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Uniform relations between the Gauss–Legendre nodes and weights

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Abstract

Four different relations between the Legendre nodes and weights are presented which, unlike the circle and trapezoid theorems for Gauss–Legendre quadrature, hold uniformly in the whole interval $(-1, 1)$. These properties are supported by strong asymptotic evidence. The study of these results was originally motivated by the role some of them play in certain finite difference schemes used in the discretization of the angular Fokker–Planck diffusion operator.

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1 Introduction

Given a quadrature rule $Q(f)$ for approximating an integral $I(f)$ in the interval $[-1, 1]$,

$$I(f) = \int_{-1}^1 f(x)dx \approx Q(f) = \sum_{i=1}^n w_i f(x_i),$$

the formula is said to be of Gauss–Legendre type if it has the maximum possible degree of exactness, that is, if $I(f) = Q(f)$ for f any polynomial of degree less than $2n$. Gauss–Legendre quadrature is a particular case of a more general set of quadrature rules, known as Gauss quadratures, and it is the most widely used of them. The fact that this rule has maximum degree of exactness implies that it is rapidly convergent as the number of nodes increases, in particular for integrating analytic functions.

Gauss–Legendre nodes (x_i) and weights (w_i) are important quantities appearing in numerous applications, as they are not only relevant in numerical integration but also in the approximation by barycentric interpolation at the Legendre nodes (see, for instance, the applications mentioned in [1] and [7]) and in spectral methods. In the present paper, the study of the uniform relations between the Legendre nodes and weights has been motivated by the role these (so far unproven) relations play in certain finite difference schemes used in the field of nuclear engineering, specifically for discretizing the angular Fokker–Planck diffusion operator (see [9, 12, 13]). In this paper we provide strong asymptotic evidence for such uniform results.

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In [2], some asymptotic relations between the nodes and weights of Gauss quadratures were explored, which hold for all the nodes in any fixed compact subinterval of $(-1, 1)$; see also [5] for a more recent account of this type of results. The fact that these results hold in fixed compact intervals is relevant as this means that such results may not be valid close to the endpoints of the interval of orthogonality. In particular, for the Gauss–Legendre quadrature the nodes are known to cluster at the ends of the interval $(-1, 1)$ as the degree tends to infinity, and as a consequence those results can fail (and in fact do fail) for the extreme nodes, as explained in Sect. 3.

In this paper we present four cases of asymptotic relations between nodes and weights of Gauss–Legendre quadrature which hold uniformly for all the nodes in the interval of orthogonality and they do so with a nearly constant error term (tending to zero as the degree increases). Similar relations may exist for more general quadratures, and they will be explored in a future paper.

The paper is organized as follows. In Sect. 2 we summarize known asymptotic results for the Legendre nodes and weights, both considering expansions in terms of elementary functions and in terms of Bessel functions. In Sect. 3 the circle and trapezoid theorems, first presented in [2], are revisited, and it is discussed how these relations fail for the extreme nodes and how a uniform version of the circle theorem (which holds for all the nodes) can be easily obtained. Uniform relations involving sums of weights are described in Sect. 4, which can be understood as a uniform counterpart of the trapezoid theorems; three uniform relations are described in this section. Finally, Sect. 5 describes the connection of these uniform relations with some finite difference schemes, in particular for discretizing the angular Fokker–Planck diffusion operator; the uniform relations discussed in this paper provide alternative sets of nodes to Legendre nodes which may be useful in other numerical contexts.

2 Some preliminary asymptotic results

We briefly recall some asymptotic estimates for the nodes and weights of Gauss–Legendre quadrature. We consider two types of estimations: elementary asymptotic expansions for large degree, valid in compact subintervals inside the interval of orthogonality $(-1, 1)$, and uniform expansions in terms of Bessel functions. Details on these expansions are described in [7]. In particular, we use the compound Poincaré-type expansions of [7, Sect. 2.2], valid in compact subintervals of $(-1, 1)$, and the Bessel-type expansion of [3], with additional information on the coefficients given in [7, Sect. 3]. Details on the computation of these expansions, particularly for the weights, are given in the Appendices A and B. As an alternative method for computing these asymptotic expansions for the nodes and weights we mention the reference [16] which uses a Riemann–Hilbert approach. We only compute the terms we need to prove our results; additional terms are computed in [16] by using a symbolic computation package and, as expected, our expansions coincide with the first terms in [16]. It is not the goal of the present paper to rederive asymptotic expansions for the nodes and weights, but to prove new uniform relations between them which are uniformly valid in $(-1, 1)$.

2.1 Elementary expansions

The circle and trapezoid theorems of [2] can be obtained using elementary asymptotic estimates as $n \rightarrow +\infty$ of the nodes and weights. We recall these results, and give some additional detail by not only considering the dominant term.

Instead of using as asymptotic parameter n , it is more convenient, as done in [7], to use $\kappa = n + 1/2$. Starting with the nodes, we write $x_i = \cos \theta_i$, $i = 1, \dots, n$, with

$$\theta_i = \alpha_i + \delta_i, \quad \alpha_i = \frac{\kappa + \frac{1}{4} - i}{\kappa} \pi, \quad \delta_i \sim \frac{c_1}{\kappa^2} + \frac{c_2}{\kappa^4} + \dots \quad (1)$$

Details on the coefficients c_i are given in [7, Sect. 2.2.2].

For our purpose, we only need the first term in the expansion of δ_i . We have

$$\delta_i = \frac{\cot \alpha_i}{8\kappa^2} + \mathcal{O}(\kappa^{-4}), \quad (2)$$

which coincides with the expansion in [4].

We notice that for the nodes close to the endpoints of the interval of orthogonality i is small or close to n , which means that $c_1 = \mathcal{O}(\kappa)$ because $\cot \alpha_i = \mathcal{O}(\kappa)$; similarly, $c_2 = \mathcal{O}(\kappa^3)$, and so on (see [7, Eq. (2.28)]). This indicates that the expansion for δ_i is not a valid asymptotic representation for such nodes.

Assuming now that we are not considering extreme nodes, we use (2) and get

$$x_i = \cos(\alpha_i + \delta_i) = \cos \alpha_i - \delta_i \sin \alpha_i + \mathcal{O}(\kappa^{-4}) = F(\kappa) \cos \alpha_i + \mathcal{O}(\kappa^{-4}), \quad (3)$$

where

$$F(\kappa) = 1 - \frac{1}{8\kappa^2}. \quad (4)$$

For obtaining the corresponding expansion for the weights, we must substitute the expansion for the nodes in the expression for the weights in terms of the derivative of the Legendre polynomial, using the expansion for large order of the polynomial and reexpanding the result (see Appendix A). We get the following expression for the first terms:

$$w_i = \frac{\pi}{\kappa} F(\kappa) \sin \alpha_i + \mathcal{O}(\kappa^{-5}). \quad (5)$$

2.2 Bessel-type expansions

As an alternative to the previous elementary expansions, we can consider the expansions of [3] for Jacobi polynomials and their zeros, and use the corresponding expansion for the derivative in order to compute the weights [7]. These expansions are not so easy to handle as the elementary expansions because they are given in terms of Bessel functions but they have the advantage that they are valid for all the Legendre nodes, also for those closest to ± 1 .

Particularizing the result for Jacobi polynomials of [3] to the Legendre case, the nodes are given by $x_i = \cos \theta_i$ with

$$\theta_i = \beta_i + \delta_i, \quad \beta_i = \frac{j_{n-i+1}}{\kappa}, \quad \delta_i = -\frac{1}{8\kappa^2} \frac{1 - \beta_i \cot \beta_i}{\beta_i} + \beta_i^2 \mathcal{O}(\kappa^{-3}),$$

where j_k is the k th positive zero of the Bessel function $J_0(x)$. This gives

$$x_{n-i} = F(\kappa) \cos \beta_{n-i} + \frac{1}{8\kappa^2} \frac{\sin \beta_{n-i}}{\beta_{n-i}} + \sin \beta_{n-i} \beta_{n-i}^2 \mathcal{O}(\kappa^{-3}) + \mathcal{O}(\kappa^{-4}).$$

Now, in the limit $\kappa \rightarrow +\infty$ for finite i , we have $\beta_{n-i} = j_{i+1}/\kappa = \mathcal{O}(\kappa^{-1})$ (notice that, as $i \rightarrow +\infty$, $j_{i+1} \sim i\pi$), and expanding in powers of β_i ,

$$x_{n-i} = 1 - \frac{\beta_{n-i}^2}{2} + \mathcal{O}(\kappa^{-4}) = 1 - \frac{j_{i+1}^2}{2\kappa^2} + \mathcal{O}(\kappa^{-4}). \quad (6)$$

Of course, the latter approximation cannot be accurate for the nodes close to 0. For example, for the smallest nodes $i \sim n/2$, and for such nodes and large n , $j_{n-i+1} \sim j_{n/2} \sim n\pi/2$ (see [15, Eq. 10.21.19]), and so $\beta_i \sim \pi/2 + \mathcal{O}(n^{-1})$ (corresponding to nodes close to zero); then the approximation (6) is inaccurate for such nodes. This approximation can only be used for $i \ll n$.

For the weights, we must substitute the expansion for the nodes in the expression for the weights in terms of the derivative of Legendre polynomials, using the Bessel-type expansion for this derivative, and reexpand again in inverse powers of κ (see Appendix B). We get

$$w_{n-i} = \frac{2}{\kappa^2 J_1(j_{i+1})^2} \left(1 - \frac{1}{12\kappa^2} - \frac{j_{i+1}^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4}) \right). \quad (7)$$

Similarly as commented after Eq. (6), the latter approximation is accurate for $i \ll n$.

3 The circle and trapezoid theorems

Next, we recall the results of [2] for the case of Gauss–Legendre quadrature, but giving one additional term in the expansions.

Theorem 1 *Let $[a, b] \subset (-1, 1)$, then*

1. $\frac{\kappa w_i}{\pi \sqrt{1-x_i^2}} = 1 - \frac{1}{8 \sin^2 \alpha_i \kappa^2} + \mathcal{O}(\kappa^{-4})$ for any i such that $x_i \in [a, b]$;
2. $\frac{2(x_{i+1} - x_i)}{w_{i+1} + w_i} = 1 + \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4})$ for any i such that $x_i, x_{i+1} \in [a, b]$;
3. $\frac{x_{i+1} - x_{i-1}}{2w_i} = 1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4})$ for any i such that $x_{i-1}, x_{i+1} \in [a, b]$.

Proof These relations follow from (3) and (5).

1. With $x_i = \cos \theta_i$, this is the same as proving that

$$\frac{\pi \sin \theta_i}{\kappa w_i} = 1 + \frac{1}{8 \sin^2 \alpha_i \kappa^2} + \mathcal{O}(\kappa^{-4}),$$

which follows from (5) and the fact that

$$\sin \theta_i = \sin(\alpha_i + \delta_i) = \sin(\alpha_i) + \delta_i \cos \alpha_i + \mathcal{O}(\kappa^{-4}),$$

which, using (2), gives

$$\sin \theta_i = F(\kappa) \sin \alpha_i + \frac{1}{8 \sin \alpha_i \kappa^2} + \mathcal{O}(\kappa^{-4}).$$

With this and Eq. (5), the result is proved.

2. The expansion (3) and some elementary trigonometry gives

$$\begin{aligned}x_{i+1} - x_i &= F(\kappa) (\cos \alpha_{i+1} - \cos \alpha_i) + \mathcal{O}(\kappa^{-4}) \\&= 2F(\kappa) \sin\left(\frac{\alpha_i - \alpha_{i+1}}{2}\right) \sin\left(\frac{\alpha_i + \alpha_{i+1}}{2}\right) + \mathcal{O}(\kappa^{-4}) \\&= 2F(\kappa) \sin\left(\frac{i + 1/4}{\kappa}\pi\right) \sin\left(\frac{\pi}{2\kappa}\right) + \mathcal{O}(\kappa^{-4})\end{aligned}$$

and similarly, using (5),

$$\frac{w_i + w_{i+1}}{2} = \frac{\pi}{\kappa} F(\kappa) \sin\left(\frac{i + 1/4}{\kappa}\pi\right) \cos\left(\frac{\pi}{2\kappa}\right) + \mathcal{O}(\kappa^{-5}).$$

Then

$$\frac{2(x_{i+1} - x_i)}{w_{i+1} + w_i} = \frac{2\kappa}{\pi} \tan\left(\frac{\pi}{2\kappa}\right) + \mathcal{O}(\kappa^{-4}),$$

and the first two terms in the expansion as $\kappa \rightarrow +\infty$ prove the result.

3. First, we have, using (3),

$$\begin{aligned}\frac{x_{i+1} - x_{i-1}}{2} &= F(\kappa) \sin\left(\frac{\alpha_{i-1} - \alpha_{i+1}}{2}\right) \sin\left(\frac{\alpha_{i-1} + \alpha_{i+1}}{2}\right) + \mathcal{O}(\kappa^{-4}) \\&= F(\kappa) \sin\left(\frac{\pi}{\kappa}\right) \sin \alpha_i + \mathcal{O}(\kappa^{-4}).\end{aligned}$$

Then, because $w_i = \frac{\pi}{\kappa} F(\kappa) \sin \alpha_i + \mathcal{O}(\kappa^{-5})$, we get

$$\frac{x_{i+1} - x_{i-1}}{2w_i} = \frac{\kappa}{\pi} \sin\left(\frac{\pi}{\kappa}\right) + \mathcal{O}(\kappa^{-4}),$$

and the first two terms in the expansion of the sine function give the result. \square

The first result in the previous theorem is related to the circle theorem, which states that $\frac{1}{\pi} n w_i \sim \sqrt{1 - x_i^2}$ as $n \rightarrow +\infty$, that is,

$$\lim_{n \rightarrow +\infty} \frac{n w_i}{\pi \sqrt{1 - x_i^2}} = 1$$

for any i such that x_i is inside a fixed compact subinterval of $(-1, 1)$. We see that the condition that it holds inside a compact given subinterval is important. Indeed, the extreme nodes tend to ± 1 as $n \rightarrow +\infty$, and for those the result does not hold. We observe that in the previous theorem we have

$$\frac{\kappa w_i}{\pi \sqrt{1 - x_i^2}} = 1 - \frac{1}{8 \sin^2 \alpha_i \kappa^2} + \mathcal{O}(\kappa^{-4})$$

and for $i = n$ (largest node) the second term on the right-hand side does not tend to zero because $\sin \alpha = \mathcal{O}(\kappa^{-1})$. This indicates that the elementary expansion fails for such a zero, and suggests that the circle theorem does not hold for the largest node; the same would

be true for the second largest zero, and for a finite number of zeros close to the endpoints of the interval of orthogonality. For the rest of properties in the theorem, the failure is not so evident, but the next terms in the expansions (not shown) do display such problems. These results are neither valid for the extreme zeros, although the deviation is smaller in that cases.

To see more explicitly how these results fail, we can use the asymptotics in terms of Bessel functions. For the circle theorem, we have

$$\frac{\kappa w_{n-i}}{\pi \sqrt{1 - x_{n-i}^2}} = \frac{\kappa w_{n-i}}{\pi \sin \beta_{n-i}(1 + \mathcal{O}(\kappa^{-2}))} \sim \frac{2}{\pi j_{i+1} J_1(j_{i+1})^2} < 1. \quad (8)$$

That this quantity is smaller than 1, therefore violating the circle theorem, is easy to prove (see Appendix C). Defining

$$a_i = 1 - \frac{2}{\pi j_{i+1} J_1(j_{i+1})^2}, \quad (9)$$

one has that this is a positive and decreasing sequence (Appendix C), and the circle theorem is violated maximally at the largest node, where $a_0 = 0.0177079 \dots$, while for the next node we have $a_1 = 0.0039098 \dots$

With respect to the second result of the theorem, and considering the approximations (6) and (7), we have that

$$\frac{w_{n-i} + w_{n-i-1}}{2(x_{n-i} - x_{n-i-1})} \sim \frac{2}{j_{i+2}^2 - j_{i+1}^2} \left(\frac{1}{J_1(j_{i+2})^2} + \frac{1}{J_1(j_{i+1})^2} \right) \equiv b_i + 1.$$

We have checked numerically that the values b_i constitute a positive decreasing sequence and the second result of the previous theorem is violated maximally at the largest zero, where $b_0 = 0.0002756 \dots$. Finally, for the third result we have

$$\frac{x_{n-i+1} - x_{n-i-1}}{2w_{n-i}} \sim \frac{1}{8} J_i(j_{i+1})^2 (j_{i+2}^2 - j_i^2) \equiv c_i + 1$$

and the values c_i constitute a positive decreasing sequence, as checked numerically. The third result of the previous theorem is violated maximally at the largest zero, where $c_0 = 0.00010624 \dots$

The third result is heuristically related to the trapezoidal rule in [2]. Both the second and third results of the previous theorem are mentioned as trapezoid theorems in [2].

3.1 A first uniform relation: the uniform circle theorem for Gauss–Legendre quadrature

It turns out that it is quite easy to find a uniform version of the circle theorem. We enunciate this result, although we must recognize that the proof is not complete in the sense we will discuss next.

Conjecture 1 (Uniform circle theorem) *The points $(x_i, y_i) \equiv (x_i, \kappa w_i / \pi)$, $i = 1, \dots, n$, where x_i and w_i are respectively the nodes and weights of the n -points Gauss–Legendre quadra-*

ture, lie asymptotically on the unit circle. Furthermore,

$$0 < 1 - (x_i^2 + y_i^2) < \frac{1}{4\kappa^2}, \quad i = 1, \dots, n.$$

The asymptotic evidence supporting this result is strong, as we see next. To begin with, the first part of the theorem is trivially true for the nodes in any fixed compact subinterval of $(-1, 1)$. Considering (3) and (5), we have that

$$x_i^2 + y_i^2 = F(\kappa)^2 + \mathcal{O}(\kappa^{-4}) = 1 - \frac{1}{4\kappa^2} + \mathcal{O}(\kappa^{-4}),$$

and therefore the points (x_i, y_i) lie asymptotically on the unit circle. That the same holds for the nodes close to $+1$ (or -1) can be checked by using (6) and (7), which gives

$$x_{n-i}^2 + y_{n-i}^2 = 1 - \frac{k_i}{\kappa^2} + \mathcal{O}(\kappa^{-4}), \quad k_i = j_{i+1}^2 \left(1 - \frac{4}{\pi^2 j_{i+1}^2 J_1(j_{i+1})^4} \right). \quad (10)$$

The constant k_i is positive as a consequence of the properties of a_i that are shown in Appendix C; in addition, it appears that k_i is monotonically increasing as a function of i , which we have not proven so far, and it is easy to check that

$$\lim_{i \rightarrow +\infty} k_i = \frac{1}{4} \quad (11)$$

using the asymptotic expansion for Bessel functions of large argument [15, 10.17.3], together with the McMahon expansion of the zeros j_{i+1} for large i [15, 10.21.19]. An even more direct way to check this is by using the direct expansion given in [1, Eq. (4.1)] for $J_1(j_k)^2$ for large k (precisely obtained by combining the aforementioned expansions), together with the McMahon expansion for the zeros. Substituting both expansions in the definition of k_i of Eq. (10) and reexpanding, we get

$$k_i = \frac{1}{4} - \frac{7}{16\mu_i^2} + \mathcal{O}(\mu_i^{-4}),$$

where $\mu_i = \pi(i + 3/4)$. This proves the limit (11) and suggests (but does not prove) that the sequence is increasing.

The (so far unproven) monotonicity of k_i , together with (11), implies the inequalities stated in the previous conjecture. This is a conjecture not only because we have not proved the monotonicity of the sequence $\{k_i\}$ but also because we have a separate proof for the nodes inside any fixed compact subinterval of $(-1, 1)$ and for the extreme nodes. One would need to make a unified analysis for all the nodes in order to arrive to a rigorous proof, using only the Bessel-type expansion and without the type of reexpansion considered in (6), so that the asymptotics hold for all the nodes and weights. Notice that, even with the reexpansion, we need to assume some conjectured properties of Bessel functions for which there is no proof so far (although we have managed to prove one of them, as we will see). This complete and fully rigorous analysis is appealing and highly challenging, but outside the scope of the present work.

Similar discussions can be considered for other conjectures we will present later. In all these cases, apart from the strong asymptotic evidence presented, the conjectures have

been numerically validated to high accuracy with an arbitrary precision implementation of the algorithm for Gauss–Gegenbauer quadrature of [8].

We can rewrite the inequalities in Conjecture 1 as follows

Corollary 1 *The nodes x_i and weights w_i of Gauss–Legendre quadrature satisfy*

$$\sqrt{1 - \frac{1}{4\kappa^2(1-x_i^2)}} < \frac{y_i}{\sqrt{1-x_i^2}} < 1, \quad i = 1, \dots, n.$$

This corollary shows, again, that the “classical” circle theorem does not hold for the extreme nodes because for such nodes $1 - x_i^2 = \mathcal{O}(\kappa^{-2})$.

4 Uniform relations involving sums of weights

The results we will next describe were originally motivated by the role they play in certain finite difference schemes used in the discretization of the angular Fokker–Planck diffusion operator (see Sect. 5). As we will see, the proof of these results relies in part in the trapezoid theorems and therefore can be interpreted as a uniform counterpart of those results.

We start this section by considering a set of definitions and notations.

Given the Legendre nodes $\{x_i\}_{i=1}^n$, we define the intermediate nodes $\{\bar{x}_i\}_{i=1}^{n-1}$ by

$$\bar{x}_i = \frac{x_i + x_{i+1}}{2}.$$

We observe that

$$\bar{x}_{i+1} = \bar{x}_i + \frac{x_{i+2} - x_i}{2}. \quad (12)$$

We will call these primary intermediate nodes in order to distinguish them from the secondary intermediate nodes $\{\bar{z}_i\}$ that we define as follows:

$$\bar{z}_0 = -1, \quad \bar{z}_i = \bar{z}_{i-1} + w_i, \quad i = 1, \dots, n,$$

that is,

$$\bar{z}_i = -1 + \sum_{j=1}^i w_j = 1 - \sum_{j=i+1}^n w_j, \quad (13)$$

where we have used that $\sum_{i=1}^n w_i = 2$ in the last equality. Notice that $\bar{z}_n = 1$.

Additionally, we define the secondary nodes

$$z_i = \frac{\bar{z}_{i-1} + \bar{z}_i}{2}, \quad i = 1, \dots, n,$$

that is,

$$z_i = 1 - \sum_{j=i+1}^n w_j - \frac{1}{2}w_i = -1 + \sum_{j=1}^{i-1} w_j + \frac{1}{2}w_i. \quad (14)$$

We observe that

$$z_{i+1} = z_i + \frac{w_i + w_{i+1}}{2}. \quad (15)$$

Remark 1 If $n = 2k$, $k \in \mathbb{N}$, $\bar{z}_k = 0$, $\bar{z}_{k+1} = w_{k+1}$ and then $z_{k+1} = \frac{1}{2}w_{k+1}$ is the smallest positive secondary node. On the other hand, if $n = 2k + 1$, $k \in \mathbb{N}$, then $z_{k+1} = 0$ and the smallest positive secondary node is $z_{k+2} = \frac{1}{2}(w_{k+1} + w_{k+2})$.

Of course, both the intermediate and secondary nodes are symmetrical with respect to $x = 0$.

Summarizing, we have defined the following sets of nodes: the (*primary*) *Legendre nodes* $\{x_i\}_{i=1}^n$, the *secondary nodes* $\{z_i\}_{i=1}^n$, the *primary intermediate nodes* $\{\bar{x}_i\}_{i=1}^{n-1}$ (which are trivially interlaced with the primary nodes), and the *secondary intermediate nodes* $\{\bar{z}_i\}_{i=0}^n$, which we will prove that are also interlaced with the primary nodes (and are trivially interlaced with the secondary nodes). We will prove that the secondary nodes $\{z_i\}_{i=1}^n$ approach asymptotically the primary nodes, with a very uniform error term which is $\mathcal{O}(\kappa^{-2})$, and that the same will be true with respect to the primary and secondary intermediate nodes $\{\bar{x}_i\}_{i=1}^{n-1}$ and $\{\bar{z}_i\}_{i=0}^n$.

4.1 Relation between the primary and the secondary nodes

That the secondary nodes approximate the primary nodes x_i as $n \rightarrow +\infty$ is one of the three uniform relations we will discuss in this section. We start by proving this fact for the smallest positive nodes (we do not need to consider negative nodes for obvious reasons).

Lemma 1 *Let x_i be the smallest positive node, then*

$$\frac{x_i}{z_i} = 1 + \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4}).$$

Proof If $n = 2k$, x_{k+1} is the smallest positive node and $x_k = -x_{k+1}$, $w_{k+1} = w_k$. In addition, as discussed in Remark 1, $z_{k+1} = \frac{1}{2}w_{k+1}$. Then

$$\frac{x_{k+1}}{z_{k+1}} = \frac{2x_{k+1}}{w_{k+1}} = \frac{x_{k+1} - x_k}{w_{k+1}} = 2 \frac{x_{k+1} - x_k}{w_{k+1} + w_k},$$

and considering the second result of Theorem 1 completes the proof for even n .

For $n = 2k + 1$, as discussed in Remark 1, $x_{k+1} = z_{k+1} = 0$, and the smallest positive node is x_{k+2} . Now, using (15),

$$z_{k+2} = z_{k+1} + \frac{w_{k+2} + w_{k+1}}{2} = \frac{w_{k+2} + w_{k+1}}{2},$$

then

$$\frac{x_{k+2}}{z_{k+2}} = 2 \frac{x_{k+2} - x_{k+1}}{w_{k+2} + w_{k+1}},$$

and again the second result of Theorem 1 completes the proof. \square

Lemma 2 *If, as $\kappa \rightarrow +\infty$,*

$$\frac{x_j}{z_j} = 1 + \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4})$$

for $j = m$ then the same holds for $j = m \pm 1$, provided all the nodes are inside a fixed compact subset of $(-1, 1)$.

Proof We assume that $\frac{x_m}{z_m} = 1 + \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4})$, consider the relation (15) and then use the second result of Theorem 1 to get

$$\begin{aligned} z_{m+1} &= z_m + \frac{w_m + w_{m+1}}{2} \\ &= x_m \left(1 - \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4}) \right) + (x_{m+1} - x_m) \left(1 - \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4}) \right) \\ &= x_{m+1} \left(1 - \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4}) \right). \end{aligned}$$

This proves the result for $j = m + 1$. That the same holds for $j = m - 1$ is obvious. \square

Remark 2 If n is odd $x_j = z_j = 0$ for $j = (n + 1)/2$ and for this reason one should exclude the trivial case $x_j = 0$ in the previous lemma. The same will be true for the rest of results involving ratios: when the denominator is zero, the numerator is also zero. Instead of singling out this case for each of these results, we will assume that such case is excluded.

Corollary 2 *Let $[a, b] \subset (-1, 1)$ and $x_k, z_k \in [a, b]$, then*

$$\frac{x_k}{z_k} = 1 + \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-3})$$

as $\kappa \rightarrow +\infty$.

The error term in the previous corollary is n times $\mathcal{O}(\kappa^{-4})$, which gives $\mathcal{O}(\kappa^{-3})$. However, it appears that it is in fact $\mathcal{O}(\kappa^{-4})$, as the Bessel-type expansions will indicate.

Corollary 2, similarly to Theorem 1, holds for nodes in a compact interval inside $(-1, 1)$. However, we can check that the quantities $x_i/z_i - 1$ are in fact $\mathcal{O}(\kappa^{-2})$ for all the nodes in $(-1, 1)$ and, as the next results suggest, with an asymptotic constant not larger than $\pi^2/12$. For this purpose, we use the Bessel-type expansions of Sect. 2.2.

We consider the first equality in (14) together with the expansions (6) and (7). We have

$$\frac{x_{n-i}}{z_{n-i}} - 1 = \frac{1}{\kappa^2} C_i + \mathcal{O}(\kappa^{-4}),$$

with

$$C_i = 2 \sum_{k=0}^{i-1} J_1(j_{k+1})^{-2} + J_1(j_{i+1})^{-2} - \frac{j_{i+1}^2}{2}, \quad (16)$$

where the sum is assumed to be zero for $i = 0$.

For the largest node, we have $C_0 = 0.8187877\dots$, which is quite close to the error constant for the smallest nodes, which is $C = \pi^2/12 = 0.8224670\dots$. In fact, the following conjecture appears to be true, as numerical experiments show.

Conjecture 2 *The sequence $\{C_i\}_{i=0}^{+\infty}$ is positive, increasing, and with limit $\lim_{i \rightarrow \infty} C_i = \frac{\pi^2}{12}$.*

In Appendix D, we prove that the limit $C_{+\infty}$ is finite.

Conjecture 2 leads us to the following conjecture.

Conjecture 3 *The primary and secondary nodes of Gauss–Legendre quadrature of degree n are such that*

$$0 < \frac{x_i}{z_i} - 1 < \frac{\pi^2}{12\kappa^2}, \quad i = 1, \dots, n,$$

with $\pi^2/12$ the best possible asymptotic constant.

Conjecture 3 can be used to check that the primary and secondary intermediate nodes are interlaced, that is, $\bar{z}_0 < x_1 < \bar{z}_1 < x_2 < \dots < \bar{z}_{n-1} < x_n < \bar{z}_n$.

Conjecture 4 *The primary nodes $\{x_i\}$ and the secondary intermediate nodes $\{\bar{z}_i\}$ are interlaced, at least asymptotically.*

Proof We are proving the interlacing asymptotically, that is, as $\kappa \rightarrow +\infty$, and assuming Conjecture 3. However, the result appears to hold for any n .

We are checking that in each interval $(\bar{z}_{j-1}, \bar{z}_j)$, $j = 1, \dots, n-1$ there is one primary node x_j ; because there are $n+1$ intermediate nodes (including ± 1) and n primary nodes, this proves interlacing. For proving this, and because $\bar{z}_j - \bar{z}_{j-1} = w_j$, we need to prove that $|x_j - z_j|/(w_j/2)$ is smaller than 1, where $z_j = (\bar{z}_{j-1} + \bar{z}_j)/2$ is the middle point of the interval $(\bar{z}_{j-1}, \bar{z}_j)$.

We use that $x_j/z_j - 1 < \frac{\pi^2}{12\kappa^2}$ (Conjecture 3) and then

$$|x_j - z_j| < |z_j| \frac{\pi^2}{12\kappa^2} < \frac{\pi^2}{12\kappa^2}, \quad (17)$$

and, considering the elementary asymptotic expansion for w_j , we have

$$\frac{2|x_j - z_j|}{w_j} < \frac{\pi^2}{6\kappa^2 w_j} \sim \frac{\pi}{6\kappa \sin \alpha_j},$$

which is smaller than 1 for large enough κ and fixed j . This would prove the result under the same conditions as in Theorem 1, but not for the extreme nodes.

For proving that this holds in all the interval $(-1, 1)$, we have to rely on the Bessel expansions for the extreme nodes again. The distance $|x_j - z_j|$ can be uniformly bounded in all the interval using (17); however, the length of the interval $(\bar{z}_{j-1}, \bar{z}_j)$ decreases because the positive weights w_j decrease with increasing j , and we expect that the most problematic case is for $j = n$.

Using Bessel asymptotics for w_{n-i} (Eq. (5)),

$$\frac{2|x_{n-i} - z_{n-i}|}{w_{n-i}} \lesssim \frac{\pi^2 J_1(j_{i+1})^2}{12} \equiv D_i.$$

For the last interval ($i = 0$), we have $D_0 = 0.2216664\dots$, for the following $D_1 = 0.0952253\dots$ and D_i tends to zero as i increases.

Considering the result proved in Appendix C, we have

$$D_i < \frac{\pi}{6j_{i+1}} = \mathcal{O}(i^{-1}). \quad \square$$

4.2 Relation between the primary and secondary intermediate nodes

The relation between the intermediate nodes can be shown in a similar way as in the previous section, but in this case we will use the third result in Theorem 1 instead of the second. We first prove the following

Lemma 3 *Let $\{\bar{x}_i\}$ be the smallest positive intermediate node, then*

$$\frac{\bar{x}_i}{\bar{z}_i} = 1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4}).$$

Proof Let $n = 2k$, $k \in \mathbb{N}$. By symmetry, we have that $\bar{x}_k = \bar{z}_k = 0$ and then, using (12), the smallest positive intermediate node \bar{x}_{k+1} is such that

$$\bar{x}_{k+1} = \frac{x_{k+2} - x_k}{2},$$

and, by the third result of Theorem 1,

$$\bar{x}_{k+1} = w_{k+1} \left(1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4}) \right).$$

Because $\bar{z}_{k+1} = \bar{z}_k + w_{k+1} = w_{k+1}$, the result is proved for n even.

Take now $n = 2k + 1$, $k \in \mathbb{N}$. Then $x_k = -x_{k+2}$ and $x_{k+1} = 0$ and, by the third result of Theorem 1,

$$\frac{x_{k+2} - x_k}{2w_{k+1}} = \frac{x_{k+2}}{w_{k+1}} = \frac{2\bar{x}_{k+1}}{w_{k+1}}.$$

Now, by symmetry, $\bar{z}_k = -\bar{z}_{k+1}$ and, because $\bar{z}_{k+1} = \bar{z}_k + w_{k+1}$, $\bar{z}_{k+1} = w_{k+1}/2$. Therefore

$$\frac{x_{k+2} - x_k}{2w_{k+1}} = \frac{\bar{x}_{k+1}}{\bar{z}_{k+1}},$$

and, applying the third result of Theorem 1 to the left-hand side, we have the desired result. \square

Lemma 4 *If, as $\kappa \rightarrow +\infty$,*

$$\frac{\bar{x}_j}{\bar{z}_j} = 1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4})$$

for $j = m$ then the same holds for $j = m \pm 1$, provided all the nodes are inside a fixed compact subset of $(-1, 1)$.

Proof Considering the property (12), we have

$$\bar{x}_{m+1} = \bar{x}_m + \frac{x_{m+2} - x_m}{2}.$$

Now, because we are assuming that $\frac{\bar{x}_m}{\bar{z}_m} = 1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4})$, using the third result of Theorem 1 yields

$$\bar{x}_{m+1} = \bar{z}_m \left(1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4}) \right) + w_{m+1} \left(1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4}) \right)$$

and, because $\bar{z}_{m+1} = \bar{z}_m + w_{m+1}$, the result is proved for $j = m + 1$. \square

As a consequence, and similarly as we proved for the primary and secondary nodes in the previous section, we have

Corollary 3 *Let $[a, b] \subset (-1, 1)$ and $x_k, z_k \in [a, b]$, then*

$$\frac{\bar{x}_k}{\bar{z}_k} = 1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-3})$$

as $k \rightarrow +\infty$.

And the same comments following Corollary 2 apply here.

Using the Bessel-type expansions, we can confirm, similarly as in the previous section, that the relation between primary and secondary intermediate nodes holds uniformly in all the interval $(-1, 1)$, and not only in fixed compact subsets.

Considering the second equality in (13), together with the expansions (6) and (7), we have

$$\frac{\bar{x}_{n-i}}{\bar{z}_{n-i}} - 1 = \frac{1}{\kappa^2} E_i + \mathcal{O}(\kappa^{-4}), \quad i = 1, 2, \dots,$$

with

$$E_i = 2 \sum_{k=1}^i J_1(j_k)^{-2} - \frac{j_i^2}{4} - \frac{j_{i+1}^2}{4}. \quad (18)$$

For the largest intermediate node ($i = 1$), we have $D_1 = -1.6428507\dots$, which is quite close to the error constant for the smallest nodes, which is $E_i = -\pi^2/12 = -1.6449340\dots$. In fact, the following conjecture appears to be true, as numerical experiments show.

Conjecture 5 *The sequence $\{E_i\}_{i=1}^{+\infty}$ is negative, decreasing, and with limit $\lim_{i \rightarrow +\infty} E_i = -\frac{\pi^2}{6}$.*

That the limit is finite can be proved similarly as it is proved in Appendix D that the limit $C_{+\infty}$ is finite. We omit the proof for brevity.

The previous result leads to the following conjecture.

Conjecture 6 *The primary and secondary intermediate nodes of Gauss–Legendre quadrature of degree n are such that*

$$0 < 1 - \frac{\bar{x}_i}{\bar{z}_i} < \frac{\pi^2}{6\kappa^2}, \quad i = 1, \dots, n-1,$$

with $\pi^2/6$ the best possible asymptotic constant.

4.3 Relation between the first order partial moments and the intermediate nodes

Let us now define $\alpha_0 = 0$, $\alpha_i = \alpha_{i-1} - 2x_i w_i$, that is,

$$\alpha_{n-i} = 2 \sum_{k=0}^{i-1} x_{n-k} w_{n-k} = 2 \sum_{k=i+1}^n x_k w_k.$$

Notice that the previous two sums are equal because $x_{n-k+1} = -x_k$ and $w_{n-k+1} = w_k$, $k = 1, \dots, n$, which also implies that the first-order moment is zero, that is, $\sum_{k=1}^n x_k w_k = 0$. For the same reason, $\alpha_i = \alpha_{n-i}$, $i = 0, \dots, n$.

We propose the following conjecture relating the first-order partial moments α_i with the secondary intermediate nodes.

Conjecture 7 *The following holds for all the secondary intermediate nodes and partial moments:*

$$0 < \frac{\alpha_i}{1 - (\bar{z}_i)^2} - 1 < \frac{\pi^2}{12\kappa^2},$$

where the constant $\frac{\pi^2}{12}$ is the best possible.

The asymptotic evidence supporting this conjecture is not as solid as for the case of Conjecture 3, as it will be solely based on Bessel asymptotics for large nodes, and assuming another unproved property for Bessel functions. However, later we discuss how this can be also seen as a consequence of the asymptotic relation between primary and secondary nodes; for this purpose, we solve an initial value problem relating both results.

Now we see how the Bessel-type expansions suggest the validity of Conjecture 7. Taking into account (6) and (7), we have

$$x_{n-k} w_{n-k} = \frac{2}{\kappa^2 j_1(j_{k+1})^2} \left(1 - \frac{1}{12\kappa^2} - \frac{2j_{k+1}^2}{3\kappa^2} \right) + \mathcal{O}(\kappa^{-5}),$$

and therefore

$$\alpha_{n-i} = \frac{4G(\kappa)S_i^{(1)}}{\kappa^2} - \frac{8S_i^{(2)}}{3\kappa^4} + \mathcal{O}(\kappa^{-5}),$$

where $G(\kappa) = 1 - \frac{1}{12\kappa^2}$ and

$$S_i^{(1)} = \sum_{k=0}^{i-1} \frac{1}{j_1(j_{k+1})^2}, \quad S_i^{(2)} = \sum_{k=0}^{i-1} \frac{j_{k+1}^2}{j_1(j_{k+1})^2}.$$

On the other hand, considering again (7) gives

$$\bar{z}_{n-i} = 1 - \sum_{k=0}^{i-1} w_{n-k} = 1 - \left(\frac{2G(\kappa)S_i^{(1)}}{\kappa^2} - \frac{S_i^{(2)}}{3\kappa^4} \right) + \mathcal{O}(\kappa^{-5}).$$

With these two expansions, we get

$$\frac{\alpha_{n-i}}{1 - (\bar{z}_{n-i})^2} = 1 + \left(S_i^{(1)} - \frac{S_i^{(2)}}{2S_i^{(1)}} \right) \kappa^{-2} + \mathcal{O}(\kappa^{-4}),$$

which proves that $\frac{\alpha_{n-i}}{1 - (\bar{z}_{n-i})^2} - 1 = \mathcal{O}(\kappa^{-2})$, at least for the large zeros (such that $j_i \ll \kappa$ holds).

It turns out that the constants

$$K_i = S_i^{(1)} - \frac{S_i^{(2)}}{2S_i^{(1)}} \quad (19)$$

are bounded for any $i \in \mathbb{N}$, as numerical experiments show. We propose the following conjecture.

Conjecture 8 *The sequence $\{K_i\}_{i=1}^\infty$ is monotonically increasing, positive, and*

$$\lim_{i \rightarrow +\infty} K_i = \frac{\pi^2}{12}$$

We observe that $K_1 = C_0 = 0.8187877 \dots$, as could be expected because

$$\frac{\alpha_{n-1}}{1 - (\bar{z}_{n-1})^2} = \frac{2x_n w_n}{1 - (1 - w_n)^2} = \frac{x_n}{1 - w_n/2} = \frac{x_n}{z_n}.$$

On the other hand, because $K_{+\infty} = \pi^2/12 = 0.8224 \dots$, we observe that the sequence $\{K_i\}$, as happened with $\{C_i\}$, has very small variation. The convergence of the $\{K_i\}$ sequence appears to be fast, and K_{100} already approximates $\pi^2/12$ with 6 exact digits.

A consequence of Conjecture 7 is that, considering n even, and because by symmetry $\bar{z}_{n/2} = 0$, we have that

$$\alpha_{n/2} = 2 \sum_{x_i > 0} x_i w_i = 1 + \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4}).$$

On the other hand, for n odd, we have $0 = x_k = z_k = \bar{z}_k^{(w)} - \frac{1}{2}w_k$ for $k = (n+1)/2$ and then

$$\begin{aligned} \alpha_k &= 2 \sum_{x_i > 0} x_i w_i = \left(1 - \frac{w_k^2}{4} \right) \left(1 + \frac{\pi^2}{12\kappa^2} + \mathcal{O}(\kappa^{-4}) \right), \\ &= 1 - \frac{\pi^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4}). \end{aligned}$$

These later results, as well as the rest of asymptotic relations between nodes and weights, can be numerically checked to high accuracy with an arbitrary precision implementation of the algorithm for Gauss–Gegenbauer quadrature of [8].

4.3.1 A complementary observation that supports Conjecture 7

Notice that $D(x) = 1 - x^2$ is the solution of the following initial value problem (IVP):

$$\begin{cases} y' = -2x \text{ in } (-1, 1), \\ y(-1) = 0. \end{cases} \quad (20)$$

Our goal is to prove the following observation, which demonstrates that proving that $\max_{0 \leq i \leq n} |D(\bar{z}_i) - \alpha_i| = \mathcal{O}(n^{-2})$ (cf. Conjecture 7) is as difficult as proving Conjecture 3, but not more.

Observation 1 *Under Conjecture 3,*

$$\max_{0 \leq i \leq n} |D(\bar{z}_i) - \alpha_i| = \mathcal{O}(n^{-2}). \quad (21)$$

To this aim, we are going to solve the IVP (20) on the mesh of intermediate nodes $\{\bar{z}_i\}_{i=0}^n$ by means of a convenient numerical method of order 2 which will compute the first-order partial moment α_i as the approximation of $D(\bar{z}_i)$. Let us start trying the midpoint rule:

$$\begin{cases} y_0 = 0, \\ y_{i+1} = y_i - 2h_i(\bar{z}_i + h_i/2) \text{ for } i = 0, \dots, n-1, \end{cases} \quad (22)$$

where $h_i = w_{i+1}$ is the distance between \bar{z}_i and \bar{z}_{i+1} .

Since $\bar{z}_i + h_i/2 = z_{i+1}$, the scheme (22) does not use the desired formula $y_{i+1} = y_i - 2w_{i+1}x_{i+1}$, but rather $y_{i+1} = y_i - 2w_{i+1}z_{i+1}$. This problem can be easily fixed by considering instead the following adjustment:

$$\begin{cases} y_0 = 0, \\ y_{i+1} = y_i - 2h_i(\bar{z}_i + h_i^*/2) \text{ for } i = 0, \dots, n-1, \end{cases} \quad (23)$$

where $h_i^* = 2(x_{i+1} - \bar{z}_i)$. This scheme computes $y_i = \alpha_i$ for $i = 0, \dots, n$, whereupon the reasoning is complete and proves Observation 1. The statement in Conjecture 3 is needed to guarantee that the step-sizes h_i^* and h_i are close enough so that the scheme (23) still has order 2. A detailed proof is given in Appendix E.

5 Applications in finite difference schemes

The initial motivation for the study of these properties was the analysis of convergence of a number of finite difference schemes used in the discretization of the angular Fokker–Planck diffusion operator, of particular relevance in the context of nuclear engineering. The properties discussed in this paper appear as necessary conditions for the convergence with order 2 of some of these methods [12]. Although these properties are of intrinsic interest, next we briefly explain why they are important for the analysis of such finite difference schemes. These properties were previously either assumed correct or simply overlooked, and the present paper fills this gap by providing strong asymptotic evidence that they hold.

Let us define $D(x) = 1 - x^2$ and suppose that we want to discretize the operator

$$\Delta_{\text{FP}} f(x) = (D(x)f'(x))', \quad \text{with } x \in [-1, 1], \quad (24)$$

by using, for each natural n , the mesh formed by the Gauss–Legendre nodes x_i . This is a natural choice which acquires special meaning if one must solve a PDE of which the above operator is a part and there are quantities of interest defined by means of integrals of functions involving the solution. To accomplish the discretization, Haldy and Ligou

[9] used as support the secondary intermediate nodes \bar{z}_i , $i = 0, \dots, n$, defined in (13), and, going through the intermediate step

$$\Delta_{\text{FP}}f(x_i) \approx \frac{D(\bar{z}_i)f'(\bar{z}_i) - D(\bar{z}_{i-1})f'(\bar{z}_{i-1})}{w_i}, \quad (25)$$

they finally employed

$$\Delta_{\text{FP}}f(x_i) \approx \frac{D(\bar{z}_i)\frac{f(x_{i+1})-f(x_i)}{x_{i+1}-x_i} - D(\bar{z}_{i-1})\frac{f(x_i)-f(x_{i-1})}{x_i-x_{i-1}}}{w_i} \quad (26)$$

for $i = 1, \dots, n$, where terms containing the undefined nodes x_0 and x_{n+1} are multiplied by zero and must be ignored.

Since $w_i = \bar{z}_i - \bar{z}_{i-1}$, the idea behind (25) and (26) is clear as soon as one thinks of the centered formula of two points for the first derivative. It is then apparent that the formula (26) will perform better if

1. x_i is close to z_i , the midpoint of $[\bar{z}_{i-1}, \bar{z}_i]$ (see Conjecture 3), and
2. \bar{z}_i is close to \bar{x}_i , the midpoint of $[x_i, x_{i+1}]$ (see Conjecture 6).

In particular, the interlacing property stated in Corollary 4 is needed.

On the other hand, we have Morel's scheme [13], which is obtained by substituting in (26) $D(\bar{z}_{i-1})$ and $D(\bar{z}_i)$ by the first-order partial moments α_{i-1} and α_i , respectively. It is natural to think that α_i must be close to $D(\bar{z}_i)$ (see Conjecture 7) so as not to lose accuracy.

Experimentally, both schemes converge with order 2. The proof of this fact, which uses the properties just mentioned, can be found in [12].

In these methods, a motivation for using nodes defined as sum of weights (what we call secondary nodes and secondary intermediate nodes) was to preserve the zeroth and first moment properties, that is,

$$\int_{-1}^1 \Delta_{\text{FP}}f(x) dx = 0, \quad (27)$$

$$\int_{-1}^1 x \Delta_{\text{FP}}f(x) dx = -2 \int_{-1}^1 xf(x) dx, \quad (28)$$

in the discrete setting. Haldy–Ligou's scheme preserves the zeroth moment, while Morel's scheme preserves both.

We refer to [12] for further details of the analysis of those finite differences schemes, for which the use of the uniform properties described in this paper is crucial. The reader might also like to consult references [14, 17, 18] to see that Morel's scheme is still in use.

Although we are not aware of additional specific numerical methods, apart from [9] and [13], where the properties discussed in this paper are used (probably because they were unknown), the secondary nodes can be useful in other numerical applications because they are closely related to Legendre nodes, as we have proved. We observe that in finite difference methods based on Legendre nodes, the differences between the nodes are prone to severe rounding errors, particularly significant at the extremes of $(-1, 1)$, where the nodes tend to cluster. As pointed out by Laurie [11, p. 215]: “For careful work, one should store as floating-point numbers not the nodes, but the gaps between them”. Alternatively, the differences between secondary nodes are sums of positive weights, which

can be accurately computed either by iterative methods [8] or by asymptotic methods [8] (even for a very large number of nodes); no cancellations occur in this case.

For a better understanding of the uses of the secondary nodes in approximation, it will be interesting to analyze the Lebesgue constants corresponding to those nodes, both numerically and asymptotically. Some preliminary numerical tests indicate that the Lebesgue functions are very similar for the primary and secondary nodes and that their asymptotic behavior is essentially the same. This will be the object of further study.

Appendix A: Elementary expansion for the weights

For obtaining the first term of the elementary asymptotic expansion for the weights, we start from Eqs. (4.3), (4.4), (4.5), and (2.20) of [7] to write

$$w_i = \frac{\pi}{\kappa} \sin \theta_i H_\kappa(\theta_i)^{-2}, \quad (29)$$

where

$$H_\kappa(\theta) = \left(1 + \frac{m_2(\theta)}{\kappa^2} + \mathcal{O}(\kappa^{-4})\right) \sin \chi + \left(\frac{n_1(\theta)}{\kappa} + \mathcal{O}(\kappa^{-3})\right) \cos \chi,$$

with $\chi = \kappa\theta - \frac{\pi}{4}$ and

$$m_2(\theta) = \frac{1}{384} \frac{24 - 3 \cos^2 \theta}{\sin^2 \theta}, \quad n_1(\theta) = -\frac{1}{8} \cot \theta.$$

Now, for obtaining an expansion for the weights, we must substitute the expansion (1) in (29) and reexpand in powers of κ^{-2} . For our purpose, it will be enough to use the terms explicitly shown.

In the expression for m_2 and n_1 it will be enough to replace θ_i by α_i . Now, we have

$$\chi_i = \kappa\theta_i - \frac{\pi}{4} = \left(n - i + \frac{1}{2}\right)\pi + d_i, \quad d_i = \frac{\cot \alpha_i}{8\kappa},$$

and with this

$$\sin \chi_i = (-1)^{n-i} \left(1 - \frac{d_i^2}{2} + \mathcal{O}(\kappa^{-4})\right), \quad \cos \chi_i = -(-1)^{n-i} d_i + \mathcal{O}(\kappa^{-3}).$$

Substituting the expansions,

$$\begin{aligned} (-1)^{n-i} H_\kappa(\theta_i) &= 1 + \frac{m_2(\alpha_i)}{\kappa^2} - \frac{d_i^2}{2} - \frac{d_i n_1(\alpha_i)}{\kappa} + \mathcal{O}(\kappa^{-4}) \\ &= 1 + \frac{1}{16\kappa^2 \sin^2 \alpha_i} + \mathcal{O}(\kappa^{-4}). \end{aligned}$$

Therefore

$$H_\kappa(\theta_i)^{-2} = 1 - \frac{1}{8\kappa^2 \sin^2 \alpha_i} + \mathcal{O}(\kappa^{-4}). \quad (30)$$

Finally, we have

$$\begin{aligned}\sin \theta_i &= \sin(\alpha_i + \delta_i) = \sin(\alpha_i) + \delta_i \cos(\alpha_i) + \mathcal{O}(\kappa^{-4}) \\ &= \sin \alpha_i \left(1 + \frac{1}{8\kappa^2 \sin^2 \alpha_i} - \frac{1}{8\kappa^2} \right)\end{aligned}\quad (31)$$

and, substituting (30) and (31) into (29), get

$$w_i = \frac{\pi}{\kappa} F(\kappa) \sin \alpha_i + \mathcal{O}(\kappa^{-5}), \quad (32)$$

with $F(\kappa)$ defined in (4). This coincides with the expansion [16, A.8], which is obtained by different means (using the Riemann–Hilbert approach).

Appendix B: Bessel-type expansion for the weights

For obtaining the Bessel-type expansions for the Gauss–Legendre weights, we start by combining Eqs. (4.2), (4.4), (4.6), and (3.10) of [7], to write

$$w_i = \frac{2 \sin \theta_i}{\kappa^2 \theta_i} H_\kappa(\theta_i)^{-2}, \quad (33)$$

where

$$H_\kappa(\theta) = J_1(\kappa\theta)Y(\theta) - \frac{1}{2\theta\kappa}J_0(\kappa\theta)Z(\theta),$$

with $Y(\theta)$ and $Z(\theta)$ admitting asymptotic expansions in powers of κ^{-2} , namely

$$Y(\theta) \sim \sum_{m=0}^{+\infty} \frac{Y_m(\theta)}{\kappa^{2m}}, \quad Z(\theta) \sim \sum_{m=0}^{+\infty} \frac{Z_m(\theta)}{\kappa^{2m}}.$$

Because $\theta_i = \beta_i + \delta_i$ with $\delta_i = \mathcal{O}(\kappa^{-2})$, we have $Y(\theta_i) = 1 + Y_1(\beta_i)\kappa^{-2} + \mathcal{O}(\kappa^{-4})$ and $Z(\theta_i) = 1 + \mathcal{O}(\kappa^{-2})$. For our purposes, we will only need to know that $Y_0(\theta) = Z_0(\theta) = 1$ and that $Y_1(\beta_i) = \frac{1}{48} + \mathcal{O}(\beta_i^2)$ as $\beta_i \rightarrow 0$.

On the other hand, $\kappa\theta_i = b_i + d_i$, with $b_i = j_{n-i+1}$ and then $J_0(b_i) = 0$; in addition, using the differentiation formulas [15, 10.6.2], we have $J'_1(b_i) = -J_1(b_i)/b_i$, $J''_1(b_i) = (2/b_i^2 - 1)J_1(b_i)$, $J'_0(b_i) = -J_1(b_i)$ and then

$$\begin{aligned}J_1(\kappa\theta_i) &= J_1(b_i) \left(1 - \frac{d_i}{b_i} + \frac{d_i^2}{b_i^2} - \frac{1}{2}d_i^2 + \mathcal{O}(d_i^3) \right), \\ J_0(\kappa\theta_i) &= J_1(b_i) \left(-d_i + \frac{d_i^2}{2b_i} + \mathcal{O}(d_i^3) \right).\end{aligned}$$

Putting this together and using that $Y_0(\theta) = Z_0(\theta) = 1$ gives

$$H_\kappa(\theta_i) = J_1(b_i) \left(1 - \frac{1}{2} \frac{d_i}{b_i} + \frac{d_i^2}{4b_i^2} - \frac{1}{2}d_i^2 + \frac{Y_1(\beta_i)}{\kappa^2} + \mathcal{O}(\kappa^{-4}) + \mathcal{O}(d_i^3) \right). \quad (34)$$

From this, we can proceed to compute the first terms of the asymptotic expansion as $k \rightarrow +\infty$, without any restriction on the values of β_i . We are next simplifying the expansion

by further assuming that $\beta_i = j_{n-i+1}/\kappa \ll 1$, which holds for the largest zeros, but not for the zeros close to the origin. Under this approximation, $\beta_i = \mathcal{O}(\kappa^{-1})$, $d_i = \mathcal{O}(\kappa^{-2})$. Additionally, using Eq. (3.12) of [7], in this limit we have $Y_1(\beta_i) = \frac{1}{48} + \mathcal{O}(\kappa^{-2})$. We neglect all the terms in (34) except the first two and the dominant contribution from Y_1 , yielding

$$H_\kappa(\theta_i) = J_1(b_i) \left(1 - \frac{1}{2} \frac{d_i}{b_i} + \frac{1}{48\kappa^2} + \mathcal{O}(\kappa^{-4}) \right).$$

Then

$$\kappa \theta_i H_\kappa(\theta)^2 = (b_i + d_i) F_\kappa(\theta_i)^2 = b_i J_1(b_i)^2 \left(1 + \frac{1}{24\kappa^2} + \mathcal{O}(\kappa^{-4}) \right),$$

which we insert into Eq. (33) to get

$$w_i = \frac{2 \sin \theta_i}{b_i \kappa J_1(b_i)^2} \left(1 - \frac{1}{24\kappa^2} + \mathcal{O}(\kappa^{-4}) \right).$$

Now, because we are considering that $\beta_i = \mathcal{O}(\kappa^{-1})$, we have

$$\begin{aligned} \sin \theta_i &= \sin(\beta_i + \delta_i) = \sin \beta_i + \delta_i \cos \beta_i + \mathcal{O}(\delta_i^2) \\ &= \beta_i \left(1 - \frac{1}{6} \beta_i^2 - \frac{1}{24\kappa^2} + \mathcal{O}(\kappa^{-4}) \right) \end{aligned}$$

and, finally,

$$w_{n-i} = \frac{2}{\kappa^2 J_1(j_{i+1})^2} \left(1 - \frac{1}{12\kappa^2} - \frac{j_{i+1}^2}{6\kappa^2} + \mathcal{O}(\kappa^{-4}) \right). \quad (35)$$

This last approximation is accurate for $i \ll n$, and coincides with the expansion [16, A.6].

Appendix C: Proof of a property of Bessel functions

Previously, we used the property that

$$a_i = 1 - \frac{2}{\pi j_{i+1} J_1(j_{i+1})^2}, \quad i = 0, 1, \dots$$

is a positive decreasing sequence. We prove a more general result, using a variant of Sonin's theorem (see Lemma 3.3 in [10]).

Theorem 2 *Let $w(x)$ be a solution of $w''(x) + A(x)w(x) = 0$ in some interval where $A'(x) > 0$ (respectively $A'(x) < 0$), then the values of $w'(x)^2$ increase (respectively decrease) when they are evaluated at the successive zeros of $w(x)$ (in increasing order).*

Proof Let $f(x) = w'(x)^2 + A(x)w(x)^2$, which has derivative $f'(x) = A'(x)w(x)^2$ (only zero at the zeros of $w(x)$). Then $f(x)$ has the same monotonicity as $A(x)$ and, because at the zeros of $w(x)$ we have $f(x) = w'(x)^2$, the result is proved. \square

Next we apply the previous result to the Bessel differential equation.

Corollary 4 Let $v_v(x) = \sqrt{x}y'_v(x)$, with $y_v(x)$ any solution of the Bessel equation $(x^2y''_v(x) + xy'_v(x) + (x^2 - v^2)y_v(x) = 0)$ and let c_i , $i = 1, 2, \dots$ be the positive zeros of $y_v(x)$ in increasing order. The sequence $v_v(c_i)^2$ is strictly decreasing if $|v| < 1/2$, strictly increasing if $|v| > 1/2$, and constant if $|v| = 1/2$.

Proof The function $w_v(x) = \sqrt{x}y_v(x)$ is a solution of the differential equation $w''(x) + A(x)w(x) = 0$ with

$$A(x) = 1 - \frac{v^2 - 1/4}{x^2}.$$

With this, and considering the previous theorem, we deduce that $w'_v(c_i)^2$ increases with i if $|v| > 1/2$ (because $A'(x) > 0$), decreases if $|v| < 1/2$ ($A'(x) < 0$), and is constant if $|v| = 1/2$ ($A'(x) = 0$). Now, because $w'_v(c_i) = v_v(c_i)$, the monotonicity properties of the sequence $v_v(c_i)^2$ are proved. \square

Any solution of the Bessel equation, up to a constant multiplicative factor, can be written as

$$C_v(x) = \cos \alpha J_v(x) - \sin \alpha Y_v(x), \quad (36)$$

for some $\alpha \in [0, \pi)$, where $J_v(x)$ and $Y_v(x)$ are the Bessel functions of the first and second kinds, respectively [15]. For any fixed value of α , at the zeros c_i of $C_v(c_i)$ we have $C'_v(c_i) = -C_{v+1}(c_i)$ on account of [15, 10.6.2], and therefore the previous corollary implies the next result.

Corollary 5 The sequence $c_i C_{v+1}(c_i)^2$ is strictly increasing if $|v| > 1/2$, strictly decreasing if $|v| < 1/2$, and constant if $|v| = 1/2$.

In the next discussion, we will need the asymptotic expansions for $C_v(x)$ for large x , as well as the expansion for c_i and large i . Combining the equations [15, 10.17.3–10.17.4], we have

$$C_v(x) \sim \left(\frac{2}{\pi x}\right)^{1/2} (\cos(\chi_v(x))P_v(x) - \sin(\chi_v(x))Q_v(x)), \quad (37)$$

where

$$\chi_v(x) = x + \alpha - \frac{v\pi}{2} - \frac{\pi}{4},$$

$$P_v(x) = \sum_{k=0}^{\infty} (-1)^k \frac{a_{2k}(v)}{x^{2k}}, \quad Q_v(x) = \sum_{k=0}^{\infty} (-1)^k \frac{a_{2k+1}(v)}{x^{2k+1}},$$

and $a_k(v) = (-2)^{-k} \left(\frac{1}{2} - k\right)_k \left(\frac{1}{2} + k\right)_k / k!$.

The dominant term in the expansion gives

$$C_v(x) \sim \left(\frac{2}{\pi x}\right)^{1/2} \cos(\chi_v(x)) (1 + \mathcal{O}(x^{-1})).$$

McMahon asymptotic expansion for the zeros c_i for large i is obtained by inversion of the asymptotic series (37), as done in [6, Sect. 3.3.1]. The leading contribution is that which makes $\cos(\chi) = 0$, that is, $c_i + \alpha - \frac{\nu\pi}{2} - \frac{\pi}{4} \sim (2i-1)\frac{\pi}{2}$, which gives $c_i \sim \left(i + \frac{\nu}{2} - \frac{1}{4}\right) - \alpha \equiv \lambda_i$. With one additional term, the expansion reads (see [6])

$$c_i = \lambda_i - \frac{4\nu^2 - 1}{8\lambda_i} + \mathcal{O}(i^{-3}). \quad (38)$$

With the previous expansions, we can prove the following

Lemma 5

$$\lim_{i \rightarrow \infty} \frac{\pi c_i}{2} C_{v+1}(c_i)^2 = 1.$$

Proof Considering that $\chi_\nu(c_i) = (2i-1)\frac{\pi}{2} + \mathcal{O}(i^{-1})$ and $\chi_{v+1}(x) = \chi_\nu(x) + \frac{\pi}{2}$, we have $\cos(\chi_{v+1}(c_i)) = (-1)^{i+1} + \mathcal{O}(i^{-1})$ and therefore

$$C_{v+1} = (-1)^{i+1} \left(\frac{2}{\pi c_i} \right)^{1/2} (1 + \mathcal{O}(i^{-1})),$$

which proves the result. \square

As a consequence of Corollary 5 and Lemma 5, we can state the following

Corollary 6 *The sequence $\{a_i\}$, $a_i = 1 - \frac{2}{\pi c_i C_{v+1}(c_i)^2}$, $0 < c_1 < c_2 < \dots$ being the positive zeros of $C_\nu(x)$, is strictly decreasing and positive if $|v| < 1/2$, strictly increasing and negative if $|v| < 1/2$, and constant if $|v| = 1/2$. Additionally, $\lim_{i \rightarrow \infty} s_i = 0$.*

The result that we have mentioned at the beginning of this Appendix is simply the case $\alpha = 0$ of the previous corollary.

Appendix D: Proof that the limit $C_{+\infty}$ is finite

We prove the convergence in a more general case. Let us define

$$C_i = 2 \sum_{k=0}^{i-1} J'_\nu(j_{k+1})^{-2} + J'_\nu(j_{i+1})^{-2} - \frac{J_{i+1}^2}{2}$$

with j_i being the i th positive zero of $J_\nu(x)$. For the case $\nu = 0$, we obtain our previous definition.

We write

$$C_{i-1} = C_0 + \sum_{k=1}^{i-1} s_k, \quad s_k = C_k - C_{k-1}.$$

We have

$$s_k = J'_\nu(j_{k+1})^{-2} + J'_\nu(j_k)^{-2} - \frac{J_{k+1}^2 - J_k^2}{2}.$$

We are checking that as $k \rightarrow +\infty$, $s_k = \mathcal{O}(k^{-2})$, which means that $\sum_{k=1}^{+\infty} s_k < +\infty$, and completes the proof.

For this purpose, using [15, 10.17.9], we have

$$J'_v(j_k)^{-2} = \frac{\pi}{2} j_k Q_v(j_k)^{-2},$$

where $Q_v(z)$ admits, as $z \rightarrow +\infty$ the expansion

$$Q_v(z) \sim \sin w \sum_{i=0}^{+\infty} (-1)^i \frac{b_{2i}}{z^{2i}} + \cos w \sum_{i=0}^{+\infty} (-1)^i \frac{b_{2i+1}}{z^{2i+1}},$$

where $w = z - \frac{\nu\pi}{2} - \frac{\pi}{4}$. Now, for large k we have [15, 10.21.19]

$$j_k = a_k + \delta_k, \quad \delta_k = \frac{1 - 4\nu^2}{8a_k} + \mathcal{O}(a_k^{-3}), \quad a_k = \left(k + \frac{\nu}{2} - \frac{1}{4}\right)\pi. \quad (39)$$

Now set $z = j_k$, $w = (k - \frac{1}{2})\pi + \delta_k$, and then $\sin w = (-1)^{k+1} \cos \delta_k$, $\cos w = (-1)^k \sin \delta_k$. With this, we get $Q_v(j_k) = 1 + \mathcal{O}(k^{-2})$ and

$$s_k = \frac{\pi}{2} (j_k + j_{k+1}) (1 + \mathcal{O}(k^{-2})) - \frac{1}{2} (j_{k+1} - j_k)(j_{k+1} + j_k).$$

Now, because of (39),

$$j_{k+1} - j_k \sim \pi + \frac{(4\nu^2 - 1)\pi}{8a_{k+1}a_k} = \pi + \mathcal{O}(k^{-2}).$$

With this, $s_k = \mathcal{O}(k^{-2})$.

Appendix E: Proof of Observation 1

In this appendix, x_i will be a generic point of the mesh, rather than the i th Gaussian node. By using standard analysis of numerical schemes for initial value problems (IVPs), we will prove convergence of order 2 for a scheme which contains (23) as a particular case.

Consider, to be solved with some numerical scheme, the scalar IVP

$$\begin{cases} y' = f(x) \text{ in } (-1, 1), \\ y(-1) = \eta \in \mathbb{R}, \end{cases} \quad (40)$$

where $f \in C^2([-1, 1])$. This problem has a unique solution $y \in C^3([-1, 1])$.

We are going to employ meshes

$$x_0 = -1 < x_1 < \cdots < x_{n-1} < x_n = 1 \quad (41)$$

such that, if $h_i = x_{i+1} - x_i$ and $H_n = \max_{0 \leq i \leq n-1} h_i$, one has

$$H_n = \mathcal{O}(n^{-1}). \quad (42)$$

On any of these meshes, define the following scheme:

$$\begin{cases} y_0 = \eta, \\ y_{i+1} = y_i + h_i f(x_i + h_i^*/2) \text{ for } i = 0, \dots, n-1, \end{cases} \quad (43)$$

where $h_i^* = h_i + d_i$, with $D_n = \max_{0 \leq i \leq n-1} |d_i|$ satisfying

$$D_n = \mathcal{O}(n^{-2}). \quad (44)$$

When $h_i = h_i^* = h = 2/n$, the scheme (43) is easily recognizable as more than one numerical method applied to problem (40). One is the midpoint rule adapted to have only one step (this can be done because f does not depend on y); another one is the modified Euler scheme, which can be seen as a member of the Runge–Kutta family with the following Butcher tableau:

$$\begin{array}{c|cc} 0 & 0 & 0 \\ 1/2 & 1/2 & 0 \\ \hline & 0 & 1 \end{array}. \quad (45)$$

Both the midpoint rule and the modified Euler scheme are known to have order 2, so the following result is quite natural.

Theorem 3 *Under the hypotheses (42) and (44), the scheme (43) is convergent of order 2, that is, $\max_{0 \leq i \leq n} |y(x_i) - y_i| = \mathcal{O}(n^{-2})$.*

The proof of Theorem 3 follows the standard approach, which is proving convergence by means of consistency and stability, but, since in this simple case function f does not depend on y , stability is trivially satisfied.

Lemma 6 *Under the hypotheses (42) and (44), the scheme (43) is consistent of order 2, that is, for any solution y of $y' = f(x)$,*

$$\max_{1 \leq i \leq n} |\tau_i| = \mathcal{O}(n^{-2}), \quad (46)$$

where $\tau_{i+1} = (y(x_{i+1}) - y(x_i))/h_i - f(x_i + h_i^*/2)$ for $i = 0, \dots, n-1$.

Proof In this proof, we will employ the notation $\|\varphi\|_\infty = \max_{x \in [-1,1]} |\varphi(x)|$ for $\varphi \in C([-1,1])$.

Notice that $\tau_{i+1} = (y(x_{i+1}) - y(x_i))/h_i - y'(x_i + h_i^*/2)$ because y is a solution of $y' = f(x)$, and recall that $y \in C^3([-1,1])$. Now use the Taylor expansions

$$y(x_{i+1}) = y(x_i) + h_i y'(x_i) + \frac{h_i^2}{2} y''(x_i) + \frac{h_i^3}{6} y'''(\xi_i) \quad (47)$$

and

$$y'(x_i + h_i^*/2) = y'(x_i) + \frac{h_i^*}{2} y''(x_i) + \frac{(h_i^*)^2}{8} y'''(\xi_i^*), \quad (48)$$

together with $h_i^* = h_i + d_i$, to write

$$\begin{aligned}\tau_{i+1} &= \left\{ y'(x_i) + \frac{h_i}{2} y''(x_i) + \frac{h_i^2}{6} y'''(\xi_i) \right\} \\ &\quad - \left\{ y'(x_i) + \frac{(h_i + d_i)}{2} y''(x_i) + \frac{(h_i + d_i)^2}{8} y'''(\xi_i^*) \right\} \\ &= \frac{h_i^2}{6} y'''(\xi_i) - \frac{d_i}{2} y''(x_i) - \frac{(h_i + d_i)^2}{8} y'''(\xi_i^*).\end{aligned}\quad (49)$$

So,

$$|\tau_{i+1}| \leq \frac{H_n^2}{6} \|y'''\|_\infty + \frac{D_n}{2} \|y''\|_\infty + \frac{(H_n^2 + 2H_n D_n + D_n^2)}{8} \|y'''\|_\infty \quad (50)$$

for $i = 0, \dots, n-1$, and, as the bound on the right-hand side does not depend on i , the result follows from the hypotheses (42) and (44). \square

Now Theorem 3 can be proved as follows.

Proof of Theorem 3 The conclusion $\max_{0 \leq i \leq n} |y(x_i) - y_i| = \mathcal{O}(n^{-2})$ will be proved if $\max_{1 \leq i \leq n} |y(x_i) - y_i| = \mathcal{O}(n^{-2})$, as $y(x_0) = y_0 = \eta$.

Due to the definition of τ_{i+1} in Lemma 6, the values $y(x_i)$ of the exact solution satisfy

$$\begin{cases} y(x_0) = \eta, \\ y(x_{i+1}) = y(x_i) + h_i(f(x_i + h_i^*/2) + \tau_{i+1}) \text{ for } i = 0, \dots, n-1, \end{cases} \quad (51)$$

while the approximate values y_i satisfy the scheme (43). Hence, we have that, for $i = 0, \dots, n-1$,

$$y(x_{i+1}) - y_{i+1} = y(x_i) - y_i + h_i \tau_{i+1}, \quad (52)$$

so

$$|y(x_{i+1}) - y_{i+1}| \leq |y(x_i) - y_i| + H_n |\tau_{i+1}|. \quad (53)$$

By induction,

$$|y(x_i) - y_i| \leq H_n \sum_{j=1}^i |\tau_j| \quad (54)$$

for $i = 1, \dots, n$, which implies

$$\max_{1 \leq i \leq n} |y(x_i) - y_i| \leq H_n \sum_{i=1}^n |\tau_i|. \quad (55)$$

The proof ends by combining (55) with the inequality

$$H_n \sum_{i=1}^n |\tau_i| \leq n H_n \max_{1 \leq i \leq n} |\tau_i|, \quad (56)$$

the hypothesis (42), and the consistency of order 2 stated in Lemma 6. \square

Notice that, under Conjecture 3, the scheme (23) converges with order 2 by virtue of Theorem 3. Indeed, the collection $\{h_i\}_{i=0}^{n-1} = \{w_i\}_{i=1}^n$ is known to satisfy (42), and Conjecture 3 implies that, for the h_i^* in (23), hypothesis (44) holds as well. So, we have in this way a detailed proof of Observation 1.

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Author contributions

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Data Availability

No datasets were generated or analysed during the current study.

Declarations

Competing interests

The authors declare no competing interests.

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