VECTOR GRÜNWALD FORMULA FOR FRACTIONAL DERIVATIVES

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Abstract. The Grünwald formula is used to numerically estimate fractional derivatives. It is an extension of the finite difference formula for integer order derivatives. This paper develops an extension of the Grünwald formula for vector fractional derivatives. This result should be useful for numerical solution of fractional partial differential equations where the space variable is a vector.

1. Introduction

Fractional derivatives have been around for centuries [22, 26] but recently they have found new applications in physics [2, 6, 7, 9, 15, 18, 19, 29], hydrology [1, 4, 5, 10, 14, 28], and finance [24, 25, 27]. Analytical solutions of ordinary fractional differential equations [22, 23] and partial fractional differential equations [8, 16] are now available in some special cases. But the solution to many fractional differential equations will have to rely on numerical methods, just like their integer-order counterparts. Numerical solutions of fractional differential equations require a numerical estimate of the fractional derivative. In one dimension, this estimate is called the Grünwald formula [20, 22, 26]. A variant of this formula has been used to develop practical numerical methods for solving certain fractional partial differential equations that model flow in porous media [21, 30]. The purpose of this paper is to develop a multivariable analogue of the Grünwald formula for estimating multidimensional fractional derivatives, so that the results in [21, 30] can be extended to two and three dimensional flow regimes.

The scalar Grünwald formula is a discrete approximation to the fractional derivative by a fractional difference quotient

$$\frac{d^\alpha f(x)}{dx^\alpha} = \lim_{h\to 0} h^{-\alpha}\Delta_h^\alpha f(x) = \lim_{h\to 0} h^{-\alpha}\sum_{m=0}^{\infty}(-1)^m\binom{\alpha}{m} f(x-mh) \tag{1.1}$$

where for noninteger $\alpha > 0$ the binomial coefficient

$$\binom{\alpha}{m} = \frac{(-1)^{m-1}\alpha\Gamma(m-\alpha)}{\Gamma(1-\alpha)\Gamma(m+1)}, \tag{1.2}$$

see for example [20, 26]. When α is a positive integer, the sum terminates at $m=\alpha$ and equation (1.1) reduces to the usual one-sided difference formula for the derivative. In this

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paper, we extend (1.1) to multivariable fractional derivatives, see Theorems 4.1 and 4.3 below.

The multivariable fractional derivative first appeared in [16] in connection with a model of anomalous diffusion. Given $f : \mathbb{R}^d \to \mathbb{R}$ and using the Fourier transform convention $\hat{f}(k) = \int e^{i\langle k,x\rangle} f(x)dx$ we specify this operator by requiring that $D_M^\alpha f(x)$ has Fourier transform

$$\left[\int_{\|\theta\|=1} (-i\langle k,\theta\rangle)^\alpha M(d\theta)\right] \hat{f}(k) \tag{1.3}$$

where $M(d\theta)$ is an arbitrary probability measure on the unit sphere $S^{d-1} = \{x \in \mathbb{R}^d : \|x\| = 1\}$. If $d = 1$ then (1.3) reduces to

$$\big(p(-ik)^\alpha + (1-p)(ik)^\alpha\big)\hat{f}(k)$$

so that

$$D_M^\alpha f(x) = p\frac{d^\alpha f(x)}{dx^\alpha} + (1-p)\frac{d^\alpha f(x)}{d(-x)^\alpha}.$$

When $\alpha = 2$ the integral in equation (1.3) reduces to

$$-\int_{\|\theta\|=1} \left(\sum_{j=1}^d k_j\theta_j\right)^2 M(d\theta) = (-ik)\cdot A(-ik) \tag{1.4}$$

where the matrix $A = (a_{ij})$ with $a_{ij} = \int \theta_i\theta_j M(d\theta)$. Then

$$D_M^\alpha f(x) = \nabla \cdot A\nabla f(x) = \sum_{i=1}^d \sum_{j=1}^d a_{ij}\frac{\partial^2 f(x)}{\partial x_i \partial x_j}.$$

The vector fractional derivative appears in the diffusion/dispersion term of evolution equations as a generalization of this Laplacian term. The fractional order α speeds up the diffusion of a cloud of particles as α decreases, and the mixing measure M governs the direction of large particle jumps, allowing an asymmetric plume.

2. Preliminary Results

In this section, we show that the multivariable fractional derivative operator $D_M^\alpha f(x)$ defined by the Fourier transform in (1.3) above, for certain functions, can be represented as a mixture of fractional directional derivatives $D_\theta^\alpha f(x)$. This will enable us in the next section to apply the scalar Grünwald formula in each radial direction. We assume throughout this section that $\alpha > 0$ is not an integer and that θ is a unit vector in $\mathbb{R}^d$.

The directional derivative $D_\theta f(x) = \langle \theta, \nabla f(x)\rangle = \sum_j \theta_j \partial f(x)/\partial x_j = dg/ds$ at $s = 0$ where $g(s) = f(x + s\theta)$. Its Fourier transform is

$$\sum_{j=1}^d \theta_j(-ik_j)\hat{f}(k) = (-i\langle k,\theta\rangle)\hat{f}(k)$$

since $(-ik_j)\hat{f}(k)$ is the Fourier transform of $\partial f(x)/\partial x_j$. The scalar fractional derivative can be defined by

$$D_+^\alpha g(s) = \frac{1}{\Gamma(n-\alpha)} \frac{d^n}{ds^n} \int_0^\infty r^{n-\alpha-1} g(s-r)dr$$

where $n = 1 + [\alpha]$ is the smallest integer greater than α, and it is easy to check that this convolution integral has Fourier transform $(-iu)^\alpha \hat{g}(u)$, see [3, 26]. The fractional order directional derivative $D_\theta^\alpha f(x)$ is defined by $D_+^\alpha g(s)$ evaluated at $s = 0$, where $g(s) = f(x + s\theta)$. Then it is clear that $D_\theta^\alpha f(x)$ has Fourier transform $(-i\langle k, \theta\rangle)^\alpha \hat{f}(k)$ which reduces to the classical case when $\alpha = 1$. Now (1.3) is revealed as a mixture of fractional directional derivatives. The next theorem will make this precise.

Definition 2.1. For any positive integer l, let $W^{l,1}(\mathbb{R}^d)$ denote the collection of functions $f \in C^l(\mathbb{R}^d)$ whose partial derivatives up to order l are in $\mathcal{L}^1(\mathbb{R}^d)$ and whose partial derivatives up to order $l-1$ vanish at infinity.

Theorem 2.2. *For $f \in W^{l,1}(\mathbb{R}^d)$ with $l = [\alpha] + 2$ we have*

$$D_M^\alpha f(x) = \int_{\|\theta\|=1} D_\theta^\alpha f(x) M(d\theta) \quad a.e. \tag{2.1}$$

Remark 2.3. If we define $D_M^\alpha f$ by (2.1), then the proof below shows

$$(D_M^\alpha f)\widehat{\ }(k) = \int_{\|\theta\|=1} (-i\langle k, \theta\rangle)^\alpha M(d\theta) \hat{f}(k)$$

so no *a.e.* is needed in (2.1).

Before we prove Theorem 2.2 we need the following technical result. Recall that the Gamma function defined for $t > 0$ by $\Gamma(t) = \int_0^\infty x^{t-1} e^{-x} dx$ can be extended to the rest of the complex plane, less the non-positive integers, by analytic continuation, and that consequently the formula $\Gamma(t+1) = t\Gamma(t)$ holds for all real t, less the non-positive integers.

Lemma 2.4. *For $f \in W^{l,1}(\mathbb{R}^d)$ with $l = [\alpha] + 2$ we have*

$$D_\theta^\alpha f(x) = \frac{-1}{\Gamma(1-\alpha)} \int_0^\infty \Big[f(x - r\theta) - \sum_{p=0}^{[\alpha]} \frac{(-r)^p}{p!} D_\theta^p f(x) \Big] \alpha r^{-\alpha-1}\, dr \tag{2.2}$$

a.e., where $[\alpha]$ denotes the integer part of α. Moreover, there exists a constant $C > 0$ (independent of θ) such that

$$\int_{\mathbb{R}^d} |D_\theta^\alpha f(x)| dx \le C \tag{2.3}$$

for all $\theta \in S^{d-1}$.

Proof. Let $g(x,\theta)$ denote the right hand side of (2.2). We first show that for some constant $C>0$ (independent of θ) we have

$$\int_{\mathbb{R}^d} |g(x,\theta)|dx \le C \tag{2.4}$$

for all $\theta \in S^{d-1}$.

Note that by Taylor expansion with integral form of the remainder we obtain

$$f(x-r\theta) - \sum_{p=0}^{[\alpha]} \frac{(-r)^p}{p!} D_\theta^p f(x) = \frac{(-1)^{[\alpha]+1}}{[\alpha]!} \int_0^r D_\theta^{[\alpha]+1} f(x-s\theta)(r-s)^{[\alpha]}\, ds \tag{2.5}$$

Write for any $\delta>0$

$$\begin{aligned}\int_{\mathbb{R}^d} |g(x,\theta)|\, dx &\le |C_\alpha| \int_{\mathbb{R}^d} \int_0^\delta \Big| f(x-r\theta) - \sum_{p=0}^{[\alpha]} \frac{(-r)^p}{p!} D_\theta^p f(x)\Big| \alpha r^{-\alpha-1}\, dr\, dx \\ &\quad + |C_\alpha| \int_{\mathbb{R}^d} \int_\delta^\infty \Big| f(x-r\theta) - \sum_{p=0}^{[\alpha]} \frac{(-r)^p}{p!} D_\theta^p f(x)\Big| \alpha r^{-\alpha-1}\, dr\, dx \\ &= |C_\alpha|(I_1+I_2)\end{aligned} \tag{2.6}$$

where $C_\alpha = -1/\Gamma(1-\alpha)$. Now by Tonelli we have

$$\begin{aligned} I_2 &\le \int_\delta^\infty \left(\int_{\mathbb{R}^d} |f(x-r\theta)|\, dx + \sum_{p=0}^{[\alpha]} \frac{r^p}{p!} \int_{\mathbb{R}^d} |D_\theta^p f(x)|\, dx \right) \alpha r^{-\alpha-1}\, dr \\ &= \|f\|_1 \int_\delta^\infty \alpha r^{-\alpha-1}\, dr + \sum_{p=0}^{[\alpha]} \frac{1}{p!} \|D_\theta^p f\|_1 \int_\delta^\infty \alpha r^{p-\alpha-1}\, dr < \infty \end{aligned} \tag{2.7}$$

since $p-\alpha-1 \le [\alpha]-\alpha-1 < -1$ for all $0 \le p \le [\alpha]$.

For I_1 we obtain by using (2.5)

$$\begin{aligned} I_1 &\le \int_{\mathbb{R}^d} \int_0^\delta \left| \frac{1}{[\alpha]!} \int_0^r D_\theta^{[\alpha]+1} f(x-s\theta)(r-s)^{[\alpha]}\, ds \right| \alpha r^{-\alpha-1}\, dr\, dx \\ &\le \frac{1}{[\alpha]!} \int_{\mathbb{R}^d} \int_0^\delta \int_0^r \left| D_\theta^{[\alpha]+1} f(x-s\theta)\right| (r-s)^{[\alpha]}\, ds\, \alpha r^{-\alpha-1}\, dr\, dx \\ &= \frac{1}{[\alpha]!} \int_0^\delta \int_0^r \int_{\mathbb{R}^d} \left| D_\theta^{[\alpha]+1} f(x-s\theta)\right|\, dx (r-s)^{[\alpha]}\, ds\, \alpha r^{-\alpha-1}\, dr \\ &= \|D_\theta^{[\alpha]+1} f\|_1 \frac{1}{[\alpha]!} \int_0^\delta \int_0^r (r-s)^{[\alpha]}\, ds\, \alpha r^{-\alpha-1}\, dr \\ &= \|D_\theta^{[\alpha]+1} f\|_1 \frac{\alpha}{([\alpha]+1)!} \int_0^\delta r^{-\alpha+[\alpha]}\, dr < \infty \quad (\text{since } -\alpha+[\alpha] > -1) \end{aligned} \tag{2.8}$$

Then (2.6) along with (2.7) and (2.8) prove (2.4).

Recall that the Fourier transform of $f(x-a)$ is $e^{i\langle k,a\rangle}\hat{f}(k)$. In view of (2.4) we compute using Fubini's theorem

$$\begin{aligned}\hat{g}(k,\theta) &= \int_{\mathbb{R}^d} e^{i\langle k,x\rangle} g(x,\theta)dx \\ &= C_\alpha \int_0^\infty \Big[e^{ir\langle k,\theta\rangle} - \sum_{p=0}^{[\alpha]} \frac{(ir\langle k,\theta\rangle)^p}{p!}\Big]\alpha r^{-\alpha-1} dr \hat{f}(k).\end{aligned}$$

By letting $t = \langle k,\theta\rangle$ we have to compute

$$J(\alpha) = \int_0^\infty \Big[e^{irt} - \sum_{p=0}^{[\alpha]} \frac{(irt)^p}{p!}\Big]\alpha r^{-\alpha-1} dr.$$

The argument is similar to the case $1 < \alpha < 2$ proved in [17], Lemma 7.3.8. We only sketch the argument. For $s > 0$ let

$$J_s(\alpha) = \int_0^\infty \Big[e^{(it-s)r} - \sum_{p=0}^{[\alpha]} \frac{((it-s)r)^p}{p!}\Big]\alpha r^{-\alpha-1} dr. \tag{2.9}$$

If $0 < \alpha < 1$ then by (7.27) in [17] we obtain

$$J_s(\alpha) = \int_0^\infty \big[e^{(it-s)r} - 1\big]\alpha r^{-\alpha-1} dr = -\Gamma(1-\alpha)(s-it)^\alpha.$$

If $\alpha > 1$ then we integrate by parts to obtain

$$\begin{aligned}J_s(\alpha) &= (it-s)\int_0^\infty \Big[e^{(it-s)r} - \sum_{p=0}^{[\alpha]-1} \frac{((it-s)r)^p}{p!}\Big] r^{-\alpha} dr \\ &= \frac{it-s}{\alpha-1} J_s(\alpha-1) \\ &= \cdots = \frac{(it-s)^{[\alpha]}}{(\alpha-1)\cdots(\alpha-[\alpha])} J_s(\alpha-[\alpha]).\end{aligned}$$

Now, since $0 < \alpha - [\alpha] < 1$, by (7.27) of [17] we have $J_s(\alpha-[\alpha]) = C_1(s-it)^{\alpha-[\alpha]}$ where $C_1 = -\Gamma(1-(\alpha-[\alpha]))$. Using the property $\Gamma(t+1) = t\Gamma(t)$ we get

$$\begin{aligned}J_s(\alpha) &= \frac{-\Gamma([\alpha]-\alpha+1)}{(\alpha-1)\cdots(\alpha-[\alpha])}(it-s)^{[\alpha]}(s-it)^{\alpha-[\alpha]} \\ &= \frac{-\Gamma([\alpha]-\alpha+1)}{(1-\alpha)\cdots([\alpha]-\alpha)}(s-it)^\alpha \\ &= -\Gamma(1-\alpha)(s-it)^\alpha.\end{aligned}$$

Note that the absolute value of the integrand in (2.9) is bounded by $C_2 r^{[\alpha]-\alpha-1}$ as $r \to \infty$ and by $C_3 r^{[\alpha]-\alpha}$ as $r \to 0$, so by dominated convergence we get $J_s(\alpha) \to J(\alpha)$ as $s \to 0$. Hence $J(\alpha) = (-it)^\alpha$ and then

$$\hat{g}(k,\theta) = (-i\langle k,\theta\rangle)^\alpha \hat{f}(k) = (D_\theta^\alpha f)\widehat{\ }(k).$$

Hence, by the uniqueness of the Fourier transform we have $D_\theta^\alpha f(x) = g(x,\theta)$ a.e. and (2.4) holds true. This concludes the proof. □

Proof of Theorem 2.2. Let $h(x) = \int_{\|\theta\|=1} D_\theta^\alpha f(x) M(d\theta)$ where $D_\theta^\alpha f(x)$ is given by (2.2) and hence $(D_\theta^\alpha f)\widehat{\ }(k) = (-i\langle k,\theta\rangle)^\alpha \hat{f}(k)$. Since by Lemma 2.4

$$\int_{\|\theta\|=1} \int_{\mathbb{R}^d} |D_\theta^\alpha f(x)|\, dx\, M(d\theta) < \infty$$

we can apply Fubini's theorem to obtain

$$\begin{aligned} \hat{h}(k) &= \int_{\mathbb{R}^d} e^{i\langle k,x\rangle} \int_{\|\theta\|=1} D_\theta^\alpha f(x)\, M(d\theta)\, dx \\ &= \int_{\|\theta\|=1} \int_{\mathbb{R}^d} e^{i\langle k,x\rangle} D_\theta^\alpha f(x)\, dx\, M(d\theta) \\ &= \int_{\|\theta\|=1} (D_\theta^\alpha f)\widehat{\ }(k)\, M(d\theta) \\ &= \int_{\|\theta\|=1} (-i\langle k,\theta\rangle)^\alpha\, M(d\theta) \hat{f}(k) = (D_M^\alpha f)\widehat{\ }(k) \end{aligned} \tag{2.10}$$

and the uniqueness of the Fourier transform yields (2.1). This concludes the proof. □

3. A multivariable Grünwald formula

In this section we derive, using Theorem 2.2 above, a multivariable analogue of the scalar Grünwald formula (1.1). Furthermore, generalizing a result in [31], a speed of convergence result is also obtained. Speed of convergence results are critical for numerical applications.

Tuan and Gorenflo [31] show that for certain functions f

$$\frac{d^\alpha f(x)}{dx^\alpha} = h^{-\alpha}\Delta_h^\alpha f(x) + O(h)$$

as $h \to 0$. We now apply a similar argument to the fractional directional derivative. Recall that the Fourier transform of $D_\theta^\alpha f(x)$ is $(-i\langle k,\theta\rangle)^\alpha \hat{f}(k)$. Further define

$$h^{-\alpha}\Delta_{h,\theta}^\alpha f(x) = h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} f(x - mh\theta) \tag{3.1}$$

Theorem 3.1. *For $f \in W^{l,1}(\mathbb{R}^d)$ with $l = [\alpha] + d + 2$*

$$D_\theta^\alpha f(x) = h^{-\alpha}\Delta_{h,\theta}^\alpha f(x) + O(h) \tag{3.2}$$

independent of $\theta \in S^{d-1}$ and $x \in \mathbb{R}^d$.

Proof. Let $\hat{f}(k) = \int e^{i\langle k,x\rangle} f(x)dx$ be the Fourier transform of $f(x)$ so that $e^{i\langle k,a\rangle}\hat{f}(k)$ is the Fourier transform of $f(x-a)$.

Note the well known result that

$$(1+z)^\alpha = \sum_{m=0}^{\infty} \binom{\alpha}{m} z^m \tag{3.3}$$

for any complex $|z| \leq 1$ and any $\alpha > 0$. Further, the binomial series is absolutely convergent (page 180, [13]).

It is readily verified that

$$\int_{\mathbb{R}^d} \left| \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} f(x - mh\theta) \right| dx \leq \|f\|_1 \sum_{m=0}^{\infty} |(-1)^m \binom{\alpha}{m}| < \infty$$

Consequently, the right hand side of (3.1) defines an element of $L^1(\mathbb{R}^d)$. Thus we can take Fourier transforms in (3.1) to obtain

$$\begin{aligned}
\left(h^{-\alpha}\Delta_{h,\theta}^\alpha f\right)^\frown(k) &= h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} e^{i\langle k, mh\theta\rangle}\hat{f}(k) \\
&= h^{-\alpha}\left(\sum_{m=0}^{\infty} \binom{\alpha}{m} (-e^{i\langle k,h\theta\rangle})^m \right) \hat{f}(k) \\
&= h^{-\alpha}\left(1 - e^{i\langle k,h\theta\rangle}\right)^\alpha \hat{f}(k) \\
&= h^{-\alpha}\left((-i\langle k,h\theta\rangle)^\alpha \left(\frac{1 - e^{i\langle k,h\theta\rangle}}{-i\langle k,h\theta\rangle} \right)^\alpha \right) \hat{f}(k) \\
&= (-i\langle k,\theta\rangle)^\alpha w(-i\langle k,h\theta\rangle)\hat{f}(k)
\end{aligned} \tag{3.4}$$

where

$$w(z) = \left(\frac{1 - e^{-z}}{z} \right)^\alpha = 1 - \frac{\alpha}{2} z + O(|z|^2).$$

Note that $|w(-ix) - 1| \leq C|x|$ for all $x \in \mathbb{R}$ for some $C > 0$. Then

$$\begin{aligned}
\left(h^{-\alpha}\Delta_{h,\theta}^\alpha f\right)^\frown(k) &= (-i\langle k,\theta\rangle)^\alpha \hat{f}(k) + (-i\langle k,\theta\rangle)^\alpha (w(-i\langle k,h\theta\rangle) - 1)\hat{f}(k) \\
&= \left(D_\theta^\alpha f\right)^\frown(k) + \hat{\varphi}(h,k)
\end{aligned} \tag{3.5}$$

where $\hat{\varphi}(h,k) = (-i\langle k,\theta\rangle)^\alpha (w(-i\langle k,h\theta\rangle) - 1)\hat{f}(k)$. Since $f \in W^{l,1}(\mathbb{R}^d)$ the Riemann-Lebesgue Lemma allows us to conclude that

$$|\hat{f}(k)| \leq M/(1 + \|k\|)^l$$

for some M ([12] Theorem 8.22) and thus

$$(1+\|k\|)^{\alpha+1}|\hat{f}(k)| \leq \frac{M(1+\|k\|)^{\alpha+1}}{(1+\|k\|)^{[\alpha]+d+2}} = \frac{M}{(1+\|k\|)^{[\alpha]-\alpha+d+1}}$$

which yields the integrability result

$$\int_{\mathbb{R}^d} (1+\|k\|)^{\alpha+1}|\hat{f}(k)|dk < \infty. \tag{3.6}$$

Now since

$$|\hat{\varphi}(h,k)| \leq \|k\|^{\alpha} C\|hk\|\,|\hat{f}(k)| \leq C\,h\,(1+\|k\|)^{\alpha+1}|\hat{f}(k)|$$

$\hat{\varphi}(h,\cdot) \in L^1(\mathbb{R}^d)$ for each h. Taking inverse Fourier transforms of

$$\hat{\varphi}(h,k) = \left(h^{-\alpha}\Delta^{\alpha}_{h,\theta} f\right)\hat{}\,(k) - \left(D^{\alpha}_{\theta} f\right)\hat{}\,(k)$$

we conclude that for some constant $c_d > 0$

$$\begin{aligned} |h^{-\alpha}\Delta^{\alpha}_{h,\theta} f(x) - D^{\alpha}_{\theta} f(x)| &= \left| c_d \int_{\mathbb{R}^d} e^{-i\langle k,x\rangle}\hat{\varphi}(h,k)\,dk \right| \\ &\leq c_d \int_{\mathbb{R}^d} |\hat{\varphi}(h,k)|\,dk \\ &\leq Kh \end{aligned} \tag{3.7}$$

for some constant K independent of $\theta \in S^{d-1}$ and $x \in \mathbb{R}^d$. This shows that

$$D^{\alpha}_{\theta} f(x) = h^{-\alpha}\Delta^{\alpha}_{h,\theta} f(x) + O(h) \tag{3.8}$$

independent of $\theta \in S^{d-1}$ and $x \in \mathbb{R}^d$ and the theorem is proven. □

As a consequence of (2.1) and (3.2) we obtain

Corollary 3.2. *For $f \in W^{l,1}(\mathbb{R}^d)$ with $l = [\alpha] + d + 2$ there exists a constant $C > 0$ independent of x such that*

$$\left| D^{\alpha}_{M} f(x) - \int_{\|\theta\|=1} h^{-\alpha}\Delta^{\alpha}_{h,\theta} f(x) M(d\theta) \right| \leq Ch. \tag{3.9}$$

Remark 3.3. The vector fractional derivative D^{α}_{M} is the negative generator of a multivariable stable semigroup on $\mathbb{R}^d$. A stable probability distribution ν on $\mathbb{R}^d$ has characteristic function

$$\hat{\nu}(k) = \exp\left(-C \int_{\|\theta\|=1} (-i\langle k,\theta\rangle)^{\alpha} M(d\theta) \right) \tag{3.10}$$

for some $C > 0$. This follows from the Lévy representation by a straightforward but lengthy calculation, see for example [17] Section 7.3. Then it follows that the generator $A_{\nu} = -D^{\alpha}_{M}$. In one variable this idea has been used to prove (1.1) by discretizing the Lévy measure of the stable probability distribution, see [20]. The same approach also works for vector fractional derivatives, but that method makes it more difficult to obtain the rate of convergence.

4. Vector Grünwald formula on a regular grid

Finite difference algorithms for solving fractional partial differential equations require a method for estimating fractional derivatives using only the function values on a regular grid. In this section, we modify the Grünwald approximation formula for vector fractional derivatives developed in Section 3 to operate on a rectangular grid, and we also establish order of convergence. In view of Corollary 3.2, for functions $f \in W^{[\alpha]+d+2,1}(\mathbb{R}^d)$, we can approximate the multivariable fractional derivative $D^\alpha_M f(x)$ uniformly in $x \in \mathbb{R}^d$ by

$$D^\alpha_M f(x) = h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \int_{\|\theta\|=1} f(x - mh\theta) M(d\theta) + O(h). \tag{4.1}$$

In order to apply this formula numerically we have to approximate $\int_{\|\theta\|=1} f(x-mh\theta)M(d\theta)$ in such a way that the order $O(h)$ in (4.1) is preserved. We will only consider the case when M is a discrete measure or when M has a Lipschitz-continuous density with respect to the surface measure on S^{d-1}. This is usually sufficient for most practical purposes. Usually the function f is only known (or stored) on a regular grid $G_h = u(h)\mathbb{Z}^d \subset \mathbb{R}^d$ for some $u(h) > 0$. Typically one has $u(h) = h$ or $u(h) = h^\beta$ for some $\beta > 0$. Since $x - mh\theta$ is not a grid point, we have to evaluate f on a grid point close to $x - mh\theta$ and then we have to control the error.

Recall that M is a probability measure on S^{d-1}.

Case I: (discrete M)

Assume that

$$M = \sum_{l=1}^{\infty} a_l \varepsilon_{\theta_l} \tag{4.2}$$

for some $a_l \geq 0$, $\|\theta_l\| = 1$, where ε_a denotes the point mass in $a \in \mathbb{R}^d$. In view of Theorem 3.1 and (4.1) we have

$$D^\alpha_M f(x) = h^{-\alpha} \sum_{l=1}^{\infty} a_l \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} f(x - mh\theta_l) + O(h) \tag{4.3}$$

uniformly in $x \in \mathbb{R}^d$ for $f \in W^{[\alpha]+d+2,1}(\mathbb{R}^d)$.

Now let $G_h = h^{1+\alpha}\mathbb{Z}^d$ be the grid of mesh size $h^{1+\alpha}$. Given any vector $v \in \mathbb{R}^d$ let $g(v) \in G_h$ denote the *nearest* grid point close to v. Then, for some constant $C_d > 0$ we have

$$\|v - g(v)\| \leq C_d h^{1+\alpha} \quad \text{for all } v \in \mathbb{R}^d. \tag{4.4}$$

Ties can be broken arbitrarily, and in fact, all of the ensuing arguments apply equally well for any function $g : \mathbb{R}^d \to G_h$ such that (4.4) holds.

Theorem 4.1. *If $f \in W^{[\alpha]+d+2,1}(\mathbb{R}^d)$ and (4.2) holds, then*

$$D_M^\alpha f(x) = h^{-\alpha} \sum_{l=1}^{\infty} a_l \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} f(x - g(mh\theta_l)) + O(h) \tag{4.5}$$

uniformly in $x \in \mathbb{R}^d$, especially in $x \in G_h$.

Proof. Since $f \in W^{[\alpha]+d+2,1}(\mathbb{R}^d)$, f is continuously differentiable and all first order partial derivatives are bounded. Hence f is Lipschitz-continuous, that is, there exists a constant $K > 0$ such that

$$|f(x) - f(y)| \le K\|x - y\| \quad \text{for all } x, y \in \mathbb{R}^d. \tag{4.6}$$

Hence, by (4.4) and (4.6), for some constant $C > 0$ and any $l \ge 1$ we have

$$\begin{aligned} & h^{-\alpha}\Big|\sum_{m=0}^{\infty}(-1)^m \binom{\alpha}{m} f(x - mh\theta_l) - \sum_{m=0}^{\infty}(-1)^m \binom{\alpha}{m} f(x - g(mh\theta_l))\Big| \\ \le & h^{-\alpha} \sum_{m=0}^{\infty} \Big|(-1)^m \binom{\alpha}{m}\Big| \cdot |f(x - mh\theta_l) - f(x - g(mh\theta_l))| \\ \le & K C_d h^{-\alpha} h^{1+\alpha} \sum_{m=0}^{\infty} \Big|(-1)^m \binom{\alpha}{m}\Big| \\ = & Ch. \end{aligned}$$

Then (4.5) follows from (4.3) and the proof is complete. ∎

Case II: (M has a Lipschitz-continuous density)
Assume that there exists a function $\psi : S^{d-1} \to \mathbb{R}_+$ which is Lipschitz-continuous, that is, for some $L > 0$

$$|\psi(\theta_1) - \psi(\theta_2)| \le L\|\theta_1 - \theta_2\| \quad \text{for all } \theta_1, \theta_2 \in S^{d-1}, \tag{4.7}$$

such that $M(d\theta) = \psi(\theta)\sigma(d\theta)$, where σ denotes the surface measure on S^{d-1}. We introduce standard polar coordinates on S^{d-1} (see, e.g., [11] p. 218). Let $X = [0, \pi)^{d-2} \times [0, 2\pi)$ and denote the elements of X by $\Phi = (\phi_1, \ldots, \phi_{d-1})$. Define the diffeomorphism

$$T(\Phi) = T(\phi_1, \ldots, \phi_{d-1}) = \begin{pmatrix} \cos\phi_1 \\ \sin\phi_1 \cos\phi_2 \\ \vdots \\ \sin\phi_1 \sin\phi_2 \cdots \sin\phi_{d-2} \cos\phi_{d-1} \\ \sin\phi_1 \sin\phi_2 \cdots \sin\phi_{d-2} \sin\phi_{d-1} \end{pmatrix}$$

and note that $\sigma(d\theta) = \lambda_{d-1}(T^{-1}(d\theta))$ where λ_{d-1} is the Lebesgue product measure on X. Further we define the standard metric on X by

$$d(\Phi, \bar\Phi) = \Big(\sum_{j=1}^{d-1} |\phi_j - \bar\phi_j|^2\Big)^{1/2}.$$

Then it is easy to see that for some constant $C > 0$

$$\|T(\Phi) - T(\bar{\Phi})\| \le Cd(\Phi, \bar{\Phi}) \quad \text{for all } \Phi, \bar{\Phi} \in X.$$

Hence, in view of (4.7) we get for some constant $C > 0$ that

$$|\psi(T(\Phi)) - \psi(T(\bar{\phi}))| \le Cd(\Phi, \bar{\Phi}) \quad \text{for all } \Phi, \bar{\Phi} \in X. \tag{4.8}$$

Note that in $\int_{\|\theta\|=1} f(x - mh\theta)M(d\theta)$ in (4.1) we integrate f over a sphere with radius mh around x. In order to get an approximation error that is $O(h)$ we need to approximate M in a way that depends on both m and h. When m is larger, the sphere of radius mh is larger, and so we need to use a finer discretization of the density to get the same accuracy. Now we define the grid points we will use to approximate the measure M. Given any $m \ge 1$ and $h > 0$ define for $1 \le i \le d-2$

$$\phi_i^{(h,m,j)} = j\frac{h^{1+\alpha}}{m} \quad \text{for } 0 \le j \le J_i(h,m) = \big[\frac{\pi m}{h^{1+\alpha}}\big] \text{ and } \phi_i^{(h,m,J_i(h,m)+1)} = \pi$$

and

$$\phi_{d-1}^{(h,m,j)} = j\frac{h^{1+\alpha}}{m} \quad \text{for } 0 \le j \le J_{d-1}(h,m) = \big[\frac{2\pi m}{h^{1+\alpha}}\big] \text{ and } \phi_i^{(h,m,J_{d-1}(h,m)+1)} = 2\pi$$

and set

$$\theta^{(h,m)}_{j_1,\dots,j_{d-1}} = T\big(\phi_1^{(h,m,j_1)}, \phi_2^{(h,m,j_2)}, \dots, \phi_{d-1}^{(h,m,j_{d-1})}\big)$$

for $0 \le j_i \le J_i(h,m) + 1$ and $1 \le i \le d-1$. Note that $\Delta\phi_i^{(h,m,j)} = \phi_i^{(h,m,j+1)} - \phi_i^{(h,m,j)} = h^{1+\alpha}/m$ for $0 \le j < J_i(h,m)$ while $0 \le \Delta\phi_i^{(h,m,j)} \le h^{1+\alpha}/m$ for $j = J_i(h,m)$. Define

$$M_{h,m} = \sum_{j_1=0}^{J_1(h,m)} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)} \psi\big(\theta^{(h,m)}_{j_1,\dots,j_{d-1}}\big)\Delta\phi_1^{(h,m,j_1)} \cdots \Delta\phi_{d-1}^{(h,m,j_{d-1})} \varepsilon_{\theta^{(h,m)}_{j_1,\dots,j_{d-1}}}. \tag{4.9}$$

Then we have

Theorem 4.2. *Assume M has a density such that (4.7) holds. Then for any $f \in W^{[\alpha]+d+2,1}(\mathbb{R}^d)$ there exists a constant $C > 0$ (independent of x and h) such that*

$$\Big|D_M^\alpha f(x) - h^{-\alpha}\sum_{m=0}^{\infty}(-1)^m \binom{\alpha}{m}\int_{\|\theta\|=1} f(x - mh\theta)M_{h,m}(d\theta)\Big| \le Ch \tag{4.10}$$

for all $x \in \mathbb{R}^d$ and $h > 0$.

Proof. In view of Theorem 2.2 we write

$$
\begin{aligned}
&\Big|D_M^\alpha f(x) - h^{-\alpha}\sum_{m=0}^{\infty}(-1)^m\binom{\alpha}{m}\int_{\|\theta\|=1} f(x-mh\theta)M_{h,m}(\theta)\Big|\\
\le&\Big|\int_{\|\theta\|=1} D_\theta^\alpha f(x)M(d\theta) - \int_{\|\theta\|=1} h^{-\alpha}\Delta_{h,\theta}^\alpha f(x)M(d\theta)\Big|\\
&+\Big|\int_{\|\theta\|=1} h^{-\alpha}\Delta_{h,\theta}^\alpha f(x)M(d\theta) - h^{-\alpha}\sum_{m=0}^{\infty}(-1)^m\binom{\alpha}{m}\int_{\|\theta\|=1} f(x-mh\theta)M_{h,m}(d\theta)\Big|\\
=&E_1(h)+E_2(h).
\end{aligned}
$$

Note that by (3.9) we already have $E_1(h) = O(h)$ uniformly in $x \in \mathbb{R}^d$. Moreover

$$
\begin{aligned}
E_2(h) &= \Big|h^{-\alpha}\sum_{m=0}^{\infty}(-1)^m\binom{\alpha}{m}\Big[\int_{\|\theta\|=1} f(x-mh\theta)M(d\theta) - \int_{\|\theta\|=1} f(x-mh\theta)M_{h,m}(d\theta)\Big]\Big|\\
&\le h^{-\alpha}\sum_{m=0}^{\infty}\Big|(-1)^m\binom{\alpha}{m}\Big|\Big|\int_{\|\theta\|=1} f(x-mh\theta)M(d\theta) - \int_{\|\theta\|=1} f(x-mh\theta)M_{h,m}(d\theta)\Big|
\end{aligned}
$$

Recall that $\sigma(d\theta) = \lambda_{d-1}(T^{-1}(d\theta))$. Now substitute $\theta = T(\Phi)$ and apply the mean value theorem for integrals $d-1$ times to obtain

$$
\begin{aligned}
&\int_{\|\theta\|=1} f(x-mh\theta)M(d\theta) = \int_X f\big(x-mhT(\Phi)\big)\psi\big(T(\Phi)\big)d\Phi\\
=&\int_0^\pi\cdots\int_0^\pi\int_0^{2\pi} f\big(x-mhT(\phi_1,\dots,\phi_{d-1})\big)\psi\big(T(\phi_1,\dots,\phi_{d-1})\big)d\phi_{d-1}d\phi_{d-2}\dots d\phi_1\\
=&\sum_{j_1=0}^{J_1(h,m)}\cdots\sum_{j_{d-1}=0}^{J_{d-1}(h,m)}\int_{\phi_1^{(h,m,j_1)}}^{\phi_1^{(h,m,j_1+1)}}\cdots\int_{\phi_{d-1}^{(h,m,j_{d-1})}}^{\phi_{d-1}^{(h,m,j_{d-1}+1)}}\\
&\qquad f\big(x-mhT(\phi_1,\dots,\phi_{d-1})\big)\psi\big(T(\phi_1,\dots,\phi_{d-1})\big)d\phi_{d-1}\dots d\phi_1\\
=&\sum_{j_1=0}^{J_1(h,m)}\cdots\sum_{j_{d-1}=0}^{J_{d-1}(h,m)}\Delta\phi_{d-1}^{(h,m,j_{d-1})}\int_{\phi_1^{(h,m,j_1)}}^{\phi_1^{(h,m,j_1+1)}}\cdots\int_{\phi_{d-2}^{(h,m,j_{d-2})}}^{\phi_{d-2}^{(h,m,j_{d-2}+1)}}\\
&\qquad f\big(x-mhT(\phi_1,\dots,\phi_{d-2},\bar\phi_{d-1}^{(j_{d-1})})\big)\psi\big(T(\phi_1,\dots,\phi_{d-2},\bar\phi_{d-1}^{(j_{d-1})})\big)d\phi_{d-2}\dots d\phi_1\\
&\vdots\\
=&\sum_{j_1=0}^{J_1(h,m)}\cdots\sum_{j_{d-1}=0}^{J_{d-1}(h,m)}\Delta\phi_1^{(h,m,j_1)}\cdots\Delta\phi_{d-1}^{(h,m,j_{d-1})}\\
&\qquad f\big(x-mhT(\bar\phi_1^{(j_1)},\dots,\bar\phi_{d-1}^{(j_{d-1})})\big)\psi\big(T(\bar\phi_1^{(j_1)},\dots,\bar\phi_{d-1}^{(j_{d-1})})\big)
\end{aligned}
$$

for some $\phi_i^{(h,m,j_i)} \le \bar\phi_i^{(j_i)} \le \phi_i^{(h,m,j_i+1)}$ and $1 \le i \le d-1$. Moreover, by (4.9)

$$\begin{aligned}
&\int_{\|\theta\|=1} f(x-mh\theta)M_{h,m}(d\theta)\\
&= \sum_{j_1=0}^{J_1(h,m)} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)} \Delta\phi_1^{(h,m,j_1)} \cdots \Delta\phi_{d-1}^{(h,m,j_{d-1})}\\
&\qquad f\big(x-mhT(\phi_1^{(m,h,j_1)},\ldots,\phi_{d-1}^{(m,h,j_{d-1})})\big)\psi\big(T(\phi_1^{(m,h,j_1)},\ldots,\phi_{d-1}^{(m,h,j_{d-1})})\big).
\end{aligned}$$

Hence

$$\begin{aligned}
&\Big|\int_{\|\theta\|=1} f(x-mh\theta)M(d\theta) - \int_{\|\theta\|=1} f(x-mh\theta)M_{h,m}(d\theta)\Big|\\
&\le \sum_{j_1=0}^{J_1(h,m)} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)} \Delta\phi_1^{(h,m,j_1)} \cdots \Delta\phi_{d-1}^{(h,m,j_{d-1})}\\
&\qquad \Big| f\big(x-mhT(\bar\phi_1^{(j_1)},\ldots,\bar\phi_{d-1}^{(j_{d-1})})\big)\psi\big(T(\bar\phi_1^{(j_1)},\ldots,\bar\phi_{d-1}^{(j_{d-1})})\big)\\
&\qquad - f\big(x-mhT(\phi_1^{(m,h,j_1)},\ldots,\phi_{d-1}^{(m,h,j_{d-1})})\big)\psi\big(T(\phi_1^{(m,h,j_1)},\ldots,\phi_{d-1}^{(m,h,j_{d-1})})\big)\Big|
\end{aligned} \tag{4.11}$$

It follows as in the proof of Theorem 4.1 that f is Lipschitz continuous, that is (4.6) holds. Moreover $\|\psi\|_\infty < \infty$ and $\|f\|_\infty < \infty$ and (4.8) holds. Using the inequality

$$|f(u)\psi(u) - f(v)\psi(v)| \le \|\psi\|_\infty |f(u)-f(v)| + \|f\|_\infty |\psi(u)-\psi(v)|$$

we obtain for some constants $C_1, C_2, C > 0$ that

$$\begin{aligned}
&\Big| f\big(x-mhT(\bar\phi_1^{(j_1)},\ldots,\bar\phi_{d-1}^{(j_{d-1})})\big)\psi\big(T(\bar\phi_1^{(j_1)},\ldots,\bar\phi_{d-1}^{(j_{d-1})})\big)\\
&\qquad - f\big(x-mhT(\phi_1^{(m,h,j_1)},\ldots,\phi_{d-1}^{(m,h,j_{d-1})})\big)\psi\big(T(\phi_1^{(m,h,j_1)},\ldots,\phi_{d-1}^{(m,h,j_{d-1})})\big)\Big|\\
&\le C_1 mh \|T(\bar\phi_1^{(j_1)},\ldots,\bar\phi_{d-1}^{(j_{d-1})})) - T(\phi_1^{(m,h,j_1)},\ldots,\phi_{d-1}^{(m,h,j_{d-1})})\| + C_2 \frac{h^{1+\alpha}}{m}\\
&\le C_1 mh \frac{h^{1+\alpha}}{m} + C_2\frac{h^{1+\alpha}}{m} \le Ch^{1+\alpha}
\end{aligned}$$

for all $m \ge 1$, $x \in \mathbb{R}^d$ and $0 < h \le 1$. Then the right hand side of (4.11) is bounded from above by

$$Ch^{1+\alpha} \sum_{j_1=0}^{J_1(h,m)} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)} \Delta\phi_1^{(h,m,j_1)} \cdots \Delta\phi_{d-1}^{(h,m,j_{d-1})} = 2\pi^{d-1} Ch^{1+\alpha}$$

for all $x \in \mathbb{R}^d$ and $0 < h \le 1$. Finally, we obtain for some constant $\bar C > 0$ that

$$E_2(h) \le h^{-\alpha} \sum_{m=0}^{\infty} \Big|(-1)^m \binom{\alpha}{m}\Big| 2\pi^{d-1} Ch^{1+\alpha} = \bar C h$$

for all $x \in \mathbb{R}^d$ and $0 < h \leq 1$. This concludes the proof. □

As in Case I we now move the evaluation of f to grid points. Recall that $g(v)$ denotes the nearest grid point close to $v \in \mathbb{R}^d$ and that (4.4) holds.

Theorem 4.3. *Under the assumptions of Theorem 4.2 we have*

$$D_M^\alpha f(x) = h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \sum_{j_1=0}^{J_1(h,m)} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)} \psi\big(\theta^{(h,m)}_{j_1,\dots,j_{d-1}}\big) f\big(x - g(mh\theta^{(h,m)}_{j_1,\dots,j_{d-1}})\big) \Delta\phi_1^{(h,m,j_1)} \cdots \Delta\phi_{d-1}^{(h,m,j_{d-1})} + O(h)$$

uniformly in $x \in \mathbb{R}^d$ (and especially in $x \in G_h$).

Proof. Using (4.4) and (4.6) we have

$$\big| f(x - mh\theta^{(h,m)}_{j_1,\dots,j_{d-1}}) - f(x - g(mh\theta^{(h,m)}_{j_1,\dots,j_{d-1}})) \big| \leq Ch^{1+\alpha}$$

and then for some $C_4 > 0$

$$\begin{aligned}
&\Big| h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \int_{\|\theta\|=1} f(x - mh\theta) M_{h,m}(d\theta) \\
&\quad - h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \sum_{j_1=0}^{J_1(h,m)} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)} \\
&\qquad \psi\big(\theta^{(h,m)}_{j_1,\dots,j_{d-1}}\big) f\big(x - g(mh\theta^{(h,m)}_{j_1,\dots,j_{d-1}})\big) \Delta\phi_1^{(h,m,j_1)} \cdots \Delta\phi_{d-1}^{(h,m,j_{d-1})} \Big| \\
&= \Big| h^{-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \sum_{j_1=0}^{J_1(h,m)} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)} \Delta\phi_1^{(h,m,j_1)} \cdots \Delta\phi_{d-1}^{(h,m,j_{d-1})} \\
&\qquad \psi\big(\theta^{(h,m)}_{j_1,\dots,j_{d-1}}\big) \Big(f\big(x - mh\theta^{(h,m)}_{j_1,\dots,j_{d-1}}\big) - f\big(x - g(mh\theta^{(h,m)}_{j_1,\dots,j_{d-1}})\big) \Big) \Big| \\
&\leq h^{-\alpha} \left| \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \right| \sum_{j_1=0}^{J_1(h,m)} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)} \Delta\phi_1^{(h,m,j_1)} \cdots \Delta\phi_{d-1}^{(h,m,j_{d-1})} \|\psi\|_\infty C h^{1+\alpha} \\
&= h^{-\alpha} \left| \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \right| 2\pi^{d-1} \|\psi\|_\infty C h^{1+\alpha} \leq C_4 h.
\end{aligned}$$

Now Theorem 4.2 together with (4.9) gives the desired result. □

Remark 4.4. If the step size h is chosen so that $\pi/h^{1+\alpha}$ is an integer, then the Grünwald approximation formula in Theorem 4.2 becomes simpler. In this case, we have

$$D_M^\alpha f(x) = h^{(1+\alpha)(d-1)-\alpha} \sum_{m=0}^{\infty} (-1)^m \binom{\alpha}{m} \frac{1}{m^{d-1}} \sum_{j_1=0}^{J_1(h,m)-1} \cdots \sum_{j_{d-1}=0}^{J_{d-1}(h,m)-1} \psi\big(\theta^{(h,m)}_{j_1,\dots,j_{d-1}}\big) f\big(x - g(mh\theta^{(h,m)}_{j_1,\dots,j_{d-1}})\big) + O(h)$$

uniformly in $x \in \mathbb{R}^d$ (and especially in $x \in G_h$).

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