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# Positivity of convolution quadratures generated by nonconvex sequences

*Positivité des quadratures de convolution générées par des séquences non convexes*

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**Abstract.** The positive definiteness of real quadratic forms of convolution type plays an important role in the stability analysis of time-stepping schemes for nonlocal models. Specifically, when these quadratic forms are generated by convex sequences, their positivity can be verified by applying a classical result due to Zygmund. The primary focus of this work is twofold. We first improve Zygmund's result and extend its validity to sequences that are almost convex. Secondly, we establish a more general inequality applicable to nonconvex sequences. Our results are then applied to demonstrate the positive definiteness of commonly used approximations for fractional integral and differential operators, including the convolution quadrature generated by the BDF2 formula. To conclude, we show that the stability of some simple time-fractional schemes can be obtained in a straightforward way.

**Résumé.** Le caractère défini positif des formes quadratiques réelles de type convolution joue un rôle important dans l'analyse de stabilité des schémas en temps pour les modèles non locaux. Plus précisément, lorsque ces formes quadratiques sont générées par des séquences convexes, leur positivité peut être vérifiée en appliquant un résultat classique dû à Zygmund. L'objectif principal de ce travail est double. Nous améliorons d'abord le résultat de Zygmund et étendons sa validité aux séquences presque convexes. Deuxièmement, nous établissons une inégalité plus générale applicable aux séquences non convexes. Nos résultats sont ensuite appliqués pour démontrer le caractère défini positif des approximations couramment utilisées pour les opérateurs intégraux et différentiels fractionnaires, y compris le quadrature de convolution générée par la formule BDF2. Pour conclure, nous montrons que la stabilité de certains schémas fractionnaires simples peut être obtenue de manière simple.

**Keywords.** Convolution quadrature, positive definiteness, nonconvex sequence, minimal convex sequence.

**Mots-clés.** Quadrature de convolution, définie positive, suite non convexe, suite convexe minimale.

**2020 Mathematics Subject Classification.** 65R20, 65M12.

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**1. Introduction**

Let  $\{\beta_j\}_{j=0}^\infty$  be a sequence of real numbers. The discrete convolution operator

$$q_n(\varphi) = \sum_{j=0}^n \beta_{n-j} \varphi_j$$

for  $\varphi := (\varphi_0, \varphi_1, \dots, \varphi_n) \in \mathbb{R}^{n+1}$ , is positive definite if

$$Q_n(\varphi) := \sum_{k=0}^n \sum_{j=0}^k \beta_{k-j} \varphi_j \varphi_k \geq c_0 \sum_{j=0}^n \varphi_j^2 \tag{1}$$

for some  $c_0 > 0$  and all  $n, \varphi$ . The constant  $c_0$  is optimal if (1) does not hold with any constant greater than  $c_0$ . The operator  $q_n$  is called weakly positive if  $c_0 = 0$ . The positive character of  $Q_n$  is a key ingredient in analyzing the stability and convergence of numerical schemes incorporating quadrature rules for integro-differential equations or time-fractional partial differential equations (see, e.g., [2, 4, 6–8, 10]). In [1], the author presented several conditions on  $\{\beta_j\}$  which ensure the positivity property (1). A sharp result is obtained in the case of completely monotone sequences. The objective of the work is to extend these results to cover nonconvex sequences.

Recall that a sequence  $\{\beta_j\}_{j=0}^\infty$  is said to be convex if  $\Delta\beta_j := \beta_{j-1} - 2\beta_j + \beta_{j+1} \geq 0$  for all  $j \geq 1$ . The sequence is called minimal if it becomes nonconvex when its first term  $\beta_0$  is replaced by any smaller number. In other words, the sequence is minimal if  $\Delta\beta_1 = 0$ . Additionally, we introduce the notion of a nearly convex sequence, defined as a sequence where, for some small integer  $M \geq 1$ , the subsequence  $\{\beta_j\}_{j=M}^\infty$  is convex.

Consider the Fourier transform of  $\{\beta_j\}_{j=0}^\infty$  given by  $\widehat{\beta}(\theta) = \sum_{j=0}^\infty \beta_j e^{ij\theta}$ , and assume that  $\widehat{\beta} \in L^1(0, 2\pi)$ . Then, by means of Parseval’s identity, we have (with  $\varphi_j = 0$  for  $j > n$ )

$$Q_n(\varphi) = \frac{1}{2\pi} \int_0^{2\pi} \widehat{\beta}(\theta) |\widehat{\varphi}(\theta)|^2 d\theta = \frac{1}{2\pi} \int_0^{2\pi} \text{Re} \widehat{\beta}(\theta) |\widehat{\varphi}(\theta)|^2 d\theta, \tag{2}$$

where the last equality holds because  $Q_n$  is real-valued. Thus,  $q_n$  is weakly positive if  $\text{Re} \widehat{\beta}(\theta) := \sum_{j=0}^\infty \beta_j \cos(j\theta)$  is nonnegative on  $(0, 2\pi)$ . To ensure positive definiteness, one needs to show that  $\text{Re} \widehat{\beta}(\theta)$  is bounded below by a positive constant. This task is in general delicate as  $\widehat{\beta}(\theta)$  might not be explicitly known or might be difficult to analyze.

For convex sequences, a sufficient condition that ensures (1) is due to Zygmund [11, Theorem (1.5), p. 183]: if the sequence  $\{\beta_j\}_{j=0}^\infty$  is convex and  $\beta_j \rightarrow 0$ , then

$$\frac{1}{2} \beta_0 + \sum_{j=1}^\infty \beta_j \cos(j\theta) \geq 0 \quad \text{for } 0 < \theta < 2\pi. \tag{3}$$

That is,

$$Q_n(\varphi) \geq \frac{\beta_0}{2} \sum_{j=0}^n \varphi_j^2. \tag{4}$$

A similar inequality was derived in [4], and related results can be found in [1, 6]. We notice that the condition  $\beta_j \rightarrow 0$  can be replaced by  $\{\beta_j\}_{j=0}^\infty$  is nonnegative and bounded (see [8, Lemma 4.3]). In this work, we derive an alternative to (4), which is applicable to nearly convex sequences.

As an illustration, we shall apply our results to the following generating sequences

$$\gamma_j = (-1)^j \binom{-\alpha}{j}, \quad j \geq 0, \tag{5}$$

$$\omega_j = ((j+1)^{1-\alpha} - j^{1-\alpha})/\Gamma(2-\alpha), \quad j \geq 0, \tag{6}$$

$$\rho_0 = \frac{1}{\Gamma(2+\alpha)}, \quad \rho_j = [(j+1)^{1+\alpha} - 2j^{1+\alpha} + (j-1)^{1+\alpha}]/\Gamma(2+\alpha), \quad j \geq 1, \tag{7}$$

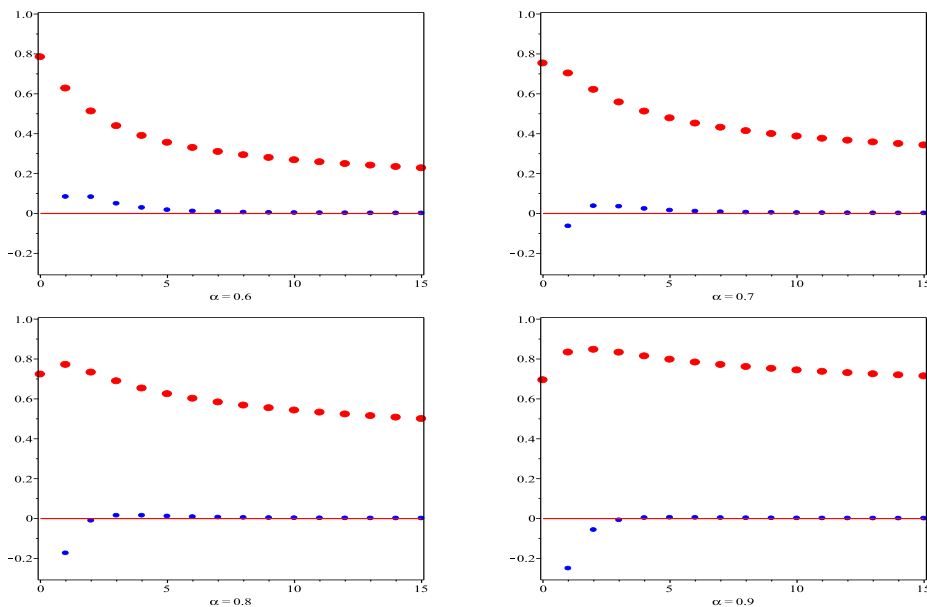
and

$$\xi_j = (-1)^j \left(\frac{2}{3}\right)^\alpha \sum_{l=0}^j 3^{-l} \binom{-\alpha}{j-l} \binom{-\alpha}{l}, \quad j \geq 0, \tag{8}$$

arising from the approximations of fractional integral and differential operators of order  $\alpha \in (0, 1)$ . The terms in (5) and (8) are the weights of convolution quadrature rules generated by Euler and BDF2 methods, respectively, for approximating a Riemann–Liouville fractional integral, see [5, 7]. On the other hand, (6) corresponds to the  $L1$ -method for approximating a Caputo fractional derivative [3]. The sequence (7) results from an integral average formula of a Riemann–Liouville fractional integral [7]. We note that  $\gamma_0 = 1$ ,  $\omega_0 = 1/\Gamma(2 - \alpha)$  and  $\xi_0 = (2/3)^\alpha$ .

While  $\{\gamma_j\}_{j=0}^\infty$  and  $\{\omega_j\}_{j=0}^\infty$  are convex for all  $\alpha$  in  $(0, 1)$ , see e.g., [1], the last two sequences  $\{\rho_j\}_{j=0}^\infty$  and  $\{\xi_j\}_{j=0}^\infty$  are convex only for some range of  $\alpha$  in  $(0, 1)$ . For instance,  $\{\rho_j\}_{j=0}^\infty$  is convex only when  $\alpha \in (0, b_1]$ , where  $b_1 \approx 0.5546$  is the root of the equation  $6 - 2^{3+\alpha} + 3^{1+\alpha} = 0$ . For this case, one can also verify that the subsequence  $\{\rho_j\}_{j=1}^\infty$  is convex for all  $\alpha$  in  $(0, 1)$ . The analysis of the convexity of  $\{\xi_j\}_{j=0}^\infty$  is quite complex. A comprehensive set of tests showed that the sequence is convex whenever  $\Delta\xi_1 \geq 0$ , leading to the conclusion that  $\{\xi_j\}_{j=0}^\infty$  is convex only when  $\alpha \in (0, b_2]$ , where  $b_2 = (19 - \sqrt{73})/16 \approx 0.6534$ . In Figure 1, we show the first few terms  $\xi_j$  and the corresponding terms  $2\Delta\xi_j$  for  $j = 1, \dots, 15$  to check for convexity for different values of  $\alpha$ .

Noting that Zygmund’s inequality (4) does not apply to the sequences  $\{\rho_j\}_{j=0}^\infty$  and  $\{\xi_j\}_{j=0}^\infty$ , one might question the feasibility of deriving a more suitable inequality to cover these cases. The aim of this study is to rigorously establish the positivity of quadratic forms generated by nearly convex sequences, including  $\{\rho_j\}_{j=0}^\infty$  and  $\{\xi_j\}_{j=0}^\infty$ . The results allow to overcome difficulties in analyzing the stability of numerical schemes for solving integro-differential and time-fractional phase-field equations.



**Figure 1.** The terms  $\xi_j$  in (8) for  $j = 0, \dots, 15$  and  $2\Delta\xi_j$  for  $j = 1, \dots, 15$ ;  $\alpha = 0.6, 0.7, 0.8, 0.9$ .

### 2. Nonoptimality of Zygmund's Inequality

Adding a positive constant  $a_0$  to the initial term of a convex sequence  $\{\beta_j\}_{j=0}^\infty$  preserves its convexity. Consequently, if we apply (3) to the new sequence, we notice that the zero lower bound in the resulting inequality can be replaced by  $a_0/2$ , indicating that (4) is not optimal. Based on this observation, we derive in the next theorem an improved lower bound, which is found to be valid for a class of nonconvex sequences.

**Theorem 1.** *Let  $\{\beta_j\}_{j=0}^\infty$  be a sequence such that  $\{\beta_j\}_{j=1}^\infty$  is nonnegative, bounded and convex. Then*

$$\sum_{k=0}^n \sum_{j=0}^k \beta_{k-j} \varphi_j \varphi_k \geq \frac{1}{2} (\beta_0 + \Delta\beta_1) \sum_{j=0}^n \varphi_j^2 \tag{9}$$

for all  $n \geq 0$  and  $\varphi \in \mathbb{R}^{n+1}$ .

**Proof.** Consider the sequence  $\{a_j\}_{j=0}^\infty$  defined by  $a_0 = 2\beta_1 - \beta_2$  and  $a_j = \beta_j$  for  $j \geq 1$ . Clearly  $\{a_j\}_{j=0}^\infty$  is nonnegative, bounded and convex. Hence, by (4),

$$\sum_{k=0}^n \sum_{j=0}^k a_{k-j} \varphi_j \varphi_k \geq \frac{a_0}{2} \sum_{j=0}^n \varphi_j^2 \tag{10}$$

for all  $n \geq 0$  and  $\varphi \in \mathbb{R}^{n+1}$ . Adding  $(\beta_0 - a_0) \sum_{j=0}^n \varphi_j^2$  to both sides of (10) yields

$$\sum_{k=0}^n \sum_{j=0}^k \beta_{k-j} \varphi_j \varphi_k \geq \left( \beta_0 - \beta_1 + \frac{\beta_2}{2} \right) \sum_{j=0}^n \varphi_j^2, \tag{11}$$

which is the desired inequality. □

When  $\{\beta_j\}_{j=0}^\infty$  is convex,  $\Delta\beta_1 \geq 0$ , and therefore (9) is an improvement over Zygmund's inequality (4). The results coincide when  $\Delta\beta_1 = 0$ , i.e., for minimal sequences. We verify that the bound  $\beta_0 + \Delta\beta_1$  is positive if  $\beta_0 > \beta_1 - \beta_2/2$  (or  $\beta_0 > a_0/2$ ), and vanishes when  $\beta_0 = \beta_1 - \beta_2/2$ . It is worth noting that within the range  $\beta_1 - \beta_2/2 < \beta_0 < 2\beta_1 - \beta_2$ , while the convexity property of convexity is violated, the positivity of the corresponding quadratic form is preserved.

In Figure 2, we compare Zygmund's constant ( $C_Z := \beta_0/2$ ), the new in (9), and the optimal constants

$$C_\gamma = \frac{1}{2\alpha} \quad \text{and} \quad C_\omega = \frac{2\text{Li}_{\alpha-1}(-1)}{(-1)\Gamma(2-\alpha)},$$

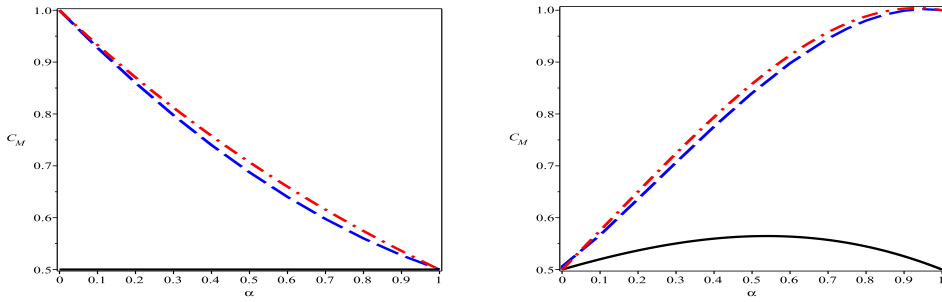
obtained in [1] for the sequences  $\{\gamma_j\}_{j=0}^\infty$  and  $\{\omega_j\}_{j=0}^\infty$ , respectively. Here,  $\text{Li}_m(z) := \sum_{j=1}^\infty \frac{z^j}{j^m}$  represents the polylogarithm function. The Figure shows that the current bound is remarkably close to the optimal bound for all values of  $\alpha$ , particularly as  $\alpha$  approaches 0 and 1. In contrast, there exists a significant disparity between Zygmund's bound and the optimal bound, particularly on one end of the interval.

Theorem 1 yields an immediate result for symmetric Toeplitz matrices, as follows.

**Corollary 2.** *Let  $\{\beta_j\}_{j=0}^\infty$  be a sequence such that  $\{\beta_j\}_{j=1}^\infty$  is nonnegative, bounded and convex. Let  $\rho_N$  denote the spectral radius of the  $N \times N$  symmetric Toeplitz matrix*

$$\begin{bmatrix} \beta_0 & \beta_1 & \beta_2 & \cdots & \beta_{N-1} \\ & \beta_0 & \beta_1 & \cdots & \beta_{N-2} \\ & & \ddots & \ddots & \vdots \\ sym & & & \beta_0 & \beta_1 \\ & & & & \beta_0 \end{bmatrix}.$$

Then,  $\rho_N \geq \Delta\beta_1$  for all  $N \geq 3$ .



**Figure 2.** Comparison of three bounds for  $\{\gamma_j\}_{j=0}^\infty$  (left) and  $\{\omega_j\}_{j=0}^\infty$  (right);  $\alpha \in (0, 1)$ . Zygmund (solid line), current (dashed line) and optimal (dot-dashed line).

The Corollary provides a simple tool for checking the positive definiteness of a symmetric Toeplitz matrix. To illustrate, consider a  $6 \times 6$  symmetric Toeplitz matrix  $A$  whose first row is  $[4 \ 2 \ 1 \ 1 \ 1 \ 1]$ . Clearly,  $A$  is not diagonally dominant, and the Gershgorin circle theorem does not yield useful information about its positive definiteness. Nevertheless, applying Corollary 2 yields  $\rho(A) \geq 1$ . We verify that  $\rho(A) \approx 1.198$ , which confirms the accuracy of the inequality (9) in the present example.

### 3. Nearly convex sequences

Let  $\{\beta_j\}_{j=0}^\infty$  be such that  $\{\beta_j\}_{j=M}^\infty$  is nonnegative, bounded and convex for some  $M \geq 1$ . Let  $f$  be a convex real-valued function defined on the interval  $[0, \infty)$  that interpolates the points  $(j, \beta_j)$ ,  $j \geq M$ . Define the sequence  $\{a_j\}_{j=0}^\infty$  by  $a_j = f(j)$  for  $j \geq 0$ . Since  $\{a_j\}_{j=0}^\infty$  is nonnegative, bounded and convex, Zygmund’s inequality implies  $\operatorname{Re} \widehat{a}(\theta) \geq a_0/2$  for all  $\theta \in (0, 2\pi)$ . Adding  $\sum_{j=0}^{M-1} (\beta_j - a_j) \cos(j\theta)$  to both sides of this inequality yields

$$\operatorname{Re} \widehat{\beta}(\theta) \geq \beta_0 - \frac{a_0}{2} + \min_{\theta} \sum_{j=1}^{M-1} (\beta_j - f(j)) \cos(j\theta). \tag{12}$$

This step simplifies the task of finding a lower bound for  $\operatorname{Re} \widehat{\beta}(\theta)$  as the last term in (12) (involving a finite sum) is more manageable compared to the original infinite series.

The distribution of the first terms of the nonconvex sequences illustrated in Figure 1 has served as our main motivation to study the case where  $\{\beta_j\}_{j=M}^\infty$  is convex for some  $M \geq 1$ . A noteworthy observation is that all the points  $(j, \beta_j)$ ,  $0 < j < M$ , lie below the line passing through the points  $(M, \beta_M)$  and  $(M + 1, \beta_{M+1})$ . We proceed to present our findings in the subsequent theorem.

**Theorem 3.** *Let  $\{\beta_j\}_{j=0}^\infty$  be a sequence such that, for some  $M \geq 1$ , the subsequence  $\{\beta_j\}_{j=M}^\infty$  is nonnegative, bounded and convex. Let  $P(t)$  denote the linear function whose graph interpolates the points  $(M, \beta_M)$  and  $(M + 1, \beta_{M+1})$ . Assume  $\beta_j \leq P(j)$  for  $j = 1, \dots, M - 1$ . then*

$$\sum_{k=0}^n \sum_{j=0}^k \beta_{k-j} \varphi_j \varphi_k \geq C_M \sum_{j=0}^n \varphi_j^2 \tag{13}$$

for all  $n \geq 0$  and  $\varphi \in \mathbb{R}^{n+1}$ , where

$$C_M = \frac{1}{2} \left( \beta_0 + \sum_{j=1}^M j^2 \Delta \beta_j \right). \tag{14}$$

**Proof.** Clearly  $P(t) = (M - t)(\beta_M - \beta_{M+1}) + \beta_M$ . Consider the sequence  $\{a_j\}_{j=0}^\infty$  defined by

$$a_j = P(j) = (M - j)(\beta_M - \beta_{M+1}) + \beta_M, \quad 0 \leq j \leq M - 1, \tag{15}$$

and  $a_j = \beta_j$  for  $j \geq M$ . Then,  $\{a_j\}_{j=0}^\infty$  is nonnegative, bounded and convex. Hence,  $\operatorname{Re} \hat{a}(\theta) \geq a_0/2$  for all  $\theta \in (0, 2\pi)$ , that is,

$$\operatorname{Re} \hat{a}(\theta) \geq \left(\frac{M}{2} + \frac{1}{2}\right)\beta_M - \frac{M}{2}\beta_{M+1}.$$

Referring to (12) and using the fact that  $\beta_j \leq a_j$  for  $j = 1, \dots, M - 1$ , we deduce

$$\operatorname{Re} \hat{\beta}(\theta) \geq \sum_{j=0}^{M-1} \beta_j - \sum_{j=0}^{M-1} a_j + \left(\frac{M}{2} + \frac{1}{2}\right)\beta_M - \frac{M}{2}\beta_{M+1}.$$

Using (15), we readily obtain

$$\sum_{j=0}^{M-1} a_j = \left(\frac{M^2}{2} + \frac{3M}{2}\right)\beta_M - \left(\frac{M^2}{2} + \frac{M}{2}\right)\beta_{M+1},$$

and as a result

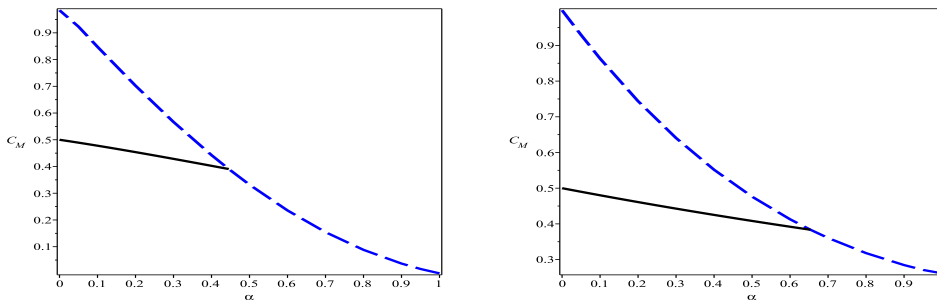
$$C_M = \sum_{j=0}^{M-1} \beta_j - \left(\frac{M^2}{2} + M - \frac{1}{2}\right)\beta_M + \frac{M^2}{2}\beta_{M+1}. \tag{16}$$

Now we show that the right hand side of (16) coincides with that of (14). Indeed, we have  $C_1 = \frac{1}{2}(\beta_0 + \Delta\beta_1)$  and we verify that

$$C_M - C_{M-1} = \frac{1}{2}M^2\Delta\beta_M, \quad M \geq 2,$$

which completes the proof. □

A comparison between the bound derived in Theorem 3 and one by Zygmund is presented in Figure 3, for  $\{\rho_j\}_{j=0}^\infty$  and  $\{\xi_j\}_{j=0}^\infty$ . Note that Zygmund's bound is only applicable for convex sequences. Further details on the convexity of  $\{\xi_j\}_{j=0}^\infty$  and the integer  $M$  are given in Table 3.



**Figure 3.** Comparison of two bounds for  $\{\rho_j\}_{j=0}^\infty$  (left) and  $\{\xi_j\}_{j=0}^\infty$  (right);  $\alpha \in (0, 1)$ . Zygmund (solid line) and  $C_M$  in (14) (dashed line).

**Table 1.** Comparison of  $C_M$  in (14) with Zygmund's constant  $C_Z$  for  $\{\xi_j\}_{j=0}^\infty$ .

| $\alpha$        | 0.4   | 0.5   | 0.6   | 0.7   | 0.8   | 0.9   | 0.95  |
|-----------------|-------|-------|-------|-------|-------|-------|-------|
| $M$             | 0     | 0     | 0     | 1     | 2     | 3     | 4     |
| $C_Z = \xi_0/2$ | 0.425 | 0.408 | 0.392 | –     | –     | –     | –     |
| $C_M$ in (14)   | 0.552 | 0.476 | 0.413 | 0.361 | 0.308 | 0.210 | 0.138 |

#### 4. Numerical Riemann–Liouville integral

We now apply our results to investigate the stability of an implicit numerical scheme for a time-fractional equation involving a fractional Riemann–Liouville integral. Recall the definition of the Riemann–Liouville integral operator with order  $\alpha > 0$  ( $0 < \alpha < 1$ ), (see, e.g., [9])

$$\mathcal{I}_t^\alpha \varphi(t) = (\omega_\alpha * \varphi)(t) = \int_0^t \omega_\alpha(t-s)\varphi(s) ds,$$

where  $\omega_\alpha(t) = t^{\alpha-1}/\Gamma(\alpha)$  and  $\Gamma(\cdot)$  is the usual Gamma function. In the following,  $\Omega \subset \mathbb{R}^d$  ( $d = 1, 2, 3$ ) is a bounded domain with a boundary  $\partial\Omega$ . We denote by  $(\cdot, \cdot)$  the usual  $L^2(\Omega)$  inner product with induced norm  $\|\cdot\|$ . For a fixed time  $T > 0$ , we divide the time interval  $[0, T]$  into a partition  $0 = t_0 < t_1 < \dots < t_N = T$  with a uniform time step  $\tau = T/N$ .

As an example, we consider the (modified) time-fractional diffusion-wave model equation

$$\partial_t \phi + \mathcal{I}_t^\gamma \phi - \kappa \mathcal{I}_t^\alpha \Delta \phi = g(x, t), \quad (x, t) \in \Omega \times (0, T], \quad \phi(x, 0) = \phi^0(x), \tag{17}$$

where  $\gamma \in (0, 1)$ ,  $\kappa > 0$  is a constant and  $g \in L^1(0, T; L^2(\Omega))$ . We assume that  $\phi(\cdot, t)$  satisfies a homogeneous Dirichlet boundary condition. We consider the implicit backward time-stepping scheme

$$\partial_\tau \phi^n + \mathcal{I}_\tau^\gamma \phi^n - \kappa \mathcal{I}_\tau^\alpha \Delta \phi^n = g^n, \quad n \geq 1, \tag{18}$$

where  $g^n = g(\cdot, t_n)$ ,  $\partial_\tau \phi^n = (\phi^n - \phi^{n-1})/\tau$ , and  $\mathcal{I}_\tau^\alpha \phi^n$  is an appropriate approximation of  $\mathcal{I}_t^\alpha \phi(t_n)$  of the form

$$\mathcal{I}_\tau^\alpha \phi^n = \tau^\alpha \sum_{j=0}^n \beta_{n-j} \phi^j,$$

with the property that the weights  $\beta_j$  satisfy (1). Taking the inner product of both sides of (18) with  $\phi^n$ , and using Green's formula, we get

$$(\partial_\tau \phi^n, \phi^n) + (\mathcal{I}_\tau^\gamma \phi^n, \phi^n) + (\kappa \mathcal{I}_\tau^\alpha \nabla \phi^n, \nabla \phi^n) = (g^n, \phi^n), \quad n \geq 1.$$

Summing over  $n$  and applying property (1), we easily obtain the following stability result

$$\|\phi^n\| \leq \|\phi^0\| + 2\tau \sum_{k=1}^n \|g^k\|.$$

#### Declaration of interests

The authors do not work for, advise, own shares in, or receive funds from any organization that could benefit from this article, and have declared no affiliations other than their research organizations.

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