

Measuring characteristic length scales of eigenfunctions of Sturm–Liouville equations in one and two dimensions

Beth A. Wingate · Mark A. Taylor

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Abstract The spatial resolution of eigenfunctions of Sturm–Liouville equations in one-dimension is frequently measured by examining the minimum distance between their roots. For example, it is well known that the roots of polynomials on finite domains cluster like $O(1/N^2)$ near the boundaries. This technique works well in one dimension, and in higher dimensions that are tensor products of one-dimensional eigenfunctions. However, for non-tensor-product eigenfunctions, finding good interpolation points is much more complicated than finding the roots of eigenfunctions. In fact, in some cases, even quasi-optimal interpolation points are unknown. In this work an alternative measure, ℓ , is proposed for estimating the characteristic length scale of eigenfunctions of Sturm–Liouville equations that does not rely on knowledge of the roots. It is first shown that ℓ is a reasonable measure for evaluating the eigenfunctions since in one dimension it recovers known results. Then results are presented in higher dimensions. It is shown that for tensor products of one-dimensional eigenfunctions in the square the results reduce trivially to the one-dimensional result. For the non-tensor product Prorior polynomials, there are quasi-optimal interpolation points (Fekete points). Comparing the minimum distance between Fekete points to ℓ shows that ℓ is a reasonably good measure of the characteristic length scale in two dimensions as well. The measure is finally applied to the non-tensor product generalized eigenfunctions in the triangle proposed by Taylor MA, Wingate BA [(2006) J Engng Math, accepted] where optimal interpolation points are unknown. While some of the eigenfunctions have larger characteristic length scales than the Prorior polynomials, others show little improvement.

Keywords Length scale · Eigenfunctions · Sturm–Liouville

B. A. Wingate (✉)
Los Alamos National Laboratory, MS D413 Computer, Computational and Statistical Sciences Division and Center
for Nonlinear Studies, Los Alamos NM 87544, USA
e-mail: wingate@lanl.gov

M. A. Taylor
Sandia National Laboratories, MS318 Exploratory Simulation Technologies, Albuquerque NM 87185, USA
e-mail: mataylo@sandia.gov

1 Introduction

Because of their spectral convergence properties, Legendre and Chebyshev polynomials are the basis of choice for non-periodic, finite domains for pseudospectral methods. However, these polynomials have higher resolution near the boundaries than their Fourier-series counterparts. The term resolution usually connotes the minimum distance between their N associated collocation points that are the roots of either the N th degree polynomial for Gauss points or the roots of the derivative of the $N + 1$ polynomial for Gauss–Lobatto points. It is well known that these points cluster near the boundary creating a minimum spacing for N points of $O(1/N^2)$, while for trigonometric polynomials (Fourier Series) of degree N the points are equally spaced with minimum spacing $O(1/N)$ [1]. As a consequence, when approximating time-dependent partial differential equations with these polynomials, as N increases the time step limit is markedly better for the Fourier series in a periodic domain than for the Legendre polynomials on the finite interval.

Improving the minimum resolution length of eigenfunctions makes prolate spheroidal wave functions (PSWFs), which have a long history in signal processing [2], interesting. Because of their more uniform resolution on the finite interval, Xiao et al. [2] suggested them as an alternative to polynomials. In one dimension, PSWFs are a one-parameter family of orthogonal functions in the interval. These are the eigenfunctions of a Sturm–Liouville equation with a bandwidth parameter, c . For $c = 0$, they are the Legendre polynomials. For larger c , their Gauss–Lobatto points are more equally spaced, indicating they oscillate more uniformly than the Legendre polynomials. For time-dependent partial differential equations with explicit time stepping algorithms this leads to a larger maximum allowable time step [2–4]. When $c > c^*$, where $c^* = (\pi/2)(N + 1/2)$ is the transition bandwidth, PSWFs exhibit a “dead-zone” [3] where the PSWFs oscillate and have exponentially small amplitudes near the endpoints of the domain. The resolution length of PSWFs in one dimension can easily be estimated by computing the minimum distance between their roots.

In dimensions greater than one, analyzing the characteristic length scales is more difficult. In quadrilateral domains, it is sensible to use tensor-product combinations of one-dimensional eigenfunctions combined with a tensor-product of collocation points. In this case, the one-dimensional theory can be applied directly. In non-tensor-product domains, such as the triangle, analyzing the resolution properties of eigenspaces generated by solving Sturm–Liouville equations is more complex. One cannot generate points from the zeros of the N th eigenfunction, since there is not a single unique eigenfunction of degree N , and the zeros are now curves instead of points. Suitable interpolation points for these eigenspaces have to be found with numerical optimization [5–7].

We analyze the characteristic length scales of the eigenfunctions of Sturm–Liouville problems by using a measure, denoted by ℓ , based on the norm of the derivative operator. We first show that this measure recovers many of the results for one-dimensional polynomials and PSWFs that were previously obtained by examining the minimum distance between their roots. We then apply this measure in two dimensions. We first show that the case of tensor products of one-dimensional eigenfunctions trivially reduce to the one-dimensional results. We then move to the triangle where the eigenfunctions are non-tensor products. First, we compare the characteristic length scale of the Prorior [8–10] polynomials to the minimum distance between their Fekete points (quasi-optimal interpolation points). Then, we apply the measure to these generalized eigenfunctions on the triangle proposed in [11], where near-optimal interpolation points are unknown. The measure ℓ indicates that the eigenspaces of the generalized eigenfunctions have larger characteristic length scales than their polynomial counterparts for some eigenfunctions, but retain small characteristic length scales for others.

The ability to study the resolution properties of an eigenspace without making use of optimal interpolation points is important for domains such as the triangle where such points are not readily known. An analysis using sub-optimal interpolation points can easily give results polluted by interpolation errors arising from the sub-optimal points, such as the well known Runge phenomenon. Therefore it is important

to have a method of estimating the characteristic length scales of the eigenfunctions that does not require the use of optimal interpolation points.

2 Computing generalized eigenfunctions of Sturm–Liouville equations

Since we apply the measure of characteristic length scales to polynomial approximations of the eigenfunctions of Sturm–Liouville equations, we briefly discuss their computation. For details about this approximation, see the cited literature.

Closed-form analytic expressions for the PSWFs in one-dimension and the generalization of the Proriol polynomials in two dimensions are not known. Instead, they are usually computed by assuming a polynomial expansion and then solving for the expansion coefficients.

The domains we will use are: $X = \{x \mid -1 \leq x \leq 1\}$ on a line, $X^2 = \{(x, y) \mid -1 \leq (x, y) \leq 1\}$ on a square, and $T_r^2 = \{(x, y) \mid -1 \leq x, y; x + y + 1 \leq 1\}$ on a right triangle. In X , the equations for the polynomial expansion coefficients can be solved analytically [2, 3, 12, 13] and in T_r^2 they have been solved numerically in [11]. In both cases, the residual of the Sturm–Liouville equation will decrease exponentially fast as the number of terms in the polynomial truncation is increased [11], and thus the truncated polynomial approximation can be made very accurate. In [3], it is shown that in X , using $M = 30 + 2N$ obtains an accuracy of 10^{-20} .

In X , the PSWFs are the eigenfunctions of the Sturm–Liouville equation,

$$\frac{d}{dx}(1 - x^2) \frac{d}{dx} \phi_n^c(x) + (\lambda_n - c^2 x^2) \phi_n^c(x) = 0, \quad x \in X, \quad \phi_n^c \in H_2^2(X), \tag{1}$$

where c is the bandwidth parameter, $H_2^2(X)$ is the Hilbert space of twice-differentiable square-integrable functions on the real line, X , $\phi_n^c(x)$ is the eigenfunction, and λ_n are the eigenvalues.

To solve this eigenvalue problem, we approximate the PSWF ϕ_n^c with a series of orthonormal polynomials. Let $P_M = \text{span}\{x^m \mid 0 \leq m \leq M\}$ be the space of polynomials in x up to degree M , and let $\{g_m(x), m = 0 \dots M\}$ be an orthonormal basis for P_M . We denote the expansion coefficients of ϕ_n^c by $(\widehat{\phi_n^c})_m$, so that

$$\phi_n^c \approx \sum_{m=0}^M (\widehat{\phi_n^c})_m g_m. \tag{2}$$

As many investigators have pointed-out, $M > N$ is required for an accurate representation of ϕ_n^c . For details about computing polynomial approximations to PSWFs, see [2, 3, 12]. In this work, all one-dimensional results are computed using the Maple(TM)¹ symbolic manipulation software and taking $M = 30 + 3N$. For the cases examined in this paper, this truncation is good enough to compute ℓ_{sv} , introduced in Sect. 4, to within three decimal places.

In X^2 , the square, we use tensor-product combinations of the one-dimensional eigenfunctions described above.

For T_r^2 , a generalization of the one-dimensional Sturm–Liouville equation was given in [11] as,

$$\begin{aligned} &\frac{\partial}{\partial x} \left((1+x) \left[(1-x) \frac{\partial}{\partial x} - (1+y) \frac{\partial}{\partial y} \right] \right) \\ &+ \frac{\partial}{\partial y} \left((1+y) \left[(1-y) \frac{\partial}{\partial y} - (1+x) \frac{\partial}{\partial x} \right] \right) \phi_n^c(x, y) + (\lambda_n - c^2 h) \phi_n^c(x, y) = 0, \end{aligned} \tag{3}$$

where

$$h = \frac{3}{16} \left(\left(x + \frac{1}{3} \right)^2 + \left(y + \frac{1}{3} \right)^2 + \left(x + y + \frac{2}{3} \right)^2 \right), \quad (x, y) \in T_r^2, \quad \phi_n^c(x, y) \in H_2^2(T_r^2). \tag{4}$$

¹ Maple is a trademark of Waterloo Maple Inc.

Here $H_2^2(T_r^2)$ is the Hilbert space of twice-differentiable functions that are square-integrable in T_r^2 . Again, we denote $\phi_n^c(x, y)$ as the eigenfunctions and λ_n as the eigenvalue. When $c = 0$, the eigenfunctions of this equation are the Proriol polynomials.

To solve this eigenvalue problem, we approximate the eigenfunctions with a series of $M + 1$ polynomials in the space of polynomials in two variables of degree d , $P_M = \{\text{span}(x^m y^n) \mid 0 \leq (m, n), m + n \leq d\}$. The dimension of this space is $M + 1 = (d + 1)(d + 2)/2$. We denote an orthonormal basis of P_M by $\{g_m(x, y), m = 0 \dots M\}$ and expand the eigenfunctions as,

$$\phi_n^c \approx \sum_{m=0}^M (\widehat{\phi_n^c})_m g_m. \tag{5}$$

For good accuracy, $M > N$ is required. Following [11] we choose M large enough so that the residual of Eq. 3 is less than 10^{-10} .

Finally, we denote the $N + 1$ dimensional eigenspace by $P_{N,c}$, where

$$P_{N,c} = \text{span}\{\phi_n^c, \quad 0 \leq n \leq N\}.$$

Note that the Sturm–Liouville equations are self-adjoint, so their eigenfunctions are orthogonal in the usual L_2 norm,

$$\|f\|^2 = \int f^2,$$

where the integration is over X, X^2 or T_e . In this paper, $\|\cdot\|$ will represent this L_2 norm, and the eigenfunctions ϕ_n^c are normalized so that $\|\phi_n^c\| = 1$.

3 Characteristic length scales of Sturm–Liouville eigenfunctions, ϕ_n^c

Let f be a differentiable function and define the characteristic length scale, $\ell(f)$, in the x -direction to be

$$\ell(f) = \frac{\|f\|}{\|\partial f / \partial x\|}. \tag{6}$$

This length scale is a measure of the variation of the gradient of the function. It is commensurate with the idea that the higher the oscillations of the function, the steeper the gradient, and subsequently, the smaller the length scale. For example the N th degree Fourier function has N troughs, N peaks, and can represent a wave number N solution on a periodic domain exactly.

As an example of computing the characteristic length scale of eigenfunctions without using optimal interpolation points, we consider the simple case of the Fourier series by examining its Sturm–Liouville equation,

$$\frac{d^2}{dx^2} \phi_n(x) + \lambda_n \phi_n(x) = 0, \quad 0 \leq x \leq 2\pi, \quad \phi_n(x) \in S_N, \tag{7}$$

where S_N is the space of trigonometric polynomials of degree $N/2$ defined as, $S_N = \text{span}\{e^{inx} \mid -N/2 \leq n \leq N/2 - 1\}$. Multiplying (7) through by ϕ_n and integrating over the domain, we find

$$\lambda_n = \frac{\|\partial \phi_n / \partial x\|^2}{\|\phi_n\|^2}. \tag{8}$$

From (6) and since $\lambda_n = n^2$, $\ell(\phi_n) = 1/n$.

4 Minimum characteristic length scale of $P_{N,c}$

We now define a minimum characteristic length scale for the space $P_{N,c}$ by considering the minimum length scale of all functions $f \in P_{N,c}$,

$$\ell_{sv} = \min_{f \in P_{N,c}} \ell(f) = \min_{f \in P_{N,c}} \frac{\|f\|}{\|\partial f / \partial x\|} \tag{9}$$

and thus

$$\frac{1}{\ell_{sv}} = \max_{f \in P_{N,c}} \frac{\|\partial f / \partial x\|}{\|f\|} = \|\partial / \partial x\|, \tag{10}$$

where $\|\partial / \partial x\|$ is the L_2 operator norm of the derivative operator in the x direction acting on $P_{N,c}$. Though we have two directions in the square and triangle (both x and y), we keep the one-dimensional measure for simplicity by examining ℓ_{sv} in one direction at a time. We denote ℓ_{sv} in the x -direction as $\|\partial / \partial x\|^{-1}$ and in the y -direction as $\|\partial / \partial y\|^{-1}$.

The length scale ℓ_{sv} is easily computed by taking the largest singular value of a properly constructed matrix B . To compute B , we start with the expansion of an arbitrary function $f \in P_{N,c}$

$$f = \sum_{n=0}^N \hat{f}_n \phi_n^c. \tag{11}$$

Now consider the polynomial expansions of ϕ_n^c from either Eq. 2 or Eq. 5. Under this approximation, ϕ_n^c is a polynomial in P_M , so its derivative is also a polynomial in P_M and thus

$$\frac{\partial \phi_n^c}{\partial x} = \sum_{m=0}^M B_{mn} g_m \quad B_{mn} = \int \frac{\partial \phi_n^c}{\partial x} g_m.$$

We note that care must be taken in computing the derivatives of polynomial approximations to eigenvalue problems [14, 15]. Applying $\partial / \partial x$ to (11) gives

$$\frac{\partial f}{\partial x} = \sum_{n=0}^N \hat{f}_n \sum_{m=0}^M B_{mn} g_m = \sum_{m=0}^M \left(\sum_{n=0}^N B_{mn} \hat{f}_n \right) g_m.$$

Applying Parseval’s theorem to this equation and to (11) gives

$$\|f\|^2 = \sum_{n=0}^N \hat{f}_n^2 \quad \left\| \frac{\partial f}{\partial x} \right\|^2 = \sum_{m=0}^M \left(\sum_{n=0}^N B_{mn} \hat{f}_n \right)^2.$$

Substituting these relations in (10) gives

$$\|\partial / \partial x\| = \max_{f \in P_{N,c}} \frac{\left(\sum_{m=0}^M \left(\sum_{n=0}^N B_{mn} \hat{f}_n \right)^2 \right)^{1/2}}{\left(\sum_{n=0}^N \hat{f}_n^2 \right)^{1/2}},$$

where the right-hand side is simply the discrete L_2 norm of the rectangular matrix B_{mn} , which is given by the largest singular value of B_{mn} . Thus, we have shown that

$$\frac{1}{\ell_{sv}} = \max \text{sv}(B_{mn}).$$

The advantage of this approach is that the minimum characteristic length scale of the eigenspace $P_{N,c}$ can be measured by simply computing the largest singular value of the matrix B_{mn} . Computing this matrix requires only evaluating inner products of polynomials.

5 Results

In this section, we present both one- and two-dimensional results. First, we apply ℓ and ℓ_{sv} to the one-dimension PSWFs and show that they reproduce known results. Next, we examine the tensor-product generalizations of one-dimensional eigenfunctions, and show they trivially reduce to the one-dimensional results. Then, in T_r^2 , we compare ℓ_{sv} to the minimum distance between their Fekete points (quasi-optimal interpolation points) and show that ℓ_{sv} can estimate the characteristic length scale just as in the one-dimensional case. Lastly, we apply the measure to the generalized eigenfunctions on the triangles where optimal interpolation points are unknown.

5.1 ℓ and ℓ_{sv} in one-dimension

We investigate the behavior of ℓ and ℓ_{sv} in one-dimension for the purpose of showing they are a reasonable means of assessing the characteristic length scales of eigenfunctions of Sturm–Liouville problems.

Figure 1 shows the results in one dimension. Panel (a) shows a graph of $\ell/\ell_{eq} = \ell(\phi_n^c)/\ell_{eq}$ versus c for values of N ranging from 4 (top curve) to 9 (bottom curve). The measure is normalized by the length scale associated with uniform resolution, $\ell_{eq} = 1/(N + 1)$. Panel (b) is similar to panel (a) except that ℓ_{sv}/ℓ_{eq} is represented on the vertical axes instead of ℓ/ℓ_{eq} . Panel (c) shows both length scales versus c/c^* where c^* is the transition bandwidth. These three panels show a rapid increase in the length scale in the neighborhood of $c/c^* \approx 3/4$. As $\ell(\phi_n^c)/\ell_{eq}$ and ℓ_{sv}/ℓ_{eq} approach unity, the mean resolution of ϕ_n approaches that of a function which oscillates uniformly. The most uniform length scales, then, occur at $c/c^* \approx 1$.

As c/c^* becomes large, the length scales become small, revealing the “dead-zone”. As is evident in panel 1 (c), ℓ_{sv}/ℓ_{eq} provides a lower bound for ℓ/ℓ_{eq} , as expected.

Panel 1 (d) shows a log–log plot of the length scale ℓ_{sv} versus N for five values of c/c^* . For $c/c^* = 0$, the slope is shallower than $O(1/N^2)$, the minimum distance between Gauss–Lobatto collocation points. This is not surprising since ℓ_{sv} is an average measure of the characteristic length scale, rather than a minimum. It also shows that the rate of decrease of the characteristic length scale is somewhat slower for $c/c^* = 1$ than it is for $c/c^* = 0$.

Previous investigators have found these results by examining waterfall plots of the PSWFs [3] or through asymptotic expansions [16, 17]. We conclude we may use this measure as a way of estimating the resolution properties of PSWFs and proceed to present two-dimensional results.

5.2 ℓ and ℓ_{sv} in two dimensions

We begin with the tensor-product generalizations on the square. Then, we look at non-tensor-product eigenfunctions, Prorior polynomials, in the triangle and compare ℓ_{sv} with the minimum spacing between Fekete points, which are quasi-optimal interpolation points. Lastly, we examine ℓ and ℓ_{sv} for non-polynomial generalizations of the Prorior eigenfunctions where even quasi-optimal interpolation points are not known.

5.2.1 Tensor products of PSWFs on the square

For squares, tensor products of one-dimensional eigenfunctions are commonly used. In this case we write the function, f , as,

$$f = \phi_n^c(x) \phi_m^c(y) \in X^2, \quad (12)$$

where ϕ_i^c are the eigenfunctions of the Sturm–Liouville problem in Eq. 1. By substituting f in the definition of $\ell(f)$, we see that $\ell(f)$ reproduces the one-dimensional results.

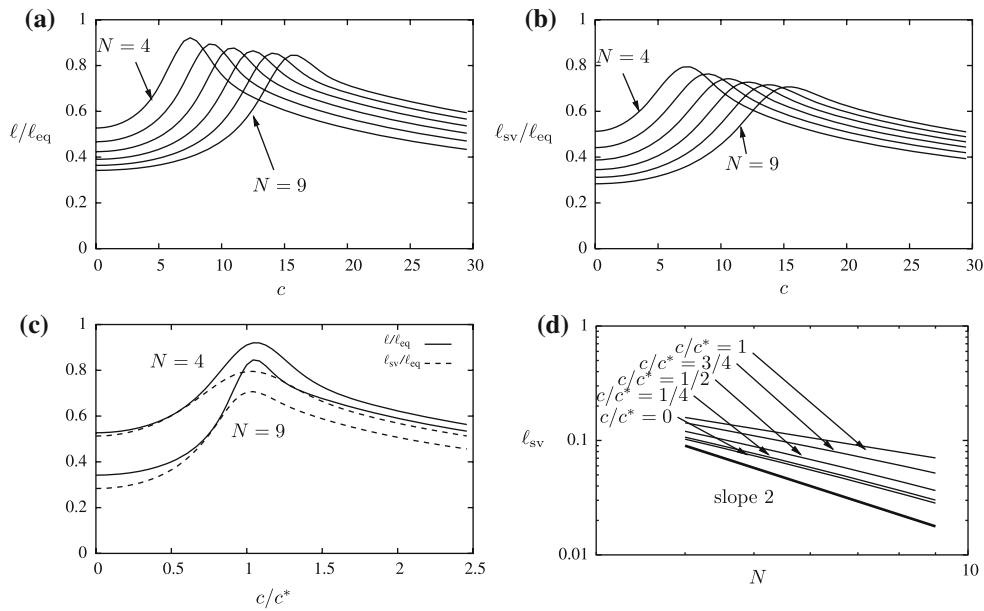


Fig. 1 (a) shows a graph of ℓ/ℓ_{eq} versus c for different maximum degrees of the PSWF in one dimension. The top curve is for the PSWF of maximum degree $N = 4$, then increases in N until it reaches $N = 9$. The measure is normalized by $\ell_{eq} = 1/(N + 1)$, the length scale associated with uniform resolution. (b) is similar to (a) except that ℓ_{sv}/ℓ_{eq} is represented on the vertical axes instead of ℓ/ℓ_{eq} . (c) shows both ℓ/ℓ_{eq} and ℓ_{sv}/ℓ_{eq} , versus c/c^* where c^* is the transition bandwidth. These three panels show a rapid increase in the length scale in neighborhood of $c/c^* \approx 3/4$. As ℓ/ℓ_{eq} and ℓ_{sv}/ℓ_{eq} approach 1, their resolution approaches that of a function which oscillates uniformly. The most uniform length scales, then, occur at $c/c^* \approx 1$. As c/c^* becomes large, the length scales become small, revealing the “dead-zone”. (d) shows a log–log plot of ℓ_{sv} versus N for five different values of c/c^* . For $c/c^* = 0$ the slope is a little shallower than $O(1/N^2)$, the minimum distance between Gauss–Lobatto collocation points. When $c/c^* \approx 1$ the slope is even shallower, showing that ℓ_{sv} is larger at higher degrees of N than the $c/c^* = 0$ case

5.2.2 Prorior eigenfunctions on the triangle

One of the motivations for proposing the measures ℓ and ℓ_{sv} of the characteristic length scale of eigenfunctions is that assessing their resolution properties by using roots of the eigenfunctions is sometimes impossible in higher dimensions. For non-tensor-product eigenfunctions, finding good interpolation points is more difficult than finding the roots of the eigenfunctions. First, for each eigenvalue there is no longer a unique eigenfunction. Instead, there is a family of eigenfunctions for each eigenvalue. Second, the zeros of the eigenfunctions are curves in space, not points. Therefore, we rely on numerically computed, quasi-optimal interpolation points, such as Fekete [5, 7] or electrostatic [6] points. However, in order to assess whether ℓ_{sv} does a reasonably good job in two dimensions, we compare it to the minimum spacing between Fekete points. Figure 2 shows a plot of ℓ_{sv} computed for the Prorior polynomials, compared to the measure of the minimum spacing between their Fekete points. The minimum distance between Fekete points is noisy at higher degrees because Fekete points are numerically computed and only approximately optimal. However, they give a distribution that is generally shallower than the square of the degree, while ℓ_{sv} is shallower still. This result is similar to the one-dimension case shown in Fig. 1(d).

5.2.3 Generalized eigenfunctions on the triangle

We now show results of applying this measure to the eigenspaces P_N^c generated by the Sturm–Liouville equation in the triangle. Figure 3 shows our results for $N = 9$. In this case, we show the length scale of the eigenfunctions with the 10 largest eigenvalues. For $c = 0$, these are the 10 Prorior polynomials of highest

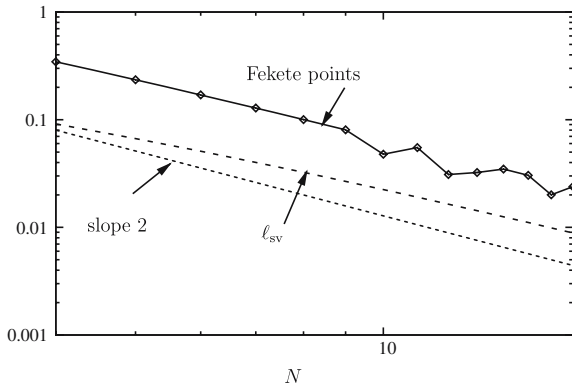


Fig. 2 This figure compares the minimum distance between Fekete points for the Proriol polynomials (top line) with the measure ℓ_{sv} (middle line). The minimum distance between Fekete points has roughly slope 2 (the lower line), while the characteristic length, ℓ_{sv} , has a shallower slope. This result is similar to the one-dimensional case for $c/c^* = 1$ in Fig. 1(d)

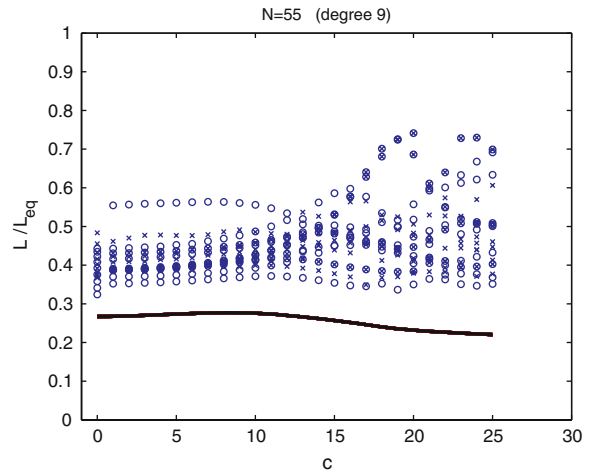


Fig. 3 The length scale $\ell(\phi_n^c)$ of the 10 eigenfunctions with largest eigenvalues in $P_{55,c}$ is shown. Circles are used for the length scale in the x -direction and crosses for the y direction. The solid line shows $\|\partial/\partial x\|^{-1}$ and $\|\partial/\partial y\|^{-1}$ which agree to within roundoff error. $L_{eq} = 1/(N+1)$ is the length scale associated with a uniform distribution of points along a line. For the case shown above the dimension of the space is $(N + 1)(N + 2)/2 = 55$, since $N = 9$

degree nine. We show the length scale in both the x - and y -direction, as well as ℓ_{sv} . We have normalized the length scales by the length scale associated with equally spaced points on the line, $L_{eq} = 1/(N + 1)$. The length scale in other directions produces similar results. While some eigenfunctions exhibit an increase in the characteristic length scale, the increase is not as proportionally large as in the one-dimensional PSWFs. More importantly, other eigenfunctions show no increase in their characteristic length scale. This suggests that for some values of c , the eigenspace $P_{N,c}$ contains modes with more uniform resolution and thus should better approximate functions such as sinusoids than $c = 0$, confirming the numerical results in [11]. But it also suggests that the space retains some of the modes with length scales as small as in the $c = 0$ case, suggesting that criteria sensitive to the minimum length scales (such as the CFL restriction on the time step) will not be improved.

6 Concluding remarks

The characteristic length scales of non-tensor-product eigenfunctions cannot usually be measured by examining the minimum distance between their roots. Furthermore, quasi-optimal interpolation points for these kinds of eigenfunctions are frequently unknown. In this paper, we have used an integral measure of the characteristic length scale, ℓ , to estimate their resolution properties. This measure has the advantage of not requiring a set of quasi-optimal interpolation points. We have shown that this measure reproduces one-dimensional results for PSWFs and two-dimensional results for Proriol polynomials, making it a candidate measure for eigenfunctions whose optimal interpolation points are not known. Finally, we applied this measure to the generalized eigenfunctions proposed by [11]. In this measure, the eigenspace contains some functions with more uniform resolution than the Proriol polynomials, but at the same time retains some eigenfunctions that have length scales as small as those contained in the Proriol polynomials.

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