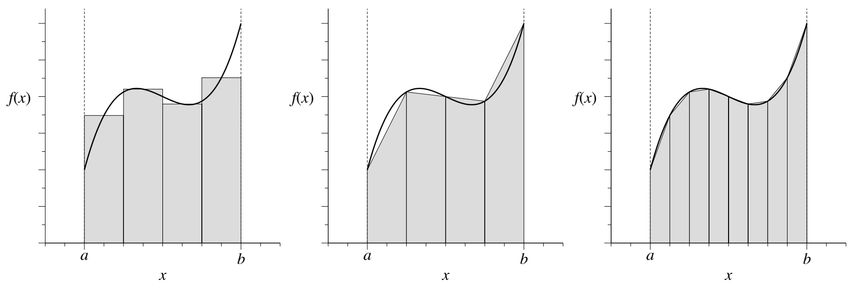
INTEGRALS



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Trapezoid rule

$$I(a,b) = \int_a^b f(x)\,\mathrm{d}x.$$

Suppose we divide the interval from a to b into N slices or steps, so that each slice has width $h = (b-a)/N$. Then the right-hand side of the kth slice falls at $a + kh$, and the left-hand side falls at $a + kh - h = a + (k-1)h$. Thus the area of the trapezoid for this slice is

$$A_k = \tfrac{1}{2}h\big[f(a+(k-1)h) + f(a+kh)\big].$$

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Trapezoid rule

$$
\begin{aligned}
I(a,b) \simeq \sum_{k=1}^{N} A_k &= \tfrac{1}{2}h \sum_{k=1}^{N} \big[f(a+(k-1)h) + f(a+kh) \big] \\
&= h\big[\tfrac{1}{2}f(a) + f(a+h) + f(a+2h) + \ldots + \tfrac{1}{2}f(b)\big] \\
&= h\left[\tfrac{1}{2}f(a) + \tfrac{1}{2}f(b) + \sum_{k=1}^{N-1} f(a+kh)\right].
\end{aligned}
$$

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```
def f(x):
    return x**4 - 2*x + 1

N = 10
a = 0.0
b = 2.0
h = (b-a)/N

s = 0.5*f(a) + 0.5*f(b)
for k in range(1,N):
    s += f(a+k*h)

print(h*s)
```

If we run the program it prints

```
4.50656
```

The correct answer is

$$\int_0^2 (x^4 - 2x + 1)\,\mathrm{d}x = \left[\tfrac{1}{5}x^5 - x^2 + x\right]_0^2 = 4.4.$$

2% error

5

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$N = 100$ and run the program again we get 4.40107,

0.02% error

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$N = 100$ and run the program again we get 4.40107,

$N = 1000$ we get 4.40001,

0.0002% error

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The trapezoidal rule is the simplest of numerical integration methods, taking only a few lines of code as we have seen, but it is often perfectly adequate for calculations where no great accuracy is required. It happens frequently in physics calculations that we don't need an answer accurate to many significant figures and in such cases the ease and simplicity of the trapezoidal rule can make it the method of choice. One should not turn up one's nose at simple methods like this; they play an important role and are used widely. Moreover, the trapezoidal rule is the basis for several other more sophisticated methods of evaluating integrals, including the adaptive methods

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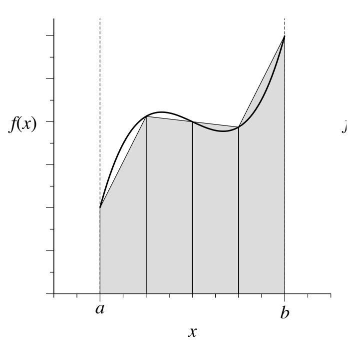
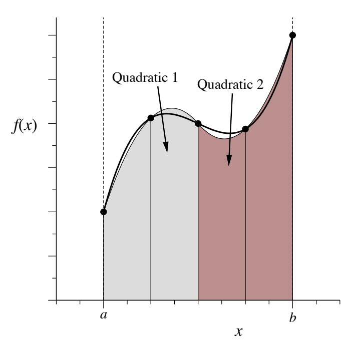
Simpson's rule





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Simpson's Rule

Suppose, as before, that our integrand is denoted $f(x)$ and the spacing of adjacent points is h. And suppose for the purposes of argument that we have three points at $x = -h$, 0, and $+h$. If we fit a quadratic $Ax^2 + Bx + C$ through these points, then by definition we will have:

$$f(-h) = Ah^2 - Bh + C, \qquad f(0) = C, \qquad f(h) = Ah^2 + Bh + C.$$

Solving these equations simultaneously for A, B, and C gives

$$A = \frac{1}{h^2}\left[\tfrac{1}{2}f(-h) - f(0) + \tfrac{1}{2}f(h)\right], \quad B = \frac{1}{2h}\left[f(h) - f(-h)\right], \quad C = f(0),$$

and the area under the curve of $f(x)$ from $-h$ to $+h$ is given approximately by the area under the quadratic:

$$\int_{-h}^{h} (Ax^2 + Bx + C)\,\mathrm{d}x = \tfrac{2}{3}Ah^3 + 2Ch = \tfrac{1}{3}h\left[f(-h) + 4f(0) + f(h)\right].$$

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Simpson's Rule

$$\int_{-h}^{h} (Ax^2 + Bx + C)\,\mathrm{d}x = \tfrac{2}{3}Ah^3 + 2Ch = \tfrac{1}{3}h\left[f(-h) + 4f(0) + f(h)\right].$$

Works for any three uniformly spaced point.

So like trapezoidal rule: divide domain into many slices and sum.

For x = a to x = b:

x = a, a+h, a+2h next a+2h, a+3h, a+4h …

$$\begin{aligned} I(a,b) \simeq\ & \tfrac{1}{3}h\left[f(a) + 4f(a+h) + f(a+2h)\right] \\ & + \tfrac{1}{3}h\left[f(a+2h) + 4f(a+3h) + f(a+4h)\right] + \ldots \\ & + \tfrac{1}{3}h\left[f(a+(N-2)h) + 4f(a+(N-1)h) + f(b)\right]. \end{aligned}$$

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Simpson's Rule

Note that the total number of slices must be even for this to work. Collecting terms together, we now have

$$\begin{aligned} I(a,b) &\simeq \tfrac{1}{3}h\big[f(a) + 4f(a+h) + 2f(a+2h) + 4f(a+3h) + \ldots + f(b)\big] \\ &= \tfrac{1}{3}h\Bigg[f(a) + f(b) + 4\sum_{\substack{k \text{ odd} \\ 1\ldots N-1}} f(a+kh) + 2\sum_{\substack{k \text{ even} \\ 2\ldots N-2}} f(a+kh)\Bigg]. \end{aligned}$$

The sums over odd and even values of k can be conveniently accomplished in Python using a for loop of the form "`for k in range(1,N,2)`" for the odd terms or "`for k in range(2,N,2)`" for the even terms.

Or:

$$I(a,b) \simeq \tfrac{1}{3}h\left[f(a) + f(b) + 4\sum_{k=1}^{N/2} f(a+(2k-1)h) + 2\sum_{k=1}^{N/2-1} f(a+2kh)\right],$$

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Simpson's Rule

As an example, suppose we apply Simpson's rule with $N = 10$ slices to

$$\int_0^2 (x^4 - 2x + 1)\,\mathrm{d}x = \left[\tfrac{1}{5}x^5 - x^2 + x\right]_0^2 = 4.4.$$

We get 4.400427, which is already accurate to 0.01%, much better that trapezoidal rule

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Errors on Integrals

Consider again an integral $\int_a^b f(x)\,\mathrm{d}x$, and let us first look at the trapezoidal rule of Eq. (5.3). To simplify our notation a little, let us define $x_k = a + kh$ as a shorthand for the positions at which we evaluate the integrand $f(x)$. We will refer to these positions as *sample points*. Now consider one particular slice of the integral, the one that falls between x_{k-1} and x_k, and let us perform a Taylor expansion of $f(x)$ about x_{k-1} thus:

$$f(x) = f(x_{k-1}) + (x - x_{k-1})f'(x_{k-1}) + \tfrac{1}{2}(x - x_{k-1})^2 f''(x_{k-1}) + \ldots$$

$$\int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x = f(x_{k-1})\int_{x_{k-1}}^{x_k} \mathrm{d}x + f'(x_{k-1})\int_{x_{k-1}}^{x_k} (x - x_{k-1})\,\mathrm{d}x + \tfrac{1}{2}f''(x_{k-1})\int_{x_{k-1}}^{x_k} (x - x_{k-1})^2\,\mathrm{d}x + \ldots$$

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Now we make the substitution $u = x - x_{k-1}$, which gives

$$\begin{aligned}\int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x &= f(x_{k-1})\int_0^h \mathrm{d}u + f'(x_{k-1})\int_0^h u\,\mathrm{d}u + \tfrac{1}{2}f''(x_{k-1})\int_0^h u^2\,\mathrm{d}u + \ldots \\ &= hf(x_{k-1}) + \tfrac{1}{2}h^2 f'(x_{k-1}) + \tfrac{1}{6}h^3 f''(x_{k-1}) + \mathrm{O}(h^4),\end{aligned}$$

where $\mathrm{O}(h^4)$ denotes the rest of the terms in the series, those in h^4 and higher, which we are neglecting.

We can do a similar expansion around $x = x_k$ and again integrate from x_{k-1} to x_k to get

$$\int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x = hf(x_k) - \tfrac{1}{2}h^2 f'(x_k) + \tfrac{1}{6}h^3 f''(x_k) - \mathrm{O}(h^4).$$

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$$\int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x = \tfrac{1}{2}h[f(x_{k-1})+f(x_k)] + \tfrac{1}{4}h^2[f'(x_{k-1})-f'(x_k)] + \tfrac{1}{12}h^3[f''(x_{k-1})+f''(x_k)] + \mathrm{O}(h^4).$$

Finally, we sum this expression over all slices k to get the full integral that we want:

$$\begin{aligned}\int_a^b f(x)\,\mathrm{d}x &= \sum_{k=1}^{N}\int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x \\ &= \tfrac{1}{2}h\sum_{k=1}^{N}[f(x_{k-1})+f(x_k)] + \tfrac{1}{4}h^2[f'(a)-f'(b)] \\ &\quad + \tfrac{1}{12}h^3\sum_{k=1}^{N}[f''(x_{k-1})+f''(x_k)] + \mathrm{O}(h^4).\end{aligned}$$

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$$\begin{aligned}\int_a^b f(x)\,\mathrm{d}x &= \sum_{k=1}^{N}\int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x \\ &= \boxed{\tfrac{1}{2}h\sum_{k=1}^{N}[f(x_{k-1})+f(x_k)]} + \tfrac{1}{4}h^2[f'(a)-f'(b)] \\ &\quad + \tfrac{1}{12}h^3\sum_{k=1}^{N}[f''(x_{k-1})+f''(x_k)] + \mathrm{O}(h^4). \qquad (5.16)\end{aligned}$$

Trapezoid Rule

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$$\int_a^b f(x)\,\mathrm{d}x = \sum_{k=1}^{N} \int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x$$
$$= \boxed{\tfrac{1}{2}h \sum_{k=1}^{N} [f(x_{k-1}) + f(x_k)]} + \tfrac{1}{4}h^2[f'(a) - f'(b)]$$
$$+ \tfrac{1}{12}h^3 \sum_{k=1}^{N} [f''(x_{k-1}) + f''(x_k)] + \mathrm{O}(h^4). \qquad (5.16)$$

Just the Trapezoid Rule

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$$\int_a^b f(x)\,\mathrm{d}x = \sum_{k=1}^{N} \int_{x_{k-1}}^{x_k} f(x)\,\mathrm{d}x$$
$$= \tfrac{1}{2}h \sum_{k=1}^{N} [f(x_{k-1}) + f(x_k)] + \tfrac{1}{4}h^2[f'(a) - f'(b)]$$
$$\boxed{+ \tfrac{1}{12}h^3 \sum_{k=1}^{N} [f''(x_{k-1}) + f''(x_k)] + \mathrm{O}(h^4).} \qquad (5.16)$$

Trapezoid Rule of the f''(x) integral

make the substitution $f(x) \to f''(x)$

$$\int_a^b f''(x)\,\mathrm{d}x = \tfrac{1}{2}h \sum_{k=1}^{N} [f''(x_{k-1}) + f''(x_k)] + \mathrm{O}(h^2).$$

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Multiplying by $\frac{1}{6}h^2$ and rearranging, we then get

$$\begin{aligned}\tfrac{1}{12}h^3 \sum_{k=1}^{N}[f''(x_{k-1}) + f''(x_k)] &= \tfrac{1}{6}h^2 \int_a^b f''(x)\,\mathrm{d}x + \mathrm{O}(h^4) \\ &= \tfrac{1}{6}h^2[f'(b) - f'(a)] + \mathrm{O}(h^4),\end{aligned}$$

since the integral of $f''(x)$ is just $f'(x)$.

$$\int_a^b f(x)\,\mathrm{d}x = \tfrac{1}{2}h \sum_{k=1}^{N}[f(x_{k-1}) + f(x_k)] + \tfrac{1}{12}h^2[f'(a) - f'(b)] + \mathrm{O}(h^4).$$

So resulting error is just:

$$\boxed{\epsilon = \tfrac{1}{12}h^2\big[f'(a) - f'(b)\big].}$$

This is the *Euler–Maclaurin formula*

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the trapezoidal rule is a *first-order* integration

accurate to $\mathrm{O}(h)$ and has an *error* $\mathrm{O}(h^2)$.

In addition to approximation error, there is also a rounding error

C is about 10^{-16} in current versions of Python.

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Thus decreases in h will only help us up to the point at which the approximation and rounding errors are roughly equal, which is the point where

$$\tfrac{1}{12}h^2\left[f'(a) - f'(b)\right] \simeq C\int_a^b f(x)\,\mathrm{d}x.$$

Rearranging for h we get

$$h \simeq \sqrt{\frac{12\int_a^b f(x)\,\mathrm{d}x}{f'(a) - f'(b)}}\,C^{1/2}.$$

Or we can set $h = (b-a)/N$ to get

$$N \simeq (b-a)\sqrt{\frac{f'(a) - f'(b)}{12\int_a^b f(x)\,\mathrm{d}x}}\,C^{-1/2}.$$

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We can do an analogous error analysis for Simpson's rule. The algebra is similar but more tedious. Here we'll just quote the results. For an integral over the interval from a to b the approximation error is given to leading order by

$$\epsilon = \tfrac{1}{90}h^4\left[f'''(a) - f'''(b)\right]. \tag{5.24}$$

Thus Simpson's rule is a third-order integration rule.

$$N = (b-a)\sqrt[4]{\frac{f'''(a) - f'''(b)}{90\int_a^b f(x)\,\mathrm{d}x}}\,C^{-1/4}.$$

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