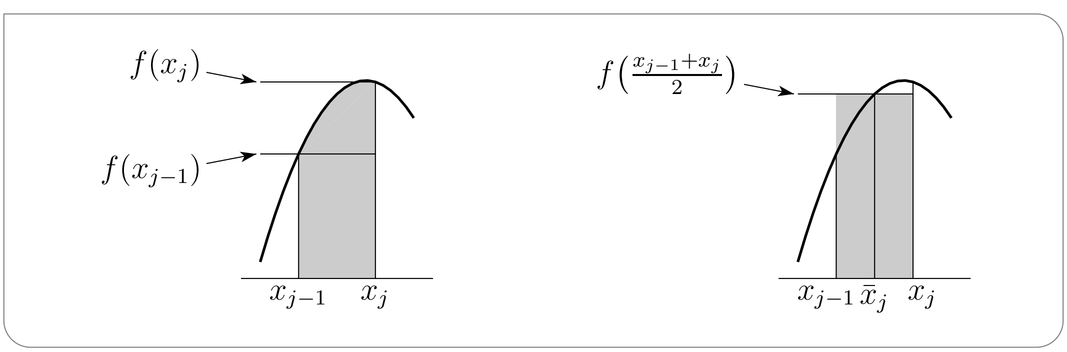
$x_1 = a + \Delta x$. The second runs from x_1 to $x_2 = a + 2\Delta x$, and so on. The last runs from $x_{n-1} = b - \Delta x$ to $x_n = b$. The corresponding decomposition of the integral is

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx$$

Each subintegral $\int_{x_{j-1}}^{x_j} f(x)\,dx$ is approximated by the area of a simple geometric figure. The three different algorithms use three different figures.

The Midpoint Rule

The integral $\int_{x_{j-1}}^{x_j} f(x)\,dx$ represents the area under the curve $y = f(x)$ with x running from x_{j-1} to x_j. The width of this region is $x_j - x_{j-1}$. The height varies over the different values that $f(x)$ takes as x runs from x_{j-1} to x_j. The midpoint rule approximates this area by



the area of a rectangle of width $x_j - x_{j-1} = \Delta x$ and height $f\big(\frac{x_{j-1}+x_j}{2}\big)$, which is the exact height at the midpoint of the range covered by x. The area of the approximating rectangle is $f\big(\frac{x_{j-1}+x_j}{2}\big)\Delta x$. To save writing, set $\bar{x}_j = \frac{x_{j-1}+x_j}{2}$. So the midpoint rule approximates each subintegral by

$$\int_{x_{j-1}}^{x_j} f(x)\,dx \approx f(\bar{x}_j)\Delta x$$

and the full integral by

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx \\ &\approx f(\bar{x}_1)\Delta x + f(\bar{x}_2)\Delta x + \cdots + f(\bar{x}_n)\Delta x\end{aligned}$$

In summary, the midpoint rule approximates

$$\int_a^b f(x)\,dx \approx \Big[f(\bar{x}_1) + f(\bar{x}_2) + \cdots + f(\bar{x}_n)\Big]\Delta x \tag{1}$$

where $\Delta x = \frac{b-a}{n}$ and

$$\begin{array}{llllll} x_0 = a & x_1 = a + \Delta x & x_2 = a + 2\Delta x & \cdots & x_{n-1} = b - \Delta x & x_n = b \\ & \bar{x}_1 = \frac{x_0+x_1}{2} & \bar{x}_2 = \frac{x_1+x_2}{2} & \cdots & \bar{x}_{n-1} = \frac{x_{n-2}+x_{n-1}}{2} & \bar{x}_n = \frac{x_{n-1}+x_n}{2} \end{array}$$

Example 1

Let's apply the midpoint rule with $n = 8$ steps to the integral $\int_0^\pi \sin x\,dx$. First note that $a = 0$, $b = \pi$, $\Delta x = \frac{\pi}{8}$ and

$$x_0 = 0 \qquad x_1 = \tfrac{\pi}{8} \qquad x_2 = \tfrac{2\pi}{8} \qquad \cdots \qquad x_7 = \tfrac{7\pi}{8} \qquad x_8 = \tfrac{8\pi}{8} = \pi$$

Consequently,

$$\bar{x}_1 = \tfrac{\pi}{16} \qquad \bar{x}_2 = \tfrac{3\pi}{16} \qquad \cdots \qquad \bar{x}_7 = \tfrac{13\pi}{16} \qquad \bar{x}_8 = \tfrac{15\pi}{16}$$

and

$$\begin{aligned}\int_0^\pi \sin x\,dx &\approx \Big[\sin(\bar{x}_1) + \sin(\bar{x}_2) + \cdots + \sin(\bar{x}_8)\Big]\Delta x \\ &= \Big[\sin(\tfrac{\pi}{16}) + \sin(\tfrac{3\pi}{16}) + \sin(\tfrac{5\pi}{16}) + \sin(\tfrac{7\pi}{16}) + \sin(\tfrac{9\pi}{16}) + \sin(\tfrac{11\pi}{16}) + \sin(\tfrac{13\pi}{16}) + \sin(\tfrac{15\pi}{16})\Big]\tfrac{\pi}{8} \\ &= \Big[0.1951 + 0.5556 + 0.8315 + 0.9808 + 0.9808 + 0.8315 + 0.5556 + 0.1951\Big] \times 0.3927 \\ &= 5.1260 \times 0.3927 \\ &= 2.013\end{aligned}$$

The exact answer is $\int_0^\pi \sin x\,dx = -\cos x\Big|_0^\pi = 2$. So with eight steps of the midpoint rule we achieved an absolute error of $|2.013 - 2| = 0.013$, a relative error of $\frac{|2.013-2|}{2} = 0.0065$ and a percentage error of $100\frac{2.013-2}{2} = 0.65\%$. The definitions of these various types of error are given in Definition 2, below.

Example 1

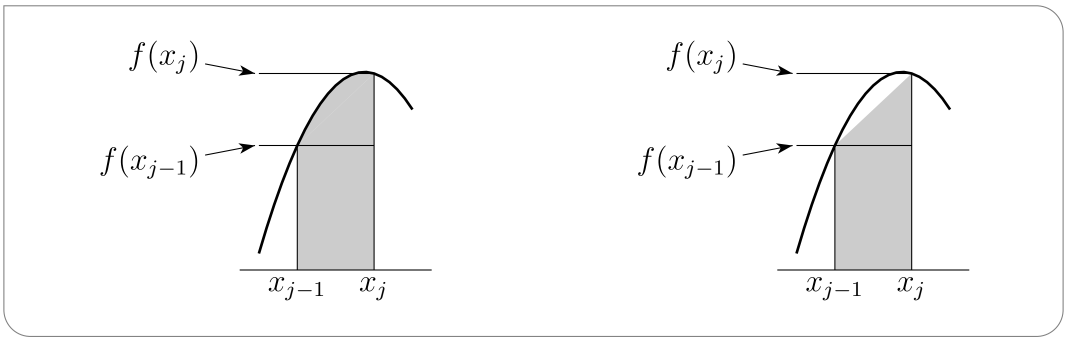
Definition 2.

Suppose that α is an approximation to A. This approximation has

- absolute error $|A-\alpha|$ and
- relative error $\frac{|A-\alpha|}{A}$ and
- percentage error $100\frac{|A-\alpha|}{A}$

The Trapezoidal Rule

The trapezoidal rule approximates $\int_{x_{j-1}}^{x_j} f(x)\,dx$ by the area of a trapezoid. A trapezoid is a four sided polygon, like a rectangle. But, unlike a rectangle, the top and bottom of a trapezoid need not be parallel. The trapezoid used to approximate $\int_{x_{j-1}}^{x_j} f(x)\,dx$ has width $x_j - x_{j-1} = \Delta x$. Its left hand side has height $f(x_{j-1})$ and its right hand side has height $f(x_j)$. The area of a trapezoid is its width times its average height. So the trapezoidal rule



approximates

$$\int_{x_{j-1}}^{x_j} f(x)\,dx \approx \tfrac{f(x_{j-1})+f(x_j)}{2}\Delta x$$

and the full integral by

$$\begin{aligned}\int_a^b f(x)\,dx &= \int_{x_0}^{x_1} f(x)\,dx \ + \int_{x_1}^{x_2} f(x)\,dx \ + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx \\ &\approx \tfrac{f(x_0)+f(x_1)}{2}\Delta x + \tfrac{f(x_1)+f(x_2)}{2}\Delta x \ + \cdots + \tfrac{f(x_{n-1})+f(x_n)}{2}\Delta x \\ &= \Big[\tfrac{1}{2}f(x_0) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \tfrac{1}{2}f(x_n)\Big]\Delta x\end{aligned}$$

In summary, the trapezoidal rule approximates

$$\int_a^b f(x)\,dx \approx \Big[\tfrac{1}{2}f(x_0) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \tfrac{1}{2}f(x_n)\Big]\Delta x \tag{2}$$

where

$$\Delta x = \tfrac{b-a}{n}, \quad x_0 = a, \quad x_1 = a + \Delta x, \quad x_2 = a + 2\Delta x, \quad \cdots, \quad x_{n-1} = b - \Delta x, \quad x_n = b$$

Example 3

As an example, we again approximate $\int_0^\pi \sin x\,dx$ but this time we use the trapezoidal rule with $n = 8$. We still have $a = 0$, $b = \pi$, $\Delta x = \frac{\pi}{8}$ and

$$x_0 = 0 \qquad x_1 = \tfrac{\pi}{8} \qquad x_2 = \tfrac{2\pi}{8} \qquad \cdots \qquad x_7 = \tfrac{7\pi}{8} \qquad x_8 = \tfrac{8\pi}{8} = \pi$$

Consequently,

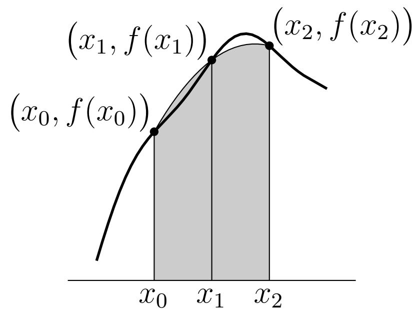
$$\begin{aligned}
&\int_0^\pi \sin x\,dx \approx \Big[\tfrac{1}{2}\sin(x_0) + \sin(x_1) + \cdots + \sin(x_7) + \tfrac{1}{2}\sin(x_8)\Big]\Delta x \\
&= \Big[\tfrac{1}{2}\sin 0 + \sin\tfrac{\pi}{8} + \sin\tfrac{2\pi}{8} + \sin\tfrac{3\pi}{8} + \sin\tfrac{4\pi}{8} + \sin\tfrac{5\pi}{8} + \sin\tfrac{6\pi}{8} + \sin\tfrac{7\pi}{8} + \tfrac{1}{2}\sin\tfrac{8\pi}{8}\Big]\tfrac{\pi}{8} \\
&= \Big[\tfrac{1}{2}\times 0 + 0.3827 + 0.7071 + 0.9239 + 1.0000 + 0.9239 + 0.7071 + 0.3827 + \tfrac{1}{2}\times 0\Big] \times 0.3927 \\
&= 5.0274 \times 0.3927 \\
&= 1.974
\end{aligned}$$

The exact answer is $\int_0^\pi \sin x\,dx = -\cos x\Big|_0^\pi = 2$. So with eight steps of the trapezoidal rule we achieved $100\frac{|1.974-2|}{2} = 1.3\%$ accuracy.

Example 3

Simpson's Rule

Simpson's rule approximates $\int_{x_0}^{x_2} f(x)\,dx$ by the area bounded by the x–axis, the parabola that passes through the three points $\big(x_0, f(x_0)\big)$, $\big(x_1, f(x_1)\big)$ and $\big(x_2, f(x_2)\big)$, the vertical line $x = x_0$ and the vertical line $x = x_2$. It then approximates $\int_{x_2}^{x_4} f(x)\,dx$ by the area between



the x–axis and the part of a parabola with $x_2 \le x \le x_4$. This parabola passes through the three points $\big(x_2, f(x_2)\big)$, $\big(x_3, f(x_3)\big)$ and $\big(x_4, f(x_4)\big)$. And so on. Because Simspon's rule does the approximation two slices at a time, *n must be even.*

To derive Simpson's rule formula, we first find the equation of the parabola that passes through the three points $\big(x_0, f(x_0)\big)$, $\big(x_1, f(x_1)\big)$ and $\big(x_2, f(x_2)\big)$. Then we find the area between the x–axis and the part of that parabola with $x_0 \le x \le x_2$. We can make the formulae look less complicated by writing the equation of the parabola in the form

$$y = A(x-x_1)^2 + B(x-x_1) + C$$

The three points $\big(x_0, f(x_0)\big)$, $\big(x_1, f(x_1)\big)$ and $\big(x_2, f(x_2)\big)$ lie on this parabola if and only if

$$\begin{aligned} A\big(x_0-x_1)^2 + B(x_0-x_1) + C &= f(x_0)\\ A\big(x_1-x_1)^2 + B(x_1-x_1) + C &= f(x_1)\\ A\big(x_2-x_1)^2 + B(x_2-x_1) + C &= f(x_2) \end{aligned}$$

Because $x_1 - x_1 = 0$, the middle equation simplifies to $C = f(x_1)$. Because $x_0 - x_1 = -\Delta x$, $x_2 - x_1 = \Delta x$ and $C = f(x_1)$, the first and third equations simplify to

$$\begin{aligned} (\Delta x)^2\, A - \Delta x\, B &= f(x_0) - f(x_1)\\ (\Delta x)^2\, A + \Delta x\, B &= f(x_2) - f(x_1) \end{aligned}$$

Adding the two equations together gives $2(\Delta x)^2\, A = f(x_0) - 2f(x_1) + f(x_2)$. Subtracting the first equation from the second gives $2\Delta x\, B = f(x_2) - f(x_0)$. We now know the desired parabola.

$$A = \tfrac{1}{2\Delta x^2}\big\{f(x_0) - 2f(x_1) + f(x_2)\big\} \qquad B = \tfrac{1}{2\Delta x}\big\{f(x_2) - f(x_0)\big\} \qquad C = f(x_1)$$

The area under the part of this parabola with $x_0 \le x \le x_2$ is

$$\begin{aligned} \int_{x_0}^{x_2} \Big[A(x-x_1)^2 + B(x-x_1) + C\Big]dx &= \int_{-\Delta x}^{\Delta x} \Big[At^2 + Bt + C\Big]dt \qquad \text{where } t = x - x_1\\ &= 2\int_0^{\Delta x} \Big[At^2 + C\Big]dt \qquad \text{since } Bt \text{ is odd and } At^2 + C \text{ is even}\\ &= 2\Big[\tfrac{1}{3}At^3 + Ct\Big]_0^{\Delta x}\\ &= \tfrac{2}{3}A(\Delta x)^3 + 2C\Delta x\\ &= \tfrac{1}{3}\Delta x\big[f(x_0) - 2f(x_1) + f(x_2)\big] + 2f(x_1)\Delta x\\ &= \tfrac{1}{3}\Delta x\big[f(x_0) + 4f(x_1) + f(x_2)\big] \end{aligned}$$

So Simpson's rule approximates

$$\int_{x_0}^{x_2} f(x)\,dx \approx \tfrac{1}{3}\Delta x\big[f(x_0) + 4f(x_1) + f(x_2)\big]$$

and

$$\int_{x_2}^{x_4} f(x)\,dx \approx \tfrac{1}{3}\Delta x\big[f(x_2) + 4f(x_3) + f(x_4)\big]$$

and so on. All together

$$\begin{aligned} \int_a^b f(x)\,dx &= \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \int_{x_4}^{x_6} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx\\ &\approx \tfrac{\Delta x}{3}\big[f(x_0) + 4f(x_1) + f(x_2)\big] + \tfrac{\Delta x}{3}\big[f(x_2) + 4f(x_3) + f(x_4)\big]\\ &\quad + \tfrac{\Delta x}{3}\big[f(x_4) + 4f(x_5) + f(x_6)\big] + \cdots + \tfrac{\Delta x}{3}\big[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\big]\\ &= \Big[f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + 2f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\Big]\tfrac{\Delta x}{3} \end{aligned}$$

In summary, Simpson's rule approximates

$$\int_a^b f(x)\,dx \approx \Big[f(x_0)+4f(x_1)+2f(x_2)+4f(x_3)+2f(x_4)+\cdots+2f(x_{n-2})+4f(x_{n-1})+f(x_n)\Big]\tfrac{\Delta x}{3} \tag{3}$$

where n is even and

$$\Delta x = \tfrac{b-a}{n},\quad x_0 = a,\quad x_1 = a+\Delta x,\quad x_2 = a+2\Delta x,\quad \cdots,\quad x_{n-1} = b-\Delta x,\quad x_n = b$$

Example 4

As an example we approximate $\int_0^\pi \sin x\,dx$ with $n = 8$, yet again. Under Simpson's rule

$$\begin{aligned}\int_0^\pi \sin x\,dx &\approx \Big[\sin(x_0)+4\sin(x_1)+2\sin(x_2)+\cdots+4\sin(x_7)+\sin(x_8)\Big]\tfrac{\Delta x}{3}\\ &= \Big[\sin(0)+4\sin(\tfrac{\pi}{8})+2\sin(\tfrac{2\pi}{8})+4\sin(\tfrac{3\pi}{8})+2\sin(\tfrac{4\pi}{8})\\ &\qquad +4\sin(\tfrac{5\pi}{8})+2\sin(\tfrac{6\pi}{8})+4\sin(\tfrac{7\pi}{8})+\sin(\tfrac{8\pi}{8})\Big]\tfrac{\pi}{8\times 3}\\ &= \Big[0+4\times 0.382683+2\times 0.707107+4\times 0.923880+2\times 1.0\\ &\qquad +4\times 0.923880+2\times 0.707107+4\times 0.382683+0\Big]\tfrac{\pi}{8\times 3}\\ &= 15.280932\times 0.130900\\ &= 2.00027\end{aligned}$$

With only eight steps of Simpson's rule we achieved $100\frac{2.00027-2}{2} = 0.014\%$ accuracy.

Example 4

This completes our derivation of the midpoint, trapezoidal and Simpson's rules for approximating the values of definite integrals. So far we have not attempted to see how efficient and how accurate the algorithms are. That's our next task.

Three Simple Numerical Integrators – Error Behaviour

Two obvious considerations in deciding whether or not a given algorithm is of any practical value are (a) the amount of computational effort required to execute the algorithm and (b) the accuracy that this computational effort yields. For algorithms like our simple integrators, the bulk of the computational effort usually goes into evaluating the function $f(x)$. The number of evaluations of $f(x)$ required for n steps of the midpoint rule is n, while the number required for n steps of the trapezoidal and Simpson's rules is $n+1$. So all three of our rules require essentially the same amount of effort – one evaluation of $f(x)$ per step.

To get a first impression of the error behaviour of these methods, we apply them to a problem that we know the answer to. The exact value of the integral $\int_0^\pi \sin x\,dx = -\cos x\big|_0^\pi$ is 2. The following table lists the error in the approximate value for this number generated by our three rules applied with three different choices of n. It also lists the number of evaluations of f required to compute the approximation.

	Midpoint		**Trapezoidal**		**Simpson's**	
n	error	# evals	error	# evals	error	# evals
10	4.1×10^{-1}	10	8.2×10^{-1}	11	5.5×10^{-3}	11
100	4.1×10^{-3}	100	8.2×10^{-3}	101	5.4×10^{-7}	101
1000	4.1×10^{-5}	1000	8.2×10^{-5}	1001	5.5×10^{-11}	1001

Observe that

- Using 101 evaluations of f worth of Simpson's rule gives an error 80 times smaller than 1000 evaluations of f worth of the midpoint rule.
- The trapezoidal rule error with n steps is about twice the midpoint rule error with n steps.
- With the midpoint rule, increasing the number of steps by a factor of 10 appears to reduce the error by about a factor of $100 = 10^2 = n^2$.
- With the trapezoidal rule, increasing the number of steps by a factor of 10 appears to reduce the error by about a factor of $10^2 = n^2$.
- With Simpson's rule, increasing the number of steps by a factor of 10 appears to reduce the error by about a factor of $10^4 = n^4$.

So it looks like

$$\begin{aligned}
\text{approx value of } \int_a^b f(x)\,dx \text{ given by } n \text{ midpoint steps } &\approx \int_a^b f(x)\,dx + K_M \tfrac{1}{n^2} \\
\text{approx value of } \int_a^b f(x)\,dx \text{ given by } n \text{ trapezoidal steps } &\approx \int_a^b f(x)\,dx + K_T \tfrac{1}{n^2} \\
\text{approx value of } \int_a^b f(x)\,dx \text{ given by } n \text{ Simpson's steps } &\approx \int_a^b f(x)\,dx + K_M \tfrac{1}{n^4}
\end{aligned}$$

with some constants K_M, K_T and K_S. It also looks like $K_T \approx 2K_M$.

To test these conjectures further, we apply our three rules with about ten different choices of n of the form $n = 2^m$ with m integer. On the next page are two figures, one containing the results for the midpoint and trapezoidal rules and the other the results for Simpson's rule. For each rule we are expecting the error e_n (that is, $|\text{exact value} - \text{approximate value}|$) with n steps to be (approximately) of the form

$$e_n = K \tfrac{1}{n^k}$$

for some constants K and k. We would like to test if this is really the case. It is not easy to tell whether or not a given curve really is a parabola $y = x^2$ or a quartic $y = x^4$. But the eye is pretty good at determining whether or not a graph is a straight line. Fortunately, there is a little trick that turns the curve $e_n = K \frac{1}{n^k}$ into a straight line – no matter what k is. Instead

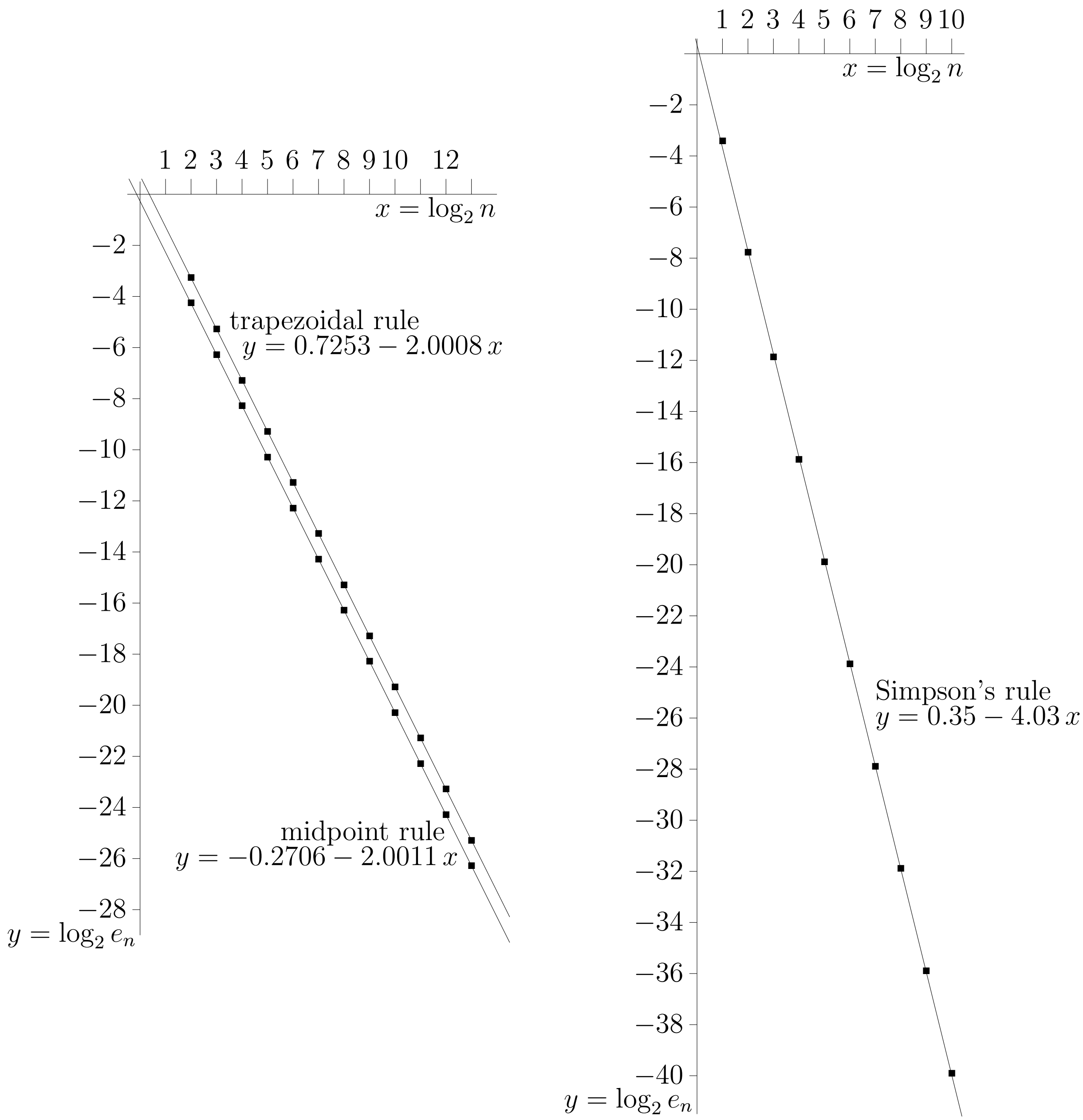


Figure 1: Error in the approximation, with n steps, to $\int_0^\pi \sin x\,dx$

of plotting e_n against n, plot $\log e_n$ against $\log n$. If $e_n = K\frac{1}{n^k}$, then $\log e_n = \log K - k \log n$. So plotting $y = \log e_n$ against $x = \log n$ gives the straight line $y = \log K - kx$, which has slope $-k$ and y–intercept $\log K$.[1]

The three graphs in Figure 1 plot $y = \log_2 e_n$ against $x = \log_2 n$ for our three rules. By definition, the base 2 logarithm, $\log_2 n$, is the power to which 2 must be raised to give n.

[1] There is a variant of this trick that works even when you don't know the answer to the integral ahead of time. Suppose that you suspect that the approximation $M_n = A + K\frac{1}{n^k}$, where A is the exact value of the integral and suppose that you don't know the values of A, K and k. Then $M_n - M_{2n} = K\frac{1}{n^k} - K\frac{1}{(2n)^k} = K\big(1-\frac{1}{2^k}\big)\frac{1}{n^k}$, so plotting $y = \log(M_n - M_{2n})$ against $x = \log n$ gives the straight line $y = \log\big[K\big(1-\frac{1}{2^k}\big)\big] - kx$.

In particular, when $n = 2^m$, $\log_2 n = \log_2 2^m = m$ is nice and simple. That's why we are using the base two logarithm. For example, applying Simpson's rule with $n = 2^5 = 32$ gives the approximate value 2.00000103, which has error $e_n = 0.00000103$. So, the data point $(x = \log_2 2^5 = 5\ ,\ y = \log_2 0.00000103 = \frac{\ln 0.00000103}{\ln 2} = -19.9)$ has been included on the Simpson's rule graph. For each of the three sets of data points, a straight line has also been plotted "through" the data points. A procedure called "linear regression" has been used to decide precisely which straight line to plot. Linear regression is not part of this course. It provides a formula for the slope and y–intercept of the straight line which "best fits" any given set of data points. From the three lines, it sure looks like $k = 2$ for the midpoint and trapezoidal rules and $k = 4$ for Simpson's rule. It also looks like the ratio between the value of K for the trapezoidal rule, namely $K = 2^{0.7253}$, and the value of K for the midpoint rule, namely $K = 2^{-0.2706}$, is pretty close to 2: $2^{0.7253}/2^{-0.2706} = 2^{0.9959}$.

The intuition, about the error behaviour, that we have just developed is in fact correct — provided the integrand $f(x)$ is reasonably smooth. Precisely, if $|f''(x)| \le M$ for all x in the domain of integration, then it turns out that

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

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

and 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 $\frac{M}{180}\frac{(b-a)^5}{n^4}$

Example 5

The integral $\int_0^\pi \sin x\,dx$ has $b - a = \pi$ and M, the largest possible value of $\left|\frac{d^2}{dx^2}\sin x\right|$ (for the midpoint and trapezoidal rules) or $\left|\frac{d^4}{dx^4}\sin x\right|$ (for Simpson's rule) is 1. So, for the midpoint rule, the error, e_n, introduced when n steps are used is bounded by

$$|e_n| \le \frac{M}{24}\frac{(b-a)^3}{n^2} = \frac{\pi^3}{24}\frac{1}{n^2} \approx 1.29\frac{1}{n^2}$$

The data in the graph in Figure 1 gives $|e_n| \approx 2^{-.2706}\frac{1}{n^2} = 0.83\frac{1}{n^2}$ which is consistent with the bound $|e_n| \le \frac{\pi^3}{24}\frac{1}{n^2}$.

Example 5

Example 6

In a typical application, one is required to evaluate a given integral to some specified accuracy. For example, if you are manufacturer and your machinery can only cut materials to an accuracy of $\frac{1}{10}^{\text{th}}$ of a millimeter, there is no point in making design specifications more accurate than $\frac{1}{10}^{\text{th}}$ of a millimeter. 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 algebraically, 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, $2x^2-1$ increases from -1 to 1, so that

$$0 \le x \le 1 \implies |2x^2-1| \le 1,\ e^{-x^2} \le 1 \implies \left|2(2x^2-1)e^{-x^2}\right| \le 2$$

So 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 6

Example 7

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 first determine how big $\frac{d^4}{dx^4}e^{-x^2}$ can get when $0 \le x \le 1$.

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

On the domain of integration $0 \le x \le 1$ so that $e^{-x^2} \le 1$. Also, for $0 \le x \le 1$,

$$3 \le 4x^4+3 \le 7 \text{ and } -12 \le -12x^2 \le 0 \quad\implies\quad -9 \le 4x^4-12x^2+3 \le 7$$

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

$$\left|4x^4-12x^2+3\right| \le 9 \implies \left|\tfrac{d^4}{dx^4}e^{-x^2}\right| \le 4 \times 9 \times 1 = 36$$

The error introduced by the n step Simpson's rule is at most $\frac{M}{180}\frac{(b-a)^5}{n^4} \le \frac{36}{180}\frac{(1-0)^5}{n^4} = \frac{1}{5n^4}$. This error is at most 10^{-6} if

$$\tfrac{1}{5n^4} \le 10^{-6} \iff n^4 \ge \tfrac{1}{5} \times 10^6 \iff n \ge \sqrt[4]{\tfrac{1}{5} \times 10^6} = 21.1$$

So 22 steps of Simpson's rule will do the job.

Example 7