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ORIGINAL PAPER

A Tikhonov-type regularization method for Caputo fractional derivative

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Abstract
Stability estimates of Hölder type for the problem of evaluating the Caputo fractional derivative are obtained. This ill-posed problem is regularized by a Tikhonov-type method, which guarantees error estimates of Hölder type. Numerical results are presented to confirm the theory.

Keywords Caputo fractional derivative · ill-posed problems · stability estimates · Tikhonov-type regularization method · error estimates

1 Introduction

Fractional differentiation, including Riemann-Liouville and Caputo derivatives, has been proposed for a long time [17, 20, 21]. Recently, Caputo fractional derivatives received great attention due to their applications in interdisciplinary research problems. Caputo fractional derivatives are usually used to model heterogeneous systems and phenomena exhibiting anomalous diffusion [14, 16, 19]. Numerous references on numerical methods for computing fractional derivatives are available [12, 13, 15,

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18, 20]. The challenge arises when the function requiring derivative calculation is not precisely defined; we only have its approximation with a known margin of error. In this scenario, utilizing traditional calculation methods is impractical because the problem is ill-posed (in the sense of Hadamard). An effective regularization method is necessary to address this challenge. Several methods have been proposed for the problems involving Caputo fractional derivative and fractional partial differential equations [4, 10]; however, they still need further enrichment. In this paper, we investigate a new regularization approach to this problem in the square-summable function space $L^2[0, T]$. The ill-posedness of the problem in $L^2[0, T]$ is discussed in more detail in Section 2. The proposed regularization method is based on the regularization of noisy data by employing the Tikhonov regularization technique combined with an appropriate modification. This modification allows us to avoid the choice of the regularization parameter, which is needed for the classical Tikhonov regularization method, and obtains an error estimate of order $\frac{1}{2}$ (see Remark 4.4).

For a fixed $T > 0$, the Caputo fractional derivative, $D^\alpha q$, of a function $q(t)$ of order α with $\alpha \in (0, 1)$ is defined by

$$D^\alpha q(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{q'(s)}{(t-s)^\alpha} ds, \ 0 \le t \le T, \tag{1}$$

where Γ is the Gamma function. In this paper, we consider the problem of evaluating $D^\alpha q$ given by (1) for $\alpha \in (0, \frac{1}{2})$ to guarantee that $D^\alpha q$ is square-summable in $[0, T]$ for each $q(t) \in C[0, T]$.

Throughout the paper, notations $\langle \cdot, \cdot \rangle$ and $\| \cdot \|$ are used to denote the regular inner product and norm in $L^2[0, T]$, respectively, i.e.

$$\langle f, g \rangle = \int_0^T f(t) g(t) dt \text{ and } \|f\| = \left(\int_0^T |f(t)|^2 dt \right)^{\frac{1}{2}}, \ \forall f, g \in L^2[0, T].$$

We assume that the exact data, $q(t)$ in (1), is unknown; but instead, we know the measured data, denoted by $q^\delta(t) \in L^2[0, T]$ satisfying

$$\|q^\delta - q\| \le \delta. \tag{2}$$

The parameter $\delta > 0$ is called the noise level. We assume further that the exact data $q(t)$ is of twice continuously differentiable function on $[0, T]$ satisfying $q(0) = q'(T) = 0$ and there exists a constant $E > 0$ such that

$$\|q''\| \le E. \tag{3}$$

The condition $q(0) = q'(T) = 0$ can be replaced by $q'(0) = q(T) = 0$ while still ensuring this method works. However, this condition is necessary to hold theoretical analysis and numerical implementation of the method. More details about this point will be discussed in Section 3 and Section 5.

The rest of the paper is organized as follows: Section 2 presents an example to demonstrate the ill-posedness of the problem in $L^2[0, T]$. Section 3 is devoted to the Stability estimate. Section 4 presents the Regularization method. The numerical part is discussed in Section 5.

2 Analysis of ill-posedness

In this section, we analyze the ill-posedness of the problem of evaluating the Caputo fractional derivative of a function in space $L^2[0, T]$. We consider

$$\begin{aligned} q_n(t) &= \frac{\sqrt{n^3}}{n^{\frac{\alpha}{2}}} \left(\frac{(\frac{t}{T})^n}{n} - \frac{(\frac{t}{T})^{2n}}{2n} \right), t \in [0, T], n = 1, 2, 3, ... \\ (t) &= 0, t \in [0, T]. \end{aligned}$$

We have for all $n = 1, 2, 3, ...$

$$\begin{aligned} &q_n(0) = 0, \\ &q_n'(t) = \frac{\sqrt{n^3}}{n^{\frac{\alpha}{2}}} \frac{1}{T} \left(\left(\frac{t}{T}\right)^{n-1} - \left(\frac{t}{T}\right)^{2n-1} \right) \geq 0, \ \forall t \in [0, T], \\ &q_n'(T) = 0. \end{aligned}$$

We notice that $q, q_n \in L^2[0, T], \ \forall n = 1, 2, 3, ...$ and

$$\begin{aligned} \|q_n - q\|^2 &= \int_0^T (q_n(s) - q(s))^2 ds \\ &= \frac{n^3}{n^\alpha} \int_0^T \left(\frac{\left(\frac{s}{T}\right)^n}{n} - \frac{\left(\frac{s}{T}\right)^{2n}}{2n} \right)^2 ds \\ &= \frac{n^3}{n^\alpha} \int_0^T \left(\frac{1}{n^2} \left(\frac{s}{T}\right)^{2n} + \frac{1}{4n^2} \left(\frac{s}{T}\right)^{4n} - \frac{1}{n^2} \left(\frac{s}{T}\right)^{3n} \right) ds \end{aligned}$$

$$\begin{aligned} &= T \frac{n}{n^\alpha} \left(\frac{1}{2n+1} \left(\frac{s}{T}\right)^{2n+1} + \frac{1}{4(4n+1)} \left(\frac{s}{T}\right)^{4n+1} - \frac{1}{3n+1} \left(\frac{s}{T}\right)^{3n+1} \right) \Big|_0^T \\ &= T \frac{n}{n^\alpha} \left(\frac{1}{2n+1} + \frac{1}{4(4n+1)} - \frac{1}{3n+1} \right) \\ &= T \frac{1}{n^\alpha} \left(\frac{1}{2+\frac{1}{n}} + \frac{1}{4(4+\frac{1}{n})} - \frac{1}{3+\frac{1}{n}} \right). \end{aligned}$$

This implies that

$$\|q_n - q\| = \frac{1}{n^{\frac{\alpha}{2}}} \sqrt{\frac{1}{2+\frac{1}{n}} + \frac{1}{4(4+\frac{1}{n})} - \frac{1}{3+\frac{1}{n}}} \sqrt{T}, \forall n = 1, 2, 3, ... \tag{4}$$

We notice that

$$\lim_{n\to\infty} \frac{\sqrt{T}}{n^{\frac{\alpha}{2}}} \sqrt{\frac{1}{2+\frac{1}{n}} + \frac{1}{4(4+\frac{1}{n})} - \frac{1}{3+\frac{1}{n}}} = 0. \tag{5}$$

From (4) and (5), we obtain

$$\|q_n - q\| \to 0 \text{ as } n \to \infty. \tag{6}$$

On the other hand, we have

$$\begin{aligned}\|D^\alpha q_n - D^\alpha q\|^2 &= \int_0^T (D^\alpha q_n(t))^2 dt \\ &= \int_0^T \left(\frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{q_n^{'}(s)}{(t-s)^\alpha} ds\right)^2 dt \\ &= \frac{1}{\Gamma^2(1-\alpha)} \int_0^T \left(\int_0^t \frac{q_n^{'}(s)}{(t-s)^\alpha} ds\right)^2 dt. \end{aligned} \tag{7}$$

With $0 < s < t$ we have $t - s > 0$ and

$$t^{n-k}s^{k-1} \geq s^{n-k}s^{k-1} = s^{n-1}, \ \forall k = 1, 2, ..., n, \forall n = 1, 2, 3, ..$$

Therefore, we obtain

$$\begin{aligned}(t^n - s^n) &= (t-s)(t^{n-1} + t^{n-2}s + t^{n-3}s^2 + ... + ts^{n-2} + s^{n-1}) \\ &\geq (t-s)(s^{n-1} + s^{n-1} + ... + s^{n-1}) \\ &= n(t-s)s^{n-1}.\end{aligned}$$

This implies that

$$t - s \leq \frac{t^n - s^n}{ns^{n-1}}. \tag{8}$$

With $0 < s < t \leq T$ we have $0 < \frac{s}{T} < \frac{t}{T} \leq 1$. Therefore $0 < \left(\frac{s}{T}\right)^n < \left(\frac{s}{T}\right)^{n-1}$ and $0 < \left(\frac{t}{T}\right)^n - \left(\frac{s}{T}\right)^n < 1$ for all $n = 1, 2, 3, ...$ We have

$$\begin{aligned}\frac{t^n - s^n}{ns^{n-1}} &= \frac{T}{n}.\frac{\left(\frac{t}{T}\right)^n - \left(\frac{s}{T}\right)^n}{\left(\frac{s}{T}\right)^{n-1}} \\ &< \frac{T}{n}.\frac{1}{\left(\frac{s}{T}\right)^{n-1}} < \frac{T}{n}.\frac{1}{\left(\frac{s}{T}\right)^n}.\end{aligned} \tag{9}$$

From (8) and (9), we have

$$t - s \leq \frac{T}{n} \cdot \frac{1}{\left(\frac{s}{T}\right)^n}, \ 0 < s < t \leq T, \forall n = 1, 2, 3, ...$$

or

$$(t - s)^\alpha \leq \frac{T^\alpha}{n^\alpha} \cdot \frac{1}{\left(\frac{s}{T}\right)^{n\alpha}}, \ 0 < s < t \leq T, \forall n = 1, 2, 3, ...$$

This implies that

$$\frac{1}{(t-s)^\alpha} \geq \frac{n^\alpha \left(\frac{s}{T}\right)^{n\alpha}}{T^\alpha}, \ 0 < s < t \leq T, \forall n = 1, 2, 3, ... \tag{10}$$

From (10) and $q_n^{'}(s) \geq 0, \ \forall s \in [0, T]$, we obtain

$$\begin{aligned}
\int_0^t \frac{q_n^{'}(s)}{(t-s)^\alpha} ds &\geq \frac{n^\alpha}{T^\alpha} \int_0^t \left(\frac{s}{T}\right)^{n\alpha} q_n^{'}(s) ds \\
&= \frac{n^\alpha}{T^\alpha} \int_0^t \frac{\sqrt{n^3}}{n^{\frac{\alpha}{2}}} \cdot \frac{1}{T} \left(\left(\frac{s}{T}\right)^{n-1} - \left(\frac{s}{T}\right)^{2n-1}\right) \left(\frac{s}{T}\right)^{n\alpha} ds \\
&= \frac{n^{\frac{\alpha}{2}} \sqrt{n^3}}{T^\alpha} \int_0^t \frac{1}{T} \left(\left(\frac{s}{T}\right)^{n(1+\alpha)-1} - \left(\frac{s}{T}\right)^{n(2+\alpha)-1}\right) ds \\
&= \frac{n^{\frac{\alpha}{2}} \sqrt{n^3}}{T^\alpha} \left(\frac{\left(\frac{s}{T}\right)^{n(1+\alpha)}}{n(1+\alpha)} - \frac{\left(\frac{s}{T}\right)^{n(2+\alpha)}}{n(2+\alpha)}\right) \Big|_0^t \\
&= \frac{n^{\frac{\alpha}{2}} \sqrt{n}}{T^\alpha} \left(\frac{\left(\frac{t}{T}\right)^{n(1+\alpha)}}{(1+\alpha)} - \frac{\left(\frac{t}{T}\right)^{n(2+\alpha)}}{(2+\alpha)}\right).
\end{aligned} \tag{11}$$

From (7) and (11), we have

$$\begin{aligned}
\|D^\alpha q_n - D^\alpha q\|^2 &\geq \frac{1}{\Gamma^2(1-\alpha)} \int_0^T \left(\frac{n^{\frac{\alpha}{2}} \sqrt{n}}{T^\alpha} \left(\frac{\left(\frac{t}{T}\right)^{n(1+\alpha)}}{(1+\alpha)} - \frac{\left(\frac{t}{T}\right)^{n(2+\alpha)}}{(2+\alpha)}\right)\right)^2 dt \\
&= \frac{n^\alpha n}{\Gamma^2(1-\alpha) T^{2\alpha}} \int_0^T \left(\frac{\left(\frac{t}{T}\right)^{n(1+\alpha)}}{(1+\alpha)} - \frac{\left(\frac{t}{T}\right)^{n(2+\alpha)}}{(2+\alpha)}\right)^2 dt \\
&= \frac{n^\alpha n}{\Gamma^2(1-\alpha) T^{2\alpha}} \int_0^T \left(\frac{\left(\frac{t}{T}\right)^{2n(1+\alpha)}}{(1+\alpha)^2} - 2\frac{\left(\frac{t}{T}\right)^{n(3+2\alpha)}}{(1+\alpha)(2+\alpha)} + \frac{\left(\frac{t}{T}\right)^{2n(2+\alpha)}}{(2+\alpha)^2}\right) dt \\
&= \frac{n^\alpha n T^{1-2\alpha}}{\Gamma^2(1-\alpha)} \Bigg(\frac{\left(\frac{t}{T}\right)^{2n(1+\alpha)+1}}{(2n(1+\alpha)+1)(1+\alpha)^2} - 2\frac{\left(\frac{t}{T}\right)^{n(3+2\alpha)+1}}{(n(3+2\alpha)+1)(1+\alpha)(2+\alpha)} \\
&\quad + \frac{\left(\frac{t}{T}\right)^{2n(2+\alpha)+1}}{(2n(2+\alpha)+1)(2+\alpha)^2} \Bigg) \Big|_0^T
\end{aligned}$$

$$
\begin{aligned}
&= \frac{n^\alpha n T^{1-2\alpha}}{\Gamma^2(1-\alpha)}\Big(\frac{1}{(2n(1+\alpha)+1)(1+\alpha)^2} - \frac{2}{(n(3+2\alpha)+1)(1+\alpha)(2+\alpha)} \\
&\qquad + \frac{1}{(2n(2+\alpha)+1)(2+\alpha)^2}\Big) \\
&= \frac{n^\alpha T^{1-2\alpha}}{\Gamma^2(1-\alpha)}\Big(\frac{1}{(2(1+\alpha)+\frac{1}{n})(1+\alpha)^2} - \frac{2}{((3+2\alpha)+\frac{1}{n})(1+\alpha)(2+\alpha)} \\
&\qquad + \frac{1}{(2(2+\alpha)+\frac{1}{n})(2+\alpha)^2}\Big).
\end{aligned}
$$

Since

$$
\begin{aligned}
\lim_{n\to\infty} \frac{n^\alpha T^{1-2\alpha}}{\Gamma^2(1-\alpha)}\Big(&\frac{1}{(2(1+\alpha)+\frac{1}{n})(1+\alpha)^2} - \frac{2}{((3+2\alpha)+\frac{1}{n})(1+\alpha)(2+\alpha)} \\
&+ \frac{1}{(2(2+\alpha)+\frac{1}{n})(2+\alpha)^2}\Big) = \infty,
\end{aligned}
$$

we obtain

$$
\left\| D^\alpha q_n - D^\alpha q \right\| \to \infty \text{ as } n \to \infty. \tag{12}
$$

From (6) and (12), we conclude that the problem of evaluating the Caputo fractional derivative of a function in space $L^2[0, T]$ is ill-posed.

3 Stability estimate

This section presents a stability estimate for the problem of evaluating the Caputo differential derivative in the space $L^2[0, T]$. We begin with discussing the stability estimate for the problem of evaluating the first-order derivative, summarized in Lemma 3.1 below.

Lemma 3.1 *Suppose that $q_i(t)$, $i = 1, 2$ are twice continuously differentiable functions in $L^2[0, T]$ satisfying $q_i(0) = q_i'(T) = 0$, $\|q_i''\| \le E$, $i = 1, 2$, and*

$$
\|q_1 - q_2\| \le \delta. \tag{13}
$$

The following estimate holds

$$
\|q_1' - q_2'\| \leqslant \sqrt{2\delta E}.
$$

Proof Set $q(t) = q_1(t) - q_2(t),\ t \in [0, T]$. Using the integration by part, we get

$$
\begin{aligned}
\int_0^T (q'(s))^2 ds = \int_0^T q'(s) dq(s) &= q'(T)q(T) - q'(0)q(0) - \int_0^T q(s)q''(s)ds \\
&= -\int_0^T q(s)q''(s)ds.
\end{aligned} \tag{14}
$$

By the Cauchy-Schwarz inequality, we have

$$\begin{aligned}\left(\int_0^T (q'(s))^2 ds\right)^2 &= \left(-\int_0^T q(s)q''(s)ds\right)^2 = \left(\int_0^T q(s)q''(s)ds\right)^2\\ &\leqslant \int_0^T |q(s)|^2 ds \int_0^T |q''(s)|^2 ds\\ &= \|q\|^2\|q''\|^2\\ &= \|q_1 - q_2\|^2\|q_1'' - q_2''\|^2\\ &\leqslant \|q_1 - q_2\|^2 \left(\|q_1''\| + \|q_2''\|\right)^2\\ &\leqslant \delta^2(2E)^2 = 4\delta^2E^2. \end{aligned} \tag{15}$$

From (14) and (15), we obtain

$$\|q_1' - q_2'\|^4 = \left(\int_0^T (q'(s))^2 ds\right)^2 \leqslant 4\delta^2E^2,$$

which is equivalent to

$$\|q_1' - q_2'\| \leqslant \sqrt{2\delta E}. \tag{16}$$

The lemma is proved. □

Theorem 3.2 *(Stability estimate) Suppose that $q_i(t)$, $i = 1, 2$ are twice continuously differentiable functions in $L^2[0, T]$ satisfying $q_i(0) = q_i'(T) = 0$, $\|q_i''\| \le E$, $i = 1, 2$, and*

$$\|q_1 - q_2\| \le \delta. \tag{17}$$

The following estimate holds

$$\|D^\alpha q_1 - D^\alpha q_2\| \le \frac{\sqrt{2}T^{1-\alpha}\sqrt{\delta E}}{\Gamma(1-\alpha)\sqrt{1-2\alpha}}.$$

Proof Set $q(t) = q_1(t) - q_2(t),\ t \in [0, T]$. We have

$$\begin{aligned}\|D^\alpha q_1 - D^\alpha q_2\|^2 &= \int_0^T \left|D^\alpha q(t)\right|^2 dt\\ &= \int_0^T \left|\frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{q'(s)}{(t-s)^\alpha}ds\right|^2 dt\\ &\le \frac{1}{\Gamma^2(1-\alpha)}\int_0^T \left(\int_0^t \frac{|q'(s)|}{(t-s)^\alpha}ds\right)^2 dt. \end{aligned} \tag{18}$$

By the Cauchy-Schwarz inequality, we have

$$
\begin{aligned}
\left(\int_0^t \frac{|q'(s)|}{(t-s)^\alpha} ds\right)^2 &= \left(\int_0^t \frac{1}{(t-s)^\alpha} |q'(s)| ds\right)^2 \\
&\leqslant \int_0^t \frac{1}{(t-s)^{2\alpha}} ds \int_0^t |q'(s)|^2 ds \\
&\leqslant \int_0^t \frac{1}{(t-s)^{2\alpha}} ds \int_0^T |q'(s)|^2 ds \\
&= \frac{t^{1-2\alpha}}{1-2\alpha} \int_0^T (q'(s))^2 ds \\
&\leqslant \frac{T^{1-2\alpha}}{1-2\alpha} \int_0^T (q'(s))^2 ds. \qquad (19)
\end{aligned}
$$

We conclude from (18), (19) and Lemma 3.1 that

$$
\begin{aligned}
\|D^\alpha q_1 - D^\alpha q_2\|^2 &\leqslant \frac{1}{\Gamma^2(1-\alpha)} \int_0^T \frac{T^{1-2\alpha}}{1-2\alpha} 2\delta E dt \\
&= 2\delta E \frac{1}{\Gamma^2(1-\alpha)} \frac{T^{2-2\alpha}}{1-2\alpha} \qquad (20)
\end{aligned}
$$

or

$$
\|D^\alpha q_1 - D^\alpha q_2\| \leq \frac{\sqrt{2} T^{1-\alpha} \sqrt{\delta E}}{\Gamma(1-\alpha)\sqrt{1-2\alpha}}.
$$

The theorem is proved. □

Remark 3.3 The following example demonstrates that if the homogeneous boundary conditions do not hold for both functions at both endpoints, then the stability results in Theorem 3.2 do not hold although other conditions are satisfied. For $T > 0$, let $f(t) = 2024t$ and $g(t) = 0, \ \forall t \in [0, T]$ then

$$
\begin{aligned}
&f(0) = g(0) = g'(T) = 0; \\
&f(T) = 2024T \neq 0, \ \ f'(T) = 2024 \neq 0.
\end{aligned}
$$

Thus, $g(t)$ satisfies the boundary condition stated in Theorem 3.2 while $f(t)$ does not satisfy. Futhermore, in this case, we see that

$$
\begin{aligned}
&\|f - g\| = 2024\sqrt{\frac{T^3}{3}} > 0; \\
&\|f' - g'\| = 2024\sqrt{T} > 0; \\
&\|D^\alpha f - D^\alpha g\| = \frac{2024}{(1-\alpha)\Gamma(1-\alpha)} \sqrt{\frac{T^{3-2\alpha}}{3-2\alpha}} > 0; \\
&f''(t) = g''(t) = 0, \ \forall t \in [0, T].
\end{aligned}
$$

Therefore, if we choose $\delta = 2024\sqrt{\frac{T^3}{3}} > 0$, $E > 0$ small enough then

$$\begin{cases} \|f - g\| \leqslant \delta \\ \|f''\| \leqslant E \\ \|g''\| \leqslant E. \end{cases} \tag{21}$$

However, we have

$$\|f' - g'\| > \sqrt{2\delta E}$$

and

$$\|D^\alpha f - D^\alpha g\| > \frac{\sqrt{2}T^{1-\alpha}\sqrt{\delta E}}{\Gamma(1-\alpha)\sqrt{1-2\alpha}},$$

which contradicts the estimate in Theorem 3.2.

4 Regularization method

As stated in the introduction, we assume that the exact data $q(t)$ is twice continuously differentiable function on $[0, T]$ satisfying $q(0) = q'(T) = 0$ and (3). We denote by V the set of such functions, that is, V is the set of all functions p that is twice continuously differentiable function on $[0, T]$ such that $p(0) = p'(T) = 0$. Obviously, $q \in V$. With this definition, V is a nontrivial subspace of $L^2[0, T]$.

Theorem 4.1 *V is a nontrivial subspace of the Hilbert space $L^2[0, T]$.*

Proof It is easy to see that V is a subspace of $L^2[0, T]$. Indeed, for any $p_1, p_2 \in V$, for any $\beta, \mu \in \mathbb{R}$, we have

$$\begin{aligned} (\beta p_1 + \mu p_2)(0) &= \beta p_1(0) + \mu p_2(0) = 0, \\ (\beta p_1 + \mu p_2)'(T) &= \beta p_1'(T) + \mu p_2'(T) = 0, \end{aligned}$$

and $\beta p_1 + \mu p_2$ is a twice continuously differentiable function. Therefore $\beta p_1 + \mu p_2 \in V$. Furthermore, consider

$$p(t) = te^{-t} + Te^{-T}t, \ 0 \le t \le T,$$

then p is a twice continuously differentiable function, $p(0) = 0$ and $p'(T) = 0$; thus, $p(t) \in V$. Therefore, V is a nontrivial subspace of the Hilbert space $L^2[0, T]$. □

The proposed regularization method aims to find an approximation to $D^\alpha q$ from the measured data $q^\delta(t)$. This approximation is expected to be $D^\alpha \overline{p}$, where $\overline{p} \in V$. Lemma 3.1 and Theorem 3.2 guarantee the stability of the first-order and the Caputo fractional derivative of $\overline{p}$ due to both $\overline{p}$ belonging to V. To find $\overline{p}$, we first consider the functional.

$$J(p) = \left(\frac{\delta}{E}\right)^2 \|p''\|^2 + \|p - q^\delta\|^2, \ p \in V. \tag{22}$$

Then, $J(p)$ is convex on V. The convexity of $J(p)$ follows immediately from the convexity of $\|p''\|^2$ and $\|p - q^\delta\|^2$.
The existence of the minimizer of $J(p)$ on V is unsure; however, let denote $I := \inf_{p \in V} J(p)$ then for each $\tau > 0$, there always exists $\overline{p} \in V$ such that

$$J(\overline{p}) \leq I + \tau\delta^2. \tag{23}$$

This function $\overline{p}$ is the one whose Caputo fractional derivative of order α is the approximation of $D^\alpha q$. The error estimate result is stated in the theorem below.

Theorem 4.2 *If $q(t)$ is twice continuously differentiable function on $[0, T]$ satisfying $q(0) = q'(T) = 0$ and (3), the measured data $q^\delta(t) \in L^2[0, T]$ satisfies (2) and $\overline{p} \in V$ satisfies (23) then*

$$\left\| D^\alpha \overline{p} - D^\alpha q \right\| \leq \frac{\sqrt{2(\tau + 2 + \sqrt{\tau + 2})} T^{1-\alpha} \sqrt{\delta E}}{\Gamma(1-\alpha)\sqrt{1 - 2\alpha}}.$$

Proof We have

$$J(\overline{p}) = \left(\frac{\delta}{E}\right)^2 \|\overline{p}''\|^2 + \|\overline{p} - q^\delta\|^2.$$

Therefore, we have

$$\begin{aligned}
\|\overline{p} - q^\delta\|^2 \leq J(\overline{p}) \leq I + \tau\delta^2 &= \inf_{p \in V} J(p) + \tau\delta^2 \\
&\leq J(q) + \tau\delta^2 \\
&= \left(\frac{\delta}{E}\right)^2 \|q''\|^2 + \|q - q^\delta\|^2 + \tau\delta^2.
\end{aligned}$$

By assumption,

$$\|q''\| \leq E, \|q^\delta - q\| \leq \delta,$$

we obtain

$$\|\overline{p} - q^\delta\|^2 \leq \left(\frac{\delta}{E}\right)^2 E^2 + \delta^2 + \tau\delta^2 = (\tau + 2)\delta^2.$$

This implies that

$$\|\overline{p} - q^\delta\| \leq \sqrt{\tau + 2}\,\delta. \tag{24}$$

From (2) and (24), we get

$$\|\overline{p} - q\| \leq \|\overline{p} - q^\delta\| + \|q^\delta - q\| \leq (1 + \sqrt{\tau + 2})\delta. \tag{25}$$

Similarly, we also have

$$\begin{aligned}\left(\frac{\delta}{E}\right)^2 \|\overline{p}''\|^2 \leq J(\overline{p}) \leq I + \tau\delta^2 &= \inf_{p\in V} J(p) + \tau\delta^2 \\ &\leq J(q) + \tau\delta^2 \\ &= \left(\frac{\delta}{E}\right)^2 \|q''\|^2 + \|q - q^\delta\|^2 + \tau\delta^2 \\ &\leq \left(\frac{\delta}{E}\right)^2 E^2 + \delta^2 + \tau\delta^2 = (\tau+2)\delta^2.\end{aligned}$$

Hence,

$$\|\overline{p}''\| \leq \sqrt{\tau+2}E. \tag{26}$$

Furthermore, we have

$$\|q''\| \leq E < \sqrt{\tau+2}E. \tag{27}$$

Combining (25), (26), (27) and applying Theorem 3.2, we obtain

$$\left\| D^\alpha \overline{p} - D^\alpha q \right\| \leq \frac{\sqrt{2(\tau + 2 + \sqrt{\tau+2})}T^{1-\alpha}\sqrt{\delta E}}{\Gamma(1-\alpha)\sqrt{1-2\alpha}}.$$

The theorem is proved. □

Remark 4.3 With $\overline{p}$ defined in Theorem 4.2, the following error estimate for the first order derivative holds

$$\left\|\overline{p}' - q'\right\| \leqslant \sqrt{2(\tau + 2 + \sqrt{\tau+2})\delta E}.$$

Proof The above error estimate is obtained straightforwardly from (25), (26), (27), and Lemma 3.1. □

Remark 4.4 The order of the error estimate in Theorem 4.2 is $\frac{1}{2}$. Indeed, the error estimate in Theorem 4.2 has the form

$$\left\| D^\alpha \overline{p} - D^\alpha q \right\| \leq C\delta^{\frac{1}{2}} \tag{28}$$

where C is a constant. Obviously, the Hölder exponent in estimate (28) is $\frac{1}{2}$. The order of our error estimate in Theorem 4.2 is the same as that in Theorem 3.1 in [4]. Furthermore, we noticed that the order of error estimate in Theorem 2.1 in [10] does not exceed $\frac{1}{2}$.

5 Numerical Implementation

In numerical implementation, we will try to avoid the role of the term $\tau\delta^2$ in (23). Employing the denseness of V in the Sobolev space H^2_{00} defined below

$$H^2_{00} := \{u \in H^2([0,T]) |\, u(0) = 0,\ u'(T) = 0\}, \tag{29}$$

with the norm $\|u\|_{H^2_{00}} := \sqrt{\|u\|^2 + \|u'\|^2 + \|u''\|^2}$, we replace $\overline{p}$ in (23) by the minimizer p^* of $J(p)$ in H^2_{00}. The existence and uniqueness of the minimizer, $p^* = \arg\min_{p\in H^2_{00}} J(p)$, is guaranteed. Before proving this claim, we first present the Lemma 5.1 below. This is an application of Friedrichs inequality (see [22], Theorem 1.9), but we here prove it for the readers' convenience.

Lemma 5.1 *There exists a constant $C > 0$ such that*

(i) $\|u\| \le C(|u(0)| + \|u'\|)$
(ii) $\|u\| \le C(|u(T)| + \|u'\|)$

for all $u \in H^1([0,T])$.

Proof We provide the proof for item (i). The proof for item (ii) can be done similarly. By contradiction, if the property is not true, there exists a sequence $(u_n) \subset H^1([0,T])$ such that

$$\|u_n\| > n(|u(0)| + \|u_n'\|) \tag{30}$$

We can choose u_n such that $\|u_n\|_{H^1} = \sqrt{\|u_n\|^2 + \|u_n'\|^2} = 1$. The sequence u_n is bounded in H^1 implies that there exists a sub-sequence, still denoted by (u_n), that converges strongly to u in $L^2([0,T])$ (due to the compact embedding of $H^1([0,T])$ in $L^2([0,T])$). Condition (30) implies that u_n' converges strongly to 0 in L^2. As a result, u_n converges in H^1. The uniqueness of the limit implies that the limit is still u. In addition, $u(0) = 0$. On the other hand, since $u_n' \to 0$ as $n \to \infty$, it deduces $u' = 0$. Thus, u is a constant. Combined with $u(0) = 0$, we obtain $u = 0$, which contradicts $\|u\|_{H^1} = 1$ (since $\|u_n\|_{H^1} = 1$ for all n). □

By applying Lemma (5.1) twice we have that, there exists $C_0, C_1 > 0$ such that for each $u \in H^2_{00}$:

$$\|u''\| \le C(|u'(T)| + \|u'\|) = C\|u'\| \tag{31}$$

$$\|u'\| \le C_1(|u(0)| + \|u\|) = C_1\|u\| \tag{32}$$

As a result, there exists $c_*, C^* > 0$ such that $c_*\|u''\| \le \|u\|_{H_{00}} \le C^*\|u''\|$, which indicates that $\|u''\|$ is a norm in H^2_{00}. We now use this property to prove the existence and uniqueness of the minimizer of $J(p)$ in H^2_{00}.

Theorem 5.2 *The functional $J(p)$ defined in (22), has a unique minimizer in H^2_{00}.*

Proof Let

$$I_H := \inf\{J(p) | p \in H^2_{00}\} \geq 0.$$

There exists $(p_n) \subset H^2_{00}$ such that $J(p_n) \to I$ as $n \to \infty$. It is easy to see that (p_n) is bounded in H^2_{00}. Indeed, by contraction, if (p_n) is unbounded, there exists a sub-sequence, still denoted by p_n, such that $\|p_n\|_H \to \infty$ as $n \to \infty$. Thus $J(p_n) \geq (\frac{\delta}{E})^2 \|p''\|^2 \to \infty$ as $n \to \infty$. The boundedness of (p_n) in H^2_{00} deduces that there exists a sub-sequence, still denoted by p_n, such that $\|p_n\|_H$ converges weakly to $p^* \in H^2_{00}$ as $n \to \infty$. By compact embedding of H^2 to L^2, $p_n - q^\delta$ converges strongly to $p^* - q^\delta$. Thus,

$$J(p^*) \leq \limsup_{n\to\infty} J(p_n) = \lim_{n\to\infty} J(p_n) = I.$$

Therefore p^* is a minimizer of J. The uniqueness of p^* is obtained straightforwardly from the strict convexity of J. □

As mentioned at the beginning of the section, $D^\alpha q^\delta$ is regularized by $D^\alpha p^*$, where p^* in Theorem 5.2 (instead of $\overline{p}$ in Theorem 4.2). The Holder-type error estimate established in Theorem 4.1 always holds. In addition, the first order derivative of q^δ is regularized by $\overline{p}$ as shown in Remark 4.3. In practice, $\overline{p}$ is replaced by p^*.

5.1 Discretization and Algorithm

Let $N > 0$ be an even integer and $\mathbf{t} = [t_n] \in \mathbb{R}^{N+1}$ such that $t_n = nh, \forall n = 0, \ldots, N$, $h = \frac{T}{N}$ be a mesh of $[0, T]$. Corresponding to a generic function $p(t)$, we denote by $\mathbf{p} = [p_n]$ a vector in $\mathbb{R}^{N+1}$ such that p_n is an approximation of $p(t_n)$ under the finite difference method. By the centered difference approximation, the approximation of $p''(t_j)$, $D^2 p_n$, is written as

$$D^2 p_n = \frac{p_{n+1} - 2p_n + p_{n-1}}{h^2}, \ \forall n = 1, \ldots, N-1.$$

At $n = 0$, the boundary condition $p(0) = 0$ implies $p_0 = 0$. At $n = N$ $(t_N = T)$, by employing the condition $p'(T) = 0$, we write the approximation of $p"(t_N)$ as

$$D^2 p_N = \frac{p'(t_{N-1}) - p'(t_N)}{-h} = \frac{p_N - p_{N-1}}{-h^2} = \frac{p_{N-1} - p_N}{h^2}.$$

We denote $\widetilde{\mathbf{p}} \in \mathbb{R}^N$, the vector obtained from $\mathbf{p}$ by removing the first entry, i.e., $\mathbf{p} = [p_1; \widetilde{\mathbf{p}}]$. Then the vector $D^2\widetilde{\mathbf{p}} \approx [p''(t_n)]$, $n = 1, \ldots, N$ is written in the form of matrix-vector multiplication as follows:

$$D^2\widetilde{\mathbf{p}} = A\widetilde{\mathbf{p}},$$

where matrix A is given by

$$A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & & & \\ 1 & -2 & 1 & & & & \\ & 1 & -2 & 1 & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & & 1 & -2 & 1 \\ & & & & 0 & 1 & -1 \end{bmatrix}.$$

The functional J is written as

$$J(\widetilde{\mathbf{p}}) = \left(\frac{\delta}{E}\right)^2 \|A\widetilde{\mathbf{p}}\|^2 + \|\widetilde{\mathbf{p}} - \widetilde{\mathbf{q}}^{\delta}\|^2 \tag{33}$$

The first task is to seek the minimizer $\widetilde{\mathbf{p}^*} \in \mathbb{R}^N$ of J:

$$\widetilde{\mathbf{p}^*} = \underset{\widetilde{\mathbf{p}} \in \mathbb{R}^N}{\arg\min}\, J\,(\widetilde{\mathbf{p}}) = \underset{\widetilde{\mathbf{p}} \in \mathbb{R}^N}{\arg\min} \left(\frac{\delta}{E}\right)^2 \|A\widetilde{\mathbf{p}}\|^2 + \|\widetilde{\mathbf{p}} - \widetilde{\mathbf{q}}^{\delta}\|^2.$$

Then, $\widetilde{\mathbf{p}^*}$ is such that

$$\big((\tfrac{\delta}{E})^2 A^T A + I\big)\widetilde{\mathbf{p}^*} - \widetilde{\mathbf{q}}^{\delta} = \mathbf{0}. \tag{34}$$

When δ/E small enough, matrix $(\frac{\delta}{E})^2 A^T A + I$ is invertible, which implies the uniqueness of $\widetilde{\mathbf{p}^*}$, $\widetilde{\mathbf{p}^*} = \big((\frac{\delta}{E})^2 A^T A + I\big)^{-1}\widetilde{\mathbf{q}}^{\delta}$.
In the following examples, we consider some particular functions $q(t)$ such that their Caputo fractional derivative can be calculated analytically. The perturbed data, $\widetilde{\mathbf{q}}^{\delta}$, is obtained from $q(t)$ by adding a random noise. In particular, $\widetilde{\mathbf{q}}^{\delta}$ is defined by:

$$q_n^{\delta} = q(t_n) + \delta_n, \;\; n = 1, \ldots, N \tag{35}$$

where δ_n, $n = 1, \ldots, N$ are uniformly distributed random numbers in $(-\delta, \delta)$. The algorithm is summarized as follows:

1. Solve equation (34), then define $\mathbf{p}^* := [0; \widetilde{\mathbf{p}^*}]$.
2. The function $p^*(t)$ is such that: $p^*(t_n) = p_n^*$ for all $n = 0, \ldots, N$.
3. Evaluate $(p^*)^{'}(t)$ at t_n by: $(p^*)^{'}(t_0) = \frac{p_1^*}{h}$, $(p^*)^{'}(t_N) = 0$, and $(p^*)^{'}(t_n) = \frac{p_{n+1}^* - p_{n-1}^*}{2h}$, $n = 1, 2, \ldots, N-1$.
4. Calculate $D^{\alpha} p^*$ using the trapezoidal rule.

Values of parameters $T = 3$, $N = 3000$, $\tau = 0$ are fixed for all examples.

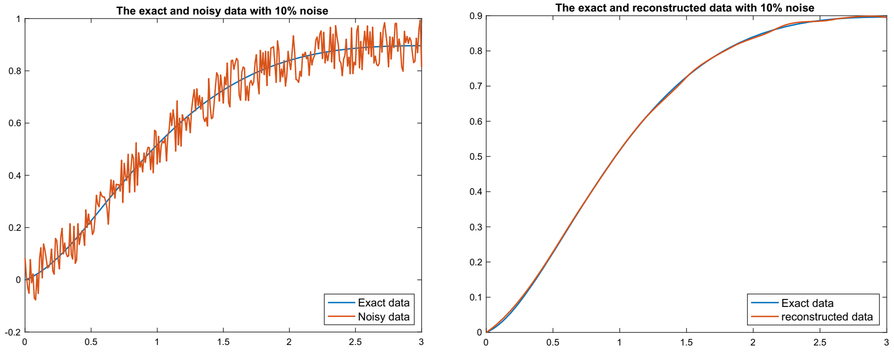

Fig. 1 An example of the noisy data and the corresponding regularized data for Example 1. Left - The noisy data with 10% noise (the zigzag orange curve) and the exact data (the smooth blue curve). Right - The regularized data (the smooth orange curve) compared to the exact data (the smooth blue curve)

5.2 Numerical examples

Example 1: In the first example, the exact data has the formula $q(t) = t^2e^{\lambda t} - ct$ where $\lambda < 0$ and c is chosen such that $q'(T) = 0$. Follow [4], $D^\alpha(t^2e^{\lambda t})$ is given by

$$D^\alpha(t^2e^{\lambda t}) = \lambda u_2 - (2\lambda t + 2)u_1 + (2t^{2-\alpha} + \lambda t^{3-\alpha})E_{1,2-\alpha}(\lambda t),$$

where

$$u_1 = \frac{1}{\Gamma(1-\alpha)}\frac{-1}{\lambda}t^{1-\alpha} + \frac{1-\alpha}{\lambda}t^{1-\alpha}E_{1,2-\alpha}(\lambda t)$$
$$u_2 = \frac{1}{\Gamma(1-\alpha)}\frac{-1}{\lambda}t^{2-\alpha} + \frac{2-\alpha}{\lambda}\left(\frac{1}{\Gamma(1-\alpha)}\frac{-1}{\lambda}t^{1-\alpha} + \frac{1-\alpha}{\lambda}t^{1-\alpha}E_{1,2-\alpha}(\lambda t)\right)$$

and $E_{a,b}(z) = \sum_{k=0}^{\infty}\frac{z^k}{\Gamma(ak+b)}$ is the two - parameter function of Mittag - Leffler type.

Thus,

$$D^\alpha q(t) = D^\alpha(t^2e^{\lambda t}) - \frac{c}{\Gamma(1-\alpha)}\frac{t^{1-\alpha}}{1-\alpha}.$$

Here we choose particularly $\lambda = -1$ and $c = -3e^{-T}$. The noisy data $\widetilde{\mathbf{q}}^\delta$ is given by (35), where δ_n, $n = 1, \ldots, N$ obtained numerically. Fig. 1 illustrates the noisy data, with noise level $\delta = 10\%$ (left) and the associated regularized data (right). The approximation $D^\alpha p^*$ $\alpha = 0.1, 0.2, 0.3, 0.49$ associated with 10% noisy data (see Fig. 2) is shown in Fig. 2. Table 1 claims the efficiency of the method, which indicates that the ℓ^2-norm relative error estimates between $D^\alpha p^*$ and $D^\alpha q$ are small enough although δ large.

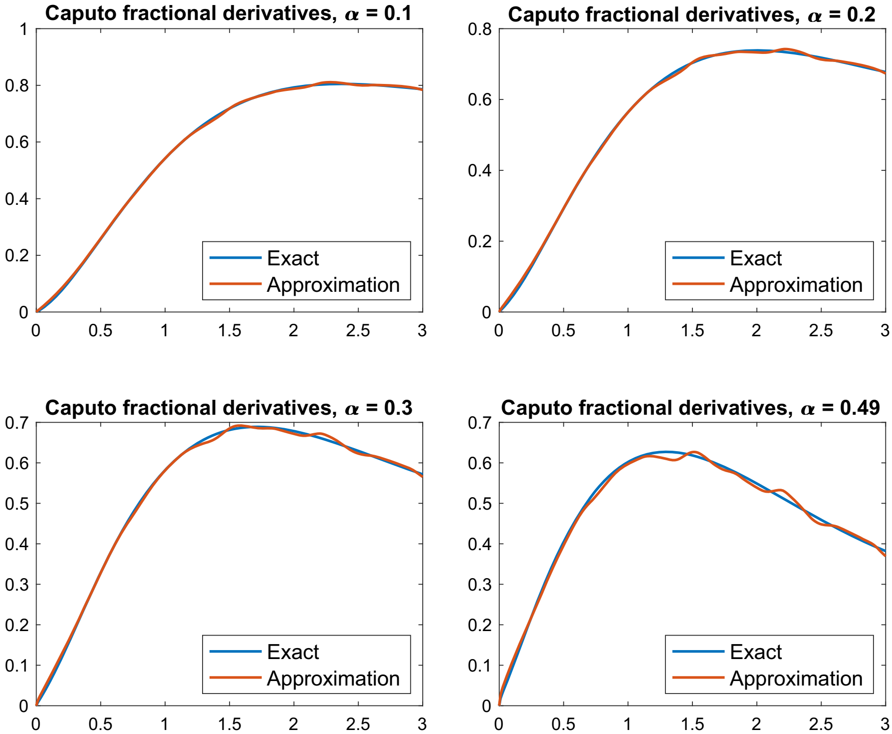

Fig. 2 Example 1: Approximations of Caputo Fractional Derivatives (CFD). For each sub-figure, the blue curve plots the CFD of the exact data, $D^\alpha q$; the orange curve plots the corresponding approximation, $D^\alpha p^*$, where the measured data is perturbed by 10% noise. Values of α are indicated in the title of each sub-figure

Example 2: In this example, we choose the exact data $q(t) = t^2 e^{-t/2} - ct^2$, where c is chosen such that $q'(T) = 0$. With the choice $T = 3$ from the beginning, $c = e^{-3/2}/4$. The noisy data q^δ is defined as same as in Example 1. The Caputo derivative of the exact data is given by

$$D^\alpha q(t) = D^\alpha (t^2 e^{-t/2}) - \frac{\Gamma(3)}{\Gamma(3-\alpha)} t^{2-\alpha},$$

where $D^\alpha (t^2 e^{-t/2})$ is provided in Example 1 that applies to $\lambda = -1/2$.

Table 1 Relative errors for Example 1 for different values of δ and α

	$\alpha = 0.1$	$\alpha = 0.2$	$\alpha = 0.3$	$\alpha = 0.49$
$\delta = 0.02$	0.0022	0.0031	0.0043	0.0065
$\delta = 0.05$	0.0044	0.0058	0.0077	0.0105
$\delta = 0.1$	0.0072	0.0092	0.0120	0.0156
$\delta = 0.2$	0.0116	0.0144	0.0180	0.0227

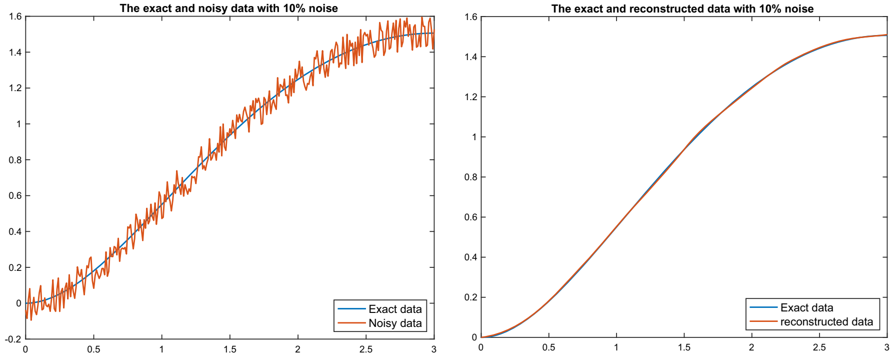

Fig. 3 An example of noisy data and the corresponding regularized data for Example 2. Left - The noisy data with 10% noise (the zigzag orange curve) compared to the exact data (the smooth blue curve). Right - The regularized data (the smooth orange curve) compared to the exact data (the smooth blue curve)

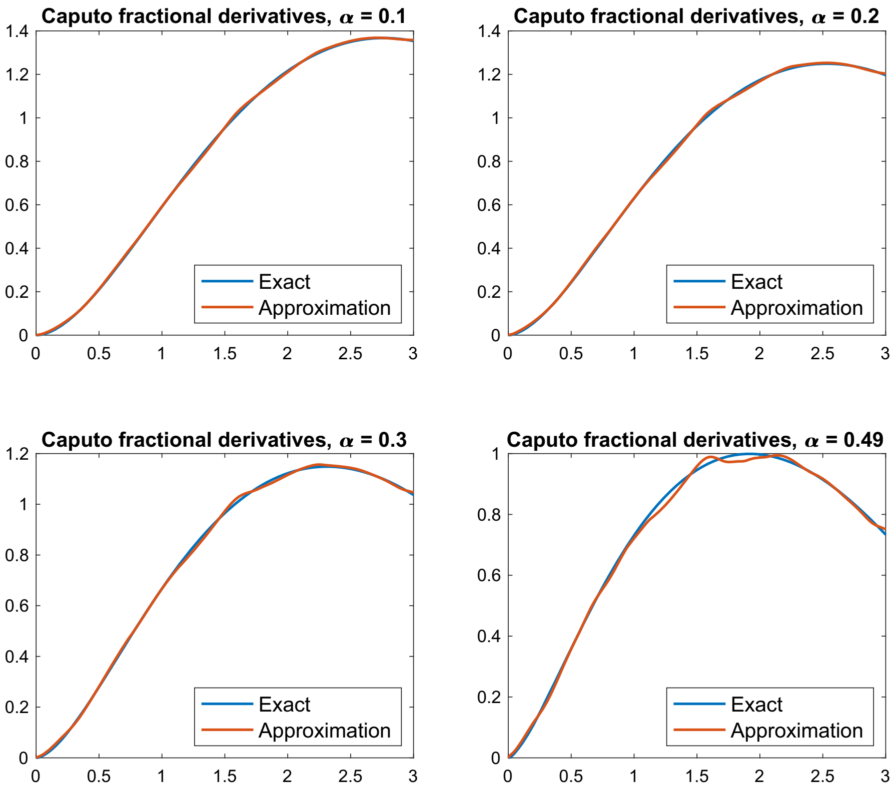

Fig. 4 Example 2: Approximations of Caputo Fractional Derivatives (CFD). For each sub-figure, the blue curve plots the CFD of the exact data, $D^\alpha q$; the orange curve plots the corresponding approximation, $D^\alpha p^*$, where the measured data is perturbed by 10% noise. Values of α are indicated in the title of each sub-figure

Table 2 Relative errors for Example 2 for different values of δ and α

	$\alpha = 0.1$	$\alpha = 0.2$	$\alpha = 0.3$	$\alpha = 0.49$
$\delta = 0.02$	0.0014	0.0019	0.0028	0.0046
$\delta = 0.05$	0.0025	0.0032	0.0044	0.0064
$\delta = 0.1$	0.0039	0.0049	0.0064	0.0086
$\delta = 0.2$	0.0068	0.0083	0.0103	0.0131

Similar to Example 1, we provide an example for the measured data, q^δ, with 10% noise and the corresponding regularized data (see Fig. 3). The approximation of the $D^\alpha q^\delta$ for $\alpha = 0.1, 0.2, 0.3, 0.49$ and the ℓ^2-norm relative error estimates are shown in Fig. 4 and Table 2, respectively.
Examples 3 and 4 below, we consider two more cases of $q(t)$. In each example, briefly illustrate 10% noisy data compared to the exact data, the regularized data, figures about the behavior of the approximation associated with various values of α, and tables showing the relative error estimate of the method.
Example 3: We choose $q(t) = 1 - \cos(2t) - ct$, where $c = 2\sin(2T)$ is chosen such that $q'(T) = 0$. The Caputo derivative of the exact data is given by

$$D^\alpha q(t) = -it^{1-\alpha}\left(E_{1,2-\alpha}(i2t) - E_{1,2-\alpha}(-i2t)\right) - \frac{c}{\Gamma(1-\alpha)}\frac{t^{1-\alpha}}{1-\alpha}, \quad \forall\, 0 < \alpha < 1.$$

Similar to Example 1, we provide an example for the measured data, q^δ, with 10% noise and the corresponding regularized data (see Fig. 5). The regularization for $D^\alpha q^\delta$, $\alpha = 0.1, 0.2, 0.3, 0.49$ and the ℓ^2-norm relative error estimates are shown in Fig. 6 and Table 3, respectively.

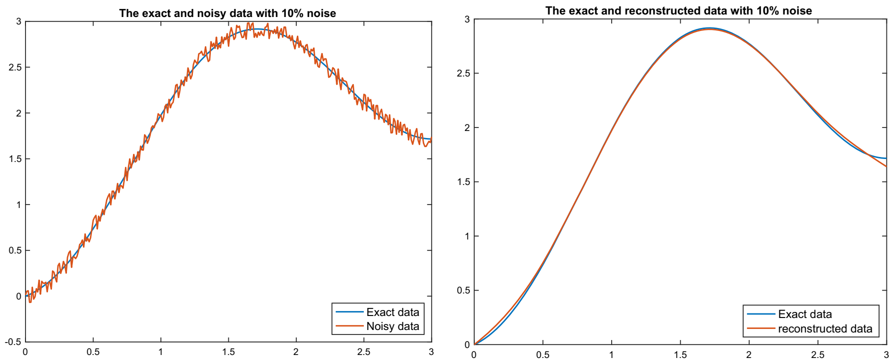

Fig. 5 An example of noisy data and the corresponding regularized data for Example 3. Left - The noisy data with 10% noise (the zigzag orange curve) compared to the exact data (the smooth blue curve). Right - The regularized data (the smooth orange curve) compared to the exact data (the smooth blue curve)

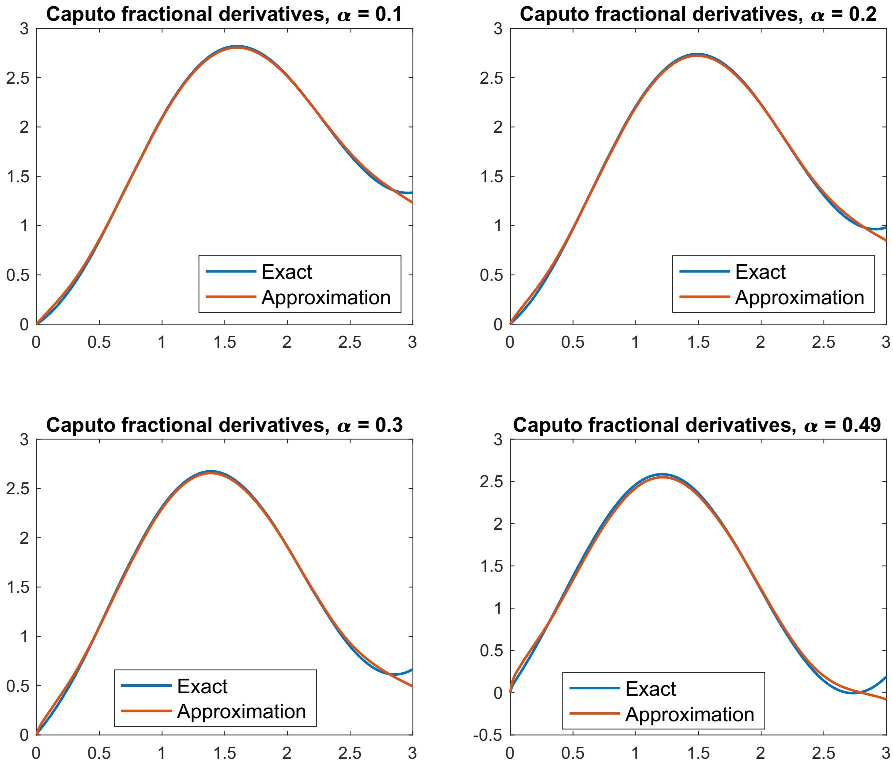

Fig. 6 Example 3: Approximations of Caputo Fractional Derivatives (CFD). For each sub-figure, the blue curve plots the CFD of the exact data, $D^\alpha q$; the orange curve plots the corresponding approximation, $D^\alpha p^*$, where the measured data is perturbed by 10% noise. Values of α are indicated in the title of each sub-figure

Example 4: In the last example, we choose the exact data $q(t) = t^2 - 6t$. The Caputo derivative of q is given by

$$D^\alpha q(t) = \frac{\Gamma(3)}{\Gamma(3-\alpha)} t^{2-\alpha} - \frac{6}{\Gamma(1-\alpha)} \frac{t^{1-\alpha}}{1-\alpha}.$$

The measured data, q^δ, with 10% noise and the corresponding regularized data is illustrated in Fig. 7. The approximation of the $D^\alpha q^\delta$ for $\alpha = 0.1, 0.2, 0.3, 0.49$ and the ℓ^2−norm relative error estimates are shown in Fig. 8 and Table 4, respectively.

Table 3 Relative errors for Example 3 for different values of δ and α

	$\alpha = 0.1$	$\alpha = 0.2$	$\alpha = 0.3$	$\alpha = 0.49$
$\delta = 0.02$	0.0014	0.0020	0.0031	0.0056
$\delta = 0.05$	0.0045	0.0060	0.0083	0.0119
$\delta = 0.1$	0.0110	0.0141	0.0183	0.0243
$\delta = 0.2$	0.0265	0.0324	0.0402	0.0502

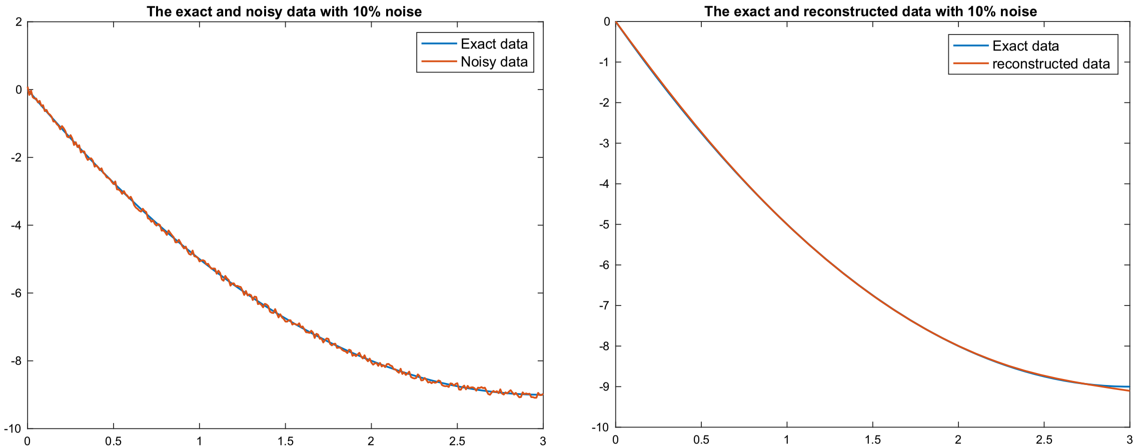

Fig. 7 Noisy data and the associated regularized data for Example 4. Left - The noisy data with 10% noise (the zigzag orange curve) compared to the exact data (the smooth blue curve). Right - The regularized data (the smooth orange curve) compared to the exact data (the smooth blue curve)

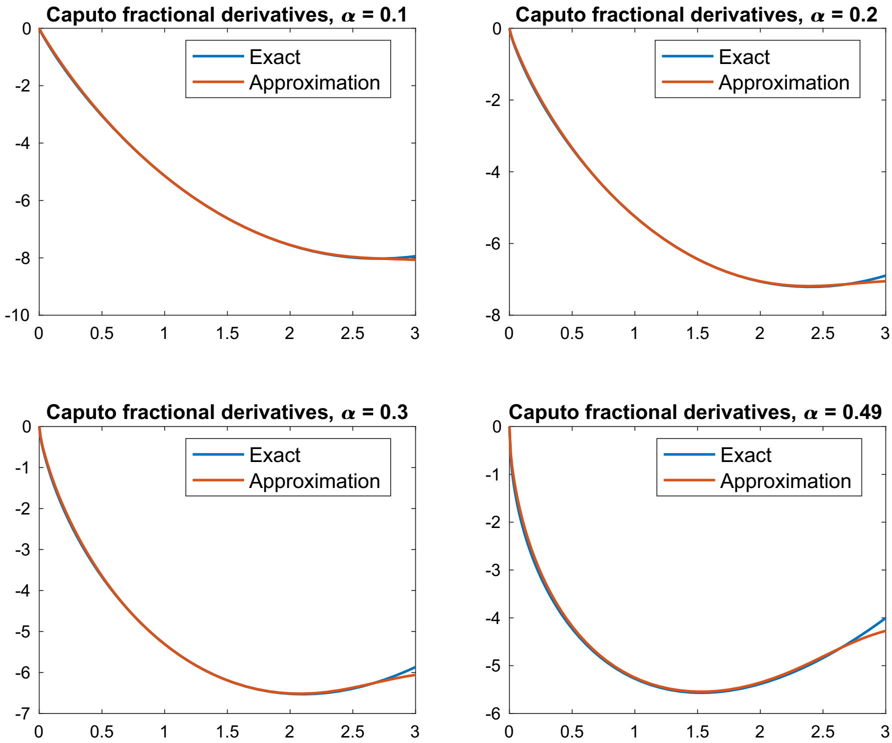

Fig. 8 Example 4: Approximations of Caputo Fractional Derivatives (CFD). In each sub-figure, the blue curve plots $D^{\alpha}q$; the orange curve plots $D^{\alpha}p^{*}$, where q^{δ} is perturbed by 10% noise. Values of α are indicated in the title of each sub-figure

Table 4 Relative errors for Example 4 for different values of δ and α

	$\alpha = 0.1$	$\alpha = 0.2$	$\alpha = 0.3$	$\alpha = 0.49$
$\delta = 0.02$	0.0008	0.0011	0.0017	0.0035
$\delta = 0.05$	0.0018	0.0024	0.0034	0.0053
$\delta = 0.1$	0.0039	0.0050	0.0067	0.0092
$\delta = 0.2$	0.0087	0.0109	0.0138	0.0179

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