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Estimation Of Numerical Integration To Improve Accuracy In Case Of Interpolation

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Abstract:

We explores the various techniques of numerical integration , focusing on methods derived from interpolation. Initially, piecewise quadratic interpolation is examined, highlighting that while higher-order splines may provide accuracy, they often incur increased computational cost without proportional benefit. Simpson's 1/3 rule, derived via quadratic interpolation, is introduced and shown to offer an error of order O(h⁴), making it efficient for equidistant data points. The method integrates third-degree polynomials exactly and is even exact for cubic due to vanishing higher derivatives.
Building on this, the use of finite difference formulas further refines the estimation, again arriving at Simpson's rule through error correction applied to the trapezoidal rule. The method of undetermined coefficients confirms this by deriving weights that make the integration exact for quadratic functions.
Richardson's extrapolation and Romberg integration are introduced as techniques for enhancing accuracy by combining estimates with different step sizes. Romberg's method recursively improves the integral's accuracy, reaching O(h⁸) precision using only the trapezoidal rule, making it highly efficient and suitable for automation.
The Newton-Cotes method, particularly the Simpson's 3/8 rule, is discussed next. Though it uses a higher-order polynomial (cubic), it surprisingly offers the same order of accuracy as the 1/3 rule (O(h⁴)). However, when applied to the same number of grid points, Simpson's 1/3 rule generally performs better in accuracy.
The Adams method is analyzed, which integrates over a single part using a polynomial derived from multiple points. Although appealing for evolving datasets due to its incremental nature, it typically produces higher errors and is less suitable for numerical integration compared to Newton-Cotes methods. Instead, Adams methods are more commonly used in solving differential equations.
Keyword: Simpson's rule; Trapezoidal rule; Pricewise quadratic interpolation; finite difference; Rechardson's extrapolation; Romberg integration; Newton-cotes method; Adams method

1.Interpolation followed by integration:

As seen in with the increase in the number of data points, it may not be a good idea to use a higher-order interpolating polynomial passing through all data points. The quadratic, cubic, or higher-order splines may be used but would typically require more computational time without a commensurate gain in accuracy.

Therefore, we assume to use piecewise quadratic interpolation,
we may write

$$\tilde{I} = \sum_{i=2,4,6,\ldots n} \int_{h_{i-1}}^{h_i} f(x_{i-2}) + (x+h_{i-1}) f[x_{i-2}, x_{i-1}]$$

$$+ x(x+h_{i-1}) f[x_{i-2}, x_{i-1}, x_i] dx$$

$$= \sum_{i=2,4,6,\ldots n} \frac{(h_{i-1}+h_i)(2h_{i-1}-h_i)}{6h_{i-1}} f(x_{i-2})$$

$$+ \frac{(h_{i-1}+h_i)^3}{6h_{i-1}h_i} f(x_{i-1}) + \frac{(h_{i-1}+h_i)(-h_{i-1}+2h_i)}{6h_i} f(x_i) \tag{1}$$

and the error as

$$E = \sum_{i=2,4,6,\ldots n} \int_{-h_{i-1}}^{h_i} x(x+h_{i-1})(x-h_i) f[x, x_{i-2}, x_{i-1}, x_i] dx \tag{2}$$

Here n is even.
If n is odd, a linear interpolation may be used in the first or last part.
However, it would lead to lower accuracy in the estimate of the integral. A better option would be to use a cubic for the three or last three parts.
But, it is difficult to apply the mean value theorem for integrals directly to equation (2) since $x(x+h_{i-1})(x-h_i)$ does not have a constant sign in the integration domain. For equidistant points, however, we use integration by parts to get

$$E_i = \int_{-h}^{h} x(x+h)(x-h) f[x, x_{i-2}, x_{i-1}, x_i] dx$$

$$= \left[f[x, x_{i-2}, x_{i-1}, x_i] \int_{-h}^{h} x(x+h)(x-h) dx \right]_{-h}^{h}$$

$$-\int_{-h}^{h}\frac{d\,f[x,x_{i-2},x_{i-1},x_i]}{dx}\int_{-h}^{h}x(x+h)(x-h)dx \quad (3)$$

It divide the integral into two parts $(-h_{i-1},0)$ and $(0,h_i)$ such that the term $x(x+h_{i-1})(x-h_i)$ has the same sign over each of these intervals. The second mean value theorem for integrals could be applied to these individual parts. However, it is seen that the presence of opposite signs over these parts would imply that the error cannot be expressed in a usable form. Also the limits on the integral involving $x(x+h)(x-h)$. While the upper limit of this integral must be x, we could have used any constant lower limit of integration in this term.

The value $-h$ is used for convenience as it makes the integral 0 for $x = -h$ as well as $x = h$. The derivative of the finite divide difference is obtained as

$$\frac{d}{dx}f[x,x_{i-2},x_{i-1},x_i] = \lim_{\varepsilon\to 0}\frac{f[x+\varepsilon,x_{i-2},x_{i-1},x_i]-f[x,x_{i-2},x_{i-1},x_i]}{x+\varepsilon-x}$$

$$=\lim_{\varepsilon\to 0}f[x+\varepsilon,x,x_{i-2},x_{i-1},x_i]=f[x,x,x_{i-2},x_{i-1},x_i]$$

Now using the relation between the finite divided difference and the function derivative, it is applicable even when some of the points coincide and get

$$f[x,x,x_{i-2},x_{i-1},x_i]=\frac{f^{iv}(\xi_i^*)}{4!}$$

in which $\xi_i^*\in(x_{i-2},x_i)$.

So that $\int_{-h}^{h}(x-h)x(x+h)dx=0$

and $\int_{-h}^{h}(x-h)x(x+h)dx$ is non-negative for all $x\in(-h,h)$ thus enabling us to use the second mean value theorem for integrals. Therefore, have

$$E_i=-\int_{-h}^{h}\frac{f^{iv}(\xi_i^*)}{4!}\int_{-h}^{h}x(x+h)(x-h)dx\;dx$$

$$=-\frac{f^{iv}(\xi_i)}{4!}\int_{-h}^{h}\frac{(x^2-h^2)^2}{4}dx=\frac{h^3 f^{iv}(\xi)}{90}$$

In which $\xi_i\in(x_{i-2},x_i)$. The estimated integral and total error are given by [equations (1) and (2)]

$$E=\frac{h}{3}\sum_{i=2,4,6,\ldots,n}[f(x_{i-2})+4f(x_{i-1})+f(x_i)]$$

$$=\frac{h}{3}\left[f(x_0)+4\sum_{i=1,3,5,\ldots,n-1}f(x_i)+2\sum_{i=2,4,6,\ldots,n-2}f(x_i)+f(x_n)\right] \quad (4)$$

and

$$E=\sum_{i=2,4,6,\ldots,n}-\frac{h^5 f^{iv}(\xi_i)}{90}=-\frac{(b-a)^5}{180n^4}\frac{\sum_{i=2,4,6,\ldots,n}f^{iv}(\xi_i)}{n/2}$$

$$=-\frac{(b-a)^5\bar{f}^{iv}}{180\,n^4} \quad (5)$$

Where $\bar{f}^{iv}$ represents the mean value of the fourth derivative of the function over the interval (*a*, *b*). If we assume that this mean value does not change significantly with change in *h*, we observe that the total error is $O(h^4)$. Sometimes, we say that the degree of precision of the quadrature scheme is 3 to indicate that all third degree polynomials would be exactly integrated but there are some fourth degree polynomial which cannot be exactly integrated. Also seen that, although we derived the formula with a quadratic interpolation, the integral would be exact even if $f(x)$ is a cubic polynomial since the fourth derivative will be identically zero. This implies that once we perform a quadratic interpolation through 3 equidistant points, and then draw the cubic interpolating polynomial utilizing an additional (equidistant) point, the net area between these two curves would be zero, no matter what the function. If we choose the constant value at the mid-point of the interval, any straight line passing through this point will result in the same area since the difference in area before and after the mid-point cancel out each other. Equation (4) is commonly called Simpson's one-third rule.

2.Using the finite difference formula:

Combining the trapezoidal rule, we estimate over two consecutive parts and using the finite difference approximation of the second derivative in the error (Eq. (3)), improved estimate of the integral over the interval (x_{i-2}, x_i), i.e. we assume that the points are equidistant. For unequal spacing, the finite difference approximation of the second derivative becomes complicated.

$$\int_{x_{i-2}}^{x_i}f(x)dx\simeq I_i=h\frac{f(x_{i-2})+f(x_{i-1})}{2}+h\frac{f(x_{i-1})+f(x_i)}{2}-2\frac{h^3}{12}\frac{f(x_{i-2})-2f(x_{i-1})+f(x_i)}{h^2} \quad (6)$$

In equation (6) the first two terms on the right-hand side are the trapezoidal rule estimates and the third term in the sum of errors in both parts. It is seen that this again results in the Simpson's 1/3 rule.

Method of undetermined coefficients Assuming an expression of the form

$$\tilde{I}_i = c_{i-2} f(x_{i-2}) + c_{i-1} f(x_{i-1}) + c_i(x_i) \quad (7)$$

in which the c's are undetermined coefficients, we require that the integral be exact for all polynomials of second degree. Taking the function as $f(x) = 1$, x, and x^2, respectively, we obtain three linear equations which can be solved to obtain the coefficients:

$$f(x)=1 \quad \Rightarrow \quad c_{i-2}+c_{i-1}+c_i = h_{i-1}+h_i$$

$$f(x)=x \quad \Rightarrow \quad -h_{i-1}\cdot c_{i-2}+0\cdot c_{i-1}+h_i\cdot c_i = \frac{-h_{i-1}^2+h_i^2}{2}$$

$$f(x)=x^2 \quad \Rightarrow \quad h_{i-1}^2\cdot c_{i-2}+0\cdot c_{i-1}+h_i^2\cdot c_i = \frac{h_{i-1}^3+h_i^3}{3} \quad (8)$$

which results in the same equation as equation (4) for equidistant points. In fact, if the points are equidistant, it may be better to write equation (7) as

$$\tilde{I}_i = [c_{i-2} f(x_{i-2}) + c_{i-1} f(x_{i-1}) + c_i f(x_i)]$$

3.Richardson's extrapolation:

From equation , the error in estimate of integral using the trapezoidal rule is equal to $-\left|(b-a)\bar{f}'' h^2\right|/12$.

If we use a step size of $2h$, and assume that the mean value of second derivative is more or less same, the error term should be four times that for the step size of h. As before, a new, and probably more accurate, value is obtained as

$$\tilde{I}_i \simeq \frac{4\left[\frac{h}{2}\{f(x_{i-2})+2f(x_{i-1})+f(x_i)\}\right]-\frac{2h}{2}[f(x_{i-2})+f(x_i)]}{3}$$

in which the first term on the right-hand side represents the trapezoidal rule estimate for the left-hand side using step size h, and the second term represents the same with step size of $2h$.

It is easy to see that we again get the Simpson's rule and the error, as shown earlier, is $O(h^4)$. One may then combine two estimates of $O(h^4)$ (e.g., one using step sizes of h and $2h$, and the other using $2h$ and $4h$) to obtain an $O(h^6)$ estimate and so on. Romberg proposed a general recursive form for this extrapolation well-suited for computer implementation which may be written as

$$\tilde{I}_{h,k+2} \simeq \frac{2^k \tilde{I}_{h,k} - \tilde{I}_{2h,k}}{2^k - 1}$$

General expressions for the error in even and odd degree polynomial interpolation.

For an even (say, $2m$) degree polynomial interpolation using $(2m+1)$ equidistant points located at $0, \pm h, \pm 2h, \ldots\ldots, mh$, the error in estimation of

$$\int_{-mh}^{mh} f(x)dx$$

is given by

$$\frac{2h^{2m+3} f^{[2m+2]}(\xi)}{(2m+2)!}\int_0^m x^2(x^2-1)(x^2-4)\ldots(x^2-m^2)dx$$

in which $\xi \in (-mh, mh)$.

For an odd (say,$2m + 1$) degree polynomial using $(2m+2)$ equidistant points located at

$\pm\frac{h}{2}, \pm\frac{3h}{2}, \ldots\ldots, \pm\frac{(2m+1)h}{2}$, the error is expressed as

$$\frac{2h^{2m+3} f^{[2m+2]}(\xi)^{m+\frac{1}{2}}}{(2m+2)}\int_0^{m+\frac{1}{2}}\left(x^2-\frac{1}{4}\right)\left(x^2-\frac{9}{4}\right)\ldots\left(x^2-\left(m+\frac{1}{2}\right)^2\right)dx$$

in which $\xi \in \left(-\left(m+\frac{1}{2}\right)h, \left(m+\frac{1}{2}\right)h\right)$.

the error in the use of the degree polynomial with $m = 0$ (linear interpolation, trapezoidal rule) is obtained as

$$\frac{2h^3 f''(\xi)}{2}\int_0^{1/2}\left(x^2-\frac{1}{4}\right)dx = -\frac{h^3 f''(\xi)}{12}$$

and that in even degree polynomial with $m = 1$ (quadratic interpolation, Simpson's rule) is obtained as

$$\frac{2h^5 f^{iv}(\xi)}{24}\int_0^1 x^2(x^2-1)dx = -\frac{h^5 f^{iv}(\xi)}{90}$$

in which $\tilde{I}_{h,k}$ represents the estimate of I of accuracy $O(h^k)$ with step size of h.

Thus, starting from trapezoidal rule estimates. $O(h^2)$, for step size of h, $2h$, $4h$, and $8h$, successive estimates could be obtained from

$$\tilde{I}_{h,4} = \frac{4\tilde{I}_{h,2} - I_{2h,2}}{3}; \tilde{I}_{2h,4} = \frac{4\tilde{I}_{2h,2} - I_{4h,2}}{3};$$

$$\tilde{I}_{4h,4} = \frac{4\tilde{I}_{4h,2} - I_{8h,2}}{3}; \tilde{I}_{h,6} = \frac{16\tilde{I}_{h,4} - I_{2h,4}}{15};$$

$$\tilde{I}_{2h,6} = \frac{16\tilde{I}_{2h,4} - I_{4h,4}}{15}; \tilde{I}_{h,8} = \frac{64\tilde{I}_{h,6} - I_{2h,6}}{63};$$

with the final result of $O(h^8)$ accuracy! This algorithm as the Romberg integration is thus a very powerful technique for performing numerical integration with very high accuracy using only a few lower accuracy estimates. Therefore, one really does not need to remember the higher accuracy formulae, only the trapezoidal rule will do! However, for unevenly spaced data it is not directly applicable.

Other techniques for obtaining a more accurate formula use higher-order interpolation and them perform the necessary integration. Two different technique could be applied at this time:

- As we did in above, we use more points to perform the higher-order interpolation and then integrate this polynomial over the domain covered by all these points.
- We use more points to obtain the higher-order interpolating polynomial and then integrate it over a single part.

The first procedure is commonly known as the *Newton-Cotes* method (i.e the trapezoidal rule and the Simpson's rule) while the second is similar to *Adams* method. We describe below these techniques using the third-order interpolating polynomial.

4.Approximation in case Newton-Cotes Method:

We assume that n is a multiple of 3. If it is not, we could be evaluated using the quadratic interpolation. We again use the fact that the integral is not affected by a translation and consider, for simplicity, the points to be equally spaced with

$x_{i-3} = -h;\ x_{i-2} = -0;\ x_{i-1} = h;\ x_i = 2h$.

Then have

$$\tilde{I} = \sum_{i=3,6,9,\ldots,n} \int_{-h}^{2h} f(x_{i-3}) + (x+h) f[x_{i-3}, x_{i-2}] + x(x+h) f[x_{i-3}, x_{i-2}, x_{i-1}] + x(x^2 - h^2) f[x_{i-3}, x_{i-2}, x_{i-1}, x_i]\, dx$$

$$= \frac{3h}{8} \sum_{i=3,6,9,\ldots,n} [f(x_{i-3}) + 3f(x_{i-2}) + 3f(x_{i-1}) + f(x_i)]$$

which is the Simpson's three-eighths rule (proposed much earlier by Newton), with the error given by

$$E = \sum_{i=3,6,9,\ldots,n} \int_{-h}^{2h} x(x^2 - h^2)(x-2h) \frac{f^{iv}(\xi_i^*)}{4!} dx$$

$$= -\frac{3}{80} h^5 \sum_{i=3,6,9,\ldots,n} f^{iv}(\xi_i) = -\frac{(b-a)^5 \bar{f}^{iv}}{80 n^4} \tag{9}$$

A comparison and it seen that Simpson's 1/3 and 3/8 rules have the same order of accuracy (h^4) but the 1/3 rule is more accurate even though it is based on a lower degree polynomial! Thus a better interpolating polynomial may dividing (b-a) into two parts for the 1/3 rule and three parts for the 3/8 rule, the 3/8 rule will be found to be more accurate. However, we feel that a true comparison should be based on the same set of grid points. If we have, say, 6 parts and we use 3 applications of 1/3 rule or 2 applications of 3/8 rule, the 1/3 rule will have smaller error but assuming, that the fourth derivative does not change much.

5.Approximation in case of Adams Method:

An interpolating polynomial over multiple parts and then integrate it over all those part, in case of the Newton-Cotes method. We know from our discussion on interpolation, the error of interpolation is likely to be small in the center of the interval and large near the ends. Earlier we would discussed the three-part case, the interpolation would be much better over the middle part and not-so-good over the corner parts. It would thus appear that a better accuracy may be obtained if we perform the integration only over the middle part. As we will see, it does not lead to a more accurate integral. The reason, as before, is that a better interpolate does not necessarily mean a more accurate integral.

In case of evolving data as new measurements become available, we would like to have updated estimates of the integral. However, if want to apply the three-part Newton- Cotes method, we have to wait for further measurements to get all three parts before we could apply the 3/8 rule.

It may be desirable to develop a technique in which as we add more points, the incremental integral could be easily obtained. It becomes even more desirable if the function value at any point depends on the value of integral at the previous times.

In Adams method, we write the integral as the sum of integrals over each part, expressed as

(take $x_{i-2} = -h;\ x_{i-1} = 0;\ x_i = h;\ x_{i+2} = 2h$)

$$\tilde{I}_i = \sum_{1,2,3,\ldots,n} \int_0^h f(x_{i-2}) + (x+h) f[x_{i-2}, x_{i-1}] + x(x+h) f[x_{i-2}, x_{i-1}, x_i] + x(x^2 - h^2) f[x_{i-3}, x_{i-2}, x_{i-1}, x_i]\, dx$$

and the error over a part is given by

$$E_i = \int_0^h (x+h)x(x-h)(x-2h) f[x, x_{i-2}, x_{i-1}, x_i, x_{i+1}]\, dx$$

Thus, while the grid points $x_{i-2}, x_{i-1}, x_i,\ and\ x_{i+1}$ are used to generate the third degree interpolating polynomial, the integration is performed only over one part. We may perform the integral over the first, middle, or the last part. Here we over the central portion of the data points used. For an evolving data, we would typically perform the integral over the last part. Also, note that for the first and the last parts of the entire data set the *central integral* formula will not be directly applicable since there is no data corresponding to x_{-1} and x_{n+1}. The resulting expression for the integral and the error over a part are

$$\widetilde{I}_i = \frac{h}{24}\left[-f(x_{i-2})+13f(x_{i-1})+13f(x_i)-f(x_{i+1})\right]$$

$$E_i = \frac{11h^5 f^{iv}(\xi_i)}{720} \quad (10)$$

The second mean value theorem for integrals is used to evaluate the error since $(x+h)x(x-h)(x-h)$ is non-negative throughout the interval (0, h) and, as before,

Disregarding the fact that equation (10) is not applicable for $i = 1$ and n, we may estimate the error in the value of the integral as

$$E = \frac{11h^5}{720}\sum_{i=1}^{n} f^{iv}(\xi_i) \simeq \frac{11(b-a)^5 \bar{f}^{iv}}{720n^4}$$

A comparison with equation (9) shows that the error is larger (and of opposite sign) than that in the Simpson's 3/8 rule. Adams methods are, therefore, generally not used for numerical integration. They are quite useful, though, for numerical solution of differential equations.

Newton Cotes method uses a parabola through x_i, x_{i+1}, x_{i+2}.

Adams method uses a parabola through x_{i-1}, x_i, x_{i+1}.

Conclusion:

Using higher-order interpolating polynomials (beyond quadratic) can introduce computational complexity without significant gain in accuracy. Piecewise quadratic interpolation leads to Simpson's 1/3 rule, which integrates cubic polynomials exactly and has an error order of $O(h^4)$. Combining the trapezoidal rule with finite difference approximations of second derivatives leads again to Simpson's 1/3 rule. Method of undetermined coefficients confirms this derivation and generalizes the approach. By using multiple step sizes and extrapolating the results, we can improve integration accuracy significantly. This recursive refinement, known as Romberg integration, can achieve accuracies as high as $O(h^8)$ using just the trapezoidal rule. However, accuracy comparisons depend on how the interval is subdivided. In contrast to Newton-Cotes, Adams method integrates the polynomial only over a single subinterval. Although it allows for easier updates with new data (useful in time-evolving systems), it tends to have larger errors and is less accurate than Newton-Cotes methods for definite integrals.

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