Arbitrary order of convergence for Riesz fractional derivative via central difference method

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Abstract

We propose a novel method to compute a finite difference stencil for Riesz derivative for arbitrary speed of convergence. This method is based on applying a pre-filter to the Grünwald-Letnikov type central difference stencil. The filter is obtained by solving for the inverse of a symmetric Vandermonde matrix and exploiting the relationship between the Taylor’s series coefficients and fast Fourier transform. The filter costs $O(N^2)$ operations to evaluate for $O(h^N)$ of convergence, where $h$ is the sampling distance. The higher convergence speed should more than offset the overhead with the requirement of the number of nodal points for a desired error tolerance significantly reduced. The benefit of progressive generation of the stencil coefficients for adaptive grid size for dynamic problems with the Grünwald-Letnikov type difference scheme is also kept because of the application of filtering. The higher convergence rate is verified through numerical experiments.

Keywords: Non-local operator, Riesz derivative, Finite difference

1. Introduction

Riesz derivative is the symmetrical version of the fractional Riemann–Liouville derivative. Fractional calculus is an important topic because fractional derivatives can account for non-local effect, which is present in many physics problems. For example, the Riesz derivative has been applied to model wave propagation in viscoelastic material and fractional electrical impedance in human skin [1, 2]. One of the most efficient methods to approximate spatial fractional derivatives is based on Grünwald-Letnikov derivatives. The development began with the derivation of the central difference scheme to approximate the Riesz potential in [3]. The order of accuracy was found to be of second order later in [4]. In [5, 6], the order of convergence was increased to 4 by applying another finite difference on the operator such that the second order term in the Maclaurin series is eliminated. Because the matrix system resulting from the fractional difference operation is not sparse, there is practically no additional cost in using a highest order approximation in a dynamic problem aside from the potential overhead in the evaluation of the coefficients for the operator. This motivates us to study methods to increase the order of approximation to an arbitrary order so that the convergence is faster, leading to reduced number of nodes required to achieve accurate results. In this paper, we propose a prefilter approach to generalise the canceling of error terms in [5, 6]. The result is a filter which maximizes the flatness of the fractional power of sinc function at the origin.

In order to understand our approach, we first discuss the development of higher order finite difference approximation using the Grünwald-Letnikov derivatives for Riesz derivative. Starting from the very basic, Grünwald-Letnikov
derivatives are obtained by applying fundamental theorem of calculus recursively as

\[
f'(x) = \lim_{h \to 0} \frac{f(x + h) - f(x)}{h}, \quad (1)
\]

\[
f''(x) = \lim_{h \to 0} \frac{f'(x + h) - f'(x)}{h} = \lim_{h \to 0} \frac{f(x + 2h) - 2f(x + h) + f(x)}{h^2}, \quad (2)
\]

\[
f'''(x) = \lim_{h \to 0} \frac{f''(x + h) - f''(x)}{h} = \lim_{h \to 0} \frac{f(x + 3h) - 3f(x + 2h) + 3f(x + h) - f(x)}{h^3}. \quad (3)
\]

\[...
\]

and so on. Shifting the difference to the centre, we have

\[
f'(x) = \lim_{h \to 0} \frac{f(x + \frac{h}{2}) - f(x - \frac{h}{2})}{h}, \quad (4)
\]

\[
f''(x) = \lim_{h \to 0} \frac{f'(x + \frac{h}{2}) - f'(x - \frac{h}{2})}{h} = \lim_{h \to 0} \frac{f(x + h) - 2f(x) + f(x - h)}{h^2}, \quad (5)
\]

\[
f'''(x) = \lim_{h \to 0} \frac{f''(x + h) - 2f'(x) + f'(x - h)}{h} = \lim_{h \to 0} \frac{f(x + \frac{3h}{2}) - 3f(x + \frac{h}{2}) + 3f(x - \frac{h}{2}) - f(x - \frac{3h}{2})}{h^3}. \quad (6)
\]

\[...
\]

Without the limits, the first Grünwald-Letnikov derivative is equivalent to first order accurate finite difference. Because of this, the subsequent derivatives are also first order accurate while the central difference version has second order of accuracy.

Grünwald-Letnikov derivatives of a function can be written as a discrete convolution of the function evaluated at the discrete points with a stencil. For the central difference, the derivatives can be expressed as

\[
D^1_h f = S_{\frac{1}{2}} (f) * \frac{1}{h} \left[ 1 \quad -1 \right], \quad (7)
\]

\[
D^2_h f = \Delta^1_h [D^1_h f] = S_{\frac{1}{2}} (f) * \frac{1}{h} \left[ 1 \quad -1 \right] * \frac{1}{h} \left[ 1 \quad -1 \right], \quad (8)
\]

\[...
\]

where the discrete convolution operator is defined as \((f * g)[n] \triangleq \sum_m f [n - m] g [m], f [n] = f (nh), S_i \) is the shift operator defined as \(S_i [f] [n] = f [n + i], \) and the array is 0 indexed. Now, let \(H_k\) be the stencil of \(k\)-th derivative. Then the \(k\)-th derivative can be written as

\[
D^k_h f = \frac{1}{h^k} \left( S_{\frac{k}{2}} (f) * H_k \right), \quad (9)
\]

with the recursive relationship

\[
H_k = H_{k-1} * \left[ 1 \quad -1 \right], \quad (10)
\]

\[
H_1 = \left[ 1 \quad -1 \right]. \quad (11)
\]
Applying discrete time Fourier transform to \( H_k \), we have

\[
\mathcal{F} \{ H_k \} = (1 - e^{-i\omega})^k = \sum_{m=0}^{k} \binom{k}{m} (-1)^m e^{-i\omega m}.
\]  

(12)

This leads to the solution \( \{ H_k \}_m = (-1)^m \binom{k}{m} \). To understand the error convergence, we replace \( m \) with \( m^{\frac{1}{2}} \) in (12) to obtain the Fourier transform of the \( k \)-th derivative of \( f \)

\[
\mathcal{F} \{ D^k_h f \} = (e^{i\omega h} - e^{-i\omega h})^k \tilde{f}(\omega) = \left(i\omega \sin \left(\frac{\omega h}{2}\right)\right)^k \tilde{f}(\omega).
\]  

(13)

Since \( \text{sinc}(x) \) can be expanded as a Maclaurin series as \( 1 + O\left(x^2\right) \) and it would converge for \( x \) from \(-\pi\) to \( \pi\), this approximation is second order accurate, assuming \( f \) is sufficiently smooth such that the magnitude of its frequency response drops significantly below the difference between 1 and the sinc function in its main lobe.

The binomial series (12) can be generalised to non-integer \( k \) for fractional derivatives, as seen in \([3, 7]\), because the magnitude of the variable in the series is not bigger than 1. Consider the Riesz derivative defined as

\[
\partial^\alpha f(x) \triangleq C_\alpha (aD^\alpha_x + bD^\alpha_y) f(x),
\]

(14)

where \( f(x) = 0 \) everywhere except \( x \in [a, b] \), \( C_\alpha = -\frac{1}{\sin \frac{\alpha \pi}{2}} \), and the left and right Riemann-Liouville fractional derivatives are defined as

\[
aD^\alpha_x f(x) \triangleq \frac{1}{\Gamma(m-a)} \frac{\partial^m}{\partial x^m} \int_a^x (x-\xi)^{m-1-a} f(\xi) \, d\xi,
\]  

(15)

\[
sD^\alpha_x f(x) \triangleq \frac{1}{\Gamma(m-a)} \frac{\partial^m}{\partial x^m} \int_x^b (\xi-x)^{m-1-a} f(\xi) \, d\xi,
\]  

(16)

where \( m = \lfloor \alpha \rfloor \). Since \( f \) can be scaled by introducing dimensionless variables, we consider \( a = 0 \), \( b = 1 \) for the Riesz derivative throughout the paper. The Riesz derivative has the frequency response \( -|\omega|^\alpha \). Therefore, for a stencil which approximates the Riesz derivative to second order of accuracy, we seek a solution of the inverse transform of \( |\omega \sin \left(\frac{\omega h}{2}\right)|^\alpha \). Let the fractional convolution kernel be \( K_\alpha \) such that

\[
\mathcal{F} \{ K_\alpha \} = \left|\omega \sin \left(\frac{\omega h}{2}\right)\right|^\alpha.
\]  

(17)

Then the solution is the Fourier series coefficient of its transform given by

\[
K_\alpha (n h) = \frac{2^n h}{2\pi h^n} \int_0^{\frac{\pi}{2^n}} \sin^n \left(\frac{\omega h}{2}\right) e^{-in\omega h} d\omega.
\]  

(18)

The coefficients are symmetrical because the frequency response is real and symmetric about the origin. Therefore, it does not matter whether the exponent is negative or not but the negative choice will be apparent later. Owing to the binomial series and Cauchy residue theorem, each biomial coefficient can be expressed in the integral form as

\[
\binom{a}{b} = \text{Res} \left( \frac{(1+z)^a}{z^{b+1}}, 0 \right) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} (1 + e^{i\omega})^a e^{-ib\omega} d\omega.
\]  

(19)

for any real \( a \) and \( b > -1 \). Eq. (18) can be rewritten in the same form to arrive at the solution as

\[
K_\alpha (n h) = \frac{(-1)^n}{2\pi h^n} \int_{-\pi}^{\pi} (1 + e^{i\omega})^a e^{-i\omega (\frac{\alpha}{2} + n)} d\omega = \frac{(-1)^n}{h^n} \left( \frac{\alpha}{2} + n \right).
\]  

(20)
This method to solve binomial related problems is known as the Egorychev method[8]. Therefore, to increase the convergence order, we propose a filter with a frequency response $G_\alpha$ such that $G_\alpha \cdot K_\alpha$ now has a response of $|\omega|^\alpha \left(1 + O\left(h^N\right)\right)$, where $N$ is the order of convergence.

This paper is organized as follows. In Section 2, we start with presenting our method, which is then followed by the details of the algorithms. In Section 3, we discuss the convergence behaviour of the method, which shows that the convergence is indeed $O\left(h^N\right)$ subject to the smoothness of the function, and we comment on the filter’s positivity and the eigenvalue problem. Numerical results are presented in Section 4 to validate the error prediction in the previous section before the conclusion in the final section.

2. Method & Algorithm

In this section, we derive the method to reduce the error of approximation of the Riesz derivative and algorithms to compute the stencil for this purpose. As discussed previously, we seek a filter to improve the flatness of the sinc function in the neighbourhood of the origin such that resulting frequency response of the finite difference operator is closer to $|\omega|^\alpha$. We expand the fractional power of the sinc function in (18) as the Maclaurin series as

$$\text{sinc} \left( \frac{\alpha}{2} \right) = 1 + \sum_{n=1}^{N_0} c_n x^{2n} + O \left(x^N\right),$$

where $N$ is the choice of convergence order, $N_0 = \left[ \frac{N}{2} \right] - 1$, $c_n = \frac{1}{\Gamma(n+1)} \left| \frac{\partial}{\partial x} \text{sinc} \left( \frac{x}{2} \right) \right|_{x=0}$. The odd coefficients are ignored because it is obvious that they are 0 for an even function. Because this series converges up to $|x| < \pi$, we know that each higher order term is always smaller in magnitude than the respective 1 lower order term below the Nyquist frequency. Then it is clear that by cancelling out the lower order ones, we will improve the flatness of this function, provided that the filter does not raise the magnitude of the coefficients of the higher order terms. Now, let us consider only the problem of eliminating the lower order terms first. Let the filter be $G_\alpha$ such that

$$\mathcal{F}\{G_\alpha\} = \tilde{G}_\alpha = \tilde{g}_0 + 2 \sum_{m=1}^{N_0} \tilde{g}_m \cos (mx).$$

The transform is a cosine series because the filter is obviously real symmetric, and there are no odd terms in the sinc expansion to cancel. Expanding each $\cos (nx)$ as Maclaurin series, we have

$$\cos (mwx) = 1 + \sum_{n=1}^{N_0} c_{n,m} x^{2n} + O \left(x^N\right),$$

where $c_{n,m} = (-1)^{n+1} \frac{\sin \alpha}{2^{n+1}}$. Let $b_n$ be the series coefficients of $\tilde{G}_\alpha$. They can be expressed in matrix form as

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ 0 & c_{1,1} & \cdots & c_{1,N_0} \\ \vdots & \ddots & \ddots & \vdots \\ 0 & c_{N_0,1} & \cdots & c_{N_0,N_0} \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \begin{bmatrix} g_0^\alpha \\ g_1^\alpha \\ \vdots \\ g_{N_0}^\alpha \end{bmatrix} = \begin{bmatrix} 1 \\ b_1 \\ \vdots \\ b_{N_0} \end{bmatrix}.$$

The coefficients of the series from the product of the two polynomials can be obtained through discrete convolution, and we set the coefficients for $n > 0$ up to $2N_h$ be 0 to eliminate the lower order terms. This can be expressed in matrix form as

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ a_1 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ a_{N_h} & a_{N_h-1} & \cdots & 1 \end{bmatrix} \begin{bmatrix} 1 \\ b_1 \\ \vdots \\ b_{N_h} \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = e_0.$$
The matrix involving $c_{nm}$ is not convenient to solve but it gives us insight of the actual problem size. We rewrite it as a larger problem, in terms of the expansion of the exponential function, leading to

\[
\begin{pmatrix}
0 & \cdots & 0 \\
(-1)^0 & \cdots & 0 \\
\vdots & \ddots & \vdots \\
0 & \cdots & (-1)^{N_h-1}
\end{pmatrix} V^T \begin{pmatrix} (-N_h, \ldots, N_h) \end{pmatrix}
= \begin{pmatrix} 1 \\
0 \\
\vdots \\
0 \\
b_{N_h}
\end{pmatrix},
\]

(26)

where $V ((x_0, x_1, \ldots, x_N))$ is the Vandermonde matrix defined as

\[
\begin{pmatrix}
x_0^0 & x_1^0 & \cdots & x_N^0 \\
x_1^0 & x_1^1 & \cdots & x_N^1 \\
\vdots & \vdots & \ddots & \vdots \\
x_0^N & x_1^N & \cdots & x_N^N
\end{pmatrix}
\]

(27)

Let $v_{ij}^\alpha = \begin{pmatrix} V^{-1} ((x_0, x_1, \ldots, x_N)) \end{pmatrix}_{ij}$, the inverse of the Vandermonde matrix can be solved using the following recurrence equations [9]

\[
v_{ik}^k = \frac{\prod_{m=0}^{k-2} (x_k - x_m)}{\prod_{m=0}^{k-1} (x_k - x_m)} \left( v_{i,k-1}^{k-1} - x_{k-1} v_{i,k-1}^{k-1} \right), \quad 0 < i \leq k, \quad k \geq 1
\]

(28)

\[
v_{0,k}^k = \frac{\prod_{m=0}^{k-2} (x_k - x_m)}{\prod_{m=0}^{k-1} (x_k - x_m)} x_k v_{0,k-1}^{k-1}
\]

(29)

and for $0 \leq j < k$

\[
v_{ij}^k = \frac{x_k v_{i,j}^{k-1} - v_{i,j}^{k-1}}{x_k - x_j}, \quad 0 < i \leq k,
\]

(30)

\[
v_{0,j}^k = \frac{x_k - v_{0,j}^{k-1}}{x_k - x_j}
\]

(31)

where $k$ is looped over $k = 0, \ldots, N$. All $v_{ij}^0$ are 0 initialised except for $v_{0,0}^0 = 1$. However, for our special case, there are some properties which can be exploited for further optimisation. In this special case, $k$ is even, and $x_{\frac{k}{2}+n} = x_{\frac{k}{2}-n} = n$ for $n = 0, \ldots, \frac{k}{2}$. Since we are only concerned about even $k$, we map $k \mapsto \frac{k}{2}$ and let the size grow 2 per step. To find the new recurrence relationship for each step, we write out the Lagrange polynomial basis as

\[
L_j^k (x) = \frac{(-1)^{k-j} \prod_{m=0}^{k-1} (x - n)}{(k + j)! (k - j)!} = \sum_{i=0}^{2k} v_{i,j+k}^{k} x^i.
\]

(32)

Each basis has the following symmetry

\[
L_j^k (x) = L_{-j}^k (-x) = \sum_{i=0}^{2k} v_{i,j-k}^{k} (-1)^j x^i,
\]

(33)

which leads to $v_{i,j+k}^{k} = v_{i,j-k}^{k}$. This relationship also arises from the fact that $g_{ij}$ is symmetric. Therefore, we need not consider the left half of the Vandermonde matrix inverse, and we can shift the indexing to the left by $N$.

The second property is

\[
\frac{v_{2i-1,j}^{k}}{v_{2i,j}^{k}} = j, \quad \text{for } i > 0, \quad 0 \leq j \leq k,
\]

(34)
so the odd terms are not required for the evaluation of future coefficients. To prove this, we write out the recurrence relationship for this special case first. For \( j = k \), we have

\[
L_k^j (x) = \frac{(x + k)(x - k + 1)}{(2k)(2k - 1)} L_{k-1}^{j-1} (x),
\]

which leads to the recurrence relationship of the coefficient after substituting in (32),

\[
v_{i,k}^j = \frac{v_{i-1,2k-1}^{j-1} + v_{i-1,2k-1}^{j-1} - k (k - 1) v_{i,k-1}^{j-1}}{(2k)(2k - 1)}, \quad \text{for } i = 2, \ldots, 2k
\]

\[
v_{0,k}^j = \frac{v_{0,k-1}^{j-1} - k (k - 1) v_{1,k-1}^{j-1}}{(2k)(2k - 1)}, \quad v_{0,k}^j = 0, \quad \text{for } k > 0,
\]

and for \( j < k \),

\[
L_j^k (x) = \frac{x^2 - k^2}{j^2 - k^2} L_{j-1}^{k-1} (x - 1),
\]

leads to

\[
v_{i,j}^k = \frac{k^2 v_{i-1,j}^{k-1} - v_{i-2,j}^{k-1}}{(k + j)(k - j)} \quad \text{for } i = 2, \ldots, 2k,
\]

\[
v_{0,j}^k = \frac{k^2 v_{0,j-1}^{k-1}}{(k + j)(k - j)}, \quad \text{for } i = 0, 1.
\]

One can verify that the property (34) is true for \( k = 1 \) using the recurrence relationships. We assume this is also true for other \( k \) up to \( N - 1 \). Then for \( k = N, j = N \), we substitute (36) into (34), we get

\[
\frac{v_{2i-1,N}^{N}}{v_{2i,N}^{N}} = \frac{v_{2i-3,N-1}^{N} + v_{2i-2,N-1}^{N} - N (N - 1) v_{2i-1,N-1}^{N-1}}{v_{2i-2,N-1}^{N} + v_{2i-1,N-1}^{N} - N (N - 1) v_{2i,N-1}^{N-1}} = N \frac{v_{2i-1,N-1}^{N-1} - (N - 1)^2 v_{2i,N-1}^{N-1}}{v_{2i-2,N-1}^{N-1} - (N - 1)^2 v_{2i,N-1}^{N-1}} = N.
\]

This is similarly proven by induction for the case \( j < N \) as such

\[
\frac{v_{2i-1,j}^{N}}{v_{2i,j}^{N}} = \frac{k^2 v_{2i-1,j}^{N-1} - v_{2i-3,j}^{N-1}}{k^2 v_{2i,j-1}^{N-1} - v_{2i-2,j}^{N-1}} = j \left( \frac{k^2 v_{2i,j}^{N-1} - v_{2i-2,j}^{N-1}}{k^2 v_{2i,j}^{N-1} - v_{2i-2,j}^{N-1}} \right) = j.
\]

For the case \( i = 1 \), one can see it is also true because from (37) and (40), we have \( v_{0,j}^k = 0 \) for all \( j > 0 \) and \( v_{0,0}^k = 1 \). Therefore, by induction, (34) is true for all \( k > 0 \). All together, these \( v_{i,j}^{N} \) at even \( i \) and right half of the Vandermonde matrix inverse constitute the inverse of the matrix product involving \( a_{n,m} \) and the diagonal matrix on the left hand side of (24).

Next, we discuss the evaluation of \( a_{i,j} \), the derivatives of the fractional power of sinc function at 0. This function is a composite function and its derivatives are given by Faà di Bruno’s formula. However, it is not convenient for use because of the involvement of combinatorics. Instead, one can simply find the corresponding Maclaurin series coefficients. They may be efficiently recovered from the inverse transform of fractional power of the fast Fourier transform of the Maclaurin series coefficients of the sinc function given by

\[
\frac{1}{(2k)!} \int_{-\infty}^{\infty} \sin^2 \left( \frac{x}{2} \right) dx = \frac{(-1)^k}{(2k + 1)!} \frac{1}{2^k},
\]

while the odd cases are all 0. To prove this, one can simply apply Cauchy residue theorem again similar to (19) for the infinite case. And because the Maclaurin series converges about the unit circle for the sinc function, the result is valid. Then to prove that this is also true for the finite case, one just has to realise that the fractional number can be split up into an integer numerator \( p \) and an integer denominator \( q \). Then there exists some transform coefficients such
that their $q$ power gives the original transform coefficients because the integer power of transform coefficients is just convolution of the coefficients with themselves an integer number of times. Therefore, the same coefficients from the infinite case can be recovered using only the finite transform coefficients. Since we would already have the transform of those coefficients, (25) can be solved by directly applying the inverse transform to the reciprocal of the transform coefficients. All in all, let $\partial_n$ be the $2n$-th Maclaurin series coefficients of the sinc function given by (43), $b_n$ in (25) are given by

$$\partial_m = \sum_{n=0}^{N_1} \alpha_n e^{i\omega_m n},$$

$$b_n = \frac{1}{2N+1} \sum_{m=0}^{2N_1} \alpha_m e^{i\omega_m n} = \frac{1}{2N+1} \left( \partial_0 + 2 \sum_{m=1}^{N} \Re \left[ \partial_m e^{i\omega_m n} \right] \right),$$

where $\omega_m = \frac{2\pi m}{2N+1}$.

To summarise, we provide the pseudo code to obtain the stencil for higher order central difference scheme for the Riesz derivative here. Algorithm 1 describes the procedure to invert the transpose of the matrix product on the left hand side of (24). The columns are scaled to better balance the scaling of the sinc Maclaurin series coefficients. Algorithm 2 outputs the right half of the stencil for $N_3$ number of elements between 0 and 1. There are $N_3 - 1$ number of elements in the output because the derivatives at the end points are not needed in dynamic problems as the boundary condition is set there. Let $k$ be the vector returned from Algorithm 2, a $(N_3 - 2) \times (N_3 - 2)$ Toeplitz matrix $D$ can be constructed from $k$ with $D_{i,j} = |k|_{i+j}$ to approximate the derivative as

$$\frac{\partial^i f(x)}{\partial[x]^i} \bigg|_{x = \frac{\pi}{N_3}} \sim \sum_{m=1}^{N_3-2} \left( D_{i-1,m-1} f(x_m) + |k|_{i,m} f(0) + |k|_{N_3-1-i,n} f(1) \right) \text{ for } n = 1, \ldots, N_3 - 2.$$  

If adaptive grid size is required, one can save the last $2N_3$ elements of $k$ before the convolution as well as the filter coefficients of $g$ for the generation of elements in higher indices. The generation of the coefficients can then be resumed, after scaling the coefficients for the larger stencil, from line 14 of Algorithm 2.

**Algorithm 1:** Inversion of integer symmetric Vandermonde matrix with each row $n$ scaled by $\prod_{k=1}^{n} k \left( k - \frac{1}{2} \right)$

1. **Input:** $N$
2. Initialise matrix $V_{i,j} \leftarrow 0$ for $i = 0 \ldots N$, $m = 0 \ldots 0$, and then $V_{0,0} \leftarrow 1$
3. for $k = 1, \ldots, N$
4. $V_{i,k} \leftarrow \left( 2n \right) \cdot |V|_{i-1,k-1} + \left( k - 1 \right) \cdot |V|_{i,k-1} \right) / \left( 2(k - 1) \right)$ for $n = 1 \ldots k$
5. $V_{i,k} \leftarrow \left| V \right|_{i-1,k-1} \cdot \left( -\frac{i(i-1)}{2k(k-1)} \right)$ for $n = 1 \ldots k - 1$
6. $V_{i,k} \leftarrow \left( 2\left| V \right|_{i-1,m} \cdot \left| V \right|_{i,k-1} \right)$ for $m = 0 \ldots k - 1$
7. $V_{i,m} \leftarrow \left( k^2 \cdot V_{i-1,m} - \left( 2n \right) \cdot |V|_{i-1,m} \right) / \left( (k - m)(k + m) \right)$ for $n = 1 \ldots k - 1, m = 0 \ldots k - 1$
8. endfor
9. return $V$

3. **Theory**

First, we study the error convergence. We follow a similar approach given in [5, 6]. A lemma for the smoothness requirement of the function is given before the error analysis. Because of this lemma, which can be considered an extension to the Riemann-Lebesgue lemma, the order requirement for derivative continuity is lower than the ones given in [5, 6].

**Lemma 1.** There exists a constant $C_0$ such that if a function $f : \mathbb{R} \rightarrow \mathbb{R}$ is $C^0$,

$$|\mathcal{F} \{ f \}(\omega)| \leq |\omega|^{-(n+2)} C_0.$$

(47)
Algorithm 2: Riesz derivative higher order central difference stencil

1 Input: $\alpha, N_h, N_x$
2 Evaluate $\tilde{a}_n$ for $n = 0, \ldots, N_h$ using (43)
3 $\tilde{a} \leftarrow$ FFT($\tilde{a}$)
4 $b \leftarrow$ IFFT ($\tilde{a}^\alpha$), superscript for element-wise power
5 $S \leftarrow -1$
6 for $n = 0 \ldots N_h$
7 $\langle b \rangle_n \leftarrow S \cdot \langle b \rangle_{n-1}$
8 $S \leftarrow -4S$
9 endfor
10 $V \leftarrow$ Algorithm 1($N_h$)
11 $g \leftarrow Vb$
12 Initialize $\langle k \rangle_0 = (N_x - 1)\rho \frac{\Gamma(\alpha+1)}{\Gamma(\frac{\alpha+1}{2})}$
13 for $k = 1, \ldots, N_x + N_h - 2$
14 $\langle k \rangle_k \leftarrow \frac{1}{2\pi} \langle k \rangle_{k-1}$
15 endfor
16 $k \leftarrow k_{\text{mirrored}}$, ‘mirrored’ implies the convolution has $k$ and $g$ mirrored to the left about position 0 as negative index elements
17 return $k$ for elements at index 0, $\ldots, N_x - 2$

Proof. Since the $k$-th derivative of $f$ is $L^1$ integrable for $k = 1, \ldots, n + 1$, according to Riemann–Lebesgue lemma, $\mathcal{F}\{f^{(k)}\}(\omega) \to 0$ as $\omega \to \infty$. Applying integration by parts to each Fourier transform of the derivatives of $f$

$$\mathcal{F}\{f^{(k)}\}(\omega) = \int_{\mathbb{R}} f^{(k)}(x) e^{-i\omega x} dx$$

$$= \frac{1}{i\omega} \left( \int_{\mathbb{R}} f^{(k+1)}(x) e^{-i\omega x} dx - \lim_{a \to \infty} \left[ f^{(k)}(x) e^{-i\omega x} \right]_a^{x} \right).$$

Clearly the boundary part vanishes for $k = 1, \ldots, n + 1$, so we have

$$|\mathcal{F}\{f\}(\omega)| = |\omega|^{-(\alpha+1)} |\mathcal{F}\{f^{(\alpha+1)}\}(\omega)|.$$  (48)

However, if we integrate by parts once more, because $f^{(\alpha+1)}$ is not continuous, the integral is broken up into a finite set of continuous regions as

$$\mathcal{F}\{f^{(\alpha)}\}(\omega) = \frac{1}{(i\omega)^\alpha} \left( \sum_{a} \int_{b_a}^{b_{a+1}} f^{(\alpha+2)}(x) e^{-i\omega x} dx - \left[ f^{(\alpha+1)}(x) e^{-i\omega x} \right]_{b_{a+1}}^{b_a} \right),$$

where each of the boundary parts does not vanish. One can see that $f^{(\alpha+1)}$ is finite from the fact that $f^{(\alpha)}$ is continuous at every point. Moreover, each part of the integrals of $f^{(\alpha+2)}$ is also finite because all those parts are $L^1$ integrals. As a result, such a constant $C_0$ exists.

**Theorem 1.** Let $|Df|_n$ be the approximation of Riesz derivative given by (46) at $0 < x_n < 1$. There exists a constant $C_0$ such that if a function $f$ is $C^\alpha$ for $0 < \alpha < 2$, the error of approximation is bounded as

$$|\varepsilon_n| = |Df|_n - \frac{\partial^\alpha f}{\partial x^\alpha}|_{x=x_n} \leq C_0 h^\alpha.$$  (51)

Proof. Let $\tilde{f}$ be the Fourier transform of $f$. According to (21), the frequency response of $Df$ near the origin is given by

$$\mathcal{F}\left\{ \sum_n \delta(x-x_n) |Df|_n \right\}(\omega) = -|\omega|^\alpha \left( 1 + O((\omega h)^\alpha) \right) \tilde{f}.$$  (52)
Then there exists a constant $C_1$ such that the error of approximation in frequency domain

$$
\hat{e}(\omega) = \mathcal{F}\left\{Df - \frac{\partial^N f}{\partial |x|^N}\right\}(\omega)
$$

(53)

satisfies

$$
|\hat{e}(\omega)| \leq C_1 |\omega|^{N+1} h^N |f(\omega)|.
$$

(54)

Now we can apply Lemma 1, and plug (47) into (54) such that the right hand side now uniformly decays with respect to $|\omega|$. Inverse transform leads to (51).

In Theorem 1, we have limited $\alpha$ to be a positive number smaller than 2, which is typical for physics problems, but it can also be generalised to higher order. The smoothness requirement means that this method does require 0 boundary condition. Because the algorithm and analysis is based on the expansion around the origin, the convergence order drops off as we approach Nyquist frequency. For demonstration, we plot the frequency response of the central difference operator divided by the response of Riesz operator given by $\text{sinc}^\alpha \left(\frac{x}{2}\right) \tilde{G}_\alpha(x)$ and the rate of convergence with respect to frequency given by

$$
r(x) = \log_2 \frac{1 - \text{sinc}^\alpha \left(\frac{x}{2}\right) \tilde{G}_\alpha(x)}{1 - \text{sinc}^\alpha \left(\frac{x}{2}\right) G_\alpha(x)},
$$

(55)

where $\tilde{G}_\alpha$ is given by (22), for $x \in [0, \pi]$ and $\alpha = 1.3$. The plots are similar for various $\alpha$, therefore we only plot them for a single value. We see in Figure 1(a) that the flatness of the curve around the origin is improved with increasing $N$. From Figure 1(b), we observe that the higher the convergence order parameter $N$ is, the greater the drop in the convergence order with respect to the normalized angular frequency. This decrease will limit the convergence rate depending on the bandwidth of the function. Despite this, a higher $N$ still results in a greater convergence order as long as the bandwidth of the function is less than 2 times the Nyquist frequency.

Because the Vandermonde matrix can be decomposed into lower and upper triangular matrices without any zero elements in the diagonal entries [10], solutions exist for any $N$. However, because the matrix system (25) does not give us control over derivatives beyond $N$-th order, there is no guarantee that this method ensures that there is no overshoot in the resulting response and the response is always ‘flatter’ than the result of a lower order one. How close the bound (54) is depends on the constant $C_1$, related to the coefficient of $(\omega h)^N$ in the expansion (52), which the formulation does not have explicit control. Nonetheless, numerical results show that there is improvement on the frequency response up to $N = 46$ without extra constraints imposed on the magnitude of higher order Maclaurin series coefficients. The proposed algorithm does become unstable at higher $N$ using double precision floating point.

The Riesz derivative is a negative definite operator, so $g$ has to be positive definite for the correct results. We do not provide a proof for this but numerical results suggest $|g_0| > \sum_{n>0} |g_n|$, which is sufficient for the filter to be positive definite because of Gershgorin circle theorem. Therefore, positivity can be checked with minimal overhead during application of the method. Moreover, because the filter response is symmetric about the point $\pi$, which also means that point is an extremum, and also because the filter should be increasing from the origin to cancel out the downward slope of the sinc function, we should expect that the filter has a response greater than 1 with a maximum at $\pi$. As for the magnitude of this maximum, which leads to the upper bound of the eigenvalue of the Toeplitz matrix in (46), if we assume that $0 < |\text{sinc} \left(\frac{x}{2}\right)|^N G_\alpha(x) \leq 1$ for all $N$ then the upper bound for the maxima is $\pi^\alpha$ and so the magnitude of the eigenvalue of the Toeplitz matrix is bounded by $(\pi N_\alpha)^\alpha$.

4. Numerical Experiment

To verify the error analysis, we apply the derivative operator to

$$
u(x) = \begin{cases} x^q (1 - x)^q, & \text{for } x \in [0, 1], \\ 0, & \text{otherwise.} \end{cases}
$$

(56)
This function belongs to $C^{q'}$ and its Riesz derivative is given in closed-form as

$$
\frac{d^q u(x)}{d|x|^q} = C_\alpha \sum_{n=0}^{q} \binom{q}{n} \frac{\Gamma(q + n + 1)}{\Gamma(q + n + 1 - \alpha)} \left( x^{q+n-\alpha} + (1-x)^{q+n-\alpha} \right).
$$

We define the error and convergence rate respectively as

$$
E_i^N = \sum_{j=1}^{N-1} \left| \tilde{u}_N \left( \frac{x_j}{\min} \right) - \frac{d^q u(x)}{d|x|^q} \left| x = \frac{x_j}{\min} \right|, \right.
$$

$$
R_i^N = \log_2 \frac{E_i^N}{E_{i+1}^N},
$$

where $\tilde{u}_N$ is the $N$ order accurate approximation of the Riesz derivative using (46), $N_{\min} = 11$, and $N_i = 2^i (N_i - 1) + 1$ is the number of nodes. The results are tabulated in Tables 1-4. From the results for $q = 6$, we see that the approximation converges at a rate close to $O(h^N)$ for all tested $N$ even though the smoothness requirement is not always met. This can be explained by the bandwidth of the polynomial being within the Nyquist frequency and tapers sufficiently fast. This allows the error from within the Nyquist frequency region to dominate and so the error reduction is as expected. We do see that with smaller $N_i$, the convergence order is more suppressed with more of the main lobe of frequency response of $u$ being in the higher end region. For $q = 10$, we see that the results converge similarly with $R_i^N$ being even more limited at higher $N$ and lower $N_i$. This is because at higher $q$, $u$ oscillates more and so the frequency response has a higher bandwidth. It appears that the error converges to a small value that is independent of the filter order and number of nodes but only dependent on $\alpha$ and $q$. Therefore, it is unlikely that this convergence barrier is a result of the error from the region in higher frequencies than Nyquist frequency either because the operator response in those areas is lifted by the filter we introduced, which would translate into lower error for higher $N$. We also cannot attribute this to the numerical errors in evaluating the stencil or the filter since the error would be multiplied by $N_i^\alpha$. It is improbable that this error barrier will become a significant factor in application but it may be investigated in future work if problems arise.

Because of the unexpected convergence for the previous problem, we look at a problem with discontinuity at the boundary. This time we let $u(x) = \cos(2\pi f x)$, $f = 11$ with compact support in $x \in [0, 1]$. The solution is given in closed-form as

$$
\frac{d^q \cos(2\pi f x)}{d|x|^q} = C_\alpha \left( D^q_{\alpha} f(x) + \partial D^q_{\alpha} f(x) \right),
$$

$$
D^q_{\alpha} f(x) = \frac{x^{-\alpha}}{2^{2-\alpha} \sqrt{\pi}} \left( (\alpha - 2)(\alpha - 1) \right) F_2 \left( 1; \frac{3-\alpha}{2}, \frac{4-\alpha}{2}; - (\pi f x)^2 \right)
$$

$$
+ (2\pi f x)^2 (\alpha - 5) \right) \left\{ F_2 \left( 2; \frac{5-\alpha}{2}, \frac{6-\alpha}{2}; - (\pi f x)^2 \right) + 8 (\pi f x)^4 \right\} \left\{ F_2 \left( 3; \frac{7-\alpha}{2}, \frac{8-\alpha}{2}; - (\pi f x)^2 \right) \right\}.
$$

The numerical results are given in Table 5 and 6. The transform of the truncated cosine function is given by the sum of two sinc functions centered at $\omega = \pm 2\pi f$. This means that when $N_i < 2f$, the main lobes are beyond Nyquist frequency. Therefore, we can see that the convergence is much more limited at lower $N_i$. Convergence rate recovers once the main lobe goes within the Nyquist frequency region. However, due to the decay rate of the sinc function being at $\omega^{-1}$, convergence is limited to $O\left(N_i^{-1}\right)$. We can conclude that for non-zero boundary condition, polynomial type approximation is more suitable as seen in [11, 12].

5. Conclusion

An efficient method to develop stencil from central difference for Riesz difference for even higher order of convergence than 4 is presented. Numerical results verify the greater convergence rates as predicted in Section 3. The error analysis is performed in the frequency domain, and because of the sinc function, Nyquist rate applies to the
convergence of the method. There is an extra cost of $O(N^2)$ operations for the evaluation of the filter and $O(NN_x)$ operations for the convolution. However, the higher convergence speed at $O(N^{-N})$ will significantly reduce the amount of nodal points required to achieve a particular error tolerance as demonstrated in numerical experiments such that the overhead will end up saving computational time and memory resources.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Tables

Table 1: $E_k$ for $q = 6$

| $\hat{N}$ | $\alpha = 0.2$ | $\alpha = 1.8$ |
|-----------|----------------|----------------|
|           | 4              | 6              | 8   | 10 | 4   | 6   | 8   | 10 |
| 0         | 8.492e-07      | 2.28e-07       | 8.90e-08 | 4.697e-08 | 0.0006732 | 0.0002419 | 0.000197 | 7.57e-05 |
| 1         | 5.639e-08      | 4.50e-09       | 5.939e-10 | 8.798e-11 | 5.104e-05 | 6.092e-06 | 9.398e-07 | 1.009e-07 |
| 2         | 3.573e-09      | 7.417e-11      | 2.629e-12 | 7.651e-14 | 3.323e-06 | 9.783e-08 | 1.983e-09 | 2.946e-10 |
| 3         | 2.225e-10      | 1.176e-12      | 1.088e-14 | 2.908e-15 | 2.046e-07 | 1.532e-09 | 8.39e-12  | 2.108e-13 |
| 4         | 1.351e-11      | 2.035e-14      | 2.966e-15 | 2.958e-15 | 1.147e-08 | 2.36e-11  | 1.428e-13 | 1.199e-13 |
| 5         | 7.416e-13      | 3.007e-15      | 2.959e-15 | 2.959e-15 | 3.772e-10 | 2.333e-13 | 1.388e-13 | 1.366e-13 |

Table 2: $R_k$ for $q = 6$

| $\hat{N}$ | $\alpha = 0.2$ | $\alpha = 1.8$ |
|-----------|----------------|----------------|
|           | 4              | 6              | 8   | 10 | 4   | 6   | 8   | 10 |
| 0         | 3.91           | 5.66           | 7.23 | 9.06 | 3.72 | 5.31 | 6.99 | 9.55 |
| 1         | 3.98           | 5.92           | 8.03 | 10.2 | 3.94 | 5.96 | 8.89 | 8.42 |
| 2         | 4.01           | 5.98           | 7.70 | 4.72 | 4.02 | 6  | 7.90 | 10.4 |
| 3         | 4.04           | 5.84           | 1.88 | -0.0247 | 4.16 | 6.02 | 5.86 | 0.814 |
| 4         | 4.19           | 2.77           | 0.00356 | -0.000493 | 4.93 | 6.66 | 0.0403 | -0.188 |

Table 3: $E_k$ for $q = 10$

| $\hat{N}$ | $\alpha = 0.2$ | $\alpha = 1.8$ |
|-----------|----------------|----------------|
|           | 4              | 6              | 8   | 10 | 4   | 6   | 8   | 10 |
| 0         | 6.193e-09      | 2.707e-09      | 1.502e-09 | 9.186e-10 | 7.223e-06 | 3.866e-06 | 2.309e-06 | 1.488e-06 |
| 1         | 4.250e-10      | 5.906e-11      | 1.100e-11 | 2.509e-12 | 6.054e-07 | 1.078e-07 | 2.327e-08 | 6.374e-09 |
| 2         | 2.721e-11      | 9.958e-13      | 5.871e-14 | 2.793e-14 | 4.073e-08 | 1.962e-09 | 1.233e-10 | 1.042e-11 |
| 3         | 1.731e-12      | 4.026e-14      | 2.686e-14 | 2.674e-14 | 2.562e-09 | 3.119e-11 | 1.589e-12 | 1.414e-12 |
| 4         | 1.322e-13      | 2.695e-14      | 2.674e-14 | 2.674e-14 | 1.518e-10 | 1.719e-12 | 1.418e-12 | 1.419e-12 |
| 5         | 3.302e-14      | 2.674e-14      | 2.674e-14 | 2.674e-14 | 7.425e-12 | 1.418e-12 | 1.419e-12 | 1.419e-12 |
Table 4: $R^2_d$ for $q = 10$

| $\alpha = 0.2$ | $\alpha = 1.8$ |
|----------------|----------------|
|                | $\alpha = 0.2$ | $\alpha = 1.8$ |
| $\hat{i}N$    | 4 | 6 | 8 | 10 | 4 | 6 | 8 | 10 |
|----------------|---|---|---|----|---|---|---|----|
| 0              | 3.87 | 5.52 | 7.09 | 8.52 | 3.58 | 5.18 | 6.63 | 7.87 |
| 1              | 3.97 | 5.89 | 7.55 | 6.49 | 3.89 | 5.77 | 7.56 | 9.26 |
| 2              | 3.97 | 4.63 | 1.13 | 0.0626 | 3.99 | 5.97 | 6.28 | 2.88 |
| 3              | 3.71 | 0.579 | 0.00646 | -3.55e-05 | 4.08 | 4.18 | 0.164 | -0.00437 |
| 4              | 2.00 | 0.0110 | -3.90e-06 | -6.71e-08 | 4.35 | 0.278 | -0.000345 | -0.000128 |

Table 5: $E^2_d$ for $\cos(2\pi f x)$, $f = 11$

| $\alpha = 1.2$ | $\alpha = 1.8$ |
|----------------|----------------|
|                | $\alpha = 1.2$ | $\alpha = 1.8$ |
| $\hat{i}N$    | 4 | 6 | 8 | 10 | 4 | 6 | 8 | 10 |
|----------------|---|---|---|----|---|---|---|----|
| 0              | 831.9 | 832.2 | 832.4 | 832.6 | 11060 | 11060 | 11070 | 11070 |
| 1              | 345.2 | 305.3 | 281.9 | 266.4 | 5915 | 5314 | 4946 | 4695 |
| 2              | 38.98 | 15.37 | 7.111 | 3.835 | 757.6 | 296.4 | 127.5 | 58.70 |
| 3              | 3.380 | 1.014 | 0.9050 | 0.9107 | 58.04 | 7.690 | 2.094 | 1.514 |
| 4              | 0.5387 | 0.4642 | 0.4651 | 0.4651 | 4.367 | 0.8183 | 0.7831 | 0.7837 |
| 5              | 0.2328 | 0.2348 | 0.2348 | 0.2348 | 0.5690 | 0.3968 | 0.3971 | 0.3971 |

Table 6: $R^2_d$ for $\cos(2\pi f x)$, $f = 11$

| $\alpha = 1.2$ | $\alpha = 1.8$ |
|----------------|----------------|
|                | $\alpha = 1.2$ | $\alpha = 1.8$ |
| $\hat{i}N$    | 4 | 6 | 8 | 10 | 4 | 6 | 8 | 10 |
|----------------|---|---|---|----|---|---|---|----|
| 0              | 1.27 | 1.45 | 1.56 | 1.64 | 0.903 | 1.06 | 1.16 | 1.24 |
| 1              | 3.15 | 4.31 | 5.31 | 6.12 | 2.96 | 4.16 | 5.28 | 6.32 |
| 2              | 3.53 | 3.92 | 2.97 | 2.07 | 3.71 | 5.27 | 5.93 | 5.28 |
| 3              | 2.65 | 1.13 | 0.960 | 0.969 | 3.73 | 3.23 | 1.42 | 0.950 |
| 4              | 1.21 | 0.983 | 0.986 | 0.986 | 2.94 | 1.04 | 0.980 | 0.981 |

Table 7: $E^2_d$ for $\cos(2\pi f x)$, $f = 11$
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Figures

(a) Relative frequency response of the central difference operator against that of Riesz derivative

(b) Spectral convergence rate given by (55)

Figure 1: Frequency response and spectral convergence rate of higher order fractional central difference method

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