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FORMULAE FOR FINITE DIFFERENCE APPROXIMATIONS, QUADRATURE AND LINEAR MULTISTEP METHODS

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Abstract

We derive finite difference formulae for approximating higher order derivatives, which are applicable to evenly or unevenly spaced grids with arbitrary order of accuracy. Using these formulae, we describe quadrature formulae and linear multistep methods for approximating integrals and numerical solution of differential equations.

1. Introduction

Finite difference approximations are often used for approximating derivatives to solve differential equations [4]. The recursion relations to calculate the weights of finite difference formulae with arbitrary order of accuracy are given in [7]. Khan et al. have presented direct formulae for the explicit forward, backward, and central difference formulae of finite difference approximations with arbitrary order for first derivative, and

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the central difference approximations for higher derivates [10-13]. General explicit formulae for first and higher order derivatives on the basis of the generalized Vandermonde determinant with arbitrary order of accuracy for approximating first and higher order derivatives are given in [14]. Some simple and conventional expressions of central difference formulae for first and second derivatives are found in [6]. This method of undetermined coefficients is limited to evenly spaced grids. A class of linear multistep methods, such as Adams-Bashforth and Adams-Moultan methods for the numerical solution of the initial value problem is based on the principle of numerical integration [1, 3, 5, 9]. The range of numerical integration formulae based on different interpolating polynomials is limited, as a rule, to finite points of interpolation. In the present study, we present finite difference formulae in terms of barycentric weights for approximating derivatives and construction of linear multistep methods to solve differential equations with simple and convenient expressions.

2. Explicit Finite Difference Approximations

2.1. Recursive formula for numerical differentiation

Let x_j, $(j = 0, 1, 2, \ldots, n)$ are $n+1$ distinct numbers in the interval $[a, b]$ together with corresponding f_j, $(j = 0, 1, 2, \ldots, n)$. Let x be any number distinct from each x_j and $f[x_0, x_1, x_2, \ldots, x_k]$ denotes k-th order divided difference of $f(x)$ at the points $x_0, x_1, x_2, \ldots, x_k$. We know that

$$\frac{f^{(k)}(x)}{k!} = f[\underbrace{x, \ldots, x}_{k+1 \text{ times}}]. \tag{2.1}$$

Expanding right hand side of (2.1) by Lagrange interpolation formula, then

$$\frac{f^{(k)}(x)}{k!} = \sum_{i=0}^{n} f[\underbrace{x, \ldots, x}_{k \text{ times}}, x_i]l_i(x) + E(x), \tag{2.2}$$

where

$$l_i(x) = \prod_{j=0,\, i\neq j}^{n} \frac{x - x_j}{x_i - x_j}, \quad i = 0 : n,$$

and

$$E(x) = \frac{f^{(n+k+1)}(\xi)}{(n+k+1)!}\, l(x),$$

where $l(x) = \prod_{j=0}^{n}(x - x_j)$ and $\xi \in [a, b]$. On the other hand, using recursive formula of divided difference [2, 5], we have

$$f[\underbrace{x, \ldots, x}_{k \text{ times}}, x_i] = -\sum_{j=0}^{k-1} \frac{f^{(j)}(x)}{j!} \frac{1}{(x_i - x)^{k-j}} + \frac{f(x_i)}{(x_i - x)^k}. \tag{2.3}$$

Substituting (2.3) in (2.2) and after simplification, we find that

$$\sum_{j=0}^{k} \frac{f^{(j)}(x)}{j!} \sum_{i=0}^{n} \frac{l_i(x)}{(x_i - x)^{k-j}} = \sum_{i=0}^{n} \frac{f(x_i) l_i(x)}{(x_i - x)^k} + E(x). \tag{2.4}$$

Setting $\rho_r(x) = \sum_{i=0}^{n} \frac{l_i(x)}{(x_i - x)^r}$, $r = 0 : k$, we obtain the following recursive formula connecting functional values f_j, $j = 0 : n$ and derivatives up to order k at x:

$$\sum_{j=0}^{k} \frac{f^{(j)}(x)}{j!} \rho_{k-j}(x) = \sum_{i=0}^{n} \frac{f(x_i) l_i(x)}{(x_i - x)^k} + E(x). \tag{2.5}$$

Note that the recursive formula (2.5) can be applied only when x is different from each x_i. Suppose that x coincide with any one of x_i (i.e., $x = x_i$), we can still use the recursive formula to estimate derivatives up to order k as follows:

$$\frac{f^{(r)}(x)}{r!} = \sum_{i=0,\, x_i \neq x}^{n} \frac{f_i l_i(x)}{(x_i - x)^r} - \sum_{j=0}^{r-1} \frac{f^{(j)}(x)}{j!} \rho_{r-j}(x), \quad r = 0 : k, \tag{2.6}$$

where

$$\rho_m(x) = \sum_{i=0,\, x_i \neq x}^{n} \frac{l_i(x)}{(x_i - x)^m}, \quad m = 0 : r, \tag{2.7}$$

and

$$l_i(x) = \prod_{j=0,\, x_i \neq x_j \neq x}^{n} \frac{x - x_j}{x_i - x_j}, \quad i = 0 : n. \tag{2.8}$$

2.2. Explicit finite difference formulae with Lagrangian coefficients

We often need approximation of derivatives for designing difference schemes to solve differential equations. Table 1 shows some examples of explicit finite difference approximations [7].

Table 1. Examples of explicit finite difference formulae

Case	Description	Examples of explicit finite difference formulae	Error level
1	Centered, regular grid	$f''(a) \approx [-\frac{1}{12} f(a-2h) + \frac{4}{3} f(a-h) - \frac{5}{2} f(a) + \frac{4}{3} f(a+h) - \frac{1}{12} f(a+2h)] / h^2$	$O(h^4)$
2	Staggered, regular grid	$f'(a) \approx [\frac{1}{24} f(a-\frac{3}{2}h) - \frac{9}{8} f(a-\frac{1}{2}h) + \frac{9}{8} f(a+\frac{1}{2}h) - \frac{1}{24} f(a+\frac{3}{2}h)] / h$	$O(h^4)$
3	Regular grid	$f'(a+h) \approx [\frac{1}{4} f(a-3h) - \frac{1}{3} f(a-2h) + 3f(a-h) - 4f(a) + \frac{25}{12} f(a+h)] / h$	$O(h^4)$

Suppose one use (2.6) to find t-th derivative of $f(x)$ at x, we get the following form of the explicit approximation:

$$\frac{f^{(t)}(x)}{t!} = \sum_{s=0}^{t-\chi} M_{t-s}(x) a_s + a_t \chi f(x), \tag{2.9}$$

where

$$\chi = \begin{cases} 1, & \text{if } x = x_i, \\ 0, & \text{if } x \neq x_i, \end{cases} \tag{2.10}$$

and

$$M_k(x) = \sum_{i=0}^{n} \frac{f_i}{(x_i - x)^k} l_i(x) + \frac{f^{(n+k+1)}(\xi_k)}{(n+k+1)!} l(x), \tag{2.11}$$

and a_s is unknown function in x. Now substituting all M's in (2.9) and after simplification, we obtain

$$\frac{f^{(t)}(x)}{t!} = \sum_{i=0}^{n} f_i l_i(x) \sum_{k=0}^{t-\chi} \frac{a_k}{(x_i - x)^{t-k}} + a_t \chi f(x) + E_D(a; x), \tag{2.12}$$

where

$$E_D(a; x) = l(x) \sum_{m=0}^{t-\chi} a_m \frac{f^{(t+n+1-m)}(\xi_m)}{(t+n+1-m)!}.$$

To find all a's, set $f(x) = 1$ in (2.12), when $t = 0$, we find $a_0 = 1$ and for $t = 1, 2, 3, \ldots$

$$\sum_{i=0}^{n} l_i(x) \sum_{s=0}^{t-1} \frac{a_s}{(x_i - x)^{t-k}} + a_t = 0.$$

Rearranging above equation and setting $\rho_r(x) = \sum_{i=0}^{n} \frac{l_i(x)}{(x_i - x)^r}$, $r = 0 : t$, we find that

$$\sum_{k=0}^{t} a_k \rho_{t-k}(x) = 0. \tag{2.13}$$

Since $a_0 = 1$, all other unknown a's can be found recursively from (2.13).

2.3. For equally spaced grids

In a few special cases (e.g., for explicit approximations on equispaced grids), the optimal weights are known in closed form. Cases 1 to 3 in Table 1 show three such examples. Let $a + ih$, $(i = -m, \ldots, -2, -1, 0, 1, 2, \ldots, n)$ are equally spaced grids. Setting $x_i = a + ih$ in (2.8) and replacing Lagrangian coefficients $l_i(a)$ by $A_i^{(m,n)}$, then

$$A_i^{(m,n)} = (-1)^{i-1} \frac{m!\, n!}{(m-i)!\,(n+i)!}. \tag{2.14}$$

It follows that

$$\rho_r(a) = \frac{1}{h^r} \sum_{i=-m,\, i\neq 0}^{n} \frac{1}{i^r} A_i^{(m,n)}.$$

Setting $\rho_r(a) = \frac{1}{h^r} W_r$, $b_k = a_k / h^k$ in (2.13) and after simplification, we have

$$b_0 = 1, \quad \sum_{k=0}^{t} b_k W_{t-k} = 0, \tag{2.15}$$

where $W_r = \sum_{i=-m,\, i\neq 0}^{n} \frac{1}{i^r} A_i^{(m,n)}$. Thus, for evenly spaced grids, (2.12) gives

$$f^{(t)}(a) = \frac{t!}{h^t} \sum_{i=-m,\, i\neq 0}^{n} A_i^{(m,n)} f_i \sum_{k=0}^{t-1} \frac{b_k}{i^{t-k}} + b_t f(a) + O(h^{n+1-t}). \tag{2.16}$$

2.4. Explicit finite difference formulae with barycentric weights

The formula given in (2.12) can be modified to even more elegant form with barycentric weights. Divide $l(x)$ on both sides of (2.8)

$$l_i(x) = l(x)\frac{w_i}{x - x_i}, \tag{2.17}$$

where

$$w_i = \prod_{j=0,\, x_i \neq x_j \neq x}^{n} \frac{1}{x_i - x_j}, \quad i = 0 : n. \tag{2.18}$$

We find that

$$\frac{\rho_r(x)}{l(x)} = \sum_{i=0}^{n} \frac{w_i}{(x_i - x)^{r+1}} = \delta_r(\text{say}). \tag{2.19}$$

Now dividing (2.13) by $l(x)$ and using (2.19), after simplification that

$$\sum_{k=0}^{t} a_k \delta_{t-k} = 0. \tag{2.20}$$

Dividing both numerator and denominator of (2.12) by $l(x)$, using (2.17) and after simplification, we obtain

$$\frac{f^{(t)}(x)}{t!} = \frac{1}{\delta_0} \sum_{i=0}^{n} f_i w_i \sum_{k=0}^{t-\chi} \frac{a_k}{(x_i - x)^{t+1-k}} + a_t \chi f(x) + E(x). \tag{2.21}$$

All the unknown a's can be found from (2.20).

3. Quadrature Formulae and Linear Multistep Methods

Table 2 shows some examples of quadrature formulae and linear multistep methods. Cases 1-2 and Case 3 are examples of Newton-Cotes integration formulae and Adams formulae for linear multistep methods.

3.1. Formula for numerical integration

Let $x_0, x_1, x_2, \ldots, x_n$ are distinct numbers on the closed interval $[x, x+h]$ and $f \in C^{(n+1)}[x, x+h]$. The problem of numerical integration is to approximate the definite integral $\int_x^{x+h} f(t)dt$. Since polynomials are easy to integrate by using Taylor series, we find that

$$\int_x^{x+h} f(t)dt = \sum_{k=0}^{n} \frac{f^{(k)}(x)}{(k+1)!} h^{k+1} + O(h^{n+2}). \tag{3.1}$$

Replacing higher order derivatives $f^{(k)}(x)$, $k = 0 : n$, using (2.12), we have

$$\int_x^{x+h} f(t)dt = \sum_{k=0}^{n} \left(\sum_{j=0}^{k-\chi} M_j a_{k-j} + a_k \chi f(x) \right) \frac{h^{k+1}}{k+1} + O(h^{n+2}).$$

Table 2. Examples of quadrature formulae and linear multistep methods

Case	Description	Examples of quadrature formulae	Error level
1	Simpson rule	$\int_x^{x+2h} f(x)dx \approx \frac{h}{3}[f(x) + 4f(x+h) + f(x+2h)]$	$O(h^5)$
2	Newton-Cotes open formula	$\int_x^{x+4h} f(x)dx \approx \frac{4h}{3}[2f(x+h) - f(x+2h) + 2(x+3h)]$	$O(h^5)$
3	Adams-Moultan corrector formula	$y_{n+1} \approx y_n + h[f_{n-3} - 5f_{n-2} + \frac{19}{24} f_{n-1} + \frac{3}{8} f_n]$	$O(h^5)$

Setting $\gamma_k = \sum_{m=0}^{n-k} a_m \frac{h^{k+m+1}}{k+m+1}$, $k = 0 : n$ and after simplification, we find that

$$\int_x^{x+h} f(t)dt = f(x)\gamma_0\chi + \sum_{k=1}^{n} M_k\gamma_k + O(h^{n+2}).$$

Substituting all the values of M's from (2.11) and after simplification, we obtain

$$\int_x^{x+h} f(t)dt = f(x)\gamma_0\chi + \sum_{i=0}^{n} f_i l_i(x) \sum_{k=\chi}^{n} \frac{\gamma_k}{(x_i - x)^k} + E_I(\gamma;\, x), \tag{3.2}$$

where χ is still defined by (2.10) and

$$E_I(\gamma;\, x) = l(x) \sum_{m=\chi}^{n} \frac{f^{(n+m+1)}(\xi_m)}{(n+m+1)!}\gamma_m + O(h^{n+2}).$$

Now dividing $l(x)$ on both numerator and denominator of (3.2), using identity (2.17) and after simplification, we get

$$\int_x^{x+h} f(t)dt = f(x)\gamma_0\chi + \frac{1}{\delta_0} \sum_{i=0}^{n} f_i w_i \sum_{k=\chi}^{n} \frac{\gamma_k}{(x_i - x)^{k+1}} + E_I(\gamma;\, x). \tag{3.3}$$

3.2. Newton-Cotes formulae

Let $x_i = a + ih$, $i = 1, 2, 3, \ldots, n (h \neq 0)$ are equally spaced grids. Now, replacing x by a and h by nh in (3.2) and after simplification, we obtain

$$\int_a^{a+nh} f(x)dx = hf_0\alpha_0 + h\sum_{i=1}^{n} (-1)^{i-1} \binom{n}{i} f_i \sum_{k=1}^{n} \frac{\alpha_k}{i^k} + O(h^{n+2}), \tag{3.4}$$

where

$$\alpha_k = \sum_{m=0}^{n-k} a_m \frac{n^{k+m+1}}{k+m+1}, \quad k = 1, 2, \ldots, n.$$

The Equation (3.4) is $(n+1)$-th point formula for *Newton-Cotes closed integration formula.*

Since the open quadrature formulae do not require the functional values at the limit points of integration, assume that $x_i = a + ih$, $i = 1, 2, \ldots, n-1$ and $h \neq 0$. Now, replacing x by a and h by nh in (3.2) and after simplification, we get

$$\int_a^{a+nh} f(x)dx = h\sum_{i=1}^{n-1}(-1)^{i-1}\binom{n-1}{i} f_i \sum_{k=1}^{n-1}\frac{\beta_k}{i^k} + O(h^n), \tag{3.5}$$

where

$$\beta_k = \sum_{m=0}^{n-1-k} a_m \frac{n^{k+m+1}}{k+m+1}, \quad k = 1, 2, \ldots, n-1.$$

The Equation (3.5) is $(n-1)$-th point formula for *Newton-Cotes open integration formula.*

3.3. Linear multistep methods

Let $x_n, x_{n-1}, x_{n-2}, \ldots, x_{n-p}$ are $p+1$ distinct numbers on the interval $[x_n, x_{n+1}]$, where $x_{n+1} = x_n + h$. If we integrate the differential equation $y' = f(x, y)$ from x_n to x_{n+1}, using (3.3) and after simplification, we find that

$$y_{n+1} = y_n + y'_n\xi_0 + \frac{1}{\delta_0}\sum_{i=1}^{p} w_i y'_{n-i} \sum_{k=1}^{p} \frac{\xi_k}{(x_{n-i} - x_n)^{k+1}} + O(h^{p+2}), \tag{3.6}$$

where

$$\xi_k = \sum_{m=0}^{p-k} a_m \frac{h^{k+m+1}}{k+m+1}, \quad k = 0, 1, 2, \ldots, p.$$

The a_m are still defined by (2.20) at the points $x_n, x_{n-1}, x_{n-2}, \ldots, x_{n-p}$. This kind of multistep formula (4.6) is known as $(p+1)$-*point predictor formula.*

If we integrate the differential equation $y' = f(x, y)$ from x_n to x_{n+1}, using (3.3) and after simplification, we find that

$$y_{n+1} = y_n + y'_{n+1}\tau_0 + \frac{1}{\delta_0}\sum_{i=1}^{p+1} w_i y'_{n+1-i} \sum_{k=1}^{p+1} \frac{\tau_k}{(x_{n+1-i} - x_{n+1})^{k+1}} + O(h^{p+3}), \tag{3.7}$$

where

$$\tau_k = \sum_{m=0}^{p+1+k} a_m \frac{h^{k+m+1}}{k+m+1}, \quad k = 0, 1, 2, \ldots, p+1.$$

This kind of multistep formula (3.7) is known as $(p+2)$*-point corrector formula.*

4. Comparison with Other Formulae

In this section, we compare the new explicit finite difference formulae, quadrature formulae, and predictor-corrector formulae with former formulae on various point distributions.

4.1. Explicit finite difference approximations

Algorithm 4.1. For any arbitrary spaced grids $x_0 < x_1 < x_2 < \ldots < x_n$, and known the function values $f(x_i)$ at $x_i (i = 0, 1, 2, \ldots, n)$, if one applies an $(n+1)$-point formula to estimate the k-th derivative of f at x, then there are five simple steps

Step 1. For $i = 0 : n$, calculate $w_i = \prod_{j=0, i\neq j, x_i \neq x_j}^{n} \frac{1}{x_i - x_j}$.

Step 2. For $m = 0 : k$, calculate $\delta_m(x) = \sum_{i=0, x_i \neq x}^{n} \frac{w_i}{(x_i - x)^{m+1}}$.

Step 3. Set $a_0 = 1$ and for $r = 1 : k$, calculate $a_r(x) = -\sum_{k=0}^{r-1} a_k \delta_{r-k}$.

Step 4. For $i = 0 : n$, calculate $c_i = \sum_{k=0}^{t-\chi} \frac{a_k}{(x_i - x)^{t+1-k}}$,

$$\text{where } \chi = \begin{cases} 1, & \text{if } x = x_i, \\ 0, & \text{if } x \neq x_i. \end{cases}$$

Step 5. Calculate $f^{(t)}(x) = t!\left(a_t f(x)\chi + \frac{1}{\delta_0}\sum_{i=0}^{n} f_i w_i c_i\right)$.

The Algorithm 4.1 requires cost of $O(n)$ flops. The quantities that have to be computed in $O(n)$ operations do not depend on the data f_i. One can easily obtain more numerical differentiation formulae for arbitrary spaced grids using Algorithm 4.1. We provide following 6-point numerical differentiation formulae of evenly spaced grids as examples for first, second, and third order derivatives, whose error levels are $O(h^5)$, $O(h^4)$, and $O(h^3)$, respectively.

$$\begin{cases} f'(a) = \frac{1}{60h}(-137f_0 + 300f_1 - 300f_2 + 200f_3 - 75f_4 + 12f_5), \\ f''(a) = \frac{1}{12h^2}(45f_0 - 154f_1 + 214f_2 - 156f_3 + 61f_4 - 10f_5), \\ f'''(a) = \frac{1}{4h^3}(-17f_0 + 71f_1 - 118f_2 + 98f_3 - 41f_4 + 7f_5), \end{cases} \tag{4.1}$$

$$\begin{cases} f'(a) = \frac{1}{60h}(-2f_{-3} + 15f_{-2} - 60f_{-1} + 20f_0 + 30f_1 - 3f_2), \\ f''(a) = \frac{1}{12h^2}(-f_{-2} + 16f_{-1} - 30f_0 + 16f_1 - f_2), \\ f'''(a) = \frac{1}{4h^3}(f_{-3} - 7f_{-2} + 14f_{-1} - 10f_0 + f_1 + f_2), \end{cases} \tag{4.2}$$

$$\begin{cases} f'(a) = \frac{1}{60h}(-12f_{-5} + 75f_{-4} - 200f_{-3} + 300f_{-2} - 300f_{-1} + 137f_0), \\ f''(a) = \frac{1}{12h^2}(-10f_{-5} + 61f_{-4} - 156f_{-3} + 214f_{-2} - 154f_{-1} + 45f_0), \\ f'''(a) = \frac{1}{4h^3}(-7f_{-5} + 41f_{-4} - 98f_{-3} + 118f_{-2} - 71f_{-1} - 17f_0). \end{cases} \tag{4.3}$$

Comparing the former formulae given in [6, 7, 10-14] with the corresponding forward, backward, and central difference formulae (4.1), (4.2), and (4.3), respectively, it could be found that they are equivalent. The above mentioned formulae are also found from (3.7), by varying the values of m and n. In particular, if $m = 0$, $n = 0$, and $m = n$, then (3.7) gives forward, backward, and central difference approximations of first and higher order derivatives. In fact, the first and second order derivative formulae in [6] are special cases of (3.7) for evenly spaced points.

For unevenly spaced grids, we choose Chebyshev point distributions. The following are some examples of the 5-points and 7-points formulae for first, second, and third order derivatives on Chebyshev points of second kind as follows:

$$\begin{cases} f'(a) \approx \frac{1}{2h}\left(-f_{-1} + \sqrt{8}f_{-\frac{1}{\sqrt{2}}} - \sqrt{8}f_{\frac{1}{\sqrt{2}}} + f_1\right), \\ f''(a) \approx \frac{1}{h^2}\left(-f_{-1} + 4f_{-\frac{1}{\sqrt{2}}} - 6f_0 + 4f_{\frac{1}{\sqrt{2}}} - f_1\right), \\ f'''(a) \approx \frac{1}{h^3}\left(-6f_{-1} + 6\sqrt{2}f_{-\frac{1}{\sqrt{2}}} - 6\sqrt{2}f_{\frac{1}{\sqrt{2}}} + 6f_1\right), \end{cases} \tag{4.4}$$

$$\begin{cases} f'(a) \approx \frac{1}{2h}\left(f_{-1} - \sqrt{\frac{16}{3}}f_{-\frac{1}{2}} + 4f_{-\frac{\sqrt{3}}{2}} - 4f_{\frac{\sqrt{3}}{2}} + \sqrt{\frac{16}{3}}f_{\frac{1}{2}} - f_1\right), \\ f''(a) \approx \frac{1}{3h^2}\left(3f_{-1} - 8f_{-\frac{1}{2}} + 24f_{-\frac{\sqrt{3}}{2}} - 38f_0 + 24f_{\frac{\sqrt{3}}{2}} - 8f_{\frac{1}{2}} + 3f_1\right), \\ f'''(a) \approx \frac{1}{h^3}\left(-16f_{-1} + 20\sqrt{3}f_{-\frac{1}{2}} - 28f_{-\frac{\sqrt{3}}{2}} + 28f_{\frac{\sqrt{3}}{2}} - 20\sqrt{3}f_{\frac{1}{2}} + 16f_1\right). \end{cases} \tag{4.5}$$

The formulae given in [14] estimate higher order derivatives only at the sampling nodes, where the new formula given in (3.11) used to estimate derivatives even when the functional values at sampling nodes are known or not known. Unlike, recursion formulae for calculation of weights given in [7], this method of approximation gives explicit formulae that use given function values at sampling nodes directly and easily to calculate numerical approximations of arbitrary order at any sampling data for the first and higher derivatives. Also, it need less calculations burden,

computing time and storage space to estimate the derivatives than the other methods stated above. It can be directly used for designing difference schemes of ODEs and PDEs and solving them.

4.2. Quadrature formulae and linear multistep methods

Algorithm 4.2. For any arbitrary spaced grids $x_0 < x_1 < x_2 < \ldots < x_n$, and known the function values $f(x_i)$ at $x_i (i = 0, 1, 2, \ldots, n)$, if one applies an $(n+1)$-point formula to estimate the integral $\int_x^{x+h} f(t)dt$, then there are six steps

Step 1. For $i = 0 : n$, calculate $w_i = \prod_{j=0, i\neq j, x_i \neq x_j}^{n} \frac{1}{x_i - x_j}$.

Step 2. For $m = 0 : n$, calculate $\delta_m(x) = \sum_{i=0, x_i \neq x}^{n} \frac{w_i}{(x_i - x)^{m+1}}$.

Step 3. For $r = 0 : n$, calculate $a_r(x) = -\sum_{k=0}^{r-1} a_k \delta_{r-k}$.

Step 4. For $k = 0 : n$, calculate $\gamma_k = \sum_{m=0}^{n-k} a_m \frac{h^{k+m+1}}{k+m+1}$.

Step 5. For $i = 0 : n$, calculate $d_i = \sum_{k=0, x_i \neq x}^{n-\chi} \frac{\gamma_k}{(x_i - x)^{k+1}}$,

$$\text{where } \chi = \begin{cases} 1, & \text{if } x = x_i, \\ 0, & \text{if } x \neq x_i. \end{cases}$$

Step 6. Calculate $\int_x^{x+h} f(t)dt = f(x)\gamma_0\chi + \frac{1}{\delta_0}\sum_{i=0}^{n} f_i w_i d_i$.

The Algorithm 4.2 requires some quantities dependent of x with cost of $O(n^2)$ flops but do not depend on the data f_i. Using this algorithm, one can easily get more formulae for arbitrary spaced grids with any degree of

accuracy. The following are some examples of Newton-Cotes closed integration formulae:

$$\begin{cases} \int_a^{a+h} f(x)dx = \frac{h}{2}(f_0 + f_1) + O(h^3), \\ \int_a^{a+2h} f(x)dx = \frac{h}{6}(f_0 + 4f_1 + f_2) + O(h^5), \\ \int_a^{a+3h} f(x)dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) + O(h^5), \\ \int_a^{a+4h} f(x)dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) + O(h^7). \end{cases} \tag{4.6}$$

Similarly, we can obtain Newton-Cotes open quadrature formulae some of them are listed below:

$$\begin{cases} \int_a^{a+2h} f(x)dx = 2hf_1 + O(h^3), \\ \int_a^{a+3h} f(x)dx = \frac{3h}{2}(f_1 + f_2) + O(h^3), \\ \int_a^{a+4h} f(x)dx = \frac{4h}{3}(2f_1 - f_2 + 2f_3) + O(h^5), \\ \int_a^{a+5h} f(x)dx = \frac{5h}{24}(11f_1 + f_2 + f_3 + 11f_4) + O(h^5). \end{cases} \tag{4.7}$$

For unevenly spaced points, we choose Chebyshev point distributions. The following are the 3-points, 4-points, and 5-points formulae on Chebysev points of second kind:

$$\begin{cases} \int_{a-h}^{a+h} f(x)dx = \frac{h}{3}(f_{-1} + 4f_0 + f_1) + O(h^5), \\ \int_{a-h}^{a+h} f(x)dx = \frac{h}{9}\left(f_{-1} + 8f_{-\frac{1}{2}} + 8f_{\frac{1}{2}} + f_1\right) + O(h^5), \\ \int_{a-h}^{a+h} f(x)dx = \frac{h}{15}\left(f_{-1} + 8f_{-\frac{1}{\sqrt{2}}} + 12f_0 + 8f_{\frac{1}{\sqrt{2}}} + f_1\right) + O(h^7). \end{cases} \tag{4.8}$$

Similarly, the following are the 1-point, 3 points, and 5-points formulae on Chebyshev points of first kind:

$$\begin{cases} \int_{a-h}^{a+h} f(x)dx = 2hf_0 + O(h^3), \\ \int_{a-h}^{a+h} f(x)dx = \frac{2h}{3}\left(f_{-\frac{1}{\sqrt{2}}} + f_0 + f_{\frac{1}{\sqrt{2}}}\right) + O(h^5), \\ \int_{a-h}^{a+h} f(x)dx = \frac{2h}{45}\left(7f_{-\frac{\sqrt{3}}{2}} + 9f_{-\frac{1}{2}} + 13f_0 + 9f_{\frac{1}{2}} + 7f_{\frac{\sqrt{3}}{2}}\right) + O(h^7). \end{cases} \tag{4.9}$$

The following are the some special formulae for linear multistep methods. If we take $p = 1, 2, 3, 4,$ we get Adams-Bashforth predictor formulae of 2-points, 3-points, 4-points, and 5-points, respectively.

$$\begin{cases} y_{n+1,p} = y_n + \frac{h}{2}(-f_{n-1} + 3f_n), \\ y_{n+1,p} = y_n + \frac{h}{12}(5f_{n-2} - 16f_{n-1} + 23f_n), \\ y_{n+1,p} = y_n + \frac{h}{24}(-9f_{n-3} + 37f_{n-2} - 59f_{n-1} + 55f_n), \\ y_{n+1,p} = y_n + \frac{h}{720}(251f_{n-4} - 1274f_{n-3} + 2616f_{n-2} - 2774f_{n-1} + 1901f_n). \end{cases} \tag{4.10}$$

Similarly, if we take $p = 0, 1, 2, 3,$ we obtain Adams-Bashforth predictor formulae of 2-points, 3-points, 4-points, and 5-points, respectively.

$$\begin{cases} y_{n+1,c} = y_n + \frac{h}{2}(f_{n+1,p} + f_n), \\ y_{n+1,c} = y_n + \frac{h}{12}(-f_{n+1,p} + 8f_n + 5f_{n-1}), \\ y_{n+1,c} = y_n + \frac{h}{24}(9f_{n+1,p} + 19f_n - 5f_{n-1} + f_{n-2}), \\ y_{n+1,c} = y_n + \frac{h}{720}(-19f_{n+1,p} + 106f_n - 264f_{n-1} + 646f_{n-2} + 251f_{n-3}). \end{cases} \tag{4.11}$$

Also, we can generate formulae for arbitrary spaced grids. The following are 3-points, 4-points, and 5-points predictor formulae obtained by taking $p = 2, 3, 4,$ respectively, to predict $y_{n+1/2}$ at $x_{n+1/2}$.

$$\begin{cases} y_{n+\frac{1}{2},p} = y_n + \frac{h}{24}(2f_{n-2} - 7f_{n-1} + 17f_n), \\ y_{n+\frac{1}{2},p} = y_n + \frac{h}{384}(-25f_{n-3} + 107f_{n-2} - 187f_{n-1} + 297f_n), \\ y_{n+\frac{1}{2},p} = y_n + \frac{h}{5760}(314f_{n-4} - 1631f_{n-3} + 3489f_{n-2} - 4061f_{n-1} + 4769f_n). \end{cases}$$

(4.12)

Similarly, the following are 3-points, 4-points, and 5-points corrector formulae obtained by taking $p = 1, 2, 3,$ respectively, to correct $y_{n+1/2}$ at $x_{n+1/2}$.

$$\begin{cases} y_{n+\frac{1}{2},c} = y_n + \frac{h}{72}(-f_{n+1/2,p} + 21f_n + 16f_{n-1}), \\ y_{n+\frac{1}{2},c} = y_n + \frac{h}{192}(f_{n+1/2,p} - 6f_n + 61f_{n-1} + 40f_{n-2}), \\ y_{n+\frac{1}{2},c} = y_n + \frac{h}{201600}(-565f_{n+1/2,p} + 3423f_n - 10255f_{n-1} + 68005f_{n-2} + 40192f_{n-3}). \end{cases}$$

(4.13)

It is easily found that these example formulae are the same as to those known corresponding numerical integration formulae based on interpolating polynomials for arbitrary spaced grids [5, 9].

5. Conclusion

In conclusion, we note that finite difference formulae, quadrature formulae, and linear multistep methods in terms of barycentric weights have been developed in this article. Firstly, we have introduced recursive formula for approximating higher order derivatives. Using this recursive formula, we have derived explicit finite difference formulae for approximating higher order derivatives in terms of Lagrange coefficients and barycentric weights for arbitrary spaced grids. Moreover, using this new explicit formula and Taylor series, we have derived numerical integration formula for approximating definite integrals. Newton-Cotes formulae and Adams formulae are special cases of this new formula.

Secondly, we have compared the new explicit finite difference formulae with other formulae. We have seen that this new formula for approximating derivatives requires very less computation time and storage space. We have shown that the forward, backward, and central difference approximations are special cases of this new formula. Similarly, we have shown the comparison of new integration formula for quadrature formulae and construction of linear multistep methods with former formulae. Former formulae for integration and linear multistep methods are limited to evenly spaced grids, but new formula presented here is quite useful on arbitrary spaced grids.

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