



# Optimal error estimates for Legendre expansions of singular functions with fractional derivatives of bounded variation

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## Abstract

We present a new fractional Taylor formula for singular functions whose Caputo fractional derivatives are of bounded variation. It bridges and “interpolates” the usual Taylor formulas with two consecutive integer orders. This enables us to obtain an analogous formula for the Legendre expansion coefficient of this type of singular functions, and further derive the optimal (weighted)  $L^\infty$ -estimates and  $L^2$ -estimates of the Legendre polynomial approximations. This set of results can enrich the existing theory for  $p$  and  $hp$  methods for singular problems, and answer some open questions posed in some recent literature.

**Keywords** Approximation by Legendre polynomials · Functions with interior and endpoint singularities · Optimal estimates · Fractional Taylor formula

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# 1 Introduction

The study of Legendre approximation to singular functions is a subject of fundamental importance in the theory and applications of  $hp$  finite element methods. We refer to the seminal series of papers by Gui and Babuška [19–21] and many other developments in, e.g., [7, 8, 37]. In particular, the very recent work of Babuška and Hakula [10] provided a review of known/unknown results and posed a few open questions on the pointwise error estimates of Legendre expansion of a typical singular function discussed in [19]:

$$u(x) = (x - \theta)_+^\mu = \begin{cases} 0, & -1 < x \leq \theta, \\ (x - \theta)^\mu, & \theta < x < 1, \end{cases} \quad |\theta| \leq 1, \quad \mu > -1. \quad (1.1)$$

One significant development along this line is the  $hp$  approximation theory in the framework of Jacobi-weighted Besov spaces [7–9, 22]. Such Besov spaces are defined through space interpolation of Jacobi-weighted Sobolev spaces with integer regularity indices using the  $K$ -method. It is important to point out that the non-uniformly Jacobi-weighted Sobolev spaces has been employed in spectral approximation theory [18, 24, 25, 37, 38].

## 1.1 Related works

Different from the Sobolev-Besov framework, Trefethen [40, 41] characterised the regularity of singular functions by using the space of absolute continuity and bounded variation (AC-BV), in the study of Chebyshev expansions of such functions. One motivative example therein is  $u(x) = |x|$  in  $\Omega = (-1, 1)$  which has the regularity:  $u, u' \in AC(\bar{\Omega})$  and  $u'' \in BV(\bar{\Omega})$  (where the integration of the norm is in the Riemann-Stieltjes (RS) sense). As a result, the maximum error of its Chebyshev expansion can attain optimal order (but can only be suboptimal in a usual Sobolev framework). There have been many follow-up works on the improved error estimates of Chebyshev approximation or more general Jacobi polynomial approximation under this AC-BV framework (see, e.g., [33, 42, 43, 46]). However, the regularity index and the involved derivatives are of integer order, so it is not suitable to best characterise the regularity of many singular functions, e.g., (1.1) and  $u(x) = |x|^\mu$  with non-integer  $\mu$ . In other words, if one naively applies the estimates, then the loss of order might occur. Nevertheless, the solutions of many singular problems (in irregular domains or with singular coefficients/operators among others) typically exhibit this kind of singularities.

To fill this gap, the authors introduced for the first time in [32] certain fractional Sobolev-type spaces and derived optimal Chebyshev polynomial approximation to functions with interior and endpoint singularities within this new framework. The study therein inspired the discovery of generalised Gegenbauer functions of fractional degree, as an analysis tool and a class of special functions with rich properties [31].

## 1.2 Our contributions

We highlight the main contributions of this work as follows.

- (i) We present a new fractional Taylor formula for AC-BV functions with fractional regularity index (see Theorem 2.1) that “interpolates” and seamlessly bridges the Taylor formulas of two consecutive integer orders. From this tool, we can derive an analogous formula for the Legendre expansion coefficient of the same class of functions, which turns out the cornerstone of all the analysis.
- (ii) We present a set of optimal Legendre approximation results in  $L^\infty$ - and  $L^2$ -norms for functions with interior or endpoint singularities. The use of a function space involving fractional integrals/derivatives to characterise regularity follows that in [32], but we further refine this framework by introducing the Caputo derivative. When the fractional regularity index takes an integer value, it reduces to the AC-BV-type space in Trefethen [40, 41] for Chebyshev approximation. We point out that the argument for the Legendre approximation herein is different from that for the Chebyshev approximation in [32].
- (iii) Babuška and Hakula [10] discussed the point-wise error estimates of the Legendre expansion for the specific function (1.1) (which was the subject of [19]) including known and unknown results. It is also of interest to study the point-wise error in the Legendre or other Jacobi cases. For example, the estimating the  $L^\infty$ -error like the Chebyshev expansion can only lead to suboptimal results for functions with the interior singularity, e.g.,  $u(x) = |x|$ , as a loss of half order occurs. It was observed numerically, but how to obtain optimal estimate appears open (see, e.g., [42]). Here, we give an answer to this, and to some conjectures in [10] as well.
- (iv) We aim at deriving sharp and optimal estimates valid for all polynomial orders. According to [10], in most applications the polynomial orders are relatively small compared to those in the asymptotic range, while the existing theory does not address the behavior of the pre-asymptotic error. As a result, our arguments and results are different from those in [46], where some asymptotic formulas were employed to derive Jacobi approximation of specific singular functions for large polynomial orders. As a final remark, this paper will be largely devoted to the  $L^\infty$ - and  $L^2$ -estimates of the finite Legendre expansions, which is the starting point to derive the approximation results for other orthogonal projections, interpolations and quadrature for singular functions. Indeed, these results can enrich the theoretical foundation of  $p$  and  $hp$  methods (cf. [11, 16, 18, 26, 37, 38]).

The rest of the paper is organised as follows. In Section 2, we derive the fractional Taylor formula for the AC-BV functions and present some preliminaries to pave the way for all forthcoming discussions. In Section 3, we obtain the main results on Legendre approximation of functions with interior singularities and extend the tools to study the endpoint singularities in Section 4.

## 2 Fractional integral/derivative formulas of GGF-Fs

In this section, we make necessary preparations for the forthcoming discussions. More precisely, we first introduce several spaces of functions that will be used to characterise the regularity of the class of functions of interest. We then recall the definition of the Riemann-Liouville (RL) fractional integrals, and present a useful RL fractional integration parts formula. Finally, we collect some relevant properties of generalised Gegenbauer functions of fractional degree (GGF-Fs), which were first introduced and studied in [31, 32].

### 2.1 Spaces of functions

Let  $\Omega = (a, b) \subset \mathbb{R}$  be a finite open interval. For real  $p \in [1, \infty]$ , let  $L^p(\Omega)$  (resp.  $W^{m,p}(\Omega)$  with  $m \in \mathbb{N}$ , the set of all positive integers) be the usual  $p$ -Lebesgue space (resp. Sobolev space), equipped with the norm  $\|\cdot\|_{L^p(\Omega)}$  (resp.  $\|\cdot\|_{W^{m,p}(\Omega)}$ ), as in Adams [1].

Let  $C(\bar{\Omega})$  be the classical space of continuous functions, and  $AC(\bar{\Omega})$  the space of absolutely continuous functions on  $\bar{\Omega}$ . It is known that every absolutely continuous function is uniformly continuous (but the converse is not true), and hence continuous (cf. [35, p. 483]). It is known that *a real function  $f(x) \in AC(\bar{\Omega})$  if and only if  $f(x) \in L^1(\Omega)$ ,  $f(x)$  has a derivative  $f'(x)$  almost everywhere on  $[a, b]$  such that  $f'(x) \in L^1(\Omega)$ , and  $f(x)$  has the integral representation:*

$$f(x) = f(a) + \int_a^x f'(t) dt, \quad \forall x \in [a, b], \quad (2.1)$$

(cf. [36, Chap. 1] and [30, p. 285]).

Let  $BV(\bar{\Omega})$  be the space of functions of bounded variation on  $[a, b]$ . We say that *a real function  $f(x) \in BV(\bar{\Omega})$ , if there exists a constant  $C > 0$  such that*

$$V(\mathbb{P}; f) := \sum_{i=0}^{k-1} |f(x_{i+1}) - f(x_i)| \leq C$$

*for every finite partition  $\mathbb{P} = \{x_0, x_1, \dots, x_k\}$  (satisfying  $x_i < x_{i+1}$  for all  $0 \leq i \leq k-1$ ) of  $[a, b]$ . Then the total variation of  $f$  on  $[a, b]$  is defined as  $V_{\bar{\Omega}}[f] := \sup\{V(\mathbb{P}; f)\}$ , where the supreme is taken over all the partitions of  $\bar{\Omega}$  (cf. [13, p. 207] or [30, Chap. X]). An important characterisation of a BV-function is the Jordan decomposition (cf. [35, Thm. 11.19]): *a function is of bounded variation if and only if it can be expressed as the difference of two increasing functions on  $[a, b]$ . As a result, every function in  $BV(\bar{\Omega})$  has at most a countable number of discontinuities, which are either jump or removable discontinuities, so it is differentiable almost everywhere. Indeed, according to [6, p. 223], if  $f \in AC(\bar{\Omega})$ , then**

$$V_{\bar{\Omega}}[f] = \int_{\Omega} |f'(x)| dx.$$

In fact, we have  $BV(\bar{\Omega}) \subset AC(\bar{\Omega}) = W^{1,1}(\Omega)$  in the sense that every  $f(x) \in AC(\bar{\Omega})$  has an almost everywhere classical derivative  $f' \in L^1(\Omega)$  (cf. (2.1)) and  $f'(x)$  is the weak derivative of  $f(x)$ . Conversely, even  $f \in W^{1,1}(\Omega)$ , modulo a

modification on a set of measure zero, is an absolutely continuous function (cf. [13, p. 206] and [15, p. 84; p. 96]).

For BV-functions, we can define the Riemann-Stieltjes (RS) integral (cf. [30, Chap. X]). A function  $f(x)$  is said to be RS( $g$ )-integrable, if  $\int_{\Omega} f dg < \infty$  for  $g \in \text{BV}(\bar{\Omega})$ . From [30, Prop. 1.3], we have that if  $f$  is RS( $g$ )-integrable, then

$$\left| \int_{\Omega} f(x) dg(x) \right| \leq \|f\|_{\infty} V_{\bar{\Omega}}[g], \quad \int_{\Omega} |dg(x)| = V_{\bar{\Omega}}[g], \quad (2.2)$$

where  $\|f\|_{\infty}$  is the  $L^{\infty}$ -norm of  $f$  on  $[a, b]$ .

In the analysis, we shall also use the splitting rule of a RS integral, which is different from the usual integral.

**Lemma 2.1** (see Carter and Brunt [17, Thm 6.1.1 & Thm 6.1.6]) *If the interval  $\Omega$  is a union of a finite number of pairwise disjoint intervals  $\Omega = \Omega_1 \cup \Omega_2 \cup \dots \cup \Omega_m$ , then*

$$\int_{\Omega} f dg = \sum_{j=1}^m \int_{\Omega_j} f dg$$

in the sense that if one side exists, then so does the other, and the two are equal. Moreover, for any function  $f$  defined at  $\theta$ , then

$$\int_{[\theta, \theta]} f dg = f(\theta)(g(\theta+) - g(\theta-)).$$

## 2.2 Formula of fractional integration by parts

Recall the formula of integration by parts involving the Riemann-Stieltjes integrals (cf. [28, (1.20)]): if  $f, g \in \text{BV}(\bar{\Omega})$ , we have

$$\int_a^b f(x) dg(x) = \{f(x)g(x)\}_{a+}^{b-} - \int_a^b g(x) df(x), \quad (2.3)$$

where we denote

$$f(x)_{a+}^{b-} = \lim_{x \rightarrow b-} f(x) - \lim_{x \rightarrow a+} f(x) = f(b-) - f(a+).$$

In particular, if  $f, g \in \text{AC}(\bar{\Omega})$ , we have

$$\int_a^b f(x)g'(x) dx + \int_a^b f'(x)g(x) dx = \{f(x)g(x)\}_a^b.$$

In what follows, we shall derive a formula of fractional integration parts from (2.3) in a weaker sense than the existing counterparts (cf. [12, 36]). For this purpose, we recap on the definition of the Riemann-Liouville fractional integral (cf. [36, p. 33, p. 44]): for any  $f \in L^1(\Omega)$ , the left-sided and right-sided Riemann-Liouville fractional integrals of real order  $\rho \geq 0$  are defined by

$$(I_{a+}^{\rho} f)(x) = \frac{1}{\Gamma(\rho)} \int_a^x \frac{f(y)}{(x-y)^{1-\rho}} dy; \quad (I_{b-}^{\rho} f)(x) = \frac{1}{\Gamma(\rho)} \int_x^b \frac{f(y)}{(y-x)^{1-\rho}} dy, \quad (2.4)$$

for  $x \in \Omega$ , where  $\Gamma(\cdot)$  is the usual Gamma function. For  $\mu \in (k-1, k]$  with  $k \in \mathbb{N}$ , the left-sided and right-side Caputo fractional derivatives of order  $\mu$  are respectively defined by

$$\left({}^C D_{a+}^{\mu} f\right)(x) = \left(I_{a+}^{k-\mu} f^{(k)}\right)(x); \quad \left({}^C D_{b-}^{\mu} f\right)(x) = (-1)^k \left(I_{b-}^{k-\mu} f^{(k)}\right)(x). \quad (2.5)$$

The following formula of fractional integration by parts plays an important role in the analysis, which can be derived from (2.3) and an argument similar to that for [32, Lemma 4.1]. We provide in Appendix B the derivation for completeness and readability.

**Lemma 2.2** Let  $\rho \geq 0$ ,  $f(x) \in L^1(\Omega)$  and  $g(x) \in AC(\bar{\Omega})$ .

(i) If  $I_{b-}^{\rho} f(x) \in BV(\bar{\Omega})$ , then

$$\int_a^b f(x) I_{a+}^{\rho} g'(x) dx = \{g(x) I_{b-}^{\rho} f(x)\}|_{a+}^{b-} - \int_a^b g(x) d\{I_{b-}^{\rho} f(x)\}. \quad (2.6)$$

(ii) If  $I_{a+}^{\rho} f(x) \in BV(\bar{\Omega})$ , then

$$\int_a^b f(x) I_{b-}^{\rho} g'(x) dx = \{g(x) I_{a+}^{\rho} f(x)\}|_{a+}^{b-} - \int_a^b g(x) d\{I_{a+}^{\rho} f(x)\}. \quad (2.7)$$

**Remark 2.1** If  $\rho = 0$ , then they reduce (2.3). It is known that the fractional integral can improve the regularity. Indeed, for  $0 < \rho < 1$  and  $u \in L^1(\Omega)$ , we have  $I_{a+}^{\rho} u, I_{b-}^{\rho} u \in L^p(\Omega)$  with  $p \in [1, \rho^{-1})$  (cf. [12, Prop.2.1]).

Compared with those in [12, 36], a weaker condition is imposed on  $f(x)$  in (2.6)–(2.7), which turns out essential in dealing with the singular functions. Moreover, for such functions, the limit values  $\lim_{x \rightarrow a+} I_{a+}^{\rho} f(x)$  in (2.6), and  $\lim_{x \rightarrow b-} I_{b-}^{\rho} f(x)$  in (2.7) might be non-zero, in contrast to a usual integral with  $\rho = 1$ . For example, for  $\rho \in (0, 1)$ , we have

$$I_{a+}^{1-\rho} (x-a)^{\rho-1} = I_{b-}^{1-\rho} (b-x)^{\rho-1} = \Gamma(\rho),$$

which follow from the explicit formulas (cf. [36]): for real  $\eta > -1$  and  $\rho \geq 0$ ,

$$I_{a+}^{\rho} (x-a)^{\eta} = \frac{\Gamma(\eta+1)}{\Gamma(\eta+\rho+1)} (x-a)^{\eta+\rho}; \quad I_{b-}^{\rho} (b-x)^{\eta} = \frac{\Gamma(\eta+1)}{\Gamma(\eta+\rho+1)} (b-x)^{\eta+\rho}. \quad (2.8)$$

In fact, we have the following more general formula, which finds useful in exemplifying some estimates to be presented later. We sketch the derivation in Appendix C.

**Proposition 2.1** Let  $f(x) = (x-a)^{\gamma} g(x)$  with real  $\gamma > -1$ , where  $g(x)$  is left continuous at  $x = a$  and Riemann integrable on  $[a, a+\delta)$  for some  $\delta > 0$ . Then, for real  $\rho > 0$ , we have

$$\lim_{x \rightarrow a^+} (I_{a+}^{\rho} f)(x) = \begin{cases} 0, & \text{if } \rho > -\gamma, \\ g(a) \Gamma(\gamma + 1), & \text{if } \rho = -\gamma, \\ \infty, & \text{if } \rho < -\gamma. \end{cases} \quad (2.9)$$

Let  $f(x) = (b - x)^{\gamma} g(x)$ ,  $\gamma > -1$ , and  $g(x)$  be right continuous at  $x = b$  and Riemann integrable on  $(b - \delta, b]$ . Then, the same result holds for the limit  $\lim_{x \rightarrow b^-} (I_{b-}^{\rho} f)(x)$  but with  $g(b)$  in place of  $g(a)$ .

### 2.3 Fractional Taylor formula

Recall this well-known formula: Let  $k \geq 1$  be an integer and let  $f(x)$  be a real function that is  $k$  times differentiable at the point  $x = \theta$ . Furthermore, let  $f^{(k)}(x)$  be absolutely continuous on the closed interval between  $\theta$  and  $x$ . Then we have

$$f(x) = \sum_{j=0}^k \frac{f^{(j)}(\theta)}{j!} (x - \theta)^j + \int_{\theta}^x \frac{f^{(k+1)}(t)}{k!} (x - t)^k dt. \quad (2.10)$$

Note that since  $f^{(k)}(x)$  is an AC-function,  $f^{(k+1)}(x)$  exists as an  $L^1$ -function.

As another building block for the analysis, we derive a fractional Taylor formula from Lemma 2.2 and (2.10).

**Theorem 2.1 (Fractional Taylor formula)** Let  $\mu \in (k - 1, k]$  with  $k \in \mathbb{N}$ , and let  $f(x)$  be a real function that is  $(k - 1)$  times differentiable at the point  $x = \theta$ .

- (i) If  $f^{(k-1)} \in AC([\theta, x])$  and  ${}^C D_{\theta+}^{\mu} f \in BV([\theta, x])$ , then we have the left-sided fractional Taylor formula

$$\begin{aligned} f(x) &= \sum_{j=0}^{k-1} \frac{f^{(j)}(\theta)}{j!} (x - \theta)^j + \frac{{}^C D_{\theta+}^{\mu} f(\theta+)}{\Gamma(\mu + 1)} (x - \theta)^{\mu} \\ &\quad + \frac{1}{\Gamma(\mu + 1)} \int_{\theta}^x (x - t)^{\mu} d\{{}^C D_{\theta+}^{\mu} f(t)\}. \end{aligned} \quad (2.11)$$

- (ii) If  $f^{(k-1)} \in AC([x, \theta])$  and  ${}^C D_{\theta-}^{\mu} f \in BV([x, \theta])$ , then we have the right-sided fractional Taylor formula

$$\begin{aligned} f(x) &= \sum_{j=0}^{k-1} \frac{f^{(j)}(\theta)}{j!} (x - \theta)^j + \frac{{}^C D_{\theta-}^{\mu} f(\theta-)}{\Gamma(\mu + 1)} (\theta - x)^{\mu} \\ &\quad - \frac{1}{\Gamma(\mu + 1)} \int_x^{\theta} (t - x)^{\mu} d\{{}^C D_{\theta-}^{\mu} f(t)\}. \end{aligned} \quad (2.12)$$

*Proof* By (2.10) (with  $k \rightarrow k - 1$ ), we have

$$f(x) = \sum_{j=0}^{k-1} \frac{f^{(j)}(\theta)}{j!} (x - \theta)^j + \frac{1}{(k - 1)!} \int_{\theta}^x (x - t)^{k-1} f^{(k)}(t) dt. \quad (2.13)$$

From (2.8), we find readily that for  $x > t$ ,

$$(x-t)^{k-1} = -\frac{(k-1)!}{\Gamma(\mu+1)} I_{x-}^{k-\mu} \left\{ \frac{d}{dt} (x-t)^\mu \right\}.$$

Thus, we can rewrite (2.13) as

$$f(x) = \sum_{j=0}^{k-1} \frac{f^{(j)}(\theta)}{j!} (x-\theta)^j - \frac{1}{\Gamma(\mu+1)} \int_{\theta}^x I_{x-}^{k-\mu} \left\{ \frac{d}{dt} (x-t)^\mu \right\} f^{(k)}(t) dt. \quad (2.14)$$

Substituting  $a$ ,  $b$ ,  $\rho$ ,  $f$  and  $g$  in (2.7) of Lemma 2.2 by  $\theta$ ,  $x$ ,  $k-\mu$ ,  $f^{(k)}(t)$  and  $(x-t)^\mu$ , respectively, we obtain that for  $x > \theta$ ,

$$\begin{aligned} & \int_{\theta}^x I_{x-}^{k-\mu} \left\{ \frac{d}{dt} (x-t)^\mu \right\} f^{(k)}(t) dt \\ &= -I_{\theta+}^{k-\mu} f^{(k)}(\theta+)(x-\theta)^\mu - \int_{\theta}^x (x-t)^\mu d\{I_{\theta+}^{k-\mu} f^{(k)}(t)\} \\ &= -{}^C D_{\theta+}^{\mu} f(\theta+)(x-\theta)^\mu - \int_{\theta}^x (x-t)^\mu d\{{}^C D_{\theta+}^{\mu} f(t)\}, \end{aligned} \quad (2.15)$$

where in the last step, we used the definition (2.5). Thus, we obtain (2.11) from (2.14)–(2.15) immediately.

The right-sided formula (2.12) can be obtained in a very similar fashion.  $\square$

**Remark 2.2** When  $\mu = k$ , the fractional Taylor formulas (2.11) and (2.12) lead to (2.10). The fractional formula can be viewed as the “interpolation” of the integer-order Taylor formulas with the regularity indexes  $k-1$  and  $k$ . Apparently, the integer-order Taylor formula (2.10) is exact for all  $f \in \mathcal{P}_k = \text{span}\{(x-\theta)^j : 0 \leq j \leq k\}$ . In the fractional case, the exactness of (2.11) is for all  $f \in \mathcal{P}_{k-1} \cup \{(x-\theta)^\mu\}$  (i.e., the remainder vanishes). We can verify this readily from (2.5) and the fundamental formula:  ${}^C D_{\theta+}^{\mu} \{(x-\theta)^\mu\} = \Gamma(\mu+1)$ . Note that the right-sided formula (2.12) is exact for all  $f \in \mathcal{P}_{k-1} \cup \{(\theta-x)^\mu\}$ .

We remark that there are several versions of fractional Taylor formulas in literature. For example, Anastassiou [3, (21)] stated the right-sided fractional Taylor formula: for real  $\mu \geq 1$ , let  $k = [\mu]$  be its integer part, and assume that  $f, f', \dots, f^{(k-1)} \in \text{AC}([x, \theta])$ . Then

$$f(x) = \sum_{j=0}^{k-1} \frac{f^{(j)}(\theta)}{j!} (x-\theta)^j + \frac{1}{\Gamma(\mu)} \int_x^{\theta} (t-x)^{\mu-1} {}^C D_{\theta-}^{\mu} f(t) dt.$$

It is seen from (2.12) and the proof that with additional BV-regularity, we can use the fractional integration by parts formula in Lemma 2.2 to obtain another explicit term involving the fractional derivative. Kolwankar and Gangal [29] presented some local fractional Taylor expansion with a different fractional derivative in the remainder.



### 3 Legendre expansions of functions with interior singularities

It is known that much of the error analysis for orthogonal polynomial approximation and associated interpolation and quadrature relies on the decay rate of the expansion coefficient (cf. [33, 45]). Remarkably, we find that the spirit in deriving the fractional Taylor formula in Theorem 2.1 can be extended to obtain an analogous formula for the Legendre expansion coefficient

$$\hat{u}_n^L = \frac{2n+1}{2} \int_{-1}^1 u(x) P_n(x) dx, \quad (3.1)$$

where  $P_n(x)$  is the Legendre polynomial of degree  $n$ . This formula lays the ground-work for all the forthcoming analysis. In fact, the argument is also different from that for the Chebyshev expansion coefficient in [32, 33, 40, 41].

#### 3.1 Fractional formula for the Legendre expansion coefficient

In what follows, we assume that  $u$  has a limited regularity with an interior singularity at  $\theta \in (-1, 1)$ , e.g.,  $u(x) = |x - \theta|^\alpha$  with  $\alpha > -1$ . Note that the results can be extended to multiple interior singularities straightforwardly.

**Theorem 3.1** *Let  $\mu \in (k-1, k]$  with  $k \in \mathbb{N}$  and let  $\theta \in (-1, 1)$ . If  $u, u', \dots, u^{(k-1)} \in AC([-1, 1])$ ,  ${}^C D_{\theta+}^\mu u \in BV([\theta, 1])$  and  ${}^C D_{\theta-}^\mu u \in BV([-1, \theta])$ , then we have the following representation of the Legendre expansion coefficient for each  $n \geq \mu + 1$ ,*

$$\begin{aligned} \hat{u}_n^L = \frac{2n+1}{2} \left\{ \left( I_{1-}^{\mu+1} P_n \right) (\theta) \left( {}^C D_{\theta+}^\mu u \right) (\theta+) + \int_{\theta}^1 \left( I_{1-}^{\mu+1} P_n \right) (x) d \left\{ {}^C D_{\theta+}^\mu u(x) \right\} \right. \\ \left. + \left( I_{-1+}^{\mu+1} P_n \right) (\theta) \left( {}^C D_{\theta-}^\mu u \right) (\theta-) - \int_{-1}^{\theta} \left( I_{-1+}^{\mu+1} P_n \right) (x) d \left\{ {}^C D_{\theta-}^\mu u(x) \right\} \right\}, \quad (3.2) \end{aligned}$$

where the fractional integrals of  $P_n(x)$  can be evaluated explicitly by

$$\begin{aligned} \left( I_{1-}^{\mu+1} P_n \right) (x) &= \frac{(1-x)^{\mu+1}}{\Gamma(\mu+2)} \frac{P_n^{(\mu+1, -\mu-1)}(x)}{P_n^{(\mu+1, -\mu-1)}(1)}, \\ \left( I_{-1+}^{\mu+1} P_n \right) (x) &= \frac{(1+x)^{\mu+1}}{\Gamma(\mu+2)} \frac{P_n^{(-\mu-1, \mu+1)}(x)}{P_n^{(\mu+1, -\mu-1)}(1)}. \end{aligned} \quad (3.3)$$

Here,  $P_n^{(\mu+1, -\mu-1)}(x)$  and  $P_n^{(-\mu-1, \mu+1)}(x)$  are the generalised Jacobi polynomials defined by the hypergeometric functions as in Szegő [39, p.64].

*Proof* Given the regularity of  $u$ , we obtain from the fractional Taylor formulas in Theorem 2.1 that for  $x \in (\theta, 1)$ ,

$$u(x) = \sum_{j=0}^{k-1} \frac{u^{(j)}(\theta)}{j!} (x - \theta)^j + \frac{{}^C D_{\theta+}^{\mu} u(\theta+)}{\Gamma(\mu + 1)} (x - \theta)^{\mu} + \frac{1}{\Gamma(\mu + 1)} \int_{\theta}^x (x - t)^{\mu} d \left\{ {}^C D_{\theta+}^{\mu} u(t) \right\}, \quad (3.4)$$

and for  $x \in (-1, \theta)$ ,

$$u(x) = \sum_{j=0}^{k-1} \frac{u^{(j)}(\theta)}{j!} (x - \theta)^j + \frac{{}^C D_{\theta-}^{\mu} u(\theta-)}{\Gamma(\mu + 1)} (\theta - x)^{\mu} - \frac{1}{\Gamma(\mu + 1)} \int_x^{\theta} (t - x)^{\mu} d \left\{ {}^C D_{\theta-}^{\mu} u(t) \right\}. \quad (3.5)$$

Substituting (3.4) and (3.5) into (3.1) leads to

$$\begin{aligned} \frac{2 \hat{u}_n^L}{2n + 1} &= \int_{-1}^1 u(x) P_n(x) dx = \sum_{j=0}^{k-1} \frac{u^{(j)}(\theta)}{j!} \int_{-1}^1 (x - \theta)^j P_n(x) dx \\ &+ \frac{{}^C D_{\theta+}^{\mu} u(\theta+)}{\Gamma(\mu + 1)} \int_{\theta}^1 (x - \theta)^{\mu} P_n(x) dx \\ &+ \frac{1}{\Gamma(\mu + 1)} \int_{\theta}^1 \left( \int_{\theta}^x (x - t)^{\mu} d \left\{ {}^C D_{\theta+}^{\mu} u(t) \right\} \right) P_n(x) dx \\ &+ \frac{{}^C D_{\theta-}^{\mu} u(\theta-)}{\Gamma(\mu + 1)} \int_{-1}^{\theta} (\theta - x)^{\mu} P_n(x) dx \\ &- \frac{1}{\Gamma(\mu + 1)} \int_{-1}^{\theta} \left( \int_x^{\theta} (t - x)^{\mu} d \left\{ {}^C D_{\theta-}^{\mu} u(t) \right\} \right) P_n(x) dx. \end{aligned} \quad (3.6)$$

From the orthogonality of the Legendre polynomials, we obtain that for  $n \geq \mu + 1 \geq k$ ,

$$\int_{-1}^1 (x - \theta)^j P_n(x) dx = 0, \quad 0 \leq j \leq k - 1. \quad (3.7)$$

We find readily that for a fixed  $\theta \in (-1, 1)$ ,

$$\int_{\theta}^1 \left( \int_{\theta}^x (x - t)^{\mu} d \left\{ {}^C D_{\theta+}^{\mu} u(t) \right\} \right) P_n(x) dx = \int_{\theta}^1 \left( \int_t^1 (x - t)^{\mu} P_n(x) dx \right) d \left\{ {}^C D_{\theta+}^{\mu} u(t) \right\}, \quad (3.8)$$

and

$$\int_{-1}^{\theta} \left( \int_x^{\theta} (t - x)^{\mu} d \left\{ {}^C D_{\theta-}^{\mu} u(t) \right\} \right) P_n(x) dx = \int_{-1}^{\theta} \left( \int_{-1}^t (t - x)^{\mu} P_n(x) dx \right) d \left\{ {}^C D_{\theta-}^{\mu} u(t) \right\}. \quad (3.9)$$

In view of the definition of the fractional integral in (2.4) and (3.7)–(3.9), we can rewrite (3.6) as

$$\begin{aligned} \frac{2\hat{u}_n^L}{2n+1} &= \left(I_{1-}^{\mu+1} P_n\right)(\theta) \left({}^C D_{\theta+}^{\mu} u\right)(\theta+) + \int_{\theta}^1 \left(I_{1-}^{\mu+1} P_n\right)(t) d\left\{{}^C D_{\theta+}^{\mu} u(t)\right\} \\ &\quad + \left(I_{-1+}^{\mu+1} P_n\right)(\theta) \left({}^C D_{\theta-}^{\mu} u\right)(\theta-) - \int_{-1}^{\theta} \left(I_{-1+}^{\mu+1} P_n\right)(t) d\left\{{}^C D_{\theta-}^{\mu} u(t)\right\}, \end{aligned} \quad (3.10)$$

which yields (3.2). The two fractional integral identities of  $P_n(x)$  in (3.3) can be obtained from the formulas of the Jacobi polynomials (cf. Szegő [39, p. 96]), due to the Bateman's fractional integral formula (cf. [4]). This ends the proof.  $\square$

We see from the above proof that the identity (3.2) is rooted in the fractional Taylor formula in Theorem 2.1. Also note that when  $\mu = k$ , the formula (3.1) takes a much simpler form. Firstly, the AC-BV regularity reduces to the setting considered by Trefethen [40, 41], Xiang and Bornemann [45] among others (where one motivative example for the framework therein is to best characterise the regularity of  $u(x) = |x|$ ). Secondly, from Szegő [39, Chap. 4], we find that for  $\mu > -2$ ,  $n \geq 0$ ,

$$P_n^{(\mu+1, -\mu-1)}(1) = \frac{\Gamma(n + \mu + 2)}{n! \Gamma(\mu + 2)}, \quad (3.11)$$

and for  $n \geq k + 1$ ,

$$P_n^{(-k-1, k+1)}(x) = \frac{(n-k-1)!(n+k+1)!}{(n!)^2} \left(\frac{x-1}{2}\right)^{k+1} P_{n-k-1}^{(k+1, k+1)}(x). \quad (3.12)$$

Thus, we can rewrite the second formula in (3.3) with  $\mu = k$  in terms of the usual Jacobi polynomial as follows

$$\left(I_{-1+}^{k+1} P_n\right)(x) = \frac{(-1)^{k+1} (n-k-1)!}{2^{k+1} n!} (1-x^2)^{k+1} P_{n-k-1}^{(k+1, k+1)}(x). \quad (3.13)$$

Following the same lines as above and using the parity of Jacobi polynomials, we can reformulate the first formula in (3.3) with  $\mu = k$  as

$$\begin{aligned} \left(I_{1-}^{k+1} P_n\right)(x) &= \frac{(n-k-1)!}{2^{k+1} n!} (1-x^2)^{k+1} P_{n-k-1}^{(k+1, k+1)}(x) \\ &= (-1)^{k+1} \left(I_{-1+}^{k+1} P_n\right)(x). \end{aligned} \quad (3.14)$$

In view of this relation, we find from (2.5) with  $\mu = k$  that (3.2) reduces to

$$\begin{aligned} \hat{u}_n^L &= \frac{2n+1}{2} \left\{ u^{(k)}(\theta+) \left(I_{1-}^{k+1} P_n\right)(\theta) + \int_{\theta}^1 \left(I_{1-}^{k+1} P_n\right)(x) d\left\{u^{(k)}(x)\right\} \right. \\ &\quad \left. - u^{(k)}(\theta-) \left(I_{1-}^{k+1} P_n\right)(\theta) + \int_{-1}^{\theta} \left(I_{1-}^{k+1} P_n\right)(x) d\left\{u^{(k)}(x)\right\} \right\} \\ &= \frac{2n+1}{2} \left\{ \int_{-1}^{\theta} + \int_{[\theta, \theta]} + \int_{\theta}^1 \right\} \left(I_{1-}^{k+1} P_n\right)(x) d\left\{u^{(k)}(x)\right\}. \end{aligned} \quad (3.15)$$

By virtue of the splitting rule in Lemma 2.1, we can summarise the formula of the Legendre expansion coefficient with  $\mu = k$  as follows.

**Corollary 3.1** *If  $u, u', \dots, u^{(k-1)} \in AC([-1, 1])$  and  $u^{(k)} \in BV([-1, 1])$  with  $k \in \mathbb{N}$ , then we have for all  $n \geq k + 1$ ,*

$$\hat{u}_n^L = \frac{2n+1}{2} \int_{-1}^1 \left( I_{1-}^{k+1} P_n \right) (x) d \left\{ u^{(k)}(x) \right\}, \quad (3.16)$$

where  $\left( I_{1-}^{k+1} P_n \right) (x)$  can be explicitly evaluated by (3.14).

It is seen from Theorem 3.1 that the decay rate of  $\hat{u}_n^L$  for  $u(x)$  with a fixed regularity index  $\mu$  is determined by the fractional integrals of  $P_n(x)$ . Indeed, we have the following bound.

**Lemma 3.1** *For  $\mu > -1/2$  and  $n \geq \mu + 1$ , we have*

$$\max_{|x| \leq 1} \left\{ \left| \left( I_{1-}^{\mu+1} P_n \right) (x) \right|, \left| \left( I_{-1+}^{\mu+1} P_n \right) (x) \right| \right\} \leq \frac{1}{2^{\mu+1} \sqrt{\pi}} \frac{\Gamma((n-\mu)/2)}{\Gamma((n+\mu+3)/2)}. \quad (3.17)$$

*Proof* According to Szegő [39, p. 62], the generalised Jacobi polynomials with real parameters  $\alpha, \beta$  are defined by the hypergeometric functions as

$$P_n^{(\alpha, \beta)}(x) = \frac{(\alpha+1)_n}{n!} {}_2F_1 \left( -n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2} \right), \quad x \in (-1, 1), \quad (3.18)$$

or alternatively,

$$P_n^{(\alpha, \beta)}(x) = (-1)^n \frac{(\beta+1)_n}{n!} {}_2F_1 \left( -n, n+\alpha+\beta+1; \beta+1; \frac{1+x}{2} \right), \quad x \in (-1, 1). \quad (3.19)$$

Recall the Euler transform identity (cf. [4, p. 95]): for  $a, b, c \in \mathbb{R}$  and  $-c \notin \mathbb{N}_0$ ,

$${}_2F_1(a, b; c; z) = (1-z)^{c-a-b} {}_2F_1(c-a, c-b; c; z), \quad |z| < 1. \quad (3.20)$$

Taking  $a = -n, b = n + \alpha + \beta + 1, c = \alpha + 1$  and  $z = (1-x)/2$  in (3.20), we obtain

$$\begin{aligned} & {}_2F_1 \left( -n, n+\alpha+\beta+1; \alpha+1; \frac{1-x}{2} \right) \\ &= \left( \frac{1+x}{2} \right)^{-\beta} {}_2F_1 \left( n+\alpha+1, -n-\beta; \alpha+1; \frac{1-x}{2} \right) \\ &= \left( \frac{1+x}{2} \right)^{-\beta} {}_2F_1 \left( -n-\beta, n+\alpha+1; \alpha+1; \frac{1-x}{2} \right). \end{aligned} \quad (3.21)$$

From (3.3), (3.18), (3.21) and  ${}_2F_1(a, b; c; 0) = 1$ , we get

$$\begin{aligned} (I_{1-}^{\mu+1} P_n)(x) &= \frac{(1-x)^{\mu+1}}{\Gamma(\mu+2)} \frac{P_n^{(\mu+1, -\mu-1)}(x)}{P_n^{(\mu+1, -\mu-1)}(1)} \\ &= \frac{(1-x)^{\mu+1}}{\Gamma(\mu+2)} {}_2F_1\left(-n, n+1; \mu+2; \frac{1-x}{2}\right) \\ &= \frac{(1-x^2)^{\mu+1}}{2^{\mu+1} \Gamma(\mu+2)} {}_2F_1\left(-n+\mu+1, n+\mu+2; \mu+2; \frac{1-x}{2}\right). \end{aligned} \quad (3.22)$$

Similarly, we can show that

$$(I_{-1+}^{\mu+1} P_n)(x) = \frac{(-1)^n (1-x^2)^{\mu+1}}{2^{\mu+1} \Gamma(\mu+2)} {}_2F_1\left(-n+\mu+1, n+\mu+2; \mu+2; \frac{1+x}{2}\right). \quad (3.23)$$

From Liu et al. [32, Definition 2.1 & (4.30)], we find that for  $\lambda \geq 1$  and  $\nu \geq 0$ ,

$$\begin{aligned} \max_{|x| \leq 1} \left\{ \left(1-x^2\right)^{\lambda-\frac{1}{2}} \left| {}_2F_1\left(-\nu, \nu+2\lambda; \lambda+\frac{1}{2}; \frac{1 \pm x}{2}\right) \right| \right\} \\ \leq \frac{\Gamma(\lambda+1/2)}{\sqrt{\pi}} \frac{\Gamma((\nu+1)/2)}{\Gamma((\nu+1)/2+\lambda)}. \end{aligned} \quad (3.24)$$

Thus, taking  $\nu \rightarrow n - \mu - 1$  and  $\lambda \rightarrow \mu + 3/2$  in (3.24), leads to

$$\begin{aligned} \max_{|x| \leq 1} \left\{ \left(1-x^2\right)^{\mu+1} \left| {}_2F_1\left(-n+\mu+1, n+\mu+2; \mu+2; \frac{1 \pm x}{2}\right) \right| \right\} \\ \leq \frac{\Gamma(\mu+2)}{\sqrt{\pi}} \frac{\Gamma((n-\mu)/2)}{\Gamma((n+\mu+3)/2)}. \end{aligned} \quad (3.25)$$

Finally the bound (3.17) follows from (3.22), (3.23) and (3.25).  $\square$

### 3.2 $L^\infty$ -estimates of Legendre orthogonal projections

With the above preparations, we are now ready to analyse the  $L^\infty$ -error estimate of the  $L^2$ -orthogonal projection:

$$u(x) = \sum_{n=0}^{\infty} \hat{u}_n^L P_n(x), \quad (\pi_N^L u)(x) = \sum_{n=0}^N \hat{u}_n^L P_n(x). \quad (3.26)$$

Below, we present the approximation results on the  $L^\infty$ -estimate and the weighted  $L^\infty$ -estimate. We shall illustrate that the former is suboptimal for functions with interior singularity, but optimal for the endpoint singularity, while the latter is optimal in both cases. Such convergence behaviors were numerically observed in [42, 44], but lack of theoretical justifications.

**Theorem 3.2** Let  $u, u', \dots, u^{(k-1)} \in AC([-1, 1])$  with  $k \in \mathbb{N}$ .

- (i) For  $\mu \in (k-1, k)$  and  $\theta \in (-1, 1)$ , if  ${}^CD_{\theta+}^\mu u \in BV([\theta, 1])$  and  ${}^CD_{\theta-}^\mu u \in BV([-1, \theta])$ , then for all  $N \geq \mu > 1/2$ ,

$$\|u - \pi_N^L u\|_{L^\infty(\Omega)} \leq \frac{1}{2^{\mu-1}(\mu-1/2)\sqrt{\pi}} \frac{\Gamma((N-\mu+1)/2)}{\Gamma((N+\mu)/2)} U_\theta^{(\mu)}, \quad (3.27)$$

and for all  $N \geq \mu$ ,

$$\left\| \left(1-x^2\right)^{\frac{1}{4}} (u - \pi_N^L u) \right\|_{L^\infty(\Omega)} \leq \frac{1}{2^{\mu-1}\mu\pi} \frac{\Gamma((N-\mu+1)/2)}{\Gamma((N+\mu+1)/2)} U_\theta^{(\mu)}, \quad (3.28)$$

where we denoted

$$U_\theta^{(\mu)} := V_{[-1,\theta]} \left[ {}^CD_{\theta-}^\mu u \right] + V_{[\theta,1]} \left[ {}^CD_{\theta+}^\mu u \right] + |{}^CD_{\theta-}^\mu u(\theta-)| + |{}^CD_{\theta+}^\mu u(\theta+)|. \quad (3.29)$$

- (ii) If  $u^{(k)} \in BV(\bar{\Omega})$  with  $\Omega = (-1, 1)$ , then the estimates (3.27)–(3.28) with  $\mu = k$  hold, but the total variation  $V_{\bar{\Omega}}[u^{(k)}]$  is in place of  $U_\theta^{(\mu)}$ .

*Proof* Using the identity in Theorem 3.1 and the bound in Lemma 3.1, we obtain from (2.2) that

$$\begin{aligned} |\hat{u}_n^L| &= \frac{2n+1}{2} \max_{x \in \bar{\Omega}} \left\{ |I_{1-}^{\mu+1} P_n(x)|, |I_{-1+}^{\mu+1} P_n(x)| \right\} U_\theta^{(\mu)} \\ &\leq \frac{(2n+1)\Gamma((n-\mu)/2)}{2^{\mu+2}\sqrt{\pi}\Gamma((n+\mu+3)/2)} U_\theta^{(\mu)}. \end{aligned} \quad (3.30)$$

We first prove the error bound (3.27). For simplicity, we denote

$$S_n^\mu := \frac{\Gamma((n-\mu)/2)}{\Gamma((n+\mu+1)/2)}, \quad \mathcal{T}_n^\mu := \frac{\Gamma((n-\mu)/2)}{\Gamma((n+\mu-1)/2)}. \quad (3.31)$$

Using the identity  $z\Gamma(z) = \Gamma(z+1)$ , we find readily that

$$\begin{aligned} \mathcal{T}_n^\mu - \mathcal{T}_{n+2}^\mu &= \frac{n+\mu-1}{2} \frac{\Gamma((n-\mu)/2)}{\Gamma((n+\mu+1)/2)} - \frac{n-\mu}{2} \frac{\Gamma((n-\mu)/2)}{\Gamma((n+\mu+1)/2)} \\ &= (\mu-1/2) \frac{\Gamma((n-\mu)/2)}{\Gamma((n+\mu+1)/2)} = (\mu-1/2) S_n^\mu. \end{aligned} \quad (3.32)$$

As  $|P_n(x)| \leq 1$ , we derive from (3.30) that

$$\begin{aligned} |(u - \pi_N^L u)(x)| &\leq \sum_{n=N+1}^{\infty} |\hat{u}_n^L| \leq \frac{U_\theta^{(\mu)}}{2^{\mu+2}\sqrt{\pi}} \sum_{n=N+1}^{\infty} \frac{(2n+1)\Gamma((n-\mu)/2)}{\Gamma((n+\mu+3)/2)} \\ &\leq \frac{U_\theta^{(\mu)}}{2^\mu\sqrt{\pi}} \sum_{n=N+1}^{\infty} \frac{\Gamma((n-\mu)/2)}{\Gamma((n+\mu+1)/2)} \\ &= \frac{U_\theta^{(\mu)}}{2^\mu(\mu-1/2)\sqrt{\pi}} \sum_{n=N+1}^{\infty} \{\mathcal{T}_n^\mu - \mathcal{T}_{n+2}^\mu\} \\ &= \frac{U_\theta^{(\mu)}}{2^\mu(\mu-1/2)\sqrt{\pi}} \{\mathcal{T}_{N+1}^\mu + \mathcal{T}_{N+2}^\mu\}. \end{aligned} \quad (3.33)$$

Since  $\mu > 1/2$ , we obtain from (A.3) immediately that

$$\mathcal{T}_{N+2}^\mu = \mathcal{R}_{\mu-1/2}^0(1 + (N - \mu)/2) \leq \mathcal{R}_{\mu-1/2}^0(1 + (N - \mu - 1)/2) = \mathcal{T}_{N+1}^\mu. \quad (3.34)$$

Therefore, we have from the above that

$$\left| \left( u - \pi_N^L u \right) (x) \right| \leq \frac{2\mathcal{T}_{N+1}^\mu U_\theta^{(\mu)}}{2^\mu(\mu - 1/2)\sqrt{\pi}} = \frac{U_\theta^{(\mu)}}{2^{\mu-1}(\mu - 1/2)\sqrt{\pi}} \frac{\Gamma((N - \mu + 1)/2)}{\Gamma((N + \mu)/2)}.$$

This leads to the error bound (3.27).

We now turn to the proof of (3.28). Recall the Bernstein inequality (cf. [5]):

$$\max_{|x| \leq 1} \left\{ \left( 1 - x^2 \right)^{\frac{1}{4}} |P_n(x)| \right\} \leq \sqrt{\frac{2}{\pi}} \left( n + \frac{1}{2} \right)^{-\frac{1}{2}}, \quad n \geq 0. \quad (3.35)$$

Thus, we infer from (3.30) and (3.35) that

$$\begin{aligned} e_N(x) &:= \left| \left( 1 - x^2 \right)^{\frac{1}{4}} \left( u - \pi_N^L u \right) (x) \right| \leq \sum_{n=N+1}^{\infty} \max_{|x| \leq 1} \left\{ \left( 1 - x^2 \right)^{\frac{1}{4}} |P_n(x)| \right\} |\hat{u}_n^L| \\ &\leq \frac{U_\theta^{(\mu)}}{2^\mu \pi} \sum_{n=N+1}^{\infty} \sqrt{\frac{n}{2} + \frac{1}{4}} \frac{\Gamma((n - \mu)/2)}{\Gamma((n + \mu + 3)/2)}. \end{aligned} \quad (3.36)$$

Considering (A.4) with  $z = z_n = (n + \mu + 1)/2$  and  $c = 1/4 - (\mu + 1)/2 (\leq 1/4)$ , we find from its monotonicity that  $\hat{\mathcal{R}}_c(z_n) \geq \hat{\mathcal{R}}_c(\infty) = 1$  (cf. (A.5)). This immediately implies

$$\frac{\sqrt{n/2 + 1/4}}{\Gamma((n + \mu + 3)/2)} \leq \frac{1}{\Gamma((n + \mu)/2 + 1)}, \quad (3.37)$$

so we can bound the summation in (3.36) by

$$\sum_{n=N+1}^{\infty} \sqrt{\frac{n}{2} + \frac{1}{4}} \frac{\Gamma((n - \mu)/2)}{\Gamma((n + \mu + 3)/2 + 1)} \leq \sum_{n=N+1}^{\infty} \frac{\Gamma((n - \mu)/2)}{\Gamma((n + \mu)/2 + 1)}. \quad (3.38)$$

Similarly, denoting

$$\hat{\mathcal{S}}_n^\mu := \frac{\Gamma((n - \mu)/2)}{\Gamma((n + \mu)/2 + 1)}, \quad \hat{\mathcal{T}}_n^\mu := \frac{\Gamma((n - \mu)/2)}{\Gamma((n + \mu)/2)}, \quad (3.39)$$

we find readily that

$$\hat{\mathcal{T}}_n^\mu - \hat{\mathcal{T}}_{n+2}^\mu = \frac{n + \mu}{2} \frac{\Gamma((n - \mu)/2)}{\Gamma((n + \mu)/2 + 1)} - \frac{n - \mu}{2} \frac{\Gamma((n - \mu)/2)}{\Gamma((n + \mu)/2 + 1)} = \mu \hat{\mathcal{S}}_n^\mu. \quad (3.40)$$

Following the same lines as in the derivation of (3.33), we can get

$$e_N(x) \leq \frac{U_\theta^{(\mu)}}{2^\mu \mu \pi} \{ \hat{\mathcal{T}}_{N+1}^\mu + \hat{\mathcal{T}}_{N+2}^\mu \} \leq \frac{2\hat{\mathcal{T}}_{N+1}^\mu}{2^\mu(\mu - 1)\pi} U_\theta^{(\mu)}, \quad (3.41)$$

where we used the property derived from (A.3) with  $\mu > 1$ , that is,

$$\hat{\mathcal{T}}_{N+2}^\mu = \mathcal{R}_{\mu-1}^0(1 + (N - \mu)/2) \leq \mathcal{R}_{\mu-1}^0(1 + (N - \mu - 1)/2) = \hat{\mathcal{T}}_{N+1}^\mu.$$

Then, the estimate (3.28) follows from (3.39) and (3.41) straightforwardly.

For  $\mu = k$ , using the identity in Corollary 3.1 to derive the bound in (3.30), and then following the same lines, we can obtain the estimates in (ii).  $\square$

Under the regularity assumption in Theorem 3.2, we infer from (A.5) and the estimates (3.27)–(3.28) the convergence behavior:

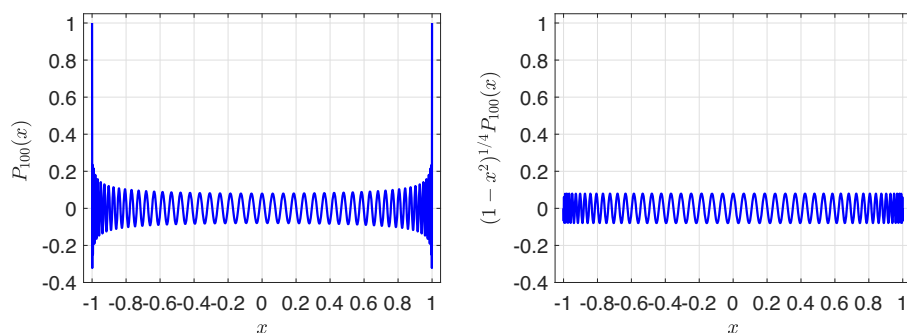
$$\begin{aligned} \|u - \pi_N^L u\|_{L^\infty(\Omega)} &= O\left(N^{-\mu+1/2}\right), \\ \|(1-x^2)^{\frac{1}{4}}(u - \pi_N^L u)\|_{L^\infty(\Omega)} &= O\left(N^{-\mu}\right), \end{aligned} \quad (3.42)$$

which exhibit a half-order convergence difference. Moreover, the estimate (3.36) implies

$$\left| (u - \pi_N^L u)(x) \right| = \left(1 - x^2\right)^{-\frac{1}{4}} O\left(N^{-\mu}\right), \quad \forall x \in [-a, a] \subset (-1, 1). \quad (3.43)$$

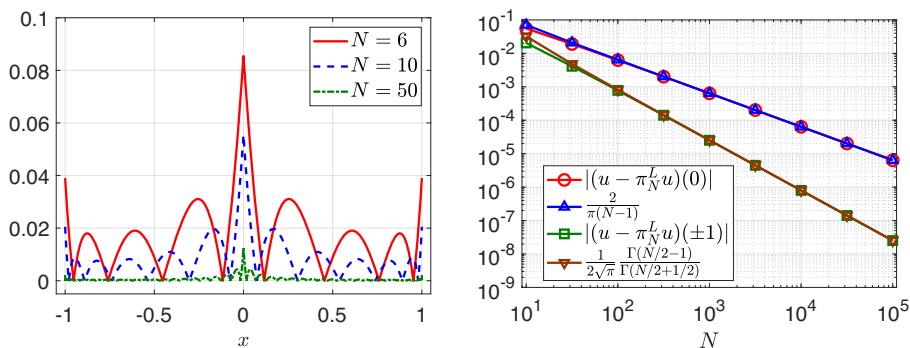
For a function with an interior singularity in  $[-a, a]$  with  $|a| < 1$ , one expects the optimal order  $O(N^{-\mu})$ . Note from (3.33) and (3.36) that the bounds essentially depend on the maximum of  $|P_n(x)|$  and  $(1-x^2)^{1/4}|P_n(x)|$ , which behave very differently near the endpoints as shown in Fig. 1. In fact,  $|P_n(x)| = O(n^{-1/2})$  for  $x \in [-a, a]$ , but it is overestimated by the bound 1 at  $x = \pm 1$ . However, from (3.35), we have  $(1-x^2)^{1/4}|P_n(x)| \leq Cn^{-1/2}$  for all  $x \in [-1, 1]$ . This is actually the cause of the lost order in the (non-weighted)  $L^\infty$ -estimate in (3.42).

With these analysis tools at hand, we further examine  $u(x) = |x|$  (as a motivative example in Trefethen [40]), for which Wang [42, 44] observed the order  $O(N^{-1})$  numerically, but the order is  $O(N^{-1/2})$  based on the error estimate of Legendre approximation in  $L^\infty$ -norm. From the pointwise error plots in Fig. 2 (left), we see the largest error occurs at the singular point  $x = 0$ . Indeed, we have the following estimates (with the proof given in Appendix D), which are sharp as shown in Fig. 2 (right).



**Fig. 1**  $P_n(x)$  and  $(1-x^2)^{\frac{1}{4}}P_n(x)$  with  $x \in [-1, 1]$  and  $n = 100$





**Fig. 2** Left:  $|u - \pi_N^L u(x)|$  with  $u(x) = |x|$  and different  $N$ . Right: Tightness of the bounds in Theorem 3.3

**Theorem 3.3** Consider  $u(x) = |x|$  for  $x \in [-1, 1]$ . Then for  $N > 2$ , we have

$$\left| (u - \pi_N^L u)(0) \right| \leq \frac{2}{\pi(N-1)}; \quad \left| (u - \pi_N^L u)(\pm 1) \right| \leq \frac{1}{2\sqrt{\pi}} \frac{\Gamma(N/2-1)}{\Gamma(N/2+1/2)}. \quad (3.44)$$

Finally, we apply the estimates to the example  $u(x) = |x|^\mu$  with  $\mu \in (k-1, k)$ . As shown in [32, Thm. 4.3],  $u, u', \dots, u^{(k-1)} \in AC(\bar{\Omega})$ ,  ${}^C D_{0+}^\mu u \in BV([0, 1])$ , and  ${}^C D_{0-}^\mu u \in BV([-1, 0])$ . Then we infer from (3.42) that the expected convergence order in  $L^\infty_{\varpi}$ -norm with  $\varpi = (1 - x^2)^{1/4}$  is  $O(N^{-\mu})$ . Indeed, the numerical results in Table 1 agree well with the prediction shown in the last row.

### 3.3 $L^2$ -estimates

As pointed out in [38, Chap. 3], the estimate of the  $L^2$ -orthogonal projection is the starting point to derive many other approximation results that provide fundamental tools for error analysis of spectral and  $hp$  methods (see, e.g., [11, 16, 23, 26, 37,

**Table 1** Convergence order of Legendre expansion for  $|x|^\mu$

$N$	Errors in $L^\infty_{\varpi}$ -norm			
	$\mu = 1.7$	Order	$\mu = 2.6$	Order
$2^3$	5.81e-03	–	2.22e-03	–
$2^4$	2.03e-03	1.52	4.38e-04	2.34
$2^5$	6.72e-04	1.60	8.01e-05	2.45
$2^6$	2.15e-04	1.65	1.40e-05	2.52
$2^7$	6.74e-05	1.67	2.37e-06	2.56
$2^8$	2.09e-05	1.69	3.97e-07	2.58
Pred.		1.70		2.60

38]). Most estimates therein are for functions in Sobolev or Besov spaces. Here, we consider functions with AC-BV regularity, thereby enriching the approximation theory.

We first highlight the fundamental importance of estimating  $L^2$ -orthogonal projection in (3.26). For  $u \in H^1(\Omega)$ , we define

$$\left(\pi_N^1 u\right)(x) = u(-1) + \int_{-1}^x \pi_{N-1}^L u'(t) dt \in \mathcal{P}_N, \quad (3.45)$$

where  $\mathcal{P}_N$  denotes the set of polynomials of degree at most  $N$ . Note that for  $N \geq 2$ , we have from the orthogonality of Legendre polynomials that

$$\left(\pi_N^1 u\right)(1) = u(-1) + \int_{-1}^1 \pi_{N-1}^L u'(t) dt = u(-1) + \int_{-1}^1 u'(t) dt = u(1).$$

Thus, we have  $\left(\pi_N^1 u\right)(\pm 1) = u(\pm 1)$ . Moreover, one verifies readily that

$$\int_{-1}^1 \left(\pi_N^1 u - u\right)'(x) v'(x) dx = 0, \quad \forall v \in \mathcal{P}_N^0 := \{v \in \mathcal{P}_N : v(\pm 1) = 0\}.$$

Therefore, (3.45) defines the  $H_0^1$ -orthogonal projection where  $u(\pm 1) = 0$ . Note that

$$\left\| \left(u - \pi_N^1 u\right)' \right\|_{L^2(\Omega)}^2 = \|u' - \pi_{N-1}^L u'\|_{L^2(\Omega)}^2, \quad (3.46)$$

so the  $H^1$ -estimate boils down to the estimate of the  $L^2$ -orthogonal projection. The high-order  $H_0^m$ -orthogonal projection is treated similarly in a recursive manner. More precisely, according to [11, p. 262], we can define the  $H_0^m$ -orthogonal projection by

$$\left(\pi_N^{m,0} u\right)(x) = \int_{-1}^x \left(\pi_{N-1}^{m-1,0} u\right)(\xi) d\xi, \quad m \geq 1,$$

where  $\pi_N^{0,0} = \pi_N^L$ . Consequently, we can estimate the projection error by using the  $L^2$ -estimate as follows

$$\left| u - \pi_N^{m,0} u \right|_{H^m(\Omega)} = \left| u' - \pi_{N-1}^{m-1,0} u' \right|_{H^{m-1}(\Omega)} = \cdots = \left\| u^{(m)} - \pi_{N-m}^L u^{(m)} \right\|_{L^2(\Omega)}.$$

On the other hand, the analysis of Gauss-type interpolation and quadrature errors is also based upon the Legendre expansion (see [38]).

With the tools in Section 3.1, we can also derive the following optimal  $L^2$ -error bound under the AC-BV regularity of  $u$ , from which we can further establish many other approximation results indispensable for analysis of spectral and  $hp$  methods for PDEs. Here, we omit such extensions.

**Theorem 3.4** Assume the conditions in Theorem 3.2 hold.

(i) For  $\mu \in (k-1, k)$  and  $-1/2 < \mu < N$ ,

$$\|u - \pi_N^L u\|_{L^2(\Omega)} \leq \sqrt{\frac{2}{(2\mu+1)\pi}} \frac{\Gamma(N-\mu)}{\Gamma(N+\mu+1)} U_\theta^{(\mu)}. \quad (3.47)$$

- (ii) For  $\mu = k$ , the estimates (3.47) hold, with the total variation  $V_{\tilde{\Omega}}[u^{(k)}]$  is in place of  $U_{\theta}^{(\mu)}$ .

*Proof* Similar to (3.34), we can use (A.3) to show that

$$\frac{\Gamma((n - \mu)/2)}{\Gamma((n + \mu + 3)/2)} \leq \frac{\Gamma((n - \mu - 1)/2)}{\Gamma((n + \mu)/2 + 1)}.$$

Then from (A.2), we derive

$$\begin{aligned} \frac{(n/2 + 1/4)\Gamma^2((n - \mu)/2)}{\Gamma^2((n + \mu + 3)/2)} &\leq \frac{\Gamma^2((n - \mu)/2)}{\Gamma((n + \mu + 3)/2)\Gamma((n + \mu + 1)/2)} \\ &\leq \frac{\Gamma((n - \mu)/2)\Gamma((n - \mu - 1)/2)}{\Gamma((n + \mu)/2 + 1)\Gamma((n + \mu + 1)/2)} \\ &= 2^{2(\mu+1)} \frac{\Gamma(n - \mu - 1)}{\Gamma(n + \mu + 1)} \\ &= \frac{2^{2(\mu+1)}}{2\mu + 1} \left( \frac{\Gamma(n - \mu - 1)}{\Gamma(n + \mu)} - \frac{\Gamma(n - \mu)}{\Gamma(n + \mu + 1)} \right). \end{aligned} \quad (3.48)$$

Then, by the orthogonality of Legendre polynomials, we derive from (3.30) and (3.48) that for  $\mu > -1/2$ ,

$$\begin{aligned} \|u - \pi_N^L u\|_{L^2(\Omega)}^2 &= \sum_{n=N+1}^{\infty} \frac{2}{2n+1} |\hat{u}_n^L|^2 \leq \frac{(U_{\theta}^{(\mu)})^2}{2^{2\mu+3}\pi} \sum_{n=N+1}^{\infty} \frac{(2n+1)\Gamma^2((n - \mu)/2)}{\Gamma^2((n + \mu + 3)/2)} \\ &\leq \frac{2(U_{\theta}^{(\mu)})^2}{(2\mu + 1)\pi} \frac{\Gamma(N - \mu)}{\Gamma(N + \mu + 1)}. \end{aligned} \quad (3.49)$$

For  $\mu = k$ , using the identity in Corollary 3.1 to derive the bound in (3.30), and then following the same lines, we can obtain the estimates in (ii).  $\square$

## 4 Legendre expansion of functions with endpoint singularities

The aforementioned AC-BV framework and main results can be extended to the study of the end-point singularities, which typically occur in underlying solutions of PDEs in various situations, for instance, irregular domains, singular coefficients and mismatch of boundary conditions among others. It is known that the Legendre expansion of a function with an endpoint singularity has a much higher convergence rate than that with an interior singularity of the same type. We illustrate this through an example which also motivates the seemingly complicated extension. To fix the idea, we focus on the left endpoint singularity but the results can be extended to the right endpoint setting straightforwardly.

#### 4.1 An illustrative example

We consider  $u(x) = (1+x)^\mu g(x)$  with  $\mu \in (k-1, k)$ ,  $k \in \mathbb{N}$  and a sufficiently smooth  $g(x)$  on  $\Omega$ . Then we can write

$$u(x) = (1+x)^\mu g(x) = \sum_{m=0}^{\infty} \frac{g^{(m)}(-1)}{m!} (1+x)^{\mu+m}. \quad (4.1)$$

Then by (2.8),

$$\begin{aligned} \left({}^C D_{-1+}^\mu u\right)(x) &= \left(I_{-1+}^{k-\mu} u^{(k)}\right)(x) \\ &= \sum_{m=0}^{\infty} \frac{\{\mu+m\}_k}{m!} g^{(m)}(-1) I_{-1+}^{k-\mu} \left\{ (1+x)^{m+\mu-k} \right\} \\ &= \sum_{m=0}^{\infty} \frac{\{\mu+m\}_k \Gamma(m+\mu-k+1)}{(m!)^2} g^{(m)}(-1) (1+x)^m, \end{aligned} \quad (4.2)$$

where  $\{a\}_k = a(a-1)\cdots(a-k+1)$  stands for the falling factorial. Here, we assume the uniform convergence of the series that allows for the differentiation. This implies  $({}^C D_{-1+}^\mu u)(x)$  is sufficiently smooth. In particular, if  $g = 1$ , then  $({}^C D_{-1+}^\mu u)(x)$  is equal to a constant.

We deduce from Theorem 3.1 with  $\theta \rightarrow -1^+$  that for  $u, u', \dots, u^{(k-1)} \in \text{AC}(\bar{\Omega})$ , and  ${}^C D_{-1+}^\mu u \in \text{BV}(\bar{\Omega})$  with  $\mu \in (k-1, k]$ , we have

$$\hat{u}_n^L = \frac{2n+1}{2} \left\{ \left({}^C D_{-1+}^\mu u\right)(-1+) \left(I_{1-}^{\mu+1} P_n\right)(-1) + \int_{-1}^1 \left(I_{1-}^{\mu+1} P_n\right)(x) d\left\{{}^C D_{-1+}^\mu u(x)\right\} \right\}. \quad (4.3)$$

In fact, we can show that  $\left(I_{1-}^{\mu+1} P_n\right)(-1) \sim n^{-2(\mu+1)}$ , so the first term decays like  $O(n^{-2\mu-1})$  (which gives the optimal convergence order for (4.1) (see Table 2), and doubles  $O(n^{-\mu-1/2})$  for the interior singularity, e.g., of  $|x|^\mu g(x)$ ).

**Lemma 4.1** For  $n \geq \mu+1 > 0$ , we have

$$\left(I_{1-}^{\mu+1} P_n\right)(-1) = \frac{(-1)^n 2^{\mu+1} \Gamma(\mu+1) \sin((\mu+1)\pi)}{\pi} \frac{\Gamma(n-\mu)}{\Gamma(n+\mu+2)}. \quad (4.4)$$

*Proof* By (3.3), we have

$$\left(I_{1-}^{\mu+1} P_n\right)(-1) = \frac{2^{\mu+1}}{\Gamma(\mu+2)} \frac{P_n^{(\mu+1, -\mu-1)}(-1)}{P_n^{(\mu+1, -\mu-1)}(1)} = \frac{(-1)^n 2^{\mu+1}}{\Gamma(\mu+2)} \frac{P_n^{(-\mu-1, \mu+1)}(1)}{P_n^{(\mu+1, -\mu-1)}(1)}, \quad (4.5)$$

where we used the parity  $P_n^{(\alpha, \beta)}(-x) = (-1)^n P_n^{(\beta, \alpha)}(x)$  valid for all real parameters  $\alpha, \beta$  (cf. Szegő [39, p.64]). Then we derive (4.4) from (3.11) and (A.1) immediately.  $\square$

**Table 2** Decay rate of  $|\hat{u}_n^L|$  with  $u = (x + 1)^\mu \sin x$

$n$	$\mu = 0.1$	Order	$\mu = 1.2$	Order	$\mu = 2.6$	Order
$2^3$	1.26e-02	–	6.86e-04	–	1.42e-04	–
$2^4$	5.59e-03	1.17	6.59e-05	3.38	1.35e-06	6.72
$2^5$	2.47e-03	1.18	6.41e-06	3.36	1.86e-08	6.18
$2^6$	1.08e-03	1.19	6.20e-07	3.37	2.60e-10	6.16
$2^7$	4.73e-04	1.19	5.94e-08	3.38	3.49e-12	6.22
Pred.		1.20		3.40		6.20

We find from Lemma 3.1 that the second term in (4.3) decays at a rate  $O(n^{-\mu-1/2})$ , if one naively works this out with this formula. However, in view of (4.2), we can continue to carry out integration by parts upon (4.3) as many as times we want, until the first boundary term in (4.3) dominates the error. This produces the optimal order  $O(n^{-2\mu-1})$  (see Table 2 for numerical illustrations where the last row is the theoretical prediction).

## 4.2 Approximation results for functions with endpoint singularities

With the above understanding, we are now ready to present the identity on the Legendre expansion coefficient from (4.3) and integration by parts. Given that the function has more regularity in this case, we make the following assumption.

**Definition 4.1 (Regularity Assumption)** For  $\mu \in (k - 1, k]$  with  $k \in \mathbb{N}$ , assume  $u, \dots, u^{(k-1)} \in AC(\bar{\Omega})$  and  $v_\mu(x) := {}^C D_{-1+}^\mu u \in BV(\bar{\Omega})$ . We further assume that  $v_\mu, \dots, v_\mu^{(m-1)} \in AC(\bar{\Omega})$  and  $v_\mu^{(m)} \in BV(\bar{\Omega})$ . Accordingly, we denote

$$U_-^{(\mu,m)} := V_{\bar{\Omega}} \left[ v_\mu^{(m)} \right] + |\sin(\mu\pi)| \sum_{l=0}^m \left| v_\mu^{(l)}(-1+) \right|. \quad (4.6)$$

For simplicity, we say  $u$  is of  $AC-BV_{\mu,m}$ -regularity.

Note that for the example (4.1),  $v_\mu$  is sufficiently smooth so we have  $m = \infty$ . Under this assumption, we can update the formula (4.3) as follows.

**Theorem 4.1** Assume that  $u$  is of  $AC-BV_{\mu,m}$ -regularity. Then for  $n \geq \mu + m + 1$ , we have

$$\hat{u}_n^L = \frac{2n+1}{2} \left\{ \sum_{l=0}^m \left( I_{1-}^{\mu+l+1} P_n \right) (-1) v_\mu^{(l)}(-1+) + \int_{-1}^1 \left( I_{1-}^{\mu+m+1} P_n \right) (x) \, d \left\{ v_\mu^{(m)}(x) \right\} \right\}, \quad (4.7)$$

where  $(I_{1-}^{\mu+l+1} P_n)(-1)$  has the explicit value given by (4.4).

*Proof* Since  $v_\mu, \dots, v_\mu^{(m-1)} \in AC(\bar{\Omega})$ , we can conduct integration by parts upon (4.3):

$$\begin{aligned} \frac{2\hat{u}_n^L}{2n+1} &= \left(I_{1-}^{\mu+1} P_n\right)(-1) v_\mu(-1) + \int_{-1}^1 \left(I_{1-}^{\mu+1} P_n\right)(x) v'_\mu(x) dx \\ &= \dots = \sum_{l=0}^{m-1} \left(I_{1-}^{\mu+l+1} P_n\right)(-1) v_\mu^{(l)}(-1) + \int_{-1}^1 \left(I_{1-}^{\mu+m} P_n\right)(x) v_\mu^{(m)}(x) dx \\ &= \sum_{l=0}^m \left(I_{1-}^{\mu+l+1} P_n\right)(-1) v_\mu^{(l)}(-1) + \int_{-1}^1 \left(I_{1-}^{\mu+m+1} P_n\right)(x) d\{v_\mu^{(m)}(x)\}, \end{aligned}$$

where the boundary values at  $x = 1$  vanish in view of (3.3), and in the last step, we used the factor  $v_\mu^{(m)} \in BV(\bar{\Omega})$  and (2.3).  $\square$

Comparing the formulas of  $\hat{u}_n^L$  in Theorem 3.1 (with  $\theta \rightarrow -1^+$ , i.e., (4.3)) and Theorem 4.1, we find they largely differ from the regularity index. We can use Lemmas 3.1 and 4.1 to deal with the fractional integrals of the Legendre polynomial. Accordingly, we can follow the same lines as in the proofs of Theorems 3.2 and 3.4 to derive the following estimates. To avoid the repetition, we skill the proof, though there is subtlety in some derivations.

**Theorem 4.2** Assume that  $u$  is of  $AC-BV_{\mu,m}$ -regularity as described in Definition 4.1. Then for  $N > m + \mu$ , we have the following estimates.

(i) For  $\mu > 0$ ,

$$\|u - \pi_N^L u\|_{L^\infty(\Omega)} \leq \left\{ \frac{1}{2^{\mu+m-1}(\mu+m-1/2)\sqrt{\pi}} \frac{\Gamma((N-\mu-m+1)/2)}{\Gamma((N+\mu+m)/2)} + \frac{2^\mu \Gamma(\mu)}{\pi} \frac{(N+1)\Gamma(N-\mu+1)}{(N+1/2)\Gamma(N+\mu+1)} \right\} U_-^{(\mu,m)}. \quad (4.8)$$

(ii) For  $\mu > -1/2$ ,

$$\|u - \pi_N^L u\|_{L^2(\Omega)} \leq \left\{ \frac{4}{(2\mu+2m+1)\pi} \frac{\Gamma(N-\mu-m)}{\Gamma(N+\mu+m+1)} + \frac{2^{6\mu+8} \Gamma^2(\mu+1)}{\pi^2(4\mu+2)} \frac{(N+1)^2 \Gamma(2N-2\mu+1)}{(2N+1)^2 \Gamma(2N+2\mu+3)} \right\}^{1/2} U_-^{(\mu,m)}. \quad (4.9)$$

**Remark 4.1** Using the Stirling's formula for the Gamma function, we can obtain the explicit convergence order in  $N$ :

$$\begin{aligned} \|u - \pi_N^L u\|_{L^\infty(\Omega)} &\leq c \left( N^{\frac{1}{2}-\mu-m} + N^{-2\mu} \right) U_-^{(\mu,m)}, \\ \|u - \pi_N^L u\|_{L^2(\Omega)} &\leq c N^{-1} \left( N^{\frac{1}{2}-\mu-m} + N^{-2\mu} \right) U_-^{(\mu,m)}, \end{aligned}$$

where  $c$  is a generic positive constant independent of  $N$  and  $u$ .

**Table 3** Convergence of Legendre expansion of  $(1+x)^\mu$ 

$N$	Errors in $L^\infty$ -norm				Errors in $L^2$ -norm			
	$\mu = 0.1$	Order	$\mu = 1.2$	Order	$\mu = 0.1$	Order	$\mu = 1.2$	Order
$2^3$	6.15e-01	–	2.27e-3	–	8.82e-3	–	2.32e-04	–
$2^4$	5.41e-01	0.18	4.87e-04	2.22	4.11e-03	1.10	2.64e-05	3.14
$2^5$	4.74e-01	0.19	9.87e-05	2.30	1.85e-03	1.15	2.75e-06	3.26
$2^6$	4.14e-01	0.20	1.94e-05	2.35	8.22e-04	1.17	2.74e-07	3.33
$2^7$	3.61e-01	0.20	3.74e-06	2.37	3.61e-04	1.19	2.67e-08	3.36
$2^8$	3.15e-01	0.20	7.15e-07	2.39	1.58e-04	1.19	2.56e-09	3.38
Pred.		0.20		2.40		1.20		3.40

In contrast to the interior singularity with a half-order loss, the  $L^\infty$ -estimate in this case is optimal. In fact, for the endpoint singularity, the largest error occurs near the boundary where  $|P_n(x)|$  attain its maximum at  $x = \pm 1$  (see Fig. 1 (left)), so the direct summation in, e.g., (3.33) will not overestimate. As an illustration, we consider  $u(x) = (1+x)^\mu$  with  $\mu \in (k-1, k)$ ,  $k \in \mathbb{N}$ . From Remark 4.1, we find  $\|u - \pi_N^L u\|_{L^\infty(\Omega)} \leq CN^{-2\mu}$  and  $\|u - \pi_N^L u\|_{L^2(\Omega)} \leq CN^{-2\mu-1}$ . We tabulate in Table 3 the errors and convergence order of Legendre approximations to  $u(x) = (x+1)^\mu$  with various  $\mu$ , which indicate the optimal convergence order as predicted (see the last row).

### 4.3 Concluding remarks

We presented a new fractional Taylor formula for singular functions whose integer-order derivatives up to  $k-1$  are absolutely continuous and Caputo fractional derivative of order  $\mu \in (k-1, k]$  is of bounded variation. It could be viewed as an “interpolation” between the usual Taylor formulas of two consecutive integer orders. We derived from this remarkable tool a similar fractional representation of the Legendre expansion of this type of functions, which became the cornerstone of the optimal error estimates for the Legendre orthogonal projection. The set of results under the fractional AC-BV framework greatly enriched the approximation theory for spectral and  $hp$  methods. It set a good example to show how the fractional calculus could impact this classic field, and seamlessly bridge between the results valid only for integer cases. Here, we merely discussed the approximation results, but hopefully it can pave the way for the analysis of and applications to singular problems in multiple dimensions. We only considered the fractional power singularity, but it is worth noting that this framework is suboptimal for log-singularities some modification of the spaces (see [32]). We shall report the works on multiple-dimensional extensions and optimal bounds for log-singularities in future works.

## Appendix A: Useful properties of Gamma function

Recall the Euler's reflection formula (cf. [4, Ch.2]):

$$\Gamma(1-a)\Gamma(a) = \frac{\pi}{\sin(\pi a)}, \quad a \neq \pm 1, \pm 2, \dots, \quad (\text{A.1})$$

and the Legendre duplication formula (cf. [34, (5.5.5)]):

$$\Gamma(2z) = \pi^{-1/2} 2^{2z-1} \Gamma(z) \Gamma(z+1/2). \quad (\text{A.2})$$

From [2, (1.1) and Thm. 10], we have that for  $0 \leq a \leq b$ , the ratio

$$\mathcal{R}_b^a(z) := \frac{\Gamma(z+a)}{\Gamma(z+b)}, \quad z \geq 0, \quad (\text{A.3})$$

is decreasing with respect to  $z$ . On the other hand, the ratio

$$\widehat{\mathcal{R}}_c(z) := \frac{1}{\sqrt{z+c}} \frac{\Gamma(z+1)}{\Gamma(z+1/2)}, \quad (\text{A.4})$$

is increasing (resp. decreasing) on  $[-1/2, \infty)$  (resp.  $(-c, \infty)$ ), if  $c \geq 1/2$  (resp.  $c \leq 1/4$ ), based on [14, Corollary 2].

In the error bounds, the ratio of two Gamma functions appears very often, so the following inequality is useful.

**Lemma A.1** *Let  $b \in (a+m, a+m+1)$  for some integer  $m \geq 0$ , and set  $b = a+m+\mu$  with  $\mu \in (0, 1)$ . Then for  $z+a > 0$  and  $z+b > 1$ , we have*

$$\begin{aligned} \frac{1}{(z+a)_m} \left( z+b - \frac{3}{2} + \left( \frac{5}{4} - \mu \right)^{1/2} \right)^{-\mu} &< \frac{\Gamma(z+a)}{\Gamma(z+b)} \\ &< \frac{1}{(z+a)_m} \left( z+b - \frac{\mu+1}{2} \right)^{-\mu}, \end{aligned} \quad (\text{A.5})$$

where the Pochhammer symbol:  $(c)_m = c(c+1) \cdots (c+m-1)$ .

*Proof* In fact, (A.5) can be derived from the bounds in [27, (1.3)]:

$$\left( x - \frac{1}{2} + \left( v + \frac{1}{4} \right)^{1/2} \right)^{v-1} < \frac{\Gamma(x+v)}{\Gamma(x+1)} < \left( x + \frac{v}{2} \right)^{v-1}, \quad x > 0, \quad v \in (0, 1). \quad (\text{A.6})$$

Indeed, using the property  $\Gamma(z+1) = z\Gamma(z)$ , we can write

$$\frac{\Gamma(z+a)}{\Gamma(z+b)} = \frac{1}{(z+a)_m} \frac{\Gamma(z+a+m)}{\Gamma(z+b)} = \frac{1}{(z+a)_m} \frac{\Gamma(z+b-\mu)}{\Gamma(z+b)}.$$

Then by (A.6) with  $x = z+b-1$  and  $v = 1-\mu$ , we obtain (A.5) immediately.  $\square$



## Appendix B: Proof of Lemma 2.2

For  $f \in L^1(\Omega)$  and  $g \in AC(\bar{\Omega})$ , changing the order of integration by the Fubini's Theorem, we derive from (2.4) that

$$\begin{aligned} \int_a^b f(x) I_{a+}^\rho g'(x) dx &= \frac{1}{\Gamma(\rho)} \int_a^b \left\{ \int_a^x \frac{g'(y)}{(x-y)^{1-\rho}} dy \right\} f(x) dx \\ &= \frac{1}{\Gamma(\rho)} \int_a^b \left\{ \int_y^b \frac{f(x)}{(x-y)^{1-\rho}} dx \right\} g'(y) dy \\ &= \frac{1}{\Gamma(\rho)} \int_a^b \left\{ \int_x^b \frac{f(y)}{(y-x)^{1-\rho}} dy \right\} g'(x) dx \\ &= \int_a^b g'(x) I_{b-}^\rho f(x) dx. \end{aligned}$$

If  $I_{b-}^\rho f(x) \in BV(\bar{\Omega})$ , we derive from (2.3) that

$$\begin{aligned} \int_a^b f(x) I_{a+}^\rho g'(x) dx &= \int_a^b g'(x) I_{b-}^\rho f(x) dx \\ &= \{g(x) I_{b-}^\rho f(x)\} \Big|_{a^+}^{b^-} - \int_a^b g(x) d\{I_{b-}^\rho f(x)\}. \end{aligned}$$

This yields (2.6).

We can derive (2.7) in a similar fashion.

## Appendix C: Proof of Proposition 2.1

Recall the first mean value theorem for the integral (cf. [47, p. 354]): Let  $f, g$  be Riemman integrable on  $[c, d]$ ,  $m = \inf_{x \in [c, d]} f(x)$ , and  $M = \sup_{x \in [c, d]} f(x)$ . If  $g$  is non-negative (or non-positive) on  $[c, d]$ , then

$$\int_c^d f(x)g(x)dx = \kappa \int_c^d g(x)dx, \quad \kappa \in [m, M]. \quad (C.7)$$

Recall that (cf. [36]): for  $\alpha > -1$  and  $\mu \in \mathbb{R}^+$ ,

$$I_{a+}^\mu (x-a)^\alpha = \frac{\Gamma(\alpha+1)}{\Gamma(\alpha+\mu+1)} (x-a)^{\alpha+\mu}. \quad (C.8)$$

For any  $x \in [a, a+\delta]$ , we derive from (2.4), (C.7) and (C.8) that

$$\begin{aligned} I_{a+}^\mu u(x) &= \frac{1}{\Gamma(\mu)} \int_a^x \frac{u(y)}{(x-y)^{1-\mu}} dy = \frac{\kappa(x)}{\Gamma(\mu)} \int_a^x \frac{(y-a)^\alpha}{(x-y)^{1-\mu}} dy \\ &= \kappa(x) I_x^\mu (x-a)^\alpha = \frac{\Gamma(\alpha+1)\kappa(x)(x-a)^{\mu+\alpha}}{\Gamma(\alpha+\mu+1)}, \end{aligned} \quad (C.9)$$

where  $\kappa(x) \in [m(x), M(x)]$ ,  $m(x) = \inf_{y \in [a, x]} v(y)$ ,  $M(x) = \sup_{y \in [a, x]} v(y)$ . We know that

$$\lim_{x \rightarrow a^+} m(x) = v(a), \quad \lim_{x \rightarrow a^+} M(x) = v(a) \Rightarrow \lim_{x \rightarrow a^+} \kappa(x) = v(a). \quad (\text{C.10})$$

From (C.9) and (C.10), we obtain (2.9). This completes the proof.

## Appendix D: Proof of Theorem 3.3

We start with the exact formula for the Legendre expansion coefficients of  $u(x) = |x|$ :

$$\hat{u}_{2j}^L = \frac{(-1)^{j+1}(j+1/4)\Gamma(j-1/2)}{\sqrt{\pi}(j+1)!}, \quad \hat{u}_{2j+1}^L = 0, \quad j \geq 1, \quad (\text{D.11})$$

which can be derived from (3.16) with  $k = 1$ , i.e.,

$$\begin{aligned} \hat{u}_n^L &= \frac{2n+1}{2} \int_{-1}^1 (I_{1-}^2 P_n)(x) \, d\left\{u^{(1)}(x)\right\} = \frac{2n+1}{2^2} (I_{1-}^2 P_n)(0) \\ &= \frac{2n+1}{2^5} {}_2F_1\left(-n+2, n+3; 3; \frac{1}{2}\right), \quad n \geq 2, \end{aligned}$$

and the value at  $z = 1/2$  (cf. [34, (15.4.28)]):

$${}_2F_1\left(a, b; \frac{a+b+1}{2}; \frac{1}{2}\right) = \frac{\sqrt{\pi} \Gamma((a+b+1)/2)}{\Gamma((a+1)/2) \Gamma((b+1)/2)}.$$

Then, we obtain from (D.11) that

$$\begin{aligned} (u - \pi_N^L u)(0) &= \sum_{j=\lceil \frac{N+1}{2} \rceil}^{\infty} \hat{u}_{2j}^L P_{2j}(0) \\ &= -\frac{1}{\pi} \sum_{j=\lceil \frac{N+1}{2} \rceil}^{\infty} \frac{(j+1/4)\Gamma(j-1/2)\Gamma(j+1/2)}{\Gamma(j+1)\Gamma(j+2)}, \end{aligned} \quad (\text{D.12})$$

where  $\lceil \frac{N+1}{2} \rceil$  is the smallest integer  $\geq \frac{N+1}{2}$ , and we used the known value (cf. [39]):

$$P_{2j}(0) = {}_2F_1\left(-2j, 2j+1; 1; \frac{1}{2}\right) = (-1)^j \frac{\Gamma(j+1/2)}{\sqrt{\pi} j!}.$$

From (A.3), we have

$$\frac{\Gamma(j+1/2)}{\Gamma(j+1)} \leq \frac{\Gamma(j)}{\Gamma(j+1/2)}. \quad (\text{D.13})$$

Thus, using (D.13) and  $\Gamma(z+1) = z\Gamma(z)$ , we obtain

$$\begin{aligned} \frac{(j+1/4)\Gamma(j-1/2)\Gamma(j+1/2)}{\Gamma(j+1)\Gamma(j+2)} &= \frac{j+1/4}{j+1} \frac{\Gamma(j-1/2)}{\Gamma(j+1)} \frac{\Gamma(j+1/2)}{\Gamma(j+1)} \\ &\leq \frac{\Gamma(j-1/2)\Gamma(j)}{\Gamma(j+1/2)\Gamma(j+1)} \\ &= \frac{1}{(j-1/2)j} \leq \frac{1}{(j-1)j} = \frac{1}{j-1} - \frac{1}{j}. \end{aligned}$$

Then

$$\begin{aligned} \sum_{j=\lceil \frac{N+1}{2} \rceil}^{\infty} \frac{(j+1/4)\Gamma(j-1/2)\Gamma(j+1/2)}{\Gamma(j+1)\Gamma(j+2)} &\leq \sum_{j=\lceil \frac{N+1}{2} \rceil}^{\infty} \left( \frac{1}{j-1} - \frac{1}{j} \right) \\ &= \frac{1}{\lceil \frac{N+1}{2} \rceil - 1} \leq \frac{2}{N-1}. \end{aligned}$$

From (D.12) and the above, we get the first result in (3.44).

We now prove the second estimate in (3.44). As  $P_n(\pm 1) = (\pm 1)^n$ , we derive from (D.11) that

$$\begin{aligned} (u - \pi_N^L u)(\pm 1) &= \sum_{j=\lceil \frac{N+1}{2} \rceil}^{\infty} \hat{u}_{2j}^L P_{2j}(\pm 1) \\ &= \sum_{j=\lceil \frac{N+1}{2} \rceil}^{\infty} \frac{(-1)^{j+1}}{\sqrt{\pi}} \frac{(j+1/4)\Gamma(j-1/2)}{\Gamma(j+2)}. \end{aligned} \quad (\text{D.14})$$

Denoting

$$\mathcal{S}_j := \frac{(-1)^{j+1}}{\sqrt{\pi}} \frac{(j+1/4)\Gamma(j-1/2)}{\Gamma(j+2)}, \quad \mathcal{T}_j := \frac{1}{2\sqrt{\pi}} \frac{\Gamma(j-3/2)}{\Gamma(j)},$$

we have

$$\begin{aligned} \mathcal{S}_j + \mathcal{S}_{j+1} &= (-1)^{j+1} \frac{3}{2\sqrt{\pi}} \frac{(j+3/4)\Gamma(j-1/2)}{\Gamma(j+3)} \\ &\leq \frac{3}{2\sqrt{\pi}} \frac{\Gamma(j-1/2)}{\Gamma(j+2)} \\ &\leq \frac{3}{4\sqrt{\pi}} \left( \frac{\Gamma(j-3/2)}{\Gamma(j+1)} + \frac{\Gamma(j-1/2)}{\Gamma(j+2)} \right) \\ &= (\mathcal{T}_j - \mathcal{T}_{j+1}) + (\mathcal{T}_{j+1} - \mathcal{T}_{j+2}), \end{aligned} \quad (\text{D.15})$$

where we noted

$$\frac{\Gamma(j-1/2)}{\Gamma(j+2)} \leq \frac{\Gamma(j-3/2)}{\Gamma(j+1)},$$

and

$$\frac{3}{4\sqrt{\pi}} \frac{\Gamma(j-3/2)}{\Gamma(j+1)} = \frac{1}{2\sqrt{\pi}} \left( j \frac{\Gamma(j-3/2)}{\Gamma(j+1)} - (j-3/2) \frac{\Gamma(j-3/2)}{\Gamma(j+1)} \right) = \mathcal{T}_j - \mathcal{T}_{j+1}.$$

Thus, from (A.3) and (D.14)–(D.15), we obtain

$$\begin{aligned}
 & \left| (u - \pi_N^L u)(\pm 1) \right| \\
 &= \left( |\mathcal{S}_{\lceil \frac{N+1}{2} \rceil} + \mathcal{S}_{\lceil \frac{N+1}{2} \rceil + 1} | \right) + \cdots + \left( |\mathcal{S}_{\lceil \frac{N+1}{2} \rceil + 2i} + \mathcal{S}_{\lceil \frac{N+1}{2} \rceil + 2i + 1} | \right) + \cdots \\
 &\leq \left\{ \left( \mathcal{T}_{\lceil \frac{N+1}{2} \rceil} - \mathcal{T}_{\lceil \frac{N+1}{2} \rceil + 1} \right) + \left( \mathcal{T}_{\lceil \frac{N+1}{2} \rceil + 1} - \mathcal{T}_{\lceil \frac{N+1}{2} \rceil + 2} \right) \right\} + \cdots \\
 &\quad + \left\{ \left( \mathcal{T}_{\lceil \frac{N+1}{2} \rceil + 2i} - \mathcal{T}_{\lceil \frac{N+1}{2} \rceil + 2i + 1} \right) + \left( \mathcal{T}_{\lceil \frac{N+1}{2} \rceil + 2i + 1} - \mathcal{T}_{\lceil \frac{N+1}{2} \rceil + 2i + 2} \right) \right\} + \cdots \\
 &= \sum_{j=\lceil \frac{N+1}{2} \rceil}^{\infty} (\mathcal{T}_j - \mathcal{T}_{j+1}) = \frac{1}{2\sqrt{\pi}} \frac{\Gamma(\lceil \frac{N+1}{2} \rceil - 3/2)}{\Gamma(\lceil \frac{N+1}{2} \rceil)} \leq \frac{1}{2\sqrt{\pi}} \frac{\Gamma(N/2 - 1)}{\Gamma(N/2 + 1/2)}.
 \end{aligned}$$

This ends the proof.

## Appendix E: Proof of Theorem 4.2

We first consider (4.8). From Lemma 3.1, we obtain that for  $\mu + m > -1/2$  and  $n \geq \mu + m + 1$ ,

$$\max_{|x| \leq 1} \left\{ \left| \left( I_{1-}^{\mu+m+1} P_n \right)(x) \right| \right\} \leq \frac{1}{2^{\mu+m+1} \sqrt{\pi}} \frac{\Gamma((n - \mu - m)/2)}{\Gamma((n + \mu + m + 3)/2)},$$

and by Lemma 4.1,

$$\begin{aligned}
 & \frac{2n+1}{2} \left| \left( I_{1-}^{\mu+l+1} P_n \right)(-1) \right| = |\sin(\mu\pi)| \widehat{C}_{n,\mu+l}, \\
 & \widehat{C}_{n,v} := 2^v \Gamma(v+1) \frac{(2n+1)\Gamma(n-v)}{\pi \Gamma(n+v+2)}.
 \end{aligned}$$

Consequently by (4.6)–(4.7),

$$|\hat{u}_n^L| \leq \left\{ \frac{1}{2^{\mu+m+2} \sqrt{\pi}} \frac{(2n+1)\Gamma((n - \mu - m)/2)}{\Gamma((n + \mu + m + 3)/2)} + \sum_{l=0}^m \widehat{C}_{n,\mu+l} \right\} U_-^{(\mu,m)}. \quad (\text{E.16})$$

Following the derivations in (3.33)–(3.34), we can get

$$\sum_{n=N+1}^{\infty} \frac{(2n+1)\Gamma((n - \mu - m)/2)}{\Gamma((n + \mu + m + 3)/2)} \leq \frac{8}{\mu + m - 1/2} \frac{\Gamma((N - \mu - m + 1)/2)}{\Gamma((N + \mu + m)/2)}, \quad (\text{E.17})$$

and

$$\sum_{n=N+1}^{\infty} \widehat{C}_{n,\mu} \leq \frac{2^\mu \Gamma(\mu)}{\pi} \frac{\Gamma(N - \mu + 1)}{\Gamma(N + \mu + 1)}. \quad (\text{E.18})$$

From direct calculation, we find

$$\begin{aligned} \sum_{l=0}^m \frac{\widehat{C}_{n,\mu+l}}{\widehat{C}_{n,\mu}} &= \sum_{l=0}^m \frac{\Gamma(n-\mu-l)}{\Gamma(n-\mu)} \frac{\Gamma(n+\mu+2)}{\Gamma(n+\mu+l+2)} \\ &= 1 + \sum_{l=1}^m \left( \prod_{i=1}^l \frac{1}{(n-\mu-i)(n+\mu+i+1)} \right) \\ &= 1 + \sum_{l=1}^m \left( \frac{1}{2(N+1)} \right)^l < \sum_{l=0}^{\infty} \left( \frac{1}{2(N+1)} \right)^l = \frac{2(N+1)}{2N+1}, \end{aligned} \quad (\text{E.19})$$

where we used the fact: for  $1 \leq i \leq l \leq m$  and  $\mu+m+1 \leq N+1 \leq n$ ,

$$\begin{aligned} (n-\mu-i)(n+\mu+i+1) &\geq (n-\mu-l)(n+\mu+l+1) \\ &\geq (n-\mu-m)(n+\mu+m+1) \\ &\geq (n-N)(n+N+1) \geq 2(N+1). \end{aligned}$$

It follows from (E.18)–(E.19) immediately that

$$\sum_{n=N+1}^{\infty} \left( \sum_{l=0}^m \widehat{C}_{n,\mu+l} \right) = \sum_{n=N+1}^{\infty} \widehat{C}_{n,\mu} \left( \sum_{l=0}^m \frac{\widehat{C}_{n,\mu+l}}{\widehat{C}_{n,\mu}} \right) \leq \frac{2^\mu \Gamma(\mu)}{\pi} \frac{(N+1)\Gamma(N-\mu+1)}{(N+1/2)\Gamma(N+\mu+1)}.$$

which, together with (E.16)–(E.17) and  $|P_n(x)| \leq 1$ , implies (4.8).

We now turn to (4.9). By the orthogonality of Legendre polynomials, we find readily from (E.16) and the Cauchy-Schwarz inequality that

$$\begin{aligned} \|u - \pi_N^L u\|_{L^2(\Omega)}^2 &= \sum_{n=N+1}^{\infty} \frac{2}{2n+1} |\hat{u}_n^L|^2 \\ &\leq \sum_{n=N+1}^{\infty} \left\{ \frac{(2n+1) \Gamma^2((n-\mu-m)/2)}{2^{2(\mu+m+1)} \Gamma^2((n+\mu+m+3)/2)} \right. \\ &\quad \left. + \frac{4\widehat{C}_{n,\mu}^2}{2n+1} \left( \sum_{l=0}^m \frac{\widehat{C}_{n,\mu+l}}{\widehat{C}_{n,\mu}} \right)^2 \right\} \left( U_-^{(\mu,m)} \right)^2. \end{aligned} \quad (\text{E.20})$$

Following the derivations in (3.48)–(3.49) with  $\mu+m$  in place of  $\mu$ , we can obtain

$$\sum_{n=N+1}^{\infty} \frac{(2n+1) \Gamma^2((n-\mu-m)/2)}{\Gamma^2((n+\mu+m+3)/2)} \leq \frac{2^{2\mu+2m+4}}{2\mu+2m+1} \frac{\Gamma(N-\mu-m)}{\Gamma(N+\mu+m+1)}.$$

Like (3.48), we can get

$$\begin{aligned} \frac{(n+1/2)\Gamma^2(n-\mu)}{\Gamma^2(n+\mu+2)} &\leq \frac{2^{4\mu+3}}{4\mu+2} \left\{ \frac{\Gamma(2n-2\mu-1)}{\Gamma(2n+2\mu+1)} - \frac{\Gamma(2n-2\mu)}{\Gamma(2n+2\mu+2)} \right\} \\ &\leq \frac{2^{4\mu+3}}{4\mu+2} \left\{ \frac{\Gamma(2n-2\mu-1)}{\Gamma(2n+2\mu+1)} - \frac{\Gamma(2n-2\mu+1)}{\Gamma(2n+2\mu+3)} \right\}. \end{aligned}$$

Similar to (3.49), we can derive

$$\begin{aligned} \sum_{n=N+1}^{\infty} \frac{2}{2n+1} \widehat{C}_{n,\mu}^2 &= \frac{2^{2\mu+2} \Gamma^2(\mu+1)}{\pi^2} \sum_{n=N+1}^{\infty} \frac{(n+1/2) \Gamma^2(n-\mu)}{\Gamma^2(n+\mu+2)} \\ &\leq \frac{2^{6\mu+5} \Gamma^2(\mu+1)}{\pi^2(4\mu+2)} \frac{\Gamma(2N-2\mu+1)}{\Gamma(2N+2\mu+3)}. \end{aligned}$$

Thus, we can obtain (4.9) from (E.20) and the above.

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## Declarations

**Conflict of interest** The authors declare no competing interests.

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