Computational Physics and Astrophysics

Numerical Intergration

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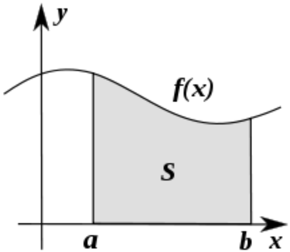
Numerical Integration

GOAL: To estimate the numerical value of the definite integral

$$I \equiv \int_a^b f(x)\,dx$$

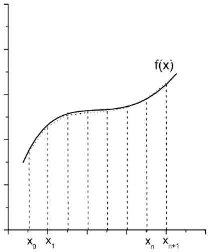


- Subdivide the range of integration $[a, b]$ into n equal subintervals $[x_{i+1}, x_i]_{i=0,\ldots,n-1}$ such that $h = (b-a)/n$ and $x_i = x_0 + i\,h$ with $x_0 = a$ and $x_n = b$.
- The integral of interest can then be rewritten as

$$I = \int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)dx = \sum_{i=0}^{n-1} I_i$$

such that

$$I_i = \int_{x_i}^{x_{i+1}} f(x)dx$$



One can also rearrange the integration to be

$$I = \int_a^b f(x)\, dx = \sum_{i=0}^{n/m-1} \int_{x_{mi}}^{x_{m(i+1)}} f(x) dx = \sum_{i=0}^{n/m-1} I_{i,m}$$

where

$$I_{i,m} = \int_{x_{mi}}^{x_{m(i+1)}} f(x) dx$$

- Our goal now is to find an approximation for $I_{i,m}$

$$I_{i,m} = \int_{x_{mi}}^{x_{m(i+1)}} f(x)dx$$

- Since the interval of integration $[x_{mi}, x_{m(i+1)}]$ contains m points, the first step is to construct a Lagrange interpolating polynomial of degree $P_m(x)$ to approximate the integrand $f(x)$.
- That is,

$$\int_{x_{mi}}^{x_{m(i+1)}} f(x)dx \approx \int_{x_{mi}}^{x_{m(i+1)}} P_m(x)dx = \int_{x_{mi}}^{x_{m(i+1)}} \sum_{j=0}^{m} f_j \, L_j(x)\, dx$$

$$= \sum_{j=0}^{m} f_j \int_{x_{mi}}^{x_{m(i+1)}} L_j(x)\, dx$$

where

$$L_j(x) = \frac{(x-x_0)(x-x_1)...(x-x_{j-1})(x-x_{j+1})...(x-x_m)}{(x_j-x_0)(x_j-x_1)...(x_j-x_{j-1})(x_j-x_{j+1})...(x_j-x_m)}$$

Trapezoidal Rule

Consider the case when $m = 1$ and for simplicity only focus on the first interval ($i = 0$). That is,

$$P_1(x) = f_0\,L_0 + f_1\,L_1$$

where

$$L_0 = \frac{x - x_1}{x_0 - x_1} \quad \text{and} \quad L_1 = \frac{x - x_0}{x_1 - x_0}$$

thus

$$\begin{aligned} P_1(x) &= \frac{x - x_1}{x_0 - x_1}\,f_0 + \frac{x - x_0}{x_1 - x_0}\,f_1 \\ &= \frac{x - x_0 - h}{-h}\,f_0 + \frac{x - x_0}{h}\,f_1 \\ &= \frac{x}{h}(f_1 - f_0) + \left(f_0 + \frac{x_0}{h}\,f_0 - \frac{x_0}{h}\,f_1\right) \end{aligned}$$

Trapezoidal Rule

$$
\begin{aligned}
\int_{x_0}^{x_1} f(x)\,dx &= \int_{x_0}^{x_1} P_1(x)\,dx \\
&= \int_{x_0}^{x_1} \left[\frac{x}{h}(f_1 - f_0) + \left(f_0 + \frac{x_0}{h}\,f_0 - \frac{x_0}{h}\,f_1\right)\right]\,dx \\
&= \frac{\left[x^2\right]_{x_0}^{x_1}}{2\,h}(f_1 - f_0) + \left(f_0 + \frac{x_0}{h}\,f_0 - \frac{x_0}{h}\,f_1\right)[x]_{x_0}^{x_1} \\
&= \frac{x_1^2 - x_0^2}{2\,h}(f_1 - f_0) + \left(f_0 + \frac{x_0}{h}\,f_0 - \frac{x_0}{h}\,f_1\right)\,h \\
&= \frac{x_1 + x_0}{2}(f_1 - f_0) + h\,f_0 + x_0\,f_0 - x_0\,f_1 \\
&= \frac{x_0 + h + x_0}{2}(f_1 - f_0) + h\,f_0 + x_0\,(f_0 - f_1) \\
&= \frac{1}{2}(f_1 + f_0)
\end{aligned}
$$

Trapezoidal Rule

Therefore

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_1 + f_0)$$

The error introduced is found from

$$E_1(x) = f(x) - P_1(x) = (x - x_0)(x - x_1)\frac{f^{(2)}(\xi)}{2!}$$

with $x_0 \leq \xi \leq x_1$. Which can be rewritten, with the help of $x = x_0 + s\,h$, as

$$E_1(s) = \frac{1}{2}s\,(s-1)\,h^2\,f^{(2)}(\xi)$$

Thus

$$\begin{aligned}\mathcal{E}_1 &= \int_{x_0}^{x_1} E_1(x)\,dx = h\int_0^1 E_1(s)\,ds = h\int_0^1 \frac{1}{2}s(s-1)h^2 f''(\xi)ds \\ &= h^3 f''(\xi)\left(\frac{s^3}{6} - \frac{s^2}{4}\right)_0^1 = -\frac{1}{12}h^3 f''(\xi)\end{aligned}$$

Newton – Cotes Formulae

Following a similar procedure, but with 3 and 4 points, one gets

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{1}{12}h^3 f^{(2)}(\xi)$$

Trapezoidal rule

$$\int_{x_0}^{x_2} f(x)dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{1}{90}h^5 f^{(4)}(\xi)$$

Simpson's rule

$$\int_{x_0}^{x_3} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3}{80}h^5 f^{(4)}(\xi)$$

Simpson's 3/8 rule

Trapezoidal rule

$$\int_{a=x_0}^{b=x_n} f(x)dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} P_1(x)dx = \sum_{i=0}^{n-1} \frac{h}{2}\left(f_i + f_{i+1}\right)$$

$$= \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + 2f_3 + \ldots + 2f_{n-2} + 2f_{n-1} + f_n\right)$$

$$= h\left(\frac{f_0}{2} + \sum_{i=1}^{n-1} f_i + \frac{f_n}{2}\right)$$

Integration Global Error:

$$\mathcal{E} = -\frac{b-a}{12} h^2 f^{(2)}(\xi) \quad \text{for} \quad x_0 \le \xi \le x_n$$

Simpson's 1/3 rule

$$\int_{a=x_0}^{b=x_n} f(x)dx = \sum_{i=0}^{n/2} \int_{x_{2i}}^{x_{2(i+1)}} P_2(x)dx = \sum_{i=0}^{n/2-1} \frac{h}{3}\left(f_{2i} + 4f_{2i+1} + f_{2i+2}\right)$$

$$= \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + \ldots + 2f_{n-2} + 4f_{n-1} + f_n\right)$$

Integration Global Error:

$$\mathcal{E} = -\frac{b-a}{180} h^4 f^{(4)}(\xi) \quad \text{for} \quad x_0 \leq \xi \leq x_n$$

Simpson's 3/8 rules

$$\int_{a=x_0}^{b=x_n} f(x)dx = \sum_{i=0}^{n/3} \int_{x_{3i}}^{x_{3(i+1)}} P_2(x)dx = \sum_{i=0}^{n/3-1} \frac{3\,h}{8} \left(f_{3i} + 3f_{3i+1} + 3f_{3i+2} + f_3\right.$$

$$= \frac{3h}{8} \left(f_0 + 3f_1 + 3f_2 + 2f_3 + ... + 2f_{n-3} + 3f_{n-2} + 3f_{n-1} + f_n\right)$$

Integration Global Error:

$$\mathcal{E} = -\frac{b-a}{80} h^4 f^{(4)}(\xi) \quad \text{for} \quad x_0 \le \xi \le x_n$$

Summary of Formulas for integration

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}\left(f_0 + 2f_1 + 2f_2 + \ldots + 2f_{n-1} + f_n\right)$$
$$- \frac{b-a}{12} h^2 f^{(2)}(\xi)$$

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + \ldots. + 2f_{n-2} + 4f_n + f_{n+1}\right)$$
$$- \frac{b-a}{180} h^4 f^{(4)}(\xi)$$ requires an even number of subintervals

$$\int_{x_0}^{x_n} f(x)dx = \frac{3h}{8}\left(f_0 + 3f_1 + 3f_2 + 2f_3 + 3f_4 + 3f_5 + \ldots. + 3f_{n-2} + 3f_{n-1} + f_n\right)$$
$$- \frac{b-a}{80} h^4 f^{(4)}(\xi)$$ requires a number of subintervals divisible by 3

Romberg integration

- Recall that the errors in numerical integration have the form $\mathcal{E} = c\,h^n$ with c a constant that depends on the derivatives of the integrand.
- Therefore, if $A \equiv \int_a^b f(x)dx$ denotes the exact value of the integral and I its numerical approximation, then $A = I + \mathcal{E}$
- Consider two evaluations of the integral A with errors such that $n = 2$. One evaluation has step h and the other a step $k\,h$. Thus,

$$
\begin{aligned}
A &= I_1 + c\,h^2 \quad \text{for step } h \\
A &= I_k + c\,(k\,h)^2 \quad \text{for step } k\,h
\end{aligned}
$$

- The solution to these equations is

$$A = \frac{k^2 I_1 - I_k}{k^2 - 1} \quad \text{and} \quad c = \frac{I_1 - I_k}{h^2(k^2 - 1)}$$

- For the general case in which the error is $O(h^n)$

$$A = \frac{k^n I_1 - I_k}{k^n - 1} \quad \text{and} \quad c = \frac{I_1 - I_k}{h^n(k^n - 1)}$$

Romberg integration

- Consider the case of the trapezoidal rule with a step h. That is

$$
\begin{aligned}
I_1 &= \sum_{i=0}^{n-1} \frac{h}{2} (f_i + f_{i+1}) \\
\mathcal{E}_1 &= -\frac{b-a}{12} h^2 f^{(2)}(\xi) = c\, h^2
\end{aligned}
$$

- And with a step $2\,h$.

$$
\begin{aligned}
I_2 &= \sum_{i=0}^{n/2-1} h\,(f_{2i} + f_{2i+2}) \\
\mathcal{E}_2 &= -\frac{b-a}{12} (2\,h)^2 f^{(2)}(\xi) = c\,(2\,h)^2
\end{aligned}
$$

Then

$$
\begin{aligned}
A &= \frac{2^2 I_1 - I_2}{2^2 - 1} = \frac{1}{3}(4\,I_1 - I_2) \\
&= \frac{1}{3}\left[4\sum_{i=0}^{n-1}\frac{h}{2}\left(f_i + f_{i+1}\right) - \sum_{i=0}^{n/2-1} h\left(f_{2i} + f_{2i+2}\right)\right] \\
&= \frac{h}{3}\left[\sum_{i=0}^{n-1} 2\left(f_i + f_{i+1}\right) - \sum_{i=0}^{n/2-1}\left(f_{2i} + f_{2i+2}\right)\right] \\
&= \frac{h}{3}\left[\sum_{i=0}^{n/2-1} 2\left(f_{2i} + 2f_{2i+1} + f_{2i+2}\right) - \sum_{i=0}^{n/2-1}\left(f_{2i} + f_{2i+2}\right)\right] \\
&= \frac{h}{3}\sum_{i=0}^{n/2-1}\left(f_{2i} + 4f_{2i+1} + f_{2i+2}\right)
\end{aligned}
$$

We get the Simpson's 1/3 rule! Recall this rule has errors $\mathcal{O}(h^4)$. Therefore, there is not a free lunch. We just have eliminated the Trapezoidal error $\mathcal{O}(h^2)$ in favor of the Simpson error $\mathcal{O}(h^4)$.

Splines and integration

For every interval $[x_i, x_{i+1}]$, approximate the integrand by a cubic spline. That is

$$\int_{x_0}^{x_n} f(x)dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} \left[a_i(x-x_i)^3 + b_i(x-x_i)^2 + c_i(x-x_i) + d_i\right] dx$$

$$= \sum_{i=0}^{n-1} \left[\frac{a_i}{4}(x-x_i)^4 + \frac{b_i}{3}(x-x_i)^3 + \frac{c_i}{2}(x-x_i)^2 + d_i(x-x_i)\right]_{x_i}^{x_{i+1}}$$

$$= \sum_{i=0}^{n-1} \left[\frac{a_i}{4}(x_{i+1}-x_i)^4 + \frac{b_i}{3}(x_{i+1}-x_i)^3 + \frac{c_i}{2}(x_{i+1}-x_i)^2 + d_i(x_{i+1}-x_i)\right]$$

$$= \frac{h^4}{4}\sum_{i=0}^{n-1} a_i + \frac{h^3}{3}\sum_{i=0}^{n-1} b_i + \frac{h^2}{2}\sum_{i=0}^{n-1} c_i + h\sum_{i=0}^{n-1} d_i$$