

A NOTE ON DECONVOLUTION WITH COMPLETELY MONOTONE SEQUENCES AND DISCRETE FRACTIONAL CALCULUS

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Abstract. We study in this work convolution groups generated by completely monotone sequences related to the ubiquitous time-delay memory effect in physics and engineering. In the first part, we give an accurate description of the convolution inverse of a completely monotone sequence and show that the deconvolution with a completely monotone kernel is stable. In the second part, we study a discrete fractional calculus defined by the convolution group generated by the completely monotone sequence $c^{(1)} = (1, 1, 1, \dots)$, and show the consistency with time-continuous Riemann-Liouville calculus, which may be suitable for modeling memory kernels in discrete time series.

1. Introduction. Many models have been proposed for the ubiquitous time-delay memory effect in physics and engineering: the generalized Langevin equation model for particles in heat bath ([7, 18]), linear viscoelasticity models for soft matter ([2, 12]), linear dielectric susceptibility model [1, 15] for polarization to name a few. In these models, the response due to memory is given by the one-side convolution $\int_0^t g(t-s)v(s) ds$ following linearity, time-translation invariance and causality [11, Chap. 1], where g is the memory kernel and v is the source of memory. Causality means that the output cannot precede the input so that $g(t) = 0$ for $t < 0$. The Titchmarsh's theorem states that the Fourier transform $G(\omega)$ of g is analytic in the upper half plane, and that the real and imaginary parts of G satisfy the Kramers-Kronig relation [11, 16]. Based on the principle of the fading memory [12], we consider g to be completely monotone, which by the Bernstein theorem can be expressed as the superposition of (may be infinitely many) decaying exponentials (see [14, 17] for more details). If the kernel g is given by the algebraically decaying completely monotone kernels $g = \frac{\theta(t)}{\Gamma(\gamma)} t^{\gamma-1}$ where $\theta(t)$ is the Heaviside step

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function and $\gamma \in (0, 1)$, we are then led to the fractional integrals and the corresponding fractional derivatives, which have already been used widely in engineering for modeling memory effects [4].

In practice, the data we collect are at discrete times and we have the one-sided discrete convolution $a * c$ (see equation (2.2)). The convolution kernel c is a completely monotone sequence (see Definition 2.1) if it is the value of g at the discrete times [17]. If c is completely monotone, it is shown in [10] that there exist $c^{(r)}$, $r \in \mathbb{R}$, such that $c^{(r)} * c^{(s)} = c^{(r+s)}$ and $c^{(1)} = c$, i.e. there exists a convolution group generated by the completely monotone sequence. If $0 \leq r \leq 1$, $c^{(r)}$ is completely monotone. Further, $c^{(0)} = \delta_d := (1, 0, 0, \dots)$, is the convolution identity. The most interesting sequence is $c^{(-1)}$, the convolution inverse, which can be used for deconvolution. Since the data are discrete, it would also be interesting to define discrete fractional calculus using the one-sided discrete convolution.

In this short note, we first investigate the convolution inverse of a completely monotone sequence c in Section 2. We show that the ℓ_1 norm is bounded and the deconvolution is stable in any ℓ^p space. Based on this, some preliminary ideas are explored for deconvolution. In Section 3, we define a discrete fractional calculus using a discrete convolution group generated by the completely monotone sequence $c^{(1)} = (1, 1, 1, \dots)$ and show that it is consistent with the time-continuous Riemann-Liouville calculus (see (3.1)).

2. Deconvolution for a completely monotone kernel. In this section, we investigate the property of convolution inverse of a completely monotone sequence and deconvolution with completely monotone sequences.

DEFINITION 2.1. A sequence $c = \{c_k\}_{k=0}^\infty$ is completely monotone if $(I - S)^j c_k \geq 0$ for any $j \geq 0, k \geq 0$ where $S c_j = c_{j+1}$.

A sequence is completely monotone if and only if it is the moment sequence of a Hausdorff measure (a finite nonnegative measure on $[0, 1]$) ([17]). Another description is given as follows ([10, 13]):

LEMMA 2.2. A sequence c is completely monotone if and only if the generating function $F_c(z) = \sum_{j=0}^\infty c_j z^j$ is a Pick function that is analytic and nonnegative on $(-\infty, 1)$.

Note that a function $f : \mathbb{C}_+ \mapsto \mathbb{C}$ (where \mathbb{C}_+ denotes the upper half plane, not including the real line) is Pick if it is analytic such that $\text{Im}(z) > 0 \Rightarrow \text{Im}(f(z)) \geq 0$.

Consider the one-sided convolution equation

$$a * c = f, \tag{2.1}$$

where the convolution kernel c is a completely monotone sequence and $c_0 > 0$. The discrete convolution is defined as

$$(a * c)_k = \sum_{n_1 \geq 0, n_2 \geq 0} \delta_k^{n_1+n_2} a_{n_1} c_{n_2}, \tag{2.2}$$

and δ_m^n is the Kronecker delta. This convolution is associative and commutative. Let $F_c(z)$ be the generating function of c :

$$F_c(z) = \sum_{n=0}^{\infty} c_n z^n. \tag{2.3}$$

Then, $F_{a*c}(z) = F_a(z)F_c(z)$. Given c , the convolution inverse $c^{(-1)}$ is the sequence that satisfies $c * c^{(-1)} = c^{(-1)} * c = \delta_d := (1, 0, 0, \dots)$. The generating function of the convolution inverse $c^{(-1)}$ is $1/F_c(z)$. If we find the convolution inverse of c , the convolution equation (2.1) can be solved.

2.1. *The convolution inverse.* Now, we present our results about the convolution inverse:

THEOREM 2.3. Suppose c is completely monotone and $c_0 > 0$. Let $c^{(-1)}$ be its convolution inverse. Then, $F_{c^{(-1)}}$ is analytic on the open unit disk, and thus the radius of convergence of its power series around $z = 0$ is at least 1. $c_0^{(-1)} = 1/c_0$ and the sequence $(-c_1^{(-1)}, -c_2^{(-1)}, \dots)$ is completely monotone. Furthermore, $0 \leq -\sum_{k=1}^{\infty} c_k^{(-1)} \leq \frac{1}{c_0}$.

Proof. The first claim follows from that $F_c(z)$ has no zeros in the unit disk [10].

By Lemma 2.2, $F_c(z)$ is Pick and it is positive on $(-\infty, 1)$. $F_c(-\infty) = 0$ if the corresponding Hausdorff measure does not have an atom at 0 (i.e. the sequence c is minimal. See [17, Chap. IV. Sec. 14] for the definition). Since $F_c(-\infty)$ could be zero, we consider

$$G_\epsilon(z) = \frac{1}{\epsilon} - \frac{1}{\epsilon + F_c(z)}, \quad \epsilon > 0.$$

It is easy to verify that G_ϵ is a Pick function, analytic and nonnegative on $(-\infty, 1)$.

Suppose G_ϵ is the generating function of $d = (d_0^\epsilon, d_1^\epsilon, \dots)$. By Lemma 2.2, this sequence is completely monotone. Then,

$$H_\epsilon(z) = \frac{1}{z} [G_\epsilon(z) - G_\epsilon(0)] = \frac{F_c(z) - F_c(0)}{z(\epsilon + F_c(0))(\epsilon + F_c(z))},$$

is the generating function of the shifted sequence (d_1^ϵ, \dots) , which is completely monotone. Hence, H_ϵ is also a Pick function, nonnegative and analytic on $(-\infty, 1)$.

Taking the pointwise limit of H_ϵ as $\epsilon \rightarrow 0$, we find the limit function

$$H(z) = \frac{F_c(z) - F_c(0)}{zF_c(0)F_c(z)} \tag{2.4}$$

to be nonnegative on $(-\infty, 1)$. By the expression of H , it is also analytic since $F_c(z)$ is never zero on $\mathbb{C} \setminus [1, \infty)$. Finally, since $\text{Im}(H_\epsilon(z)) \geq 0$ for $\text{Im}(z) > 0$, then $\text{Im}(H(z))$, as the limit, is nonnegative. It follows that the sequence corresponding to H is also completely monotone. If c is in ℓ^1 , $0 < H(1) = \frac{F_c(1) - F_c(0)}{F_c(0)F_c(1)} < \frac{1}{c_0}$. If $F_c(1) = \|c\|_1 = \infty$, we fix $z_0 \in (0, 1)$, and then for any $z \in (z_0, 1)$, we have $0 < H(z) \leq \frac{F_c(z)}{zF_c(0)F_c(z)} = \frac{1}{z_0 c_0}$. $H(z)$ is increasing in z since the sequence corresponding to H is completely monotone and therefore nonnegative. Letting $z \rightarrow 1^-$, by the monotone convergence theorem, we have $H(1) \leq \frac{1}{z_0 c_0}$. Taking $z_0 \rightarrow 1$, $H(1) \leq \frac{1}{c_0}$.

Further, $H(z)$ is the generating function of $-(c_1^{(-1)}, c_2^{(-1)}, \dots)$ since $1/F_c(z)$ is the generating function of $c^{(-1)} = (c_0^{(-1)}, c_1^{(-1)}, \dots)$. The second claim therefore follows. \square

As a corollary of Theorem 2.3, we find that the deconvolution with a completely monotone sequence is stable:

COROLLARY 2.4. Equation (2.1) can be solved stably. In particular, $\forall f \in \ell^p$, there exists a unique $a \in \ell^p$ such that $a * c = f$ and $\|a\|_p \leq \frac{2}{c_0} \|f\|_p$.

The claim follows directly from the fact that $\|c^{-1}\|_1 \leq 2/c_0$ and Young’s inequality. We omit the proof.

2.2. *Computing convolution inverse and deconvolution.* To solve the convolution equation (2.1), we can use the algorithm in [10] to find the convolution group $c^{(r)}$. Then, the solution is computed as $a = c^{(-1)} * f$. The algorithm for $c^{(r)}$ reads

- Determine the canonical sequence b that satisfies $(n + 1)c_{n+1} = \sum_{k=0}^n c_{n-k}b_k$.
- Compute $c^{(r)}$ by $(n + 1)c_{n+1}^{(r)} = r \sum_{k=0}^n c_{n-k}^{(r)}b_k$.

For a completely monotone sequence, the canonical sequence satisfies $b_k \geq 0$ ([5]). If $c_0 = 1$, computing the canonical sequence is straightforward

$$b_n = (n + 1)c_{n+1} - \sum_{k=0}^{n-1} c_{n-k}b_k. \tag{2.5}$$

Note that $F_b(z) = F'_c(z)/F_c(z)$. If $c_0 = 1$, $c_0^{(-1)} = 1$ and $|c_{n+1}^{(-1)}| \leq \frac{1}{n+1} \sum_{k=0}^n |c_{n-k}^{(-1)}|b_k$. It’s clear by induction that $|c_{n+1}^{(-1)}| \leq c_{n+1}$. For general c_0 , we can apply the above argument to c/c_0 and have the pointwise bound: $|c_k^{(-1)}| \leq \frac{1}{c_0} |c_k|$.

Now, let us show a simple example to illustrate the deconvolution with completely monotone sequences. Every completely monotone sequence is the moment sequence of a Hausdorff measure. Fix M as a big integer and denote $h = 1/M$. $x_i = (i - 1/2)h$. Consider the discrete measures

$$\mathcal{C}_M = \left\{ \mu : \mu = h \sum_{i=1}^M \lambda_i \delta(x - x_i), \lambda_i \geq 0 \right\}. \tag{2.6}$$

The weak star closure $(\langle \mu, f \rangle = \int_{[0,1]} f d\mu$ where $f \in C[0, 1])$ of $\bigcup_{M \geq 1} \mathcal{C}_M$ is the set of all Hausdorff measures. Due to this fact, we can generate completely monotone sequences using

$$d_n = \sum_{i=1}^M h \lambda_i x_i^n, \quad n = 0, 1, 2, \dots, \tag{2.7}$$

where $\lambda_i > 0$ are generated randomly (for example uniformly from $[0, 1]$).

In Fig. 1 (a), we have a sequence which is of square shape; in Fig. 1 (b), we plot the convolution between the sequence in (a) and the completely monotone sequence obtained using (2.7). Fig. 1 (c) shows the solution $a * c = f$ by convolving the sequence in Fig. 1(b) with $c^{(-1)}$. The original sequence is recovered accurately.

If the sequence c is no longer completely monotone, the generating function of $c^{(-1)}$ may have a small radius of convergence and an iterative method may be desired to

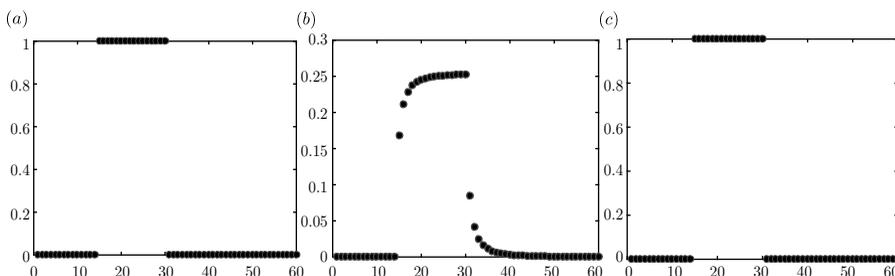


FIG. 1. A simple example of deconvolution

solve (2.1). Consider approximating the sequence c by a completely monotone sequence $d = \{d_n\}$ of the form in equation (2.7). Writing d in matrix form, we have

$$d = \frac{1}{m} A\lambda = A\eta, \tag{2.8}$$

where $\eta = \frac{1}{m}\lambda$. A simple iterative method then reads:

$$a^{p+1} = f * d^{(-1)} - a^p * [(c - d) * d^{(-1)}], \quad p = 0, 1, 2, \dots, \tag{2.9}$$

where a^0 is arbitrary. Clearly, the iteration converges if $\|(c - d) * d^{(-1)}\|_1 < 1$. A sufficient condition is therefore

$$\|d^{(-1)}\|_1 \|c - d\|_1 \leq \frac{2}{\|\eta\|_1} \|c - A\eta\|_1 < 1, \tag{2.10}$$

because d is completely monotone and $d_0 = \|\eta\|_1$. As long as we can find a solution η to this optimization problem, the iterative method can be applied to solve the convolution equation (2.1).

3. A discrete convolution group and discrete fractional calculus. In this section, we introduce a special discrete convolution group generated by a completely monotone sequence and define discrete fractional calculus. We show that the discrete fractional calculus is consistent with the Riemann-Liouville fractional calculus ([4, 6, 8]) with appropriate time scaling. The discrete convolution group proposed may be suitable for modeling memory effects in discrete time series.

The traditional Riemann-Liouville fractional calculus for a function in $C^1[0, T], T > 0$ with index $|\alpha| \leq 1$ is defined as

$$(J_\alpha f)(t) = \begin{cases} \frac{1}{\Gamma(\alpha)} \int_0^t (t-s)^{\alpha-1} f(s) ds, & \alpha > 0, \\ f(t), & \alpha = 0, \\ \frac{1}{\Gamma(1+\alpha)} \frac{d}{dt} \int_0^t \frac{f(s)}{(t-s)^{|\alpha|}} ds, & \alpha \in (-1, 0), \\ f'(t), & \alpha = -1. \end{cases} \tag{3.1}$$

In [8], a slightly different Riemann-Liouville calculus is proposed. The new definition introduces some singularities at $t = 0$ such that the resulted Riemann-Liouville calculus forms a group. However, for $t > 0$, the modified definition of a smooth function agrees with the traditional definition.

To motivate the discrete fractional calculus, we take a grid $t_i = ik : i = 0, 1, 2, \dots$ where k is the step size. Evaluating f at the grid points yields a sequence $a = \{a_i\}_{i=0}^\infty$, $a_i = f(ik)$. Using numerical approximations ([9]) for the fractional calculus, we find the following sequence for fractional integral J_γ , $0 < \gamma \leq 1$:

$$(c_\gamma)_j = \frac{1}{\gamma\Gamma(\gamma)}((j+1)^\gamma - j^\gamma).$$

Then, $J_\gamma f \approx k^\gamma c_\gamma * a$. The sequences $\{c_\gamma\}$ do not form a convolution semi-group. However, each sequence generates a convolution group. Let $\{c_\gamma^{(\alpha)} : \alpha \in \mathbb{R}\}$ be the group generated by c_γ , with $c_\gamma^{(\gamma)} = c_\gamma$. It is desirable that $\{c_\gamma^{(\alpha)} : \alpha \in \mathbb{R}\}$ can be used to define discrete fractional calculus.

We focus on the case $\gamma = 1$ and we have $c^{(1)} := c_1^{(1)} = (1, 1, \dots)$, with generating function $F_1(z) = (1 - z)^{-1}$. The convolution group generated by $c^{(1)}$ is denoted by $c^{(\alpha)} := c_1^{(\alpha)} : \alpha \in \mathbb{R}$ and the generating function is $F_\alpha(z) = (1 - z)^{-\alpha}, \forall \alpha \in \mathbb{R}$. $c^{(\alpha)}, 0 < \alpha \leq 1$ are completely monotone.

DEFINITION 3.1. For a sequence $a = (a_0, a_1, \dots)$, we define the discrete fractional operators $I_\alpha : \mathbb{R}^\mathbb{N} \mapsto \mathbb{R}^\mathbb{N}$ as $a \mapsto I_\alpha a := c^{(\alpha)} * a$.

Clearly, $\{I_\alpha : \alpha \in \mathbb{R}\}$ form a group.

3.1. *Consistency with the time continuous fractional calculus.* In this subsection, we show that the discrete fractional calculus is consistent with Riemann-Liouville fractional calculus if $|\alpha| \leq 1$.

Given a function time-continuous function $f(t)$, we pick a time step $k > 0$ and define the sequence a with $a_i = f(ik)$ ($i = 0, 1, 2, \dots$). We consider

$$T_\alpha f = k^\alpha I_\alpha a. \tag{3.2}$$

We now show that for $t > 0$ $(T_\alpha f)_n$ converges to $J_\alpha f(t)$ as $k = t/n \rightarrow 0^+$:

THEOREM 3.2. Suppose $f \in C^2[0, \infty)$. Fix $t > 0$, and define $k = t/n$. Then, $|(T_\alpha f)_n - (J_\alpha f)(t)| \rightarrow 0$ as $n \rightarrow \infty$ for $|\alpha| \leq 1$.

We first introduce some useful lemmas and then prove this theorem. The following is from [3]:

LEMMA 3.3. The m -th term of $c^{(\alpha)}$ has the following asymptotic behavior as $m \rightarrow \infty$:

$$c_m^{(\alpha)} \sim \frac{m^{\alpha-1}}{\Gamma(\alpha)} \left(1 + \frac{\alpha(\alpha-1)}{2m} + O\left(\frac{1}{m^2}\right) \right), \tag{3.3}$$

for $\alpha \neq 0, -1, -2, \dots$

LEMMA 3.4. For $|\alpha| < 1$, let $A_m = \sum_{i=0}^m c_i^{(\alpha)}$ be the partial sum of $c^{(\alpha)}$ and R be the convolution between $c^{(\alpha)}$ and $(1, 2, \dots)$. Then, as $m \rightarrow \infty$, we have:

$$A_m = \frac{m^\alpha}{\Gamma(1+\alpha)} \left(1 + O\left(\frac{1}{m}\right) \right), \quad R_m = \sum_{i=0}^m (m-i)c_i^{(\alpha)} = \frac{m^{1+\alpha}}{\Gamma(2+\alpha)} \left(1 + O\left(\frac{1}{m}\right) \right). \tag{3.4}$$

Proof. $\alpha = 0$ is trivial. Suppose $\alpha \neq 0$. $A = \{A_m\}_{m=0}^\infty$ is the convolution between $c^{(\alpha)}$ and $c^{(1)}$ and $A = c^{(\alpha+1)}$ by the group property. Similarly, since $c^{(2)} = (1, 2, 3, \dots)$, $R := \{R_m\}_{m=0}^\infty = c^{(\alpha+2)}$. Applying Lemma 3.3 yields the claims. \square

Proof of Theorem 3.2. Below, we only show the consistency and we are not trying to find the best estimate for the convergence rate.

$\alpha = 0$, $(T_0 f)_n = f(t)$ and the claim is trivial.

CASE 1 ($\alpha > 0$). If $\alpha = 1$, $(T_\alpha f)_n = \sum_{m=0}^n k f(t - mk)$. It is well known that $|(T_\alpha f)_n - \int_0^t f(s) ds| = O(k)$.

Consider $0 < \alpha < 1$. Let $n \gg 1$, $1 \ll M \ll n$ and $t_M = (M - 1)k$. We break the summation for $(T_\alpha f)_n$ at $m = M$ and apply Lemma 3.3 for the terms with $m \geq M$:

$$(T_\alpha f)_n = k^\alpha \sum_{m=0}^{M-1} c_m^{(\alpha)} f((n - m)k) + k^\alpha \sum_{m=M}^n \frac{m^{\alpha-1}}{\Gamma(\alpha)} f((n - m)k) + O(M^{\alpha-1} k^\alpha).$$

Since $f((n - m)k) = f(t) - f'(\xi)mk$ and $f(t - s) = f(t) - f'(\tilde{\xi})s$, by Lemma 3.4,

$$\begin{aligned} & \left| k^\alpha \sum_{i=0}^{M-1} c_m^{(\alpha)} f((n - m)k) - \frac{1}{\Gamma(\alpha)} \int_0^{t_M} f(t - s) s^{\alpha-1} ds \right| \\ & \leq |f(t)| \left| k^\alpha \sum_{m=0}^{M-1} c_m^{(\alpha)} - \frac{t_M^\alpha}{\Gamma(1 + \alpha)} \right| \\ & \quad + \sup |f'| M k^{\alpha+1} \sum_{m=0}^{M-1} c_m^{(\alpha)} + C \sup |f'| \int_0^{t_M} s^\alpha ds \\ & \leq C(M^{\alpha-1} k^\alpha + M^{1+\alpha} k^{1+\alpha}). \end{aligned}$$

Finally, by the error for rectangle rule for quadrature,

$$\begin{aligned} & \left| k^\alpha \sum_{m=K}^n \frac{m^{\alpha-1}}{\Gamma(\alpha)} f((n - m)k) - \int_{t_M}^t \frac{f(t - s)}{\Gamma(\alpha)} s^{\alpha-1} ds \right| \\ & \leq Ck \sup_{s \in (t_M, t)} \frac{d}{ds} (f(t - s) s^{\alpha-1}) \leq C(Mk)^{\alpha-2} k. \end{aligned}$$

Choosing $M \sim k^{-1/2}$, we find $M^{\alpha-1} k^\alpha \sim k^{(1+\alpha)/2}$, $(Mk)^{1+\alpha} \sim k^{(1+\alpha)/2}$ and $M^{\alpha-2} k^{\alpha-1} \sim k^{\alpha/2}$. Then, as $k \rightarrow 0$,

$$\left| (T_\alpha f)_n - \frac{1}{\Gamma(\alpha)} \int_0^t (t - s)^{\alpha-1} f(s) ds \right| \leq C(k^{(1+\alpha)/2} + k^{\alpha/2}) \rightarrow 0.$$

CASE 2 ($-1 \leq \alpha < 0$). If $\alpha = -1$, $c^{(\alpha)} = (1, -1, 0, 0, \dots)$. It is then clear that:

$$(T_{-1} f)_n = k^{-1} (f(nk) - f((n - 1)k)) = f'(nk) + O(k) = J_{-1} f(t) + O(k).$$

Consider that $\alpha \in (-1, 0)$ and $\gamma = |\alpha|$. The continuous Riemann-Liouville fraction derivative (3.1) equals

$$\begin{aligned} (J_{-\gamma} f)(t) &= \frac{f(0)}{\Gamma(1 - \gamma)} t^{-\gamma} + \frac{1}{\Gamma(1 - \gamma)} \int_0^t \frac{f'(s)}{(t - s)^\gamma} ds \\ &= \frac{f(t - k/b)}{k^\gamma} + \frac{1}{\Gamma(1 - \gamma)} \left[\int_{t-k/b}^t \frac{f'(s)}{(t - s)^\gamma} ds - \gamma \int_{k/b}^t \frac{f(t - s)}{s^{\gamma+1}} ds \right], \end{aligned}$$

where b is chosen such that $b^\gamma = \Gamma(1 - \gamma) = -\gamma\Gamma(-\gamma) \geq 1$. Since

$$k^{-\gamma}f(t) - k^{-\gamma}f(t - k/b) = O(k^{1-\gamma})$$

and

$$\int_{t-k/b}^t \frac{f'(s)}{(t-s)^\gamma} ds = O(k^{1-\gamma}),$$

we find

$$\begin{aligned} & |(T_{-\gamma}f)_n - (J_{-\gamma}f)(t)| \tag{3.5} \\ & \leq \left| \frac{1}{k^\gamma} \sum_{i=1}^n c_i^{(-\gamma)} f((n-i)k) + \frac{\gamma}{\Gamma(1-\gamma)} \int_{k/b}^t \frac{f(t-s)}{s^{\gamma+1}} ds \right| + O(k^{1-\gamma}). \end{aligned}$$

We first show that the right hand side of (3.5) goes to zero for constant and linear functions. By the first equation of (3.4) in Lemma 3.4 and noting $b^\gamma = -\gamma\Gamma(-\gamma)$, we have

$$k^{-\gamma} \sum_{i=1}^n c_i^{(-\gamma)} = k^{-\gamma} \left(\frac{n^{-\gamma}}{\Gamma(1-\gamma)} - 1 \right) + O\left(\frac{1}{(nk)^\gamma n} \right) = \frac{1}{\Gamma(-\gamma)} \int_{k/b}^t \frac{1}{s^{\gamma+1}} ds + O(k). \tag{3.6}$$

Hence, the right hand side of (3.5) goes to zero for constant functions. Similarly, by the second equation of (3.4), $k^{-\gamma} \sum_{i=1}^n c_i^{(-\gamma)} (n-i)k - \frac{1}{\Gamma(-\gamma)} \int_{k/b}^t \frac{t-s}{s^{\gamma+1}} ds = O((k/b)^{1-\gamma})$, and then

$$\left| k^{-\gamma} \sum_{i=1}^n c_i^{(-\gamma)} ik - \frac{1}{\Gamma(-\gamma)} \int_{k/b}^t s^{-\gamma} ds \right| = t \times O(k) + O((k/b)^{1-\gamma}) = O(k^{1-\gamma}). \tag{3.7}$$

The right hand side of (3.5) goes to zero for linear functions. Combining (3.6) and (3.7), we can assume without loss of generality that $f(t) = f'(t) = 0$ in equation (3.5) (actually, one can consider the function $\tilde{f}(s) = f(s) - f(t) - f'(t)(s-t)$).

Choose M such that $1 \ll M \ll n$ and set $t_M = (M-1)k$ again.

We first estimate the integral for $s \in (k/b, t_M)$ and the summation from 1 to $M-1$. Since $f(t) = f'(t) = 0$, one has $|f(t-s)| \leq Cs^2$, and hence

$$\left| \int_{k/b}^{t_M} \frac{f(t-s)}{s^{\gamma+1}} ds \right| \leq C \int_{k/b}^{t_M} s^{1-\gamma} ds \leq C(Mk)^{2-\gamma}.$$

Similarly, since $f(nk) = f'(nk) = 0$ and $c_i^{(-\gamma)}$ is negative for $i \geq 1$,

$$\left| k^{-\gamma} \sum_{i=1}^{M-1} c_i^{(-\gamma)} f((n-i)k) \right| \leq Ck^{2-\gamma} \sum_{i=1}^{M-1} i^2 |c_i^{(-\gamma)}| \leq CMk^{2-\gamma} \left| \sum_{i=1}^{M-1} ic_i^{(-\gamma)} \right| \leq C(Mk)^{2-\gamma}.$$

Note that (3.7) also implies $|\sum_{i=1}^{M-1} ic_i^{(-\gamma)}| = O(M^{1-\gamma})$, which has been used for the last inequality.

Now, we move onto the summation from M to n , and $s \in (t_M, t)$. By Lemma 3.3 and applying the error analysis for rectangle rule of quadrature,

$$\begin{aligned} & \left| k^{-\gamma} \sum_{i=M}^n c_i^{(-\gamma)} f((n-i)k) - \frac{1}{\Gamma(-\gamma)} \int_{t_M}^t \frac{f(t-s)}{s^{\gamma+1}} ds \right| \\ & \leq \left| k^{-\gamma} \sum_{i=M}^n \left(c_i^{(-\gamma)} - \frac{i^{-1-\gamma}}{\Gamma(-\gamma)} \right) f((n-i)k) \right| \\ & \quad + \left| k^{-\gamma} \sum_{i=M}^n \frac{i^{-1-\gamma}}{\Gamma(-\gamma)} f((n-i)k) - \frac{1}{\Gamma(-\gamma)} \int_{t_M}^t \frac{f(t-s)}{s^{\gamma+1}} ds \right| \\ & \leq CM^{-1-\gamma}k^{-\gamma} + (Mk)^{-2-\gamma}k. \end{aligned}$$

Taking $M = k^{-\epsilon - \frac{1+\gamma}{2+\gamma}}$ for some small $\epsilon > 0$, $(Mk)^{-2-\gamma}k$, $(Mk)^{2-\gamma}$ and $M^{-1-\gamma}k^{-\gamma}$ all tend to zero as $k \rightarrow 0$. Hence, the right hand side of (3.5) goes to zero for all $C^2[0, \infty)$ functions. \square

REMARK 3.5. In the case $\alpha = -1$ and $f(0) \neq 0$, $(T_\alpha f)_0 = \frac{f(0)}{k}$. This actually approximates the singular term $\delta(t)f(0)$ in the modified Riemann-Liouville derivative $J_{-1}f$ in [8].

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REFERENCES

- [1] W. Cai, *Computational methods for electromagnetic phenomena*, Cambridge University Press, Cambridge, 2013. Electrostatics in solvation, scattering, and electron transport; With a foreword by Weng Cho Chew. MR3027264
- [2] B. D. Coleman and W. Noll, *Foundations of linear viscoelasticity*, Rev. Modern Phys. **33** (1961), 239–249, DOI 10.1103/RevModPhys.33.239. MR0158605
- [3] P. Flajolet and R. Sedgewick, *Analytic combinatorics*, Cambridge University Press, Cambridge, 2009. MR2483235
- [4] R. Gorenflo and F. Mainardi, *Fractional calculus: integral and differential equations of fractional order*, Fractals and fractional calculus in continuum mechanics (Udine, 1996), CISM Courses and Lect., vol. 378, Springer, Vienna, 1997, pp. 223–276. MR1611585
- [5] B. G. Hansen and F. W. Steutel, *On moment sequences and infinitely divisible sequences*, J. Math. Anal. Appl. **136** (1988), no. 1, 304–313, DOI 10.1016/0022-247X(88)90133-3. MR972601
- [6] A. A. Kilbas, H. M. Srivastava, and J. J. Trujillo, *Theory and applications of fractional differential equations*, North-Holland Mathematics Studies, vol. 204, Elsevier Science B.V., Amsterdam, 2006. MR2218073
- [7] R. Kubo, *The fluctuation-dissipation theorem*, Reports on progress in physics **29** (1966), no. 1, 255.
- [8] L. Li and J.-G. Liu, *A generalized definition of Caputo derivatives and its application to fractional ODEs*, arXiv Preprint arXiv:1612.05103v2 (2017).
- [9] Y. Lin and C. Xu, *Finite difference/spectral approximations for the time-fractional diffusion equation*, J. Comput. Phys. **225** (2007), no. 2, 1533–1552, DOI 10.1016/j.jcp.2007.02.001. MR2349193
- [10] J.-G. Liu and R. L. Pego, *On generating functions of Hausdorff moment sequences*, Trans. Amer. Math. Soc. **368** (2016), no. 12, 8499–8518, DOI 10.1090/tran/6618. MR3551579
- [11] H. M. Nussenzveig, *Causality and dispersion relations*, Academic Press, New York-London, 1972. Mathematics in Science and Engineering, Vol. 95. MR0503032
- [12] G. Del Piero and L. Deseri, *On the concepts of state and free energy in linear viscoelasticity*, Arch. Rational Mech. Anal. **138** (1997), no. 1, 1–35, DOI 10.1007/s002050050035. MR1463802

- [13] S. Ruscheweyh, L. Salinas, and T. Sugawa, *Completely monotone sequences and universally prestarlike functions*, *Israel J. Math.* **171** (2009), 285–304, DOI 10.1007/s11856-009-0050-9. MR2520111
- [14] R. L. Schilling, R. Song, and Z. Vondraček, *Bernstein functions*, 2nd ed., De Gruyter Studies in Mathematics, vol. 37, Walter de Gruyter & Co., Berlin, 2012. Theory and applications. MR2978140
- [15] O. Stenzel, *The physics of thin film optical spectra*, Springer, 2005.
- [16] J. S. Toll, *Causality and the dispersion relation: logical foundations*, *Phys. Rev. (2)* **104** (1956), 1760–1770. MR0083623
- [17] D. V. Widder, *The Laplace Transform*, Princeton Mathematical Series, v. 6, Princeton University Press, Princeton, N. J., 1941. MR0005923
- [18] R. Zwanzig, *Nonequilibrium statistical mechanics*, Oxford University Press, New York, 2001. MR2012558