Simpson's formula for unequally-spaced grid

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1 3-point formula

We first derive 3-point formula of simpson [1]. By an appropriate shift of independent variable (say x here), we can always set the midpoint of the three to be $x = 0$. Let's assume other 2 to be $x = -\eta$ and $x = \xi$ (η and ξ are assumed to be positive). Denote $f(0) = f_0$, $f(-\eta) = f_{-\eta}$ and $f(\xi) = f_\xi$. A function $f(x)$ is approximated to be a parabora in $x[-\eta, \xi]$ as

$$f(x) = ax(x+b) + f_0 + \mathcal{O}[x^3]. \tag{1}$$

Here a and b are coefficients to be determined by the condition that $(-\eta, f_{-\eta})$ and (ξ, f_ξ) are on the parabora

$$\begin{aligned} f_{-\eta} &= -a\eta(-\eta+b) + f_0 && (2) \\ f_\xi &= a\xi(\xi+b) + f_0. && (3) \end{aligned}$$

These equation for a, b are solved as

$$\begin{aligned} a &= \frac{f_{-\eta}}{\eta(\eta+\xi)} - \frac{f_0}{\eta\xi} + \frac{f_\xi}{\xi(\xi+\eta)} && (4) \\ ab &= \frac{f_\xi - f_0}{\xi} - \xi\left(\frac{f_{-\eta}}{\eta(\eta+\xi)} - \frac{f_0}{\eta\xi} + \frac{f_\xi}{\xi(\xi+\eta)}\right). && (5) \end{aligned}$$

Then the integration S of $f(x)$ in $[-\eta, \xi]$ is approximated as

$$\begin{aligned} S &:= \int_{-\eta}^{\xi} \left[ax(x+b) + f_0 + \mathcal{O}(x^3)\right] && (6) \\ &= (\xi+\eta)\left[f_0 + \frac{ab}{2}(\xi-\eta) + \frac{a}{3}(\xi^2 - \xi\eta + \eta^2)\right] + \mathcal{O}(\max(\xi^4, \eta^4)) && (7) \\ &= \frac{\xi+\eta}{6}\left[\left(2 - \frac{\xi}{\eta}\right) f_{-\eta} + \frac{(\xi+\eta)^2}{\eta\xi} f_0 + (2 - \frac{\eta}{\xi}) f_\xi\right] + \mathcal{O}(\max(\xi^4, \eta^4)) && (8) \\ & && (9) \end{aligned}$$

2 Integration formula

Once we get the 3-point formula, the formula for general domain is straightforward to obtain.

Suppose we want to compute integration of function $f(x)$ from $x = a$ to $x = b$. Assume we are given $n+1$ unequally-spaced grid points x_j, where $x_0 = a$ and $x_n = b$.

Then using Eq.(9), we obtain approximation formula of $S = \int_a^b f(x)dx)$ as

$$S = \sum_{j=1}^{n-1} S_j + \text{error} \tag{10}$$

where S_j $(1 \leq j \leq n-1)$ is defined as

$$S_j = \frac{x_{j+1} - x_{j-1}}{6}\left[(2-\lambda_j)f_{j-1} + \frac{(x_{j+1}-x_{j-1})^2}{(x_{j+1}-x_j)(x_j - x_{j-1})}f_j + (2-\lambda_j^{-1})f_{j+1}\right]. \tag{11}$$

Here $\lambda := (x_{j+1} - x_j)/(x_j - x_{j-1})$ and $f_j := f(x_j)$ etc.

The error term is generally constrained by

$$\text{error} \leq \mathcal{O}(\max|\Delta\mathrm{x}|^3) \tag{12}$$

and in the special case of equally-spaced grid, it is higher.

References

[1] N.Shklov, The American Mathematical Monthly, 67, 1022 (1960)