A unified explicit form for difference formulas for fractional and classical derivatives

W. A. Gunarathna\textsuperscript{a}, H. M. Nasir\textsuperscript{b},\textsuperscript{*}, W. B. Daundasekera\textsuperscript{c}

\textsuperscript{a}Department of Physical Sciences, Rajarata University, Sri Lanka
\textsuperscript{b}FracDiff Research Group, Department of Mathematics, Sultan Qaboos University, Muscat, Sultanate of Oman
\textsuperscript{c}Department of Mathematics, University of Peradeniya, Peradeniya, Sri Lanka

Abstract

A unified explicit form for difference formulas to approximate the fractional and classical derivatives is presented. The formula gives finite difference approximations for any classical derivatives with a desired order of accuracy at nodal point in the computational domain. It also gives Grünwald type approximations for fractional derivatives with arbitrary order of approximation at any point. Thus, this explicit unifies approximations of both types of derivatives. Moreover, for classical derivatives, it provides various finite difference formulas such as forward, backward, central, staggered, compact, non-compact etc. Efficient computations of the coefficients of the difference formulas are also presented that lead to automating the solution process of differential equations with a given higher order accuracy. Some basic applications are presented to demonstrate the usefulness of this unified formulation.

Keywords: Fractional derivative, Shifted Grünwald approximation, Lubich Generators, compact finite difference formula, boundary value problem

1. Introduction

Fractional calculus has a history that goes back to L’Hospital, Leibniz and Euler [1, 2]. A historical account of early works on fractional calculus can be found, for eg., in [3]. Fractional integral and fractional derivative are extensions of the integer-order (or we call classical) integrals and derivatives to a real or complex order. Various definitions of fractional derivatives have been proposed in the past, among which the Riemann-Liouville, Grünwald-Letnikov and Caputo derivatives are common and established.

\textsuperscript{*}Corresponding author

Email addresses: anura@as.rjt.ac.lk (W. A. Gunarathna), nasirh@squ.edu.om (H. M. Nasir), nasirmh11@yahoo.com (H. M. Nasir), wbd@pdn.ac.lk (W. B. Daundasekera)

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Recently, fractional calculus found its way into the application domain in science and engineering \[1, 3, 6, 7, 8\]. Fractional derivative is also found to be more suitable to describe anomalous transport in an external field derived from the continuous time random walk \[9\], resulting in a fractional diffusion equation (FDE). The FDE involves fractional derivatives either in time, in space or in both variables.

Difference approximation in the form of an infinite series is a widely used tool for numerically solving problems involving FDEs. The weights of the approximation formula are obtained from the coefficients of a generator \(W_1(z) = (1 - z)^\alpha\) expressed in a power series form \[10\]. A shifted form of the difference approximation was proposed in \[11\] to remedy some stability issues in solving space-fractional diffusion equations. Both difference approximations and its shifted form are known to be of the first-order accuracy (see Section 2 for details).

For higher order approximations, Lubich \[12\] obtained some generators in the form of power of polynomials or rational polynomials. The coefficients of the expansion of the generators provide the coefficients for the approximation with higher order accuracy without shift. Shifted forms with these coefficients give only the first order approximations regardless of their higher orders in non-shifted forms.

Recently, generators for higher order approximations with shifts have been obtained by Nasir and Nafa \[13\] and applied to fractional diffusion equations with second-order accuracy, and a third-order approximation was obtained from the second order approximation and used for numerical approximations in \[14\].

The generators of these approximations are usually obtained manually by hand calculations, solving a system equations or by symbolic computations and this processes are specific to the problem at hand.

However, most of the scientific researches searching for mathematical patterns are aimed at automating the relevant scientific processes so that the task may be performed for more general problems with minimal human intervention \[15\]. In this regard, in numerical approximations and solution processes, especially in discretized numerical calculus, it is desirable to have general formulas for the approximation of derivatives that can be automated to be selected in approximation processes.

The present authors \[16\] have obtained an explicit form for generators that gives approximations for fractional derivatives with shifts retaining their higher orders. This form generalises the Lubich form with shift and hence the Lubich form becomes a special case with no shift.

Interestingly, this explicit form also gives coefficients for finite difference formulas (FDFs) for classical derivatives as demonstrated in \[16\]. However, it gives higher order compact FDFs for the first derivative only. Here, a compact FDF means the FDF which uses a minimum number of function values at the discrete grid points. For higher classical derivatives, the resulting FDFs are not compact although they are valid for FDFs.
Usually, the derivation of the weights for the FDFs for classical derivatives involves linear combinations of the Taylor series expansions of a function at various grid points about the point of derivative. For higher order accuracy requirements, this leads to uncontrollable hand calculations, solving large system of linear equations or heavy symbolic computations [17]. Besides, this technique is not suitable for fractional derivatives as the latter involves function values at infinite grid points, due to its non-local nature.

Explicit forms for finite difference formulas for classical derivatives have appeared in the past (see for eg. [18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28]). However, all of them are focussed on the classical derivatives only.

In this paper, we extend the explicit form developed in [16] to a more general unified explicit form that gives more new approximations for fractional derivatives and various finite difference formulas for any classical derivative. The formulation also provides error coefficients of the approximation for the first few terms.

We also present an algorithm to efficiently compute the coefficients of the unified difference formulas. This enables one to compute the coefficients in exact form where necessary and real coefficients with efficiency.

This paper is arranged as follows: We start with preliminary preparations in Section 2. The unified explicit form is given in Section 3. Efficient computational strategies are described in Section 4. Various difference formulas for classical and fractional derivatives are given in Section 5 demonstrating the unified nature of the explicit form. Applications of the difference formulas are presented in Section 6 and finally, Section 7 draws some conclusions.

2. Preliminaries and terminologies

We list here relevant materials and define terminologies relation to the subject of this paper.

Let \( f(x) \) be a sufficiently smooth function defined on a real domain \( \mathbb{R} \).

**Definition 1.** The left(−) and right(+) Riemann-Liouville (R-L) fractional derivatives of real order \( \alpha > 0 \) are defined as

\[
\text{RL}D_x^{-\alpha}f(x) = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dx^n} \int_{-\infty}^{x} \frac{f(\eta)}{(x - \eta)^{\alpha+1-n}} d\eta, \tag{1}
\]

and

\[
\text{RL}D_x^{+\alpha}f(x) = \left(-1\right)^n \frac{d^n}{dx^n} \int_{x}^{\infty} \frac{f(\eta)}{(\eta - x)^{\alpha+1-n}} d\eta \tag{2}
\]

respectively, where \( n = [\alpha] + 1 \), an integer with \( n - 1 < \alpha < n \) and \( \Gamma(\cdot) \) denotes the gamma function.
Definition 2. The left Caputo fractional derivative of order $\alpha > 0$ are defined analogously to (1) by
\[
C D_x^{-\alpha} f(x) = \frac{1}{\Gamma(n-\alpha)} \int_{-\infty}^{x} f^{(n)}(\eta) \frac{(x-\eta)^{\alpha+1-n}}{(x-\eta)^{\alpha+1-n}} d\eta.
\] (3)
The right Caputo derivative is defined analogously to (2).

Definition 3. The left/right Grünwald-Letnikov (G-L) definitions are given respectively by
\[
GL D_x^{\pm \alpha} f(x) = \lim_{h \to 0} \frac{1}{h^\alpha} \sum_{k=0}^{\infty} (-1)^k \binom{\alpha}{k} f(x \mp kh),
\] (4)
where the Grünwald weights, $g_k^{(\alpha)} = (-1)^k \binom{\alpha}{k} = (-1)^k \frac{\Gamma(\alpha+1)}{\Gamma(\alpha-k+1)}$ are the coefficients of the series expansion of the Grünwald generator
\[
W_1(z) = (1 - z)^\alpha = \sum_{k=0}^{\infty} g_k^{(\alpha)} z^k.
\]
These definitions of fractional derivatives are equivalent under certain smoothness conditions on $f(x)$ [10]. Therefore, we denote them commonly as $D_{x}^{\alpha} f(x)$ when the conditions are met.

Definition 4 (Difference approximations). For left and right fractional derivative of order $\alpha > 0$, we define
1. The Grünwald approximation (GA)
\[
\delta_{\pm h}^{\alpha} f(x) = \frac{1}{h^\alpha} \sum_{k=0}^{\infty} g_k^{(\alpha)} f(x \mp kh),
\] (5)
2. The shifted Grünwald approximation (ShGA) [11] with shift $r$
\[
\delta_{\pm h,r}^{\alpha} f(x) = \frac{1}{h^\alpha} \sum_{k=0}^{\infty} g_k^{(\alpha)} f(x \mp (k - r)h),
\] (6)
where $h > 0$ is the step size between discrete points in the domain referenced from $x$. Hence, the difference approximations are defined on a uniform grid points $x_k = x - kh, k \in \mathbb{Z}$.

The approximation order of GA and ShGA is one for integer shifts [11].
\[
\delta_{\pm h,r}^{\alpha} f(x) = D_{x}^{\alpha} f(x) + O(h).
\]
For a generalization of the shifted Grünwald approximation, we define the following.
**Definition 5.** Let \( w_k \) be a sequence of real numbers with it generating function
\[
W(z) = \sum_{k=0}^{\infty} w_k z^k.
\]
Define a shifted difference formula
\[
\Delta_h^{\alpha, p, r} f(x) = \frac{1}{h^\alpha} \sum_{k=0}^{\infty} w_k^{(\alpha)} f(x \mp (k - r)h).
\]
(7)
We say that
1. \( W(z) \) approximates the fractional derivatives \( D_x^{\alpha, x} \) if
\[
\lim_{h \to 0} \Delta_h^{\alpha, p, r} f(x) = D_x^{\alpha, x} f(x),
\]
(8)
2. \( W(z) \) approximates the fractional derivatives \( D_x^{\alpha, x} \) with order \( p \) if
\[
\lim_{h \to 0} \Delta_h^{\alpha, p, r} f(x) = D_x^{\alpha, x} f(x) + O(h^p).
\]
(9)
We call these approximations (8) and (9) the **Grünwald type approximations** (GTAs), \( W(z) \) the **Grünwald type generator** (GTG) and \( w_k \) the **Grünwald type weights** (GTWs).

A set of GTGs for higher order GTAs was established in Lubich [12] by utilizing the characteristic polynomials of linear multistep methods (LMMs) for classical initial value problems. Particularly, a set of generators in the form of \( W_p(z) = (P_p(z))^{\alpha} \) was obtained from the backward difference LMM for orders \( 1 \leq p \leq 6 \) and is listed in Table 1. For \( p = 1 \), it gives the Grünwald generator \( W_1(z) \).

\[
\begin{array}{c|c|c}
 p & P_p(z) & p & P_p(z) \\
\hline
 1 & 1 - z & 4 & \frac{25}{12} - 4z + 3z^2 - \frac{4}{3}z^3 + \frac{1}{4}z^4 \\
 2 & \frac{3}{2} - 2z + \frac{3}{2}z^2 & 5 & \frac{147}{60} - 5z + 5z^2 - \frac{10}{3}z^3 + \frac{5}{4}z^4 - \frac{1}{5}z^5 \\
 3 & \frac{11}{6} - 3z + \frac{3}{2}z^2 - \frac{1}{3}z^3 & 6 & \frac{147}{60} - 6z + \frac{15}{2}z^2 - \frac{20}{3}z^3 + \frac{15}{4}z^4 - \frac{6}{5}z^5 + \frac{1}{6}z^6 \\
\end{array}
\]

Table 1: Polynomials \( P_p(z) \) for Lubich generators \( W_p(z) = (P_p(z))^{\alpha} \)

**Definition 6.** We call the generators given in Table 1 for orders \( 2 \leq p \leq 6 \) as the **Lubich generators** and their weights the **Lubich weights**.

The Lubich generators are to be used without shift to obtain their respective higher approximation orders. Applying the Lubich weights with non-zero shifts reduces the approximation orders to one [13], [16], [29].
Nasir and Nafa [29] obtained a generator $W_{2,r}(z)$ for an order 2 approximation whose weights can be used with shift without reducing the order:

$$W_{2,r}(z) = \left( \frac{3}{2} - \frac{r}{\alpha} \right) + \left( -2 + \frac{2r}{\alpha} \right) z + \left( \frac{1}{2} - \frac{r}{\alpha} \right)^\alpha. \quad (10)$$

An equivalent characterization for a GTA of order $p$ with shift $r$ was established by the authors in [29] and is given in Proposition 1.

**Proposition 1.** (Theorem 1 [14, 29]) Let $\alpha > 0$, $n = [\alpha] + 1$, a non-negative integer $m$ be given. Let a function $f(x) \in C^{m+n+1}(\mathbb{R})$ and $D^k f(x) = \frac{d^k}{dx^k} f(x) \in L_1(\mathbb{R})$ for $0 \leq k \leq m + n + 1$. Then, a generator $W(z)$ approximates the fractional derivatives $D^{\alpha \pm} f(x)$ with order $p$ and shift $r$, $1 \leq p \leq m$, if and only if

$$G(z) = \frac{1}{z^\alpha} W(e^{-z}) e^{rz} = 1 + O(z^p). \quad (11)$$

Moreover, if $G(z) = 1 + \sum_{l=p}^{\infty} a_l z^l$, where $a_l \equiv a_l(\alpha, r)$, then we have

$$\Delta^{\alpha \pm}_{h, p, r} f(x) = D^{\alpha \pm}_{x \pm} f(x) + h^p a_p D^{\alpha + p}_{x \pm} f(x) + h^{p+1} a_{p+1} D^{\alpha + p+1}_{x \pm} f(x) + \cdots + h^m a_m D^{\alpha + m}_{x \pm} f(x) + O(h^{m+1}). \quad (12)$$

This characterization theorem was used in [16] to obtain an explicit form for generators of the form $W(z) = (\beta_0 + \beta_1 z + \cdots + \beta_p z^p)^\alpha$ for an approximation of order $p$ with shift $r$.

**Proposition 2.** (Theorem 3 [16]) The generator of the form

$$W_{p,r}(z) = (\beta_0 + \beta_1 z + \cdots + \beta_p z^p)^\alpha \quad (13)$$

approximates the fractional derivatives $D^{\alpha \pm} f(x)$ with order $p$ and shift $r$ if and only if the coefficients $\beta_j$ are given by

$$\beta_j = - \left( \sum_{m=0}^{p} \prod_{\substack{l=0 \atop l \neq m, j}}^{p} (\lambda - j) \right) \left( \prod_{m=0 \atop m \neq j}^{p} \frac{1}{j - m} \right), j = 0, 1, 2, \cdots, p, \quad (14)$$

where $\lambda = r/\alpha$, and the leading error coefficient is given by

$$R = \frac{1}{(p+1)} \sum_{j=0}^{p} (\lambda - j)^{p+1} \beta_j. \quad (15)$$

Using this explicit form, the authors in [16] have constructed generators of the form (13), for orders $1 \leq p \leq 6$ with shifts and the first five of the generators are listed in Table 2.

When there is no shift ($r = 0$), these generators $W_{p,0}(z)$ reduce to Lubich generators in Table 1. Moreover, for order $p = 1$ it recides to the Grünwald generator $W_1(z)$.
Definition 7. We call the generators given in Table 2 for orders $2 \leq p \leq 6$ the Lubich type generators and their weights the Lubich type weights.

We mention that the Lubich type generators also give finite difference formulas for classical derivatives with integer derivative order $\alpha$. However, we point out that the Lubich type operators give compact finite difference formula for the first order derivative only. For other higher derivatives, we get valid finite difference formulas with non-compact form.

### 3. A unified explicit form

In this section, we extend the explicit form (14) appeared in [16] to a more general form that covers compact finite difference formulas for higher order classical derivatives as well and some new Lubich type generators for fractional derivatives.

For this, we introduce a base differential order $d$, a positive integer, to express the fractional derivative as

$$D_x^\alpha = (D_x^d)^{\frac{\alpha}{d}},$$

and consider approximating the fractional derivative by a Lubich type generator of the form

$$W(z) = (\beta_0 + \beta_1 z + \cdots + \beta_N z^N)^{\frac{\alpha}{d}} = (P(z))^{\frac{\alpha}{d}}, \quad (16)$$

where $P(z)$ corresponds to the classical derivative operator $D_x^d$.

The coefficients $\beta_j$ in (16) are to be determined based on the fractional order $\alpha$, the required approximation order $p$, and shift $r$ for the GTA. The degree $N$ of $P(z)$ will also be determined according to the choice of $p$ and $d$. Then, we have the following theorem leading to our main result.

| $p$ | Coefficients $\beta_j$, $0 \leq j \leq p$ | with $\lambda = r/\alpha$ |
|-----|----------------------------------|-------------------------|
| 1   | $\beta_0 = 1$                    | $\beta_1 = -1$         |
| 2   | $\beta_0 = -\lambda + \frac{3}{2}$ | $\beta_1 = 2\lambda - 2$ |
|     | $\beta_2 = -\lambda + \frac{1}{4}$ |                        |
| 3   | $\beta_0 = \lambda^2 - 2\lambda + \frac{11}{6}$ | $\beta_1 = -\frac{2\lambda^2}{3} + 5\lambda - 3$ |
|     | $\beta_2 = \frac{5\lambda}{6} - 4\lambda + \frac{1}{3}$ | $\beta_3 = -\frac{\lambda}{3} + \lambda - \frac{1}{3}$ |
| 4   | $\beta_0 = -\lambda^3 + \frac{5\lambda^2}{4} - \frac{35\lambda}{12} + \frac{25}{12}$ | $\beta_1 = \frac{2\lambda^3}{3} - \frac{9\lambda^2}{2} + \frac{26\lambda}{3} - 4$ |
|     | $\beta_2 = -\lambda^3 + 6\lambda^2 - \frac{10\lambda}{3} + 3$ | $\beta_3 = \frac{2\lambda^3}{3} - \frac{3\lambda^2}{2} + \frac{13\lambda}{4} - 4$ |
|     | $\beta_4 = -\frac{\lambda^3}{3} + \frac{5\lambda^2}{2} - 1\lambda^2 + 1$ |
| 5   | $\beta_0 = \frac{5\lambda^4}{5} - \frac{5\lambda^3}{3} + \frac{47\lambda^2}{8} - \frac{23\lambda}{4} + \frac{13\lambda}{60}$ | $\beta_1 = -\frac{\lambda^4}{2} + \frac{7\lambda^3}{3} - \frac{21\lambda^2}{8} + \frac{7\lambda}{6} - 5$ |
|     | $\beta_2 = \frac{5\lambda^4}{8} - \frac{13\lambda^3}{3} + \frac{59\lambda^2}{4} - \frac{107\lambda}{6} + 5$ | $\beta_3 = -\frac{\lambda^4}{3} + 4\lambda^3 - \frac{49\lambda^2}{4} + 13\lambda^2 - 10\lambda$ |
|     | $\beta_4 = \frac{5\lambda^4}{8} - \frac{11\lambda^3}{3} + \frac{41\lambda^2}{8} - \frac{61\lambda}{5} + 5$ | $\beta_5 = -\frac{\lambda^4}{3} + \frac{\lambda^3}{2} - \frac{7\lambda^2}{4} + \frac{5\lambda}{3} - 1$ |

Table 2: Coefficients for $p(z) = \beta_0 + \beta_1 z + \cdots + \beta_p z^p$ for generator $W_{p,r}(z) = (p(z))^\alpha$
Theorem 1. With assumptions of Proposition 1, the generator of the form
\[ W(z) = (\beta_0 + \beta_1 z + \cdots + \beta_{N-1} z^{N-1})^{\frac{\alpha}{d}}, \]
where \( d \) is a positive integer, approximates the fractional derivatives \( D_x^\pm f(x) \) at \( x \) with order \( p \) and shift \( r \) if and only if the coefficients \( \beta_j \) satisfy the linear system
\[ \sum_{j=0}^{N-1} (\lambda - j)^k \beta_j = d \delta_{d,k}, \quad k = 0, 1, \cdots, N - 1, \quad (17) \]
where \( \lambda = \frac{rd}{\alpha} \), \( N = p + d \) and \( \delta_{d,k} \) is the Kronecker delta having value of one for \( k = d \) and zero otherwise.

Proof. In view of Proposition 1, we have \( G(z) = \frac{1}{z^\alpha} W(e^{-z}) e^{rz} = 1 + O(z^p) \). This gives
\[
G(z) = \frac{1}{z^\alpha} \left( \sum_{j=0}^{N-1} \beta_j e^{-jz} \right)^{\frac{\alpha}{d}} e^{rz} = \frac{1}{z^\alpha} \left( \sum_{j=0}^{N-1} \beta_j e^{(rd/\alpha - j)z} \right)^{\frac{\alpha}{d}} = \left( \frac{1}{z^d} \sum_{j=0}^{N-1} \beta_j e^{\lambda j z} \right)^{\frac{\alpha}{d}}.
\]
where \( \lambda_j = \lambda - j \), \( \lambda = \frac{rd}{\alpha} \) and
\[
b_k = \frac{1}{k!} \sum_{j=0}^{N} \lambda_j^k \beta_j, \quad n = 0, 1, 2, \cdots. \quad (18)
\]
Since \( G(z) \) does not have any pole singularities by virtue of (11), we have \( b_k = 0 \) for \( k = 0, 1, \cdots, d - 1 \). Moreover, since \( G(0) = 1 \), we have \( b_d = 1 \). These are the consistency condition for the GTA with generator \( W(z) \). Now, for order \( p = 1 \), these conditions give the system (17) with \( N = 1 + d \) and the proof ends.

For \( p > 1 \), \( G(z) \) reduces to
\[
G(z) = \left( 1 + \sum_{k=d+1}^{\infty} b_k z^{k-d} \right)^{\frac{\alpha}{d}} = (1 + X)^{\gamma} = 1 + O(z^p),
\]
where \( \gamma = \frac{\alpha}{d} \) and
\[
X = \sum_{k=d+1}^{\infty} b_k z^{k-d}. \quad (19)
\]
Expansion of \((1 + X)^\gamma\) gives

\[
1 + \gamma X + \frac{\gamma(\gamma - 1)}{2!}X^2 + \cdots = 1 + O(z^p). \tag{20}
\]

The term with \(z\) appears in the term \(\gamma X\) only on the left hand side of (20). This gives \(b_{d+1} = 0\). The same is true for \(b_k\) by successively comparing the coefficients of \(z^{k-d}, d < k < p + d\), to gain \(O(z^p)\) in (20).

Altogether, we have \(b_k = \delta_{d,k}\), \(k = 0, 1, 2, \ldots, p + d - 1\) which yield the linear system (17) with (18) and \(N = p + d\).

The linear system (17) can be expressed in matrix form

\[
V(\lambda_0, \lambda_1, \cdots, \lambda_{N-1})b = d, \tag{21}
\]

with \(b = [\beta_0, \beta_1, \cdots, \beta_{N-1}]^T, \ d = [0, 0, \cdots, d!, 0, \cdots, 0]^T\), where \(d!\) is at the \(d\)th position, and the Vandermonde matrix \(V \equiv V(\lambda_0, \lambda_1, \cdots, \lambda_{N-1})\) whose columns are \([1, \lambda_k, \lambda_k^2, \cdots, \lambda_k^{N-1}]^T, k = 0, 1, \cdots, N - 1\), with its determinant

\[
|V| = \prod_{0 \leq n < m \leq N-1} (\lambda_m - \lambda_n). \tag{22}
\]

Our main result is that the coefficients \(\beta_j, 0 \leq j < N\) of \(b\) in (21) can be explicitly expressed as given in the following theorem.

**Theorem 2.** Let \(\alpha > 0\), a positive integer \(d \geq 1\) and \(f(x)\) be a sufficiently smooth function such that \(D^\alpha x f(x)\) is defined. For a Grünwald type approximation (7) for \(D^\alpha x f(x)\) of order \(p\) and shift \(r\) with the generator in the form (16), the coefficients \(\beta_j\) are given by

\[
\beta_j = \frac{N_j}{D_j}, \quad j = 0, 1, \cdots, N - 1, \tag{23}
\]

where \(N = p + d\) and

\[
N_j = \sum_{0 \leq m_1 < m_2 < \cdots < m_{p-1} \leq N - 1 \atop m_i \neq j, 1 \leq i \leq p-1} \prod_{k=0}^{p-1} (\lambda - m_k), \quad D_j = \frac{(-1)^d}{d!} \prod_{m=0 \atop m \neq j}^{N-1} (j - m). \tag{24}
\]

Moreover, the leading and some successive error coefficients \(R_m\) of the approximation are given by

\[
R_m = \frac{\alpha}{m!d} \sum_{j=0}^{N-1} (\lambda - j)^m \beta_j, \quad m = N, N + 1, \cdots, N + p. \tag{25}
\]
Proof. Solving the Vandermonde system \((21)\) by Cramer’s rule, we get

\[
\beta_j = \frac{|V_j(d)|}{|V|}, \quad j = 0, 1, \ldots, N - 1, \tag{26}
\]

where \(|V| = |V(\lambda_0, \lambda_1, \ldots, \lambda_{N-1})|\) and \(V_j(d)\) is the matrix obtained from \(V\) by replacing its \(j\)th column with \(d\).

For evaluating the determinant \(|V_j(d)|\), observe that the \(j\)th column has only one non-zero entry \(d\) at the \(d\)th place. Hence, pivoting with the \(j\)th column, we have \(|V_j(d)| = (-1)^{j+d}|V_{j,d}|\), where \(|V_{j,d}|\) is the determinant of the matrix obtained from removing the \(j\)th column and \(d\)th row from \(V\), and is given by (see Appendix A)

\[
|V_j(d)| = (-1)^{j+d}d! \prod_{m>n, m, n \neq j} (\lambda_m - \lambda_n)N_j.
\]

Rearranging the Vandermonde determinant \((22)\) as

\[
|V| = \prod_{0 \leq n < m \leq N-1, m, n \neq j} (\lambda_m - \lambda_n)(-1)^j \prod_{m=0}^{N-1} (\lambda_m - \lambda_j)
\]

and substituting in \((23)\), we have \((23)\) with \(\lambda_m - \lambda_j = j - m\).

For the leading and subsequent error terms, note that \((19)\) is reduced to

\[
X = b_N z^p + b_{N+1} z^{p+1} + \cdots + b_{N+p-1} z^{2p-1} + \cdots.
\]

In \((20)\), the terms with \(z^k, k = p, p + 1, \ldots, 2p - 1\) appear only in \(X\). Thus, the error coefficients are given by

\[
R_m = \gamma b_m = \frac{\alpha}{m!d} \sum_{j=0}^{N-1} (\lambda - j)^m \beta_j, \quad N \leq m < N + p.
\]

The numerator and denominator terms of the coefficients \(\beta_j\) can be easily and efficiently evaluated despite their complicated expressions. Moreover, for rational parameters of \(\alpha, p\) and \(r\), these terms will also be rational numbers. Therefore, finite difference coefficients for classical derivatives can be evaluated to their exact rational values.

4. Efficient evaluations

We describe the details of evaluating the coefficients of the unified formulation. The denominators and numerators terms of the coefficients \(\beta_j\) are evaluated separately.
Separation of the evaluation of numerators and denominators allows one to implement the explicit expression efficiently and to express the coefficients in exact fractional form where possible, that is, when \( \lambda \) is an integer or a rational number.

4.1. Evaluating the denominator

The denominator is evaluated in recursive form for efficient computation as follows: The denominator of the coefficient \( \beta_j \) given in (24) can be expressed as

\[
D_j = \frac{(-1)^d}{d!} \prod_{m=0}^{N-1} (j - m) = \frac{(-1)^{p-1-j}}{d!} j!(N - 1 - j)!
\]

This can be described by the recursive form

\[
D_0 = \prod_{m=d+1}^{N-1} (-m), \quad D_j = \frac{-j}{N - j} D_{j-1}, \quad j = 1, 2, \ldots, N - 1.
\]

Hence, the algorithm for the denominator is as follows:

**Algorithm 1.** Compute the denominators

1. Compute \( D_0 \):

   \[
   D_0 \leftarrow -mD_0, \quad \text{for } m = d + 1, d + 2, \ldots, N - 1.
   \]

2. Compute \( D_j \):

   \[
   D_j \leftarrow \frac{-j}{N - j} D_{j-1}, \quad \text{for } j = 1, 2, \ldots, N - 1.
   \]

Since the denominator is independent of any shift \( r \) and derivative order \( \alpha \), it can be evaluated once and used for various shifts and order \( \alpha \).

4.2. Evaluating the numerator

An efficient algorithm for evaluating the numerators can be devised once we identify the sum-product term in (24) as elementary symmetric polynomials (ESPs) \( S(X_j, p - 1) \) in the set

\[
X_j = \{\lambda_k = \lambda - k : \ 0 \leq k \leq N - 1, k \neq j\}.
\]

The ESPs can be efficiently computed by the recursive relations described in [Appendix B](#). We use the operations (B.1) and (B.2) to obtain the required coefficients \( S(X_j, p - 1), j = 0, 1, \ldots, N - 1 \).

Note that each numerator in \( \beta_j \) has the ESP on distinct sets \( A_j \). In fact, \( S(X_j, p - 1) \) is the coefficient of \( x^{N-1-(p-1)} = x^d \) in the monomial

\[
M_j(x) = \prod_{m=0, m \neq j}^{N-1} (x + x_m)
\]
of degree $N - 1$ that can be expressed in the recursive form

$$M_0(x) = \prod_{m=1}^{N-1} (x + x_m), \quad M_j(x) = M_{j-1}(x) \frac{x + x_{j-1}}{x + x_j}.$$ 

The polynomials $M_j(x)$ can be computed by combining the two recurrence relations in (B.1) and (B.2) as follows:

Let

$$M_{j-1}(x) = \sum_{k=0}^{N-1} p_k x^k, \quad M_j(x) = \sum_{k=0}^{N-1} q_k x^k.$$ 

and denote their coefficient vectors as $p$ and $q$ respectively. Then, the algorithm to compute the numerators is devised as follows:

**Algorithm 2.** Computing the numerator terms $N_j$.

1. Compute $M_0(x)$:
   $p_0 = 1,$
   For $m = 1, 2, \cdots, N - 1$, with $p_{-1} = 0,$
   $$p_k \leftarrow p_{k-1} + x_m p_k, \quad k = m, m - 1, \cdots, 0.$$ 
   $$N_0 = S(X_0, p - 1) = p_d.$$ 
2. Compute $M_j(x)$:
   For $j = 1, 2, \cdots, N - 1$, with $p_N = q_N = 0,$
   $$q_k \leftarrow p_k + x_{j-1} p_{k+1} - x_j q_{k+1}, \quad k = N - 1, N - 2, \cdots, 0.$$ 
   $$p \leftarrow q.$$ 
   $$N_j = S(X_j, p - 1) = q_d.$$ 

4.3. **Evaluation of Error**

The leading and subsequent error coefficients are evaluated directly as the expression involves on a sum. From (25), we have the following algorithm:

**Algorithm 3.** Computing the error coefficient of order $m, p \leq m \leq 2p$.

Given $\beta_j = N_j/D_j$ for $j = 0, 1, \cdots, N - 1$,

1. $E \leftarrow 0,$
   For $j = 0, 1, \cdots, N - 1$, $E \leftarrow E + \lambda^{m+d} \beta_j,$
2. $R_m \leftarrow \frac{\alpha}{(m+d)!} E.$
4.4. Operation count

The direct evaluation of the numerator part in (24) computes the sum-product form with all possible combinations. The operation counts for computing the numerator part with base differential order \(d\) and approximation order \(p\) are \(MN\) additions and \(MN(p-1)\) multiplications, where \(M = \frac{N-1}{p-1}\) and \(N = p + d\). For small values of \(N\), this count is reasonably small. However, for large \(N\), the operation count uncontrollably increases. For example, the number of additions and multiplications for computing the numerator for a 10-th order derivative with approximation order 10 by FDNum are 1847560 and 16628040 respectively.

However, the efficient computation described above computes the same numerator in only 968 additions and the same amount of multiplications.

5. Difference formulas

We use the unified explicit form in this paper to construct approximating Lubich type generators with a given base differential order for the left and right fractional derivatives along with their leading error coefficients. We also list some finite difference formulas of various types that can be constructed from the unified formulation.

5.1. Difference approximations for fractional derivatives

When the base differential operator is the first derivative operator \(D = d/dx\) with base differential order \(d = 1\), we obtain the Lubich type generators obtained in [29] with shift \(r\) and are given in Table 2. When there is no shift \((r = 0)\), this gives the Lubich generators in Table 1. Hence, our unified formulation is a further generalization of the Lubich type generators and the Lubich generators for the approximation of fractional derivatives with and without shifts respectively.

When the base differential operator is of order \(d > 1\), we get new approximating generators. Tables 3 and 4 list some approximating generators with base differential orders \(d = 2\) and 3 respectively and approximation orders \(p = 1, 2, 3, 4, 5\). Note that the first order approximations in all cases turn out to be the same Grünwald generator \(W_1(z) = (1 - z)\).\(\alpha\).

The coefficients \(w_k\) of the generators can be computed from the J.C.P. Miller formula given as follows (see [30] for a proof):

\[
W(z) = \left( \sum_{j=0}^{N-1} \beta_j z^j \right)^\gamma = \sum_{k=0}^\infty w_k z^k
\]

\[
w_0 = \beta_0^\gamma, \quad w_m = \frac{1}{mw_0} \sum_{k=1}^{M} (k(\gamma + 1) - m)\beta_k w_{m-k}, \quad m = 1, 2, \cdots
\]  (27)
| $p$ | Coefficients $\beta_j, 0 \leq j \leq p + d - 1$ with $d = 2$ and $\lambda = rd/\alpha$ |
|-----|--------------------------------------------------------------------------------|
| 1   | $\beta_0 = 1$ $\beta_1 = -2$ |
|     | $\beta_2 = 1$ |
| 2   | $\beta_0 = -\lambda + 2$ $\beta_1 = 3\lambda - 5$ $\beta_3 = \lambda - 1$ |
|     | $\beta_2 = -3\lambda + 4$ |
| 3   | $\beta_0 = \frac{\lambda^4}{2^4} - \frac{5\lambda^3}{2^5} + \frac{35\lambda^2}{2^7}$ $\beta_1 = -2\lambda^2 + 9\lambda - \frac{26}{3}$ $\beta_3 = -2\lambda^2 + 7\lambda - \frac{11}{3}$ |
|     | $\beta_2 = 3\lambda^2 - 12\lambda + \frac{49}{3}$ |
|     | $\beta_4 = \frac{\lambda^2}{2^5} - \frac{3\lambda}{2^4} + \frac{11}{13}$ |
| 4   | $\beta_0 = \frac{\lambda^4}{2^4} - \frac{3\lambda^3}{2^5} - \frac{17\lambda^2}{2^7} + \frac{15}{4}$ $\beta_1 = \frac{5\lambda^4}{6} - 7\lambda^2 + \frac{71\lambda}{4} - \frac{7}{6}$ |
|     | $\beta_2 = -\frac{3\lambda^3}{2^5} + 13\lambda^2 - \frac{29\lambda}{4} + \frac{107}{6}$ $\beta_3 = \frac{5\lambda^3}{6} - 12\lambda^2 + \frac{39\lambda}{2} - 13$ |
|     | $\beta_4 = -\frac{3\lambda^2}{2^5} + \frac{11\lambda^2}{12} + \frac{41\lambda}{8} + \frac{61}{77}$ $\beta_5 = \frac{\lambda^2}{6} - \lambda^2 + \frac{7\lambda}{2} - \frac{5}{6}$ |
| 5   | $\beta_0 = \frac{\lambda^4}{2^4} - \frac{3\lambda^3}{2^5} + \frac{17\lambda^2}{12} - \frac{49\lambda^2}{8} - \frac{49}{8} + \frac{203}{45}$ $\beta_1 = -\frac{\lambda^4}{4} + \frac{10\lambda^3}{4} - \frac{31\lambda^2}{4} + 29\lambda - \frac{87}{4}$ |
|     | $\beta_2 = \frac{\lambda^3}{2^5} - \frac{3\lambda^3}{12} + \frac{17\lambda^2}{4} - \frac{46\lambda^2}{8} + \frac{117}{4} + \frac{203}{45}$ $\beta_3 = -\frac{\lambda^3}{2} + 10\lambda^2 - \frac{31\lambda^2}{2} + 62\lambda - \frac{254}{3}$ |
|     | $\beta_4 = \frac{\lambda^2}{2^5} - \frac{5\lambda^2}{12} + \frac{107\lambda^2}{4} - \frac{307\lambda^2}{8} + \frac{33}{2}$ $\beta_5 = -\frac{\lambda^2}{4} + \frac{8\lambda^3}{3} - \frac{19\lambda^3}{2} + 13\lambda - \frac{27}{5}$ |
|     | $\beta_6 = \frac{\lambda}{2^5} - \frac{5\lambda^2}{12} + \frac{17\lambda^2}{4} - \frac{15\lambda}{8} + \frac{147}{190}$ |

Table 3: Coefficients for polynomial $p(z) = (\beta_0 + \beta_1z + \beta_2z^2 + \beta_3z^3 + \beta_4z^4 + \beta_5z^5 + \beta_6z^6 + \beta_7z^7 + \beta_8z^8 + \beta_9z^9)$ for generator $W_{p,d}(z) = (p(z))^{\alpha/d}$ with base differential order $d = 2$ and $\lambda = rd/\alpha$.

where $M = \min(m, N)$.

The Grünwald type approximation for the left or right fractional derivative is then given by (7).

5.2. Finite difference formulas

The finite difference formulas for classical derivatives comes in various shapes and flavours. Forward, backward and central finite differences are well-known. There are also finite difference forms that gives derivatives at any specified grid point. We call them shifted finite difference forms. In addition, there are finite difference forms that give derivatives at a point between two adjacent points. These are called staggered finite difference forms. There are compact finite difference forms that use the minimum number of grid points for a specified order of accuracy. In contrast, there are also non-compact finite difference forms.

Our proposed algorithm gives all these forms for specified choices of input parameters of $d, p$ and $r$. In the following, we list the input parameters and their output finite difference forms in some details.

5.3. Compact finite difference forms

Compact finite difference forms are those that use the minimum number of grid points for a specified derivative order and order of approximation and are
commonly used in applications. There are known compact finite difference forms such as forward (right), backward (left) and central (symmetric). There are also other compact forms in shifted and staggered formulations. The presented algorithm gives all these forms.

In the presented algorithm, the input parameters for compact finite difference forms for a classical derivative \( \alpha \) is chosen to be equal to the base order \( d \). The required order of approximation can be independently chosen. The number of grid points for all the compact finite difference forms for a differential order \( d \) and approximation order \( p \) is \( N = p + d \). All the different forms are obtained through the choice of the shift parameter \( r \) as given in Table 5.

Table 4: Coefficients for polynomial \( p(z) = (\beta_0 + \beta_1 z + \cdots + \beta_{p+d-1} z^{p+d-1}) \) for generator \( W_{p,d}(z) = (p(z))^{d/\alpha} \) with base differential order \( d = 3 \) and \( \lambda = rd/\alpha \)

| \( p \) | Coefficients \( \beta_j, 0 \leq j \leq p + d - 1 \) |
|---|---|
| 1 | \( \beta_0 = 1 \) |
| \( \beta_1 = -3 \) |
| \( \beta_2 = 3 \) |
| \( \beta_3 = -1 \) |
| 2 | \( \beta_0 = -\lambda + \frac{4}{7} \) |
| \( \beta_1 = 4\lambda - 9 \) |
| \( \beta_2 = -6 \lambda + 12 \) |
| \( \beta_3 = 4\lambda - 7 \) |
| 3 | \( \beta_0 = \frac{\lambda}{2} - 3\lambda + \frac{47}{8} \) |
| \( \beta_1 = -5\lambda^2 + 14\lambda - \frac{71}{4} \) |
| \( \beta_2 = 5\lambda^2 - 26\lambda + \frac{29}{3} \) |
| \( \beta_3 = -5\lambda^2 + 24\lambda - \frac{19}{2} \) |
| \( \beta_4 = \frac{5\lambda^2}{2} - 11\lambda + \frac{41}{3} \) |
| \( \beta_5 = -\lambda^2 + 2\lambda - \frac{7}{3} \) |
| 4 | \( \beta_0 = -\frac{4\lambda}{3} + \frac{17\lambda^3}{6} - \frac{26\lambda}{6} + \frac{48}{8} \) |
| \( \beta_1 = \lambda^3 - 10\lambda^2 + 31\lambda - 29 \) |
| \( \beta_2 = -\frac{5\lambda^3}{2} + \frac{95\lambda^2}{4} - \frac{137\lambda}{2} + \frac{461}{8} \) |
| \( \beta_3 = \frac{10\lambda^3}{3} - 30\lambda^2 + \frac{242\lambda}{3} - 62 \) |
| \( \beta_4 = -\frac{5\lambda^3}{2} + \frac{95\lambda^2}{4} - \frac{107\lambda}{2} + \frac{307}{8} \) |
| \( \beta_5 = \lambda^3 - 8\lambda^2 + 19\lambda - 13 \) |
| \( \beta_6 = -\frac{3\lambda^3}{4} + \frac{5\lambda^2}{2} - \frac{17\lambda}{4} + \frac{15}{5} \) |
| 5 | \( \beta_0 = \frac{2\lambda^3}{3} - \frac{2\lambda^2}{3} + \frac{2\lambda}{3} - \frac{28\lambda}{6} + \frac{92\lambda}{6} \) |
| \( \beta_1 = -\frac{7\lambda^2}{3} + \frac{9\lambda^2}{2} - \frac{295\lambda^2}{6} + \frac{111\lambda}{2} - \frac{635}{6} \) |
| \( \beta_2 = \frac{2\lambda^3}{3} - 13\lambda^3 + \frac{135\lambda^2}{3} - 142\lambda + \frac{382}{24} \) |
| \( \beta_3 = -\frac{35\lambda^2}{6} + \frac{125\lambda^3}{2} - \frac{125\lambda^2}{2} + \frac{1219\lambda}{6} - \frac{389}{3} \) |
| \( \beta_4 = \frac{35\lambda^2}{6} - \frac{20\lambda^3}{3} + \frac{565\lambda^2}{6} - 176\lambda + \frac{2042}{24} \) |
| \( \beta_5 = -\frac{7\lambda^2}{3} + \frac{23\lambda^2}{2} - \frac{207\lambda^4}{4} + \frac{185\lambda^2}{12} + \frac{268}{5} \) |
| \( \beta_6 = \frac{7\lambda^3}{3} - \frac{111\lambda^3}{3} + \frac{95\lambda^4}{6} - \frac{82\lambda}{3} + \frac{1849}{120} \) |

Table 5: Choice of shift parameters for compact finite difference forms.
by $h^\alpha$.

The error term takes the leading error coefficient from the explicit form for the error multiplied by $h^p f^{(p)}(\xi)$, where $\xi$ is a point between the grid points.

For example, the central compact finite difference form for the derivative of order $\alpha = 3$ with base $d = 3$ and approximation order $p = 4$ and shift $r = 3$ in Table 6 is read as

$$\frac{d^3}{dx^3} f_0 = \frac{1}{h^3} \left( - \frac{1}{8} f_3 + f_2 - \frac{13}{8} f_1 + \frac{13}{8} f_{-1} - f_{-2} + \frac{1}{8} f_{-3} \right) - \frac{7}{120} h^4 f^{(4)}(\xi),$$

where $f_k = f(x_c + kh)$ and $c$ is the fractional part of $r$.

Note that $0 \leq c < 1$ with non-zero value for non-integer shift $r$ – the staggered case and zero for integer shifts. Thus, the last row of Table 6 is read as

$$\frac{d^2}{dx^2} f_{0.5} = \frac{1}{h^2} \left( \frac{3}{16} f_{1.5} + \frac{41}{48} f_{0.5} - \frac{67}{24} f_{-1.5} + \frac{19}{8} f_{-2.5} - \frac{35}{48} f_{-3.5} + \frac{5}{48} f_{-4.5} \right) + \frac{341}{5760} h^4 f^{(4)}(\xi).$$

| $d$ | $\alpha$ | $p$ | $r$ | Coefficients for Compact forms | Error | Names |
|-----|----------|-----|-----|-------------------------------|-------|-------|
| 1   | 1        | 3   | 0   | $(\frac{11}{6}), -3, \frac{3}{2}, -\frac{1}{3}$ | $-\frac{1}{3}$ | Left |
| 3   | 3        | 4   | 3   | $-\frac{1}{8}, 1, -\frac{13}{8}, (0), \frac{13}{8}, -1, \frac{1}{8}$ | $\frac{7}{120}$ | Central |
| 2   | 2        | 4   | 1   | $\frac{5}{6}, (-\frac{5}{3}), -\frac{1}{3}, \frac{7}{8}, -1, \frac{7}{12}$ | $\frac{11}{180}$ | Shifted |
| 3   | 3        | 4   | 6   | $-\frac{15}{8}, 13, -\frac{407}{8}, 62, -\frac{461}{8}, 29, (\frac{49}{8})$ | $-\frac{29}{45}$ | Right |
| 2   | 2        | 4   | 1.5 | $\frac{3}{16}, (\frac{11}{48}), -\frac{67}{24}, \frac{19}{8}, -\frac{35}{48}, \frac{5}{48}$ | $\frac{341}{5760}$ | Staggered |

Table 6: Some Compact finite difference forms

5.4. Non-compact finite difference forms

In contrast to the compact finite difference forms, non-compact finite difference forms use more grid points than that of the compact forms. All the various finite difference forms described in compact forms are also available in the non-compact forms with the same choices of the shift $r$.

The non-compact finite difference forms are obtained by choosing the base order $d$ such that $\alpha = \gamma d$ for some integer $\gamma > 1$. The coefficients $\beta_j$ for the polynomial $p(z) = \sum_{j=0}^{\gamma d} \beta_j z^j$ are first computed by using the unified explicit form in (24). The generator for the non-compact form is then given by $W(z) = (p(z))^\gamma$. 

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and is expanded to obtain the non-compact coefficients. The expansion can be performed by the J. C. P. Miller recurrence formula as was done in the fractional derivative case.

For example, the non-compact finite difference formula for second derivative \( (\alpha = 2) \) of approximation order \( p = 3 \) with \( d = 1 \neq \alpha \) and shift \( r = 1 \) has the coefficients and leading error coefficient computed from the unified formulation as

\[
\{\beta_k\} = \left( \frac{23}{24}, \frac{-7}{8}, \frac{-1}{8}, \frac{1}{24} \right), \quad R_3 = \frac{1}{12}
\]

Therefore, the generator for the approximate formula is given with power \( \gamma = \alpha/d = 2 \) as

\[
W(z) = \left( \frac{23}{24} - \frac{7}{8}z - \frac{1}{8}z^2 + \frac{1}{24}z^3 \right)^2
\]

\[
= \frac{529}{576} - \frac{161}{96}z + \frac{101}{192}z^2 + \frac{43}{144}z^3 - \frac{11}{192}z^4 - \frac{1}{96}z^5 + \frac{1}{576}z^6.
\]

Hence, the non-compact finite difference formula with its error term is given by

\[
\frac{d^2}{dx^2} f_0 = \frac{1}{h^2} \left( \frac{529}{576} f_1 - \frac{161}{96} f_0 + \frac{101}{192} f_{-1} + \frac{43}{144} f_{-2} - \frac{11}{192} f_{-3} - \frac{1}{96} f_{-4} + \frac{1}{576} f_{-5} \right) + \frac{1}{12} h^3 f^{(3)}(\xi).
\]

6. Numerical tests

In order to demonstrate the usefulness of the presented unified explicit formulation, we present here some numerical examples. Analysis of these applications is beyond the scope of this paper and will be considered in the future.

6.1. Boundary value problem

As a simple application, consider the boundary value problem:

\[
\frac{d^2}{dx^2} u(x) = f(x), \quad a \leq x \leq b, \quad u(a) = u_a, \quad u(b) = u_b.
\]

Consider the computational domain \( a = x_0 < x_1 < \cdots < x_N = b \) with uniform discretization of the domain \([a, b]\) with subinterval size \( h = x_{i+1} - x_i \). Usually, the second derivative is approximated by the central difference formula of order 2 for each internal point. That is, with \( u_i = u(x_i) \) and \( f_i = f(x_i) \),

\[
\frac{d^2}{dx^2} u(x_i) = f(x_i), \quad i = 1, 2, \cdots, N - 1
\]
is approximated as

\[ \frac{1}{h^2} (u_{i-1} - 2u_i + u_{i+1}) = f_i + O(h^2), \quad i = 1, 2, \cdots, N - 1. \] (30)

The resulting tridiagonal matrix equation is solved, after imposing the boundary conditions, for the discrete solution \( u_i \) which approximates \( u(x_i) \) with \( O(h^2) \) error.

Now that we have the explicit form (23) for any order of accuracy \( p \) with \( N = p + d \) grid points, we may approximate (29) by a higher order approximation through (7). Since \( \alpha = 2 \), we choose \( d = 2 \), so that \( \alpha/d = 1 \). We have from (16),

\[ W(z) = \beta_0 + \beta_1 z + \cdots + \beta_{N-1} z^{N-1}, \]

where \( \beta_j = \beta_j(r) \), \( j = 0, 1, \cdots, N - 1 \) with shift \( r \). Each equation in (29) is approximated with shift \( r = i \). The approximation of (29) is then given by

\[ \frac{1}{h^2} \sum_{j=0}^{N-1} \beta_j(i) u_j = f_i + O(h^{N-1}), \quad i = 1, 2, \cdots, N - 1. \] (31)

Note that the order of this approximation is \( N - d \) and hence, the higher the number of nodes, the higher the order of approximation. Matrix form of this system is given by \( BU = F \), where we set \( U = [\hat{u}_0, \hat{u}_1, \cdots, \hat{u}_N]^T \), \( F = [f_1, f_2, \cdots, f_{N-1}]^T \), and the matrix \( B \) is given by

\[ B_{i,j} = \beta_j(i), \quad i = 1, 2, \cdots, N - 1, \quad j = 0, 1, \cdots, N. \]

The entries of the matrix \( B \) are given by (23) and are automatically computed by the algorithms for \( \beta_j \). Imposing boundary conditions, the system reduces to

\[ \hat{B}\hat{u} = F - B_0 \hat{u}_0 - B_N \hat{u}_N, \] (32)

where \( \hat{B} = [B_1, B_2, \cdots, B_{N-1}] \), where \( B_k \) are columns of \( B \), \( \hat{U} = [\hat{u}_1, \hat{u}_2, \cdots, \hat{u}_{N-1}]^T \), and \( \hat{u}_k \approx u_k \). Solving (32) yields the approximate solution.

**Example 1.** We apply the above numerical schemes to the following boundary value problem:

\[ \frac{d^2}{dx^2} u(x) = -\sin(x), \quad -1 < x < 1, \] (33)

\[ u(-1) = \sin(-1), \quad u(1) = \sin(1). \]

for which the exact solution is \( u(x) = \sin(x) \).

In order to compare and see the effectiveness of the automation and accuracy of the unified explicit forms, the problem is solved first by using the well-known central difference formula of order 2 for the second derivative and then by using
the highest order compact finite difference formulas that use the full set of nodal values of the solution vector.

Table 7 shows the maximum absolute errors for the central difference method (30) and the proposed method in (31). As the order of the proposed method increases with the size of the discrete domain, precision errors occur for higher order approximations as the accuracy of the solution surpasses the machine precision—see orders 30, 62 and 126 in Table 7. In order to make sure that these errors are indeed due to accuracy overwhelming the machine precision, we computed the same methods with high precision arithmetic with 300 decimal digits accuracy. In this case, the errors disappear and the absolute maximum errors continue to reduce.

Although we solve the resulting matrix equation by the standard classical solvers, the solution process may be efficiently performed seeing that the matrix has a centro-symmetric structure. This has not been considered here and is thus open.

| $N$ | Step size $h$ | Order 2 Central | Proposed Higher Order Explicit Methods |
|-----|--------------|----------------|---------------------------------------|
| 4   | 0.5          | 2.3370e-01     | 2 | 0.00123815 |
| 8   | 0.25         | 5.3029e-02     | 6 | 1.85125e-07 |
| 16  | 0.125        | 1.2951e-02     | 14 | 5.55112e-15 |
| 32  | 0.0625       | 3.2190e-03     | 30 | 4.71049 |
| 64  | 0.03125      | 8.0358e-04     | 62 | (Precision error) |
| 128 | 0.015625     | 2.0082e-04     | 126 | (Precision error) |

Table 7: Maximum errors for Example 1: Order 2 Central difference and the proposed method

6.2. Fractional boundary value problem

The use of the difference approximations for fractional derivatives is an ongoing research. Therefore, the use of the unified explicit formulation is yet to be explored. Nevertheless, we present here a simple example of fractional boundary value problem that uses the difference formula with base differential order $d = 2$.

**Example 2.** Consider the fractional boundary value problem

$$D^\alpha y(x) = \frac{\Gamma(4 + x)}{6} x^3, 0 < x < 1, \quad 1 < \alpha < 2 \quad (34)$$
$$u(0) = 0, \quad u(1) = 1.$$

The exact solution is $y(x) = x^{3+\alpha}$.

The domain $[0,1]$ is discretized with points $x_j = jh, j = 0, 1, \cdots, N$ and the fractional derivative is approximated by the order $p = 2$ approximation with base order $d = 2$ and shift $r = 1$ from Table 3. The weights $w_k$ we computed by using the J.C.P. Miller relation in (27). The resulting system

$$BY = F$$
Table 8: Maximum errors and convergence orders for Example 2 using the unified explicit formula with $d = 2$, $p = 2$

| $N$ | Error $\alpha = 1.33$ | Order | Error $\alpha = 1.34$ | Order | Error $\alpha = 1.6$ | Order |
|-----|-----------------|-------|-----------------|-------|-----------------|-------|
| 8   | 2.7899e-02     | -     | 2.7899e-02     | -     | 1.7790e-02     | -     |
| 16  | 6.1767e-03     | 2.1707e+00 | 5.7018e-03     | 2.1871e+00 | 4.4935e-03     | 7.0856e-05 |
| 32  | 1.4568e-03     | 2.0840e+00 | 1.3175e-03     | 2.1136e+00 | 1.1292e-03     | 1.9925e+00 |
| 64  | 3.5663e-04     | 2.0303e+00 | 3.1401e-04     | 2.0690e+00 | 7.0856e-05     | 1.9983e+00 |
| 128 | 1.4568e-03     | 2.0840e+00 | 1.3175e-03     | 2.1136e+00 | 1.1292e-03     | 1.9925e+00 |
| 256 | 3.5663e-04     | 2.0303e+00 | 3.1401e-04     | 2.0690e+00 | 7.0856e-05     | 1.9983e+00 |
| 512 | 1.4568e-03     | 2.0840e+00 | 1.3175e-03     | 2.1136e+00 | 1.1292e-03     | 1.9925e+00 |
| 1024| 3.5663e-04     | 2.0303e+00 | 3.1401e-04     | 2.0690e+00 | 7.0856e-05     | 1.9983e+00 |
| 2048| 1.4568e-03     | 2.0840e+00 | 1.3175e-03     | 2.1136e+00 | 1.1292e-03     | 1.9925e+00 |
| 4096| 3.5663e-04     | 2.0303e+00 | 3.1401e-04     | 2.0690e+00 | 7.0856e-05     | 1.9983e+00 |

is solved after imposing the boundary conditions.

Table 8 lists the maximum errors and convergence orders for $\alpha = 1.33, 1.34, 1.6$. The order 2 accuracy is obtained for $\alpha > 4/3$, which has been confirmed by numerical tests with more $\alpha$ values and can be justified by the convergence of the series of the generator as follows. The generator $W_{2,2}(z)$ for $p = 2, d = 2$ is given by (see Table 3)

$$W_{2,2}(z) = (\beta_0 + \beta_1 z + \beta_2 z^2 + \beta_3 z^3)^{\alpha/2} = (1 - z)^\alpha (\beta_0 + \beta_3 z)^{\alpha/2},$$

where $\beta_0 = 2 - \lambda, \beta_1 = -5 + 3\lambda, \beta_2 = 4 - 3\lambda, \beta_3 = -1 + \lambda$ with $\lambda = rd/\alpha = 2r/\alpha$. The series expansion of $W_{2,2}(z)$ converges when the series of both factors $(1 - z)^\alpha$ and $(\beta_0 + \beta_3 z)^{\alpha/2}$ converges – that is, when $|z| \leq 1$ and $|\beta_3/\beta_0| < 1$.

This gives $|\beta_3/\beta_0| < 1$ and resolves to $4r/3 < \alpha$. Moreover, for real valued expansion of the second factor, it requires $\beta_0 > 0$ which leads to $r < \alpha$. For $r = 1$, these give $\alpha > 4/3$.

Further properties and analysis of the higher order approximation formulas for fractional derivatives are open to be considered.

7. Conclusion

A unified explicit form for the difference formulas for classical and fractional order derivatives was presented. This formulation gives various finite difference formulas such as left, right, central, shifted, compact and staggered finite difference formulas of an arbitrary order for classical derivatives. The formulation also gives Grünwald type difference approximation of any order for fractional derivatives.

From this unified formulation, some new type of difference formulas for fractional derivatives were also obtained.

Basic examples of applications were presented to demonstrate the effect of these
Appendix A. Vandermonde type Determinants

In this appendix, we establish the determinant of the matrix obtained in Section 3.

Lemma 1. It is known that, for a finite sequence of $q+1$ parameters $x_0, x_1, \cdots, x_q$, the determinant of the Vandermonde matrix $V(x_0, x_1, \cdots, x_q)$ of size $(q+1)$ is given by

$$ |V| = |V(x_0, x_1, \cdots, x_q)| = \begin{vmatrix} 1 & 1 & 1 & \cdots & 1 \\ x_0 & x_1 & x_2 & \cdots & x_q \\ x_0^2 & x_1^2 & x_2^2 & \cdots & x_q^2 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ x_0^q & x_1^q & x_2^q & \cdots & x_q^q \end{vmatrix} = \prod_{0 \leq i < j \leq q} (x_j - x_i). $$

Lemma 2. Let a variant of the Vandermonde matrix with $q+1$ parameters be defined as

$$ U_k(x_0, x_1, \cdots, x_q) = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_0 & x_1 & \cdots & x_q \\ x_0^2 & x_1^2 & \cdots & x_q^2 \\ \cdots & \cdots & \cdots & \cdots \\ x_0^{k-1} & x_1^{k-1} & \cdots & x_q^{k-1} \\ x_0^{k+1} & x_1^{k+1} & \cdots & x_q^{k+1} \\ \cdots & \cdots & \cdots & \cdots \\ x_0^{q+1} & x_1^{q+1} & \cdots & x_q^{q+1} \end{bmatrix}, $$

where, from the $k$-th row onward, the powers of the parameters are increased by one. Then, the determinant of $U_k$, which is of size $(q+1)$, is given by

$$ |U_k| = \prod_{0 \leq i < j \leq q} (x_j - x_i) \left( \sum_{\sigma \in B} \prod_{l \in \sigma} x_l \right) = |V| \left( \sum_{\sigma \in B} \prod_{l \in \sigma} x_l \right), \quad (A.1) $$

where $B$ is the set of all combinations of $q+1-k$ elements chosen from the index set $A = \{0, 1, 2, \cdots, q\}$ given by $B = \{\sigma = (m_1, m_2, \cdots, m_{q+1-k}) : m_k \in A\}$.

Proof. It is clear that $|U_k|$ is a homogeneous polynomial of total degree $1 + 2 + \cdots + (k-1) + (k+1) + \cdots + (q+1) = (q+1)(q+2)/2 - k$. Moreover, for $i \neq j$, by replacing $x_i$ with $x_j$, we have $|U_k| = 0$ and thus $(x_i - x_j)$ are factors
of $|U_k|$. There are $q(q + 1)/2$ such factors as in the Vandermonde determinant $|V|$. Hence,

$$|U_k| = \prod_{0 \leq i < j \leq q} (x_j - x_i)P(x_0, x_1, \ldots, x_q),$$

where $P$ is a homogeneous polynomial of total degree $(q + 1)(q + 2)/2 - k - q(q + 1)/2 = q + 1 - k$.

Since there are $q + 1$ parameters, $P$ will have \(\binom{q + 1}{q + 1 - k}\) terms of products of combinations of $q + 1 - k$ elements chosen from the $q + 1$ parameters. Thus, $P$ has the form

$$P = C \left( \sum_{\sigma \in A} \prod_{i \in \sigma} x_i \right).$$

The homogeneity of $P$ forces the constant coefficients of the product terms to be the same. Equating one of the terms of $|U_k|$, we see that $C = 1$.

**Lemma 3.** The determinant $|V_j(b)|$ in (26) of Theorem 2 is given by

$$|V_j(d)| = (-1)^{j+d} d! \prod_{\substack{m > n \\ m, n \neq j}} (\lambda_m - \lambda_n)N_j,$$

where $N_j$ is given in (24).

**Proof.** Since the matrix $V_j(d)$ is obtained from the Vandermonde matrix $V$ by replacing the $j$th column by the vector $d$, the parameter $\lambda_j$ is removed from the list \(\{\lambda_0, \lambda_2, \ldots, \lambda_{N-1}\}\). Performing the determinant evaluation with the $j$th column, we have

$$|V_j(d)| = (-1)^{j+d} d! \begin{vmatrix} 1 & 1 & \cdots & 1 \\ \lambda_0 & \lambda_1 & \cdots & \lambda_q \\ \lambda_0^2 & \lambda_1^2 & \cdots & \lambda_q^2 \\ \cdots & \cdots & \cdots & \cdots \\ \lambda_0^{d-1} & \lambda_1^{d-1} & \cdots & \lambda_q^{d-1} \\ \lambda_0^{d+1} & \lambda_1^{d+1} & \cdots & \lambda_q^{d+1} \\ \cdots & \cdots & \cdots & \cdots \\ \lambda_0^{q+1} & \lambda_1^{q+1} & \cdots & \lambda_q^{q+1} \end{vmatrix}.$$

The determinant is in the form of the variant determinant in Lemma 2. Hence, we have

$$|V_j(d)| = (-1)^{j+d} d! |V| \left( \sum_{\sigma \in B} \prod_{i \in \sigma} \lambda_i \right)$$

$$= (-1)^{j+d} d! |V| \sum_{\substack{0 \leq m_1 < m_2 < \cdots < m_{p-1} \leq N-1 \\ m_i \neq j, 1 \leq i \leq p-1 \\ k=0}} \prod_{k=0}^{p-1} \lambda_{m_k},$$

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where $\sigma$ are the combinations of $N - 1 - d = p - 1$ elements from the $N - 1$ parameter set $A_j = \{\lambda_m : 0 \leq m \leq N - 1\} \setminus \{\lambda_j\}$.

Now, the last sum-product term is $N_j$ and $|V| = \prod_{m,n \neq j} (\lambda_m - \lambda_n)$ ends the proof. \qed

Appendix B. Elementary symmetric polynomials

The elementary symmetric polynomials on a finite set $X$ of parameters are defined as follows:

**Definition 8.** Let $X = \{x_0, x_1, \cdots, x_{N-1}\}$ be a set of $N$ parameters and $B_k$ be the set of all combinations $\sigma$ of $k$ parameters chosen from $X$. Then

$$S(X, k) = \sum_{\sigma \in B_k} \prod_{i \in \sigma} x_i = \sum_{0 \leq i_1 < i_2 < \cdots < i_k \leq N-1} x_{i_1} x_{i_2} \cdots x_{i_k}. $$

It is interesting to note that the monomial

$$L(x) = \prod_{k=0}^{N-1} (x + x_k)$$

has the expanded form given by

$$L(x) = \sum_{k=0}^{N} S(X, k)x^{N-k}$$

with $S(X, 0) = 1$. The elementary symmetric polynomials can thus be obtained from the coefficients of powers of the expanded $L(x)$.

The product in $L(x)$ can be performed recursively by multiplying the factors $(x + x_k)$ successively as follows:

1. Let $L_{-1}(x) = 1$.
2. Define $L_k(x) = L_{k-1}(x)(x + x_k)$, $k = 0, 1, \cdots, N - 1$.
3. If $L_{k-1}(x) = p_0 + p_1 x + \cdots + p_{k-1} x^{k-1}$ and $L_k(x) = q_0 + q_1 x + \cdots + q_k x^k$, then, by setting $p_{-1} = p_k = 0$, the coefficients $q_m$ are related by

$$q_m = p_{m-1} + x_k p_m, \quad m = 0, 1, 2, \cdots, k. \quad (B.1)$$

Conversely, one can obtain $L_{k-1}(x)$ from $L_k(x)$ through

$$p_{m-1} = q_m - x_k p_m, \quad m = k, k - 1, \cdots, 2, 1, 0, \quad (B.2)$$

where $q_{-1}$ is the remainder when dividing $L_k(x)$ by $(x + x_k)$ which is zero since $(x + x_k)$ is a factor of $L_k(x)$. Hence, the recursion can be computed only for $m = k, k - 1, \cdots, 2, 1$. 

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