

**Extrapolation to the Limit  
for Numerical Fractional Differentiation**

MSC(1991): 65B05, 65D25

**1. Introduction**

Let  $f$  be given on  $\mathbb{R}$ . The Grünwald-Letnikov difference operator of positive order  $\alpha$  is defined by the formula ([3])

$$(\Delta_h^\alpha f)(x) = \sum_{j=0}^{\infty} (-1)^j \binom{\alpha}{j} f(x - jh), \quad h > 0, \quad x \in \mathbb{R}. \quad (1)$$

Under some conditions the operator  $h^{-\alpha} \Delta_h^\alpha f$  has been proved to converge to the Weyl fractional differentiation  $D_+^\alpha f$  as  $h \rightarrow 0$  ([3]). On the Weyl fractional differentiation  $D_+^\alpha$

$$(D_+^\alpha f)(x) = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dx^n} \int_{-\infty}^x (x - t)^{n - \alpha - 1} f(t) dt, \quad x \in \mathbb{R}, \quad n = [\alpha] + 1, \quad (2)$$

one may consult ([1, 3]). The operator  $D_+^\alpha$  is the left-inverse to the Weyl integral operator  $I_{-\infty}^\alpha$  defined by

$$(I_{-\infty}^\alpha u)(t) = \frac{1}{\Gamma(\alpha)} \int_{-\infty}^t (t - x)^{\alpha - 1} u(x) dx, \quad t \in \mathbb{R}, \quad \alpha > 0, \quad (3)$$

and hence, formally,  $u = D_+^\alpha f$  solves the Weyl integral equation  $I_{-\infty}^\alpha u = f$ . In [4] and [5] we have shown how the operator  $h^{-\alpha} \Delta_h^\alpha$  can be used not only for approximately solving this equation and the analogous Abel integral equation if the data are smooth but also for obtaining a regularized solution if instead of the exact data function an error-perturbed function  $\tilde{f}$  is given, deviating from  $f$  by a positive  $\epsilon$  in a suitable norm. The essence of our regularization method was to balance the discretization error  $h^{-\alpha} \Delta_h^\alpha f - D_+^\alpha f$  (whose order is given by the leading term of its asymptotic expansion in powers of  $h$ ) and the error resulting from the inexactness of the data (that is  $O(h^{-\alpha}\epsilon)$ ) by an appropriate choice of the steplength  $h$ , the aim being to obtain an optimal bound of the total error.

In the present paper our goal is another one, namely, to show that the error committed by approximating  $(D_+^\alpha f)(x)$  by  $h^{-\alpha} (\Delta_h^\alpha f)(x)$  possesses an asymptotic expansion in integer powers of the steplength  $h$  (as  $h \rightarrow 0$ ) if  $f$  is in  $C^\infty$  (a terminating one if  $f$  has only a finite degree of smoothness), and to derive a similar result (an expansion in even powers of  $h$ ) for the shifted operator

$$(\bar{\Delta}_h^\alpha f)(x) = \sum_{j=0}^{\infty} (-1)^j \binom{\alpha}{j} f(x + \alpha h/2 - jh), \quad h > 0, \quad (4)$$

that reduce to the standard central difference operators if  $\alpha$  is a positive integer. Thanks to the existence of such asymptotic expansions one can then apply the well-known method of "extrapolation to the limit" (that has its origins in the ideas of Richardson extrapolation, the Aitken acceleration of convergence, the Neville algorithm for interpolation, and that is

algorithmically analogous to the Romberg scheme for numerical integration) for improving the order of convergence. Because Henrici's booklet [2] in its chapter 12 exemplifies this method in a particularly lucid way in its application to numerical differentiation (of approximating  $f'(x)$ ) we use it as a reference text.

## 2. Extrapolation to the limit

Let  $f \in C^{[\alpha]+n+1}(\mathbb{R})$  and all derivatives of  $f$  up to the order  $[\alpha] + n + 2$  belong to  $L_1(\mathbb{R})$ . Then the Fourier transform

$$\hat{\varphi}(x) = \int_{\mathbb{R}} \varphi(t) \exp(ixt) dt$$

of the Grünwald–Letnikov difference operator (1) exists and has the form

$$(\widehat{\Delta}_h^\alpha f)(x) = (1 - \exp(ixh))^\alpha \hat{f}(x) \quad (5)$$

(see [3]). Let the function  $(\frac{1-\exp(-x)}{x})^\alpha$  have the Taylor expansion

$$\left(\frac{1 - \exp(-x)}{x}\right)^\alpha = \sum_{k=0}^{\infty} a_k x^k, \quad (6)$$

that converges in some vicinity of 0. It is easy to see that  $a_0 = 1$ ,  $a_1 = -\alpha/2$ . Therefore,

$$h^{-\alpha}(\widehat{\Delta}_h^\alpha f)(x) = (-ix)^\alpha \left(1 + \sum_{k=1}^{n-1} a_k (-ixh)^k\right) \hat{f}(x) + \hat{\varphi}(x, h), \quad (7)$$

where

$$\hat{\varphi}(x, h) = \left[ \left(\frac{1 - \exp(ixh)}{-ixh}\right)^\alpha - \sum_{k=0}^{n-1} a_k (-ixh)^k \right] (-ix)^\alpha \hat{f}(x). \quad (8)$$

Since the function  $(\frac{1-\exp(ix)}{-ix})^\alpha$  is bounded on  $\mathbb{R}$ , it is not difficult to see that there exists a universal constant  $C$  such that

$$\left| \left(\frac{1 - \exp(ix)}{-ix}\right)^\alpha - \sum_{k=0}^{n-1} a_k (-ix)^k \right| \leq C|x|^n.$$

Therefore,

$$|\hat{\varphi}(x, h)| \leq Ch^n |x|^{\alpha+n} |\hat{f}(x)|.$$

From the conditions imposed on  $f$  we conclude that  $(1 + |x|)^{[\alpha]+n+2} \hat{f}(x)$  is bounded on  $\mathbb{R}$ . Hence  $|x|^{\alpha+n} |\hat{f}(x)| \in L_1(\mathbb{R})$ . Consequently,

$$|\varphi(x, h)| \leq Ch^n,$$

where  $\varphi(x, h)$  is the inverse Fourier transform of the function  $\hat{\varphi}(x, h)$ , and the constant  $C$  does not depend on  $x$ . Since

$$(-ix)^{\alpha+k} \hat{f}(x) = (\widehat{D}_+^{\alpha+k} f)(x), \quad k = 0, 1, \dots, n-1, \quad (9)$$

(see [3]), we have

$$h^{-\alpha}(\Delta_h^\alpha f)(x) = (D_+^\alpha f)(x) - \frac{\alpha h}{2} (D_+^{\alpha+1} f)(x) + \sum_{k=2}^{n-1} a_k (D_+^{\alpha+k} f)(x) h^k + O(h^n) \quad (10)$$

uniformly on  $\mathbb{R}$ . Therefore we have proved

**Theorem 1.** Let  $\alpha$  be a positive number,  $f \in C^{[\alpha]+n+1}(\mathbb{R})$ , all derivatives of  $f$  up to the order  $[\alpha] + n + 2$  exist and belong to  $L_1(\mathbb{R})$ . Then formula (10) holds uniformly on  $\mathbb{R}$ .

Formula (10) is the base of the method of extrapolation to the limit (see [2]). Therefore, one can apply it to the Grünwald–Letnikov difference operator to obtain the convergence rate with arbitrary high order  $h^k$ ,  $k = 1, \dots, n$ . In particular,

$$h^{-\alpha} \frac{q^{-\alpha} (\Delta_{qh}^\alpha f)(x) - q (\Delta_h^\alpha f)(x)}{1 - q}, \quad 0 < q < 1, \quad q \text{ fixed}, \quad (11)$$

converges to  $(D_+^\alpha f)(x)$  with order  $h^2$ .

**Remark 1.** Instead of the infinite sum (1) one can take a finite sum with the same accuracy. Indeed, from the conditions imposed on  $f$  we have that  $f$  is uniformly bounded on  $\mathbb{R}$ , therefore,

$$\sum_{j=m}^{\infty} (-1)^j \binom{\alpha}{j} f(x - jh) = O(m^{-\alpha}),$$

since, by Stirling's formula,

$$\binom{\alpha}{j} = O(j^{-\alpha-1}).$$

Consequently,

$$\begin{aligned} h^{-\alpha} (\Delta_{h,m}^\alpha f)(x) &= h^{-\alpha} \sum_{j=0}^m (-1)^j \binom{\alpha}{j} f(x - jh) \\ &= (D_+^\alpha f)(x) - \frac{\alpha h}{2} (D_+^{\alpha+1} f)(x) + \sum_{k=2}^{n-1} a_k (D_+^{\alpha+k} f)(x) h^k + O(h^n), \end{aligned} \quad (12)$$

if  $m$  is a big enough natural number,  $m \geq ch^{-n/\alpha}$  with an arbitrary positive constant  $c$ .

**Remark 2.** Since both sides of (10) and (12) do not depend on the values of the function  $f$  on the right half-line  $(x, \infty)$ , Theorem 1, Remark 1 and all above conclusions are still valid, if  $f$  is given on the left half-line  $(-\infty, a)$  instead of  $\mathbb{R}$ , and all estimates hold uniformly on this half-line.

### 3. The shifted Grünwald–Letnikov difference operator

Although extrapolation to the limit can give convergence rate of order  $h^k$ ,  $k$  –arbitrary, if  $f$  is a smooth enough function, in case  $k = 2$  a simpler formula can be applied. This is a generalization of the symmetric difference operator

$$\frac{f(x + h/2) - f(x - h/2)}{h}. \quad (13)$$

We consider the shifted Grünwald–Letnikov difference operator (4) that reduces to (13) when  $\alpha = 1$ . We have

$$(\widehat{\Delta}_h^\alpha f)(x) = (\exp(-ixh/2) - \exp(ixh/2))^\alpha \hat{f}(x) = (-2i \sin(xh/2))^\alpha \hat{f}(x). \quad (14)$$



In this scheme the column with second index  $j$  will converge with order  $O(h^{j+1})$  if  $j+1 \leq n$  with  $n$  as in formula (12).

Let us take the function

$$f(x) = \begin{cases} x^4 & \text{if } 0 < x \leq 2 \\ 0 & \text{if } x \leq 0 \end{cases},$$

Let  $\alpha = 0,5$ . Then

$$(D_+^{0,5} f)(x) = \frac{\Gamma(5)}{\Gamma(4,5)} x^{4,5} \approx 2.06332190554 x^{3,5}, \quad 0 \leq x \leq 2.$$

Since  $f^{(4)} \in L_1(-\infty, 2)$  we see, using Remark 2, that in Theorem 1 one can take  $n = 2$ , so that the column with second index 1 of our scheme will converge with order 2 to the precise value.

Taking now  $x = 1$ ,  $h = 10^{-1}$ ,  $q = 0.5$ , we obtain, using formula (1), the tableau

1.89197399493					
1.97537598845	2.05877798197				
2.01877113509	2.06216628173	2.06329571498			
2.04090083363	2.06303053217	2.06331861565	2.06332188717		
2.05207479333	2.06324875303	2.06332149332	2.06332190443	2.06332190558	
2.05768918603	2.06330357873	2.06332185396	2.06332190549	2.06332190556	
2.06050325251	2.06331731899	2.06332189908	2.06332190551	2.06332190551	
2.06191200541	2.06332075831	2.06332190475	2.06332190556	2.06332190557	

We number these columns successively by 0,1,2,3,4 (second index). Since  $f(x) \equiv 0$  for  $x \leq 0$  the series for calculating the column with second index 0 terminates when  $x - 2^{-m} j h \leq 0$ .

To exhibit the convergence orders we have calculated the error ratios. Using our knowledge of the exact value (to eleven decimal places) 2.06332190554 we can first determine the errors and then the ratios of successive errors. For example, the errors of the first two entries in column 0 are 0.1713 and 0.08795 (to four significant decimals) and their ratio is 1.948. Continuing in this way we obtain the tableau of error ratios as follows

1.948				
1.974	3.931			
1.987	3.967	7.963		
1.993	3.984	7.979	16.55	
1.997	3.991	7.991	22.2	
1.998	3.996	7.985	-5	
1.999	3.999	8.177	1	

Since already column 3 is essentially produced by rounding noise we do not show column 4 of this tableau. However, the preceding columns hint impressively towards successive convergence orders 1, 2, 3, and in column 3 there is a weak hint that it may converge with order 4.

**Remark 3.** Although Theorem 1 gives the convergence rate of order 2 of column 1 of the first tableau, it cannot guarantee the higher convergence rate of the following columns.

The phenomenon will be explained in a forthcoming work, where the extrapolation to the limit for the Abel numerical fractional differentiation will be studied. In our case the Weyl fractional differentiation of the function  $x^4$  on  $(0, 2)$  coincides with the Abel fractional differentiation of  $x^4$  that is in  $C^\infty(0, 2)$ .

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