Journal of Computational Physics 229 (2010) 2046–2060

Contents lists available at ScienceDirect

Journal of Computational Physics

journal homepage: www.elsevier.com/locate/jcp

Galerkin orthogonal polynomials

Philip W. Livermore *

Institute of Geophysics and Planetary Physics, Scripps Institution of Oceanography, UCSD, La Jolla, CA 92093-0225, USA

ARTICLE INFO

Article history:
Received 19 May 2009
Received in revised form 12 November 2009
Accepted 13 November 2009
Available online 26 November 2009

Keywords:
Galerkin
Jacobi polynomials
Orthogonality
Gram-Schmidt
Spectral method
Polar coordinates
Sobolev norm

ABSTRACT

The Galerkin method offers a powerful tool in the solution of differential equations and function approximation on the real interval $[-1, 1]$. By expanding the unknown function in appropriately chosen global basis functions, each of which explicitly satisfies the given boundary conditions, in general this scheme converges exponentially fast and almost always supplies the most terse representation of a smooth solution. To date, typical schemes have been defined in terms of a linear combination of two Jacobi polynomials. However, the resulting functions do not inherit the expedient properties of the Jacobi polynomials themselves and the basis set will not only be non-orthogonal but may, in fact, be poorly conditioned. Using a Gram-Schmidt procedure, it is possible to construct, in an incremental fashion, polynomial basis sets that not only satisfy any linear homogeneous boundary conditions but are also orthogonal with respect to the general weighting function $(1-x)^{\alpha}(1+x)^{\beta}$. However, as it stands, this method is not only cumbersome but does not provide the structure for general index n of the functions and obscures their dependence on the parameters (α, β). In this paper, it is shown that each of these Galerkin basis functions, as calculated by the Gram-Schmidt procedure, may be written as a linear combination of a small number of Jacobi polynomials with coefficients that can be determined. Moreover, this terse analytic representation reveals that, for large index, the basis functions behave asymptotically like the single Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$. This new result shows that such Galerkin bases not only retain exponential convergence but expedient function-fitting properties too, in much the same way as the Jacobi polynomials themselves. This powerful methodology of constructing Galerkin basis sets is illustrated by many examples, and it is shown how the results extend to polar geometries. In exploring more generalised definitions of orthogonality involving derivatives, we discuss how a large class of differential operators may be discretised by Galerkin schemes and represented in a sparse fashion by the inverse of band-limited matrices.

1. Introduction

Spectral methods are a widely used tool in the solution of differential equations, function approximation and variational problems [1,2]. Their utility is based on the fact that if the solution sought is smooth, usually only a few terms in an expansion of global basis functions are needed to represent it to high accuracy. This efficiency comes about because the spectral coefficients, f_n, typically tend to zero faster than any algebraic power of their index n, showing either exponential or sometimes super-exponential convergence [3]. On the non periodic canonical interval $[-1, 1]$, the Jacobi polynomials are a well-known class of polynomials exhibiting spectral convergence, of which particular examples are Chebyshev polynomials of the first and second kinds, and Legendre polynomials [3]. Chebyshev polynomials are often a popular choice since, via their links with Fourier methods, they have a fast transform.

* Present address: School of Earth and Environment, University of Leeds, Leeds LS2 9JT, UK.
E-mail address: P.W.Livermore@leeds.ac.uk

0021-9991/$ - see front matter © 2009 Elsevier Inc. All rights reserved.
doi:10.1016/j.jcp.2009.11.022

When approximating a given function by a spectral expansion, the choice of which Jacobi polynomials to use can rest on the required asymptotic behaviour of the error. For example, Chebyshev polynomials of the first kind are well-known to minimise the maximum error between any function and its approximant, the so-called minimax or L^∞ norm characteristic [4,5]. Such an expedient property has led to widespread use of Chebyshev approximants in numerical computation [6]. Lesser known but, in the appropriate case no less useful, is the property that the Chebyshev polynomials of the second kind minimise the error in the L^1 norm, that is, the integrated absolute error between the function and its approximant. These properties are intimately tied to certain properties of the polynomials themselves: Chebyshev polynomials of the first kind are equal-ripple (uniform oscillations) and those of the second kind are equal-area (the area under the curve between any two consecutive zeros is constant). Lastly, Legendre polynomials minimise the error between any function and its approximant in the L^2 norm although this is not associated with any obvious graphical property of the polynomials themselves.

Physical problems almost always involve known boundary conditions which can be fully exploited in a Galerkin method [7,8,3]. Such a scheme adopts an expansion in terms of a global basis set constructed so that each member explicitly satisfies the boundary conditions; by encoding this additional information, out of all numerical methods, this approach almost always provides the most terse numerical representation. If an analytic solution of a differential equation is known but difficult to compute, it is expedient to write it in terms of a spectral expansion (for instance in Chebyshev polynomials) which, after finding the coefficients, is easy to evaluate. In this paper, we shall see such an approximation method can be extended by using an expansion in terms of an exponentially convergent orthogonal Galerkin basis. Furthermore, as in functional approximation by Jacobi polynomials, the principal error stems from the first ignored term in the expansion which can be chosen in an optimal fashion, for instance, to be quasi-equal-ripple and therefore for the approximant to minimise the L^∞ error.

Unlike a spectral expansion of a known function, the error in the solution of a differential equation or variational problem is not well approximated by the first ignored term (since the error contaminates all coefficients). It is therefore not possible to prescribe in advance, by choice of the basis set, the asymptotic behaviour of the error. However, as we shall see subsequently, Galerkin schemes remain a useful tool since, not only do they converge exponentially fast but, because the boundary conditions are already encoded, in general they converge faster than canonical spectral methods. In a traditional Galerkin method, a differential equation is discretised by imposing an orthogonality condition to the same set of basis functions. However, other variants include imposing orthogonality to a different set of functions in the so-called Petrov-Galerkin scheme and, by extending the basis sets to those of compact support, Galerkin schemes form the foundation of the finite-element method [9]. By adopting a Galerkin expansion at the outset, often subsequent analysis is eased since the boundary conditions may, essentially, be dispensed with. By contrast, in other pseudospectral schemes that could be employed to solve differential equations (e.g. Chebyshev-tau or a collocation method), the boundary conditions are carried through to the end of the calculation where they are imposed explicitly as additional rows of the discretised matrix system.

There are several particular cases where Galerkin expansions have the greatest utility. First are problems where terseness of the solution is pivotal. Such a case can arise when forming low-order models of a system, or when using symbolic computation to produce an approximation to the solution. To expedite the solution of matrix problems symbolically, the matrix size should be reduced as much as possible, a property which Galerkin methods can readily provide. Second are variational problems, where often integration by parts of the raw equations produces awkward boundary terms. Unless one is very lucky, the boundary conditions cannot be used to evaluate these terms and no further progress is possible. Within a Galerkin method, such boundary terms can always be evaluated and a matrix system then constructed [10]. Third, Galerkin methods often exhibit the lowest condition number dependence on matrix size. Such an issue may arise when solving a problem to very high resolution. For instance, although a standard Chebyshev-tau method may theoretically be capable of resolving a fine-scale solution, its numerical discretisation may be too ill-conditioned and any answer swamped with numerical error in finite precision (although, solving the system using high precision will give an accurate answer). Galerkin methods often have a low scaling of the condition number with matrix size, thus minimising the computational error and allowing high resolution in finite precision. The main drawback of Galerkin methods is that, in general, no fast-transform exists and, until now, there has been no generally accepted method of constructing the required basis sets for arbitrary boundary conditions.

Galerkin schemes are easily constructed when considering linear homogeneous boundary conditions. Note that if the given boundary conditions are not homogeneous they can always be made so with the addition of an appropriate function to the unknown solution, with the associated modification of the equations. To date, typical schemes involve forming a linear combination of a Jacobi polynomial (usually a Chebyshev polynomial, $T_n(x)$) with one of neighbouring index or some fixed low-order polynomial in order to satisfy the required conditions [11,7,3]. For example, the following are two possible choices of basis sets that satisfy the boundary condition $f'(1) = 0$:

$$\phi_n(x) = T_n(x) - n^2 T_1(x), \qquad \chi_n(x) = (n-1)^2 T_n(x) - n^2 T_{n-1}(x).$$

It is clear that $\phi_n(x)$ becomes increasingly ill-conditioned as n increases since, when normalised, $\phi_n(x) \to T_1(x) = x$ as $n \to \infty$ which is independent of n. The second case, $\chi_n(x)$, is better conditioned but forms a basis set that is neither orthogonal nor close to equal-ripple. Thus in recombining Chebyshev polynomials, many of their optimal properties have been lost.

An alternative method to construct a basis set is to use a Gram-Schmidt procedure in the following way. The lowest-degree polynomial that satisfies the boundary conditions is $\Psi_1(x) = 1$ (up to a normalisation). The next element $\Psi_2(x)$ is written as an arbitrary quadratic in x, whose coefficients are determined by imposing (i) the boundary condition and (ii) orthogonality to $\Psi_1(x) = 1$. Note that we need to jump degree from 0 to 2: there is no non-trivial linear form that will satisfy

these two conditions. In fact, for a general first order boundary condition, $\Psi_1(x)$ is linear in x which, for this particular case, reduces to a constant. We are at liberty to define orthogonality in any way we please; one such choice is the weighted integral over the domain between two functions f and g:

$$\int_{-1}^{1} f(x)g(x)w(x)dx = 0,$$

where we shall choose the arbitrary weight function as $w(x) = (1-x^2)^{-1/2}$ for reasons that will shortly become apparent. This procedure defines $\Psi_2 = 1 + 4x - 2x^2$ up to a normalisation. By defining $\Psi_3(x)$ as a cubic whose coefficients are chosen by imposing the boundary condition and orthogonality to Ψ_1 and Ψ_2, it is clear that, by continuing in this fashion, an orthogonal Galerkin set can be constructed:

$$\{1, 1 + 4x - 2x^2, 9 - 15x - 18x^2 + 17x^3, \ldots\}. \tag{1}$$

Two points are immediately apparent. First, there is no means available of determining the asymptotic properties of the basis functions. Put another way, it is impossible to know *in advance* how Ψ_n will behave without first computing it (and, in order to do so, every $\Psi_m, m \leqslant n$). Second, although guaranteed to produce an orthogonal set, there is no evident reason why an expansion in such a basis set will converge exponentially fast. In addition, although not obvious from the computations of Ψ_1, Ψ_2, Ψ_3 above, in general this approach is very cumbersome, requiring computer algebra to compute Ψ_n. This is because the polynomial coefficients grow rapidly with degree and lead to severe accuracy problems in finite precision.[1] We shall shortly return to this example after introducing some further concepts that are central to this paper.

In certain special cases Galerkin bases can be written down in closed form, for which the most basic example occurs when considering the boundary condition $f(1) = 0$. A basis set capable of representing a function on $[-1, 1]$, which vanishes at $x = 1$ and for which all members are mutually orthogonal with respect to the weight function $w(x) = (1-x)^{\alpha}(1+x)^{\beta}$ may be written as

$$\Psi_n(x) = (1-x)P_{n-1}^{(\alpha+2,\beta)}(x), \quad n \geqslant 1,$$

since $\Psi_n(1)$ clearly vanishes and, applying the standard orthogonality relation of Jacobi polynomials, we see that

$$\int \Psi_n(x)\Psi_m(x)w(x)dx = \int_{-1}^{1} P_{n-1}^{(\alpha+2,\beta)} P_{m-1}^{(\alpha+2,\beta)} (1-x)^{\alpha+2}(1+x)^{\beta}dx = h_n\delta_{nm}$$

for some constants h_n. Using the standard Jacobi-polynomial index recurrence relations (A.1) and (A.3) we can write

$$\Psi_n(x) = \sum_{i=1}^{3} c_i(n) P_{n+1-i}^{(\alpha+2,\beta)}(x), \quad n \geqslant 2, \tag{2}$$

for coefficients $c_i(n)$ which take the (unnormalised) form

$$\begin{aligned} c_1(n) &= n(\beta+\alpha+2n)(\alpha+\beta+n+2),\\ c_2(n) &= -(\beta+1+2n+\alpha)(2n^2+2n\beta+2n+2n\alpha+\beta\alpha+\alpha^2+3\alpha+2+\beta),\\ c_3(n) &= (\alpha+n+1)(\beta+n-1)(\beta+\alpha+2n+2), \end{aligned}$$

for $n \geqslant 2$ and $\Psi_1(x) = 1 - x$. Note that the c_i take on the ratio $[1, -2, 1]$ as $n \to \infty$, a property that has great significance. By applying index recurrence identity (A.3) twice, we see that

$$P_n^{(\alpha,\beta)}(x) \sim P_n^{(\alpha+2,\beta)}(x) - 2P_{n-1}^{(\alpha+2,\beta)}(x) + P_{n-2}^{(\alpha+2,\beta)}(x) \tag{3}$$

as $n \to \infty$, an expression which involves the same ratio of coefficients. It follows immediately that, up to a normalisation, $\Psi_n(x) \sim P_n^{(\alpha,\beta)}(x)$ for large n (except possibly in boundary layers). As we explore further examples in this paper, Pascal-triangle-like ratios of the c_i will continue to spring up, which point to a simple asymptotic description, as here.

Suppose now we consider constructing a second basis set, from scratch, that satisfies $f(1) = 0$ and is of the form (2). This is a severely truncated Gram-Schmidt method where the nth basis function relies on only three, rather than $n+1$, unknown coefficients which are found by imposing the boundary condition, some normalisation condition (which for the moment we ignore) and orthogonality only to the first polynomial element $1 - x$. It is clear that such a scheme must reconstruct the mutually orthogonal basis set that we first thought of; however, in contrast with a typical Gram-Schmidt construction, we only impose orthogonality with respect to one polynomial rather than all the polynomials of lesser degree. The fact that orthogonality extends to all possible pairings of basis functions is remarkable, a property termed *auto-orthogonality*.

We now extend and revisit the case considered previously with the explicit Gram-Schmidt process and the boundary condition $f'(1) = 0$. Instead of expanding in generalised polynomials as before, we look for a vastly truncated basis set of the form (2) with $\alpha = \beta = -1/2$. The coefficients c_i are found by imposing (i) the boundary condition, (ii) orthogonality with respect to $\Psi_1(x)$ and (iii) an arbitrary normalisation. It is far from evident that the set of Ψ_n so produced will be mutually

[1] This property is due to the fact, as we shall see shortly, that Ψ_n has a terse representation in terms of Jacobi polynomials whose monomial coefficients are known to increase exponentially with n.

orthogonal, since we have merely only imposed orthogonality to Ψ_1. But *auto-orthogonality* holds here also and this prescription is sufficient to generate an orthogonal set. The coefficients c_i are

$$c_1 = 4n(n-1)(2n-1)(3n^2-3n-1),$$
$$c_2 = -4n^2(n-1)(-13+12n^2),$$
$$c_3 = (2n-3)(1+2n)^2(3n^2+3n-1),$$

and take on the ratio [1, −2, 1] as $n \to \infty$. It follows from (3) that

$$\Psi_n(x) \sim P_n^{(-1/2,-1/2)}(x) = T_n(x),$$

that is, the basis functions become asymptotically similar to the Chebyshev polynomials themselves. This suggests that the basis functions converge exponentially fast, which we find to be the case, and also quasi-equal-ripple,[2] asymptotically reducing the error between any function and its approximant in the L^∞ norm. In this case, the (normalised) basis functions satisfy

$$\int_{-1}^{1} \Psi_n \Psi_m (1-x^2)^{-1/2} dx = \delta_{nm},$$

which motivated the choice of weight function in the standard Gram-Schmidt construction of (1). It is clear, however, that other choices of weight function are possible too. For instance, the weight function $w(x) = (1-x^2)^{1/2}$, corresponding to $\alpha = \beta = 1/2$, would result (with modified c_i) in basis functions that behave, as $n \to \infty$, like U_n, Chebyshev polynomials of the second kind.

This terse representation of Galerkin basis sets extends to boundary conditions of arbitrary order at either end (or both ends) of the interval $[-1, 1]$ and weight function $(1-x)^\alpha(1+x)^\beta$ for arbitrary (α, β). A proof of the construction of these auto-orthogonal basis sets along with their expedient properties is given, in so far as is currently possible, in an accompanying paper [12]. However, rather than dwell on formal proofs, it is the purpose of this paper to guide the reader through a brief tour of examples, showing how to construct such a basis set with any given set of boundary conditions.

A lengthy compendium of Galerkin basis sets that satisfy physically motivated boundary conditions is given in the technical report [13] accessible at the permanent URL http://escholarship.org/uc/item/9vk1c6cm. A quick inspection of this resource would immediately reveal that, in general, the formulae for the Jacobi coefficients, c_i, appearing in cases where either (α, β) and/or the boundary conditions (of a certain order) were kept arbitrary are extremely lengthy. We do not expect a user to type out these expressions, but merely to copy and paste as required from this online resource. The remainder of the paper is arranged as follows. In the next section, it is shown how to construct a variety of basis sets on the domain $[-1, 1]$, with boundary conditions imposed at either one end of the interval or both. In Section 3, the extension of these results to a polar geometry, where regularity of the basis functions must also be taken into account, is discussed. Lastly, in Section 4 we consider more general Sobolev-type orthogonality, involving the derivatives of functions. The last section comprises a brief discussion of the mathematical framework on which these results rest, and possible future research directions.

2. Construction of orthogonal Galerkin polynomials on [−1, 1]

In the following section, it is shown how to construct a family of orthogonal polynomials on $[-1, 1]$ that satisfy arbitrary boundary conditions involving derivatives of given maximum degree. By making a suitable linear transformation, all the results extend to the interval $[a, b]$, leaving invariant the number and the maximum derivative appearing in the boundary conditions imposed (although their precise form will change). It is only possible to specify boundary conditions at the ends of the domain: $x = \pm 1$. Brief experimentation shows that auto-orthogonality does not hold with either interior boundary conditions or replacing any homogeneous boundary condition by a homogeneous integral condition. In fact, it is useful to separate so-called one-sided boundary conditions (that is, imposed at either $x = 1$ or $x = -1$ but not both), from the general mixed so-called two-sided case. This difference is not only important in what is accessible to proof in [12], but the one-sided case affords considerable simplification of the basis set construction.

2.1. One sided boundary conditions

Consider a set of M boundary conditions involving derivatives of the function at $x = 1$ only and of degree at most $N-1$. Clearly M cannot exceed N unless there is degeneracy in the conditions. The nth basis function can be written

$$\Psi_n(x) = \sum_{i=1}^{N+1} c_i(n) P_{M+n-i}^{(\alpha+N,\beta)}(x), \quad n \geqslant N - M + 1, \tag{4}$$

but it is clear that, for $n < N - M + 1$, this form breaks down since Jacobi polynomials must have a non-negative degree. The first few basis functions must instead be found by using the explicit Gram-Schmidt process, by determining the coefficients c_i in

[2] The qualifier "quasi" refers to a Gibbs type departure from strict equal-ripple (or equivalent property) and that is confined to narrow boundary layers at each end.

$$\Psi_n(x) = \sum_{i=1}^{M+n} c_i(n) P_{i-1}^{(\alpha+N,\beta)}(x), \quad n \leqslant N-M, \tag{5}$$

and imposing the M boundary conditions, one normalisation condition, and orthogonality to Ψ_m with weight $w(x)$ for $1 \leqslant m < n$. Note that the construction of the first $N-M$ basis functions is equivalent to that in (1), but here Jacobi polynomials rather than monomials are used. It is clear that the basis set discussed in the introduction that satisfies $f'(1) = 0$ is of the above form with $N = 2, M = 1$. It is also apparent that increasing M does not change the essential structure of the basis, but merely increases the degree of all the polynomials; this is caused by providing each Ψ_n with the degrees of freedom it needs to satisfy the extra boundary conditions. The functions Ψ_n have the property that

$$\int_{-1}^{1} \Psi_n(x)\Psi_m(x)(1-x)^{\alpha}(1+x)^{\beta}dx = h_n\delta_{nm} \tag{6}$$

for some h_n determined by the choice of normalisation. In addition, the c_i have a Pascal-triangle-like asymptotic ratio leading to

$$\Psi_n(x) \sim P_{n+M-1}^{(\alpha,\beta)}(x).$$

Thus the asymptotic form of any Galerkin basis function is that of a single Jacobi polynomial. A similar construction holds if the boundary conditions are imposed only at $x = -1$. We may simply use the transformation $x \to -x$ and the fact that

$$P_n^{(\alpha,\beta)}(-x) = (-1)^n P_n^{(\beta,\alpha)}(x)$$

to swap the roles of α and β, leading to

$$\Psi_n(x) = \begin{cases} \sum_{i=1}^{M+n} c_i(n) P_{i-1}^{(\alpha,\beta+N)}(x), & 1 \leqslant n \leqslant N-M, \\ \sum_{i=1}^{N+1} c_i(n) P_{M+n-i}^{(\alpha,\beta+N)}(x), & n \geqslant N-M+1. \end{cases} \tag{7}$$

A peculiar case arises in the determination of c_i, for $n \leqslant N-M$, when the boundary conditions do not supply enough constraints on the function. For instance, $\Psi_1(x) = c_1 + c_2 P_1^{(\alpha+N,\beta)}(x)$ is not determined (even up to a normalisation) by the condition $\Psi_n''(1) = 0$. Indeed, imposing this same condition on $\Psi_2(x) = c_1 + c_2 P_1^{(\alpha+N,\beta)}(x) + c_3 P_2^{(\alpha+N,\beta)}(x)$ requires only that $c_3 = 0$, while orthogonality with respect to Ψ_1 still leaves three degrees of freedom among Ψ_1 and Ψ_2. While we could leave the undetermined c_i arbitrary, it is clear that the space of linear combinations of these functions is also spanned by $\Psi_1(x) = 1, \Psi_2(x) = P_1^{(\alpha,\beta)}(x)$, which are also orthogonal in the required manner of (6).

The reader may wonder how the coefficients c_i are calculated; we defer discussion of this until Section 2.5.

2.2. Two sided boundary conditions

By using (A.4) it is clear that (4) can be written in the symmetric form

$$\Psi_n(x) = \sum_{i=1}^{2N+1} c_i P_{M+n-i}^{(\alpha+N,\beta+N)}(x), \quad n \geqslant 2N-M+1, \tag{8}$$

where we solve for the $2N+1$ coefficients using the M boundary conditions, one normalisation condition, and $2N-M$ orthogonality conditions. The first $2N-M$ functions are constructed using the standard Gram-Schmidt procedure.

It is also apparent that the one-sided form of (7) with boundary conditions imposed only at $x = -1$ can be written in precisely the same way. It is therefore unsurprising that (8) is the most general representation required for any combination of M boundary conditions of degree $N-1$ acting at either (or both) of the endpoints.

2.3. Examples

We now consider some specific examples, taken from the compendium [13]. First, consider taking $\alpha = \beta = 1/2$ and the two conditions at $x = 1$,

$$\Psi_n''(1) = \Psi_n(1) = 0.$$

Inserting $M = 2$ and $N = 3$ into (4) we find that the (unnormalised) basis functions are

$$\Psi_n = \begin{cases} 1-x, & n = 1, \\ \sum_{i=1}^{4} c_i P_{2+n-i}^{(7/2,1/2)}(x), & n \geqslant 2, \end{cases} \tag{9}$$

where c_i are found to be (up to a normalisation)

$$
\begin{aligned}
c_1 &= 8(n-1)(n+1)^2(n+4)(2n+3)(9n^2+27n-35),\\
c_2 &= -12(n+1)(n-1)(n+4)(2n+5)(18n^3+93n^2+131n-63),\\
c_3 &= 6(n-1)(n+3)(2n+7)(2n+3)(18n^3+123n^2+251n+251),\\
c_4 &= -(n+3)(2n+7)(2n-1)(2n+5)^2(9n^2+45n+1).
\end{aligned}
$$

Note that we have removed a common factor of $n(n+5)/16$, which appears when substituting $\alpha=\beta=1/2$ into the general expression in [13]. The coefficients $[c_1,c_2,c_3,c_4]\sim 144n^7[1,-3,3,-1]$, the same ratio that appears when applying (A.3) thrice to $P_n^{(\alpha,\beta)}(x)$. It follows that

$$\Psi_n \sim P_n^{(1/2,1/2)}(x) = U_n(x),$$

the Chebyshev polynomials of the second kind, from which Ψ_n inherit optimal properties (at least asymptotically).

Second, consider the two-sided boundary conditions at $x=\pm 1$

$$\Psi_n(-1) = \Psi_n'(1) = 0,$$

with $\alpha=\beta=-1/2$. A Galerkin basis can be written

$$\Psi_n = \begin{cases} (x+1)(x-3), & n=1,\\ (x+1)(67x^2-125x+40), & n=2,\\ \sum_{i=1}^{5} c_i P_{2+n-i}^{(5/2,5/2)}(x), & n\geqslant 3, \end{cases} \tag{10}$$

where c_i are found to be (up to a normalisation)

$$
\begin{aligned}
c_1 &= 16n^2(n+1)(n+3)(n+4)(24n^3+12n^4-1-4n^2-16n),\\
c_2 &= -32n^2(n+2)(n+3)(2n+1)(2n+5)(6n^2+6n-7),\\
c_3 &= -8(n+1)(2n+3)(2n+5)(12n^6+72n^5-16n^3+116n^4-61n^2+102n+30),\\
c_4 &= 8n(n+2)(2n+1)(2n+3)^2(2n+5)(6n^2+18n+5),\\
c_5 &= (n+2)(2n+1)(2n+3)(2n+5)(2n-1)(12n^4+72n^3+140n^2+96n+15).
\end{aligned}
$$

Note that $[c_1,c_2,c_3,c_4,c_5]\sim 192\ n^9[1,0,-2,0,1]$. The same ratio is found by applying each of (A.3) and (A.4) twice to $P_n^{(\alpha,\beta)}(x)$. It follows that

$$\Psi_n \sim P_n^{(-1/2,-1/2)}(x) = T_n(x),$$

the Chebyshev polynomials of the first kind, from which Ψ_n inherit optimal properties (at least asymptotically).

Fig. 1(a) and (b) shows plots of example members of these two basis sets. The most visual characteristics are the quasi-equal-area property in (a) and the quasi-equal-ripple property in (b). In each case the basis functions are normalised according to

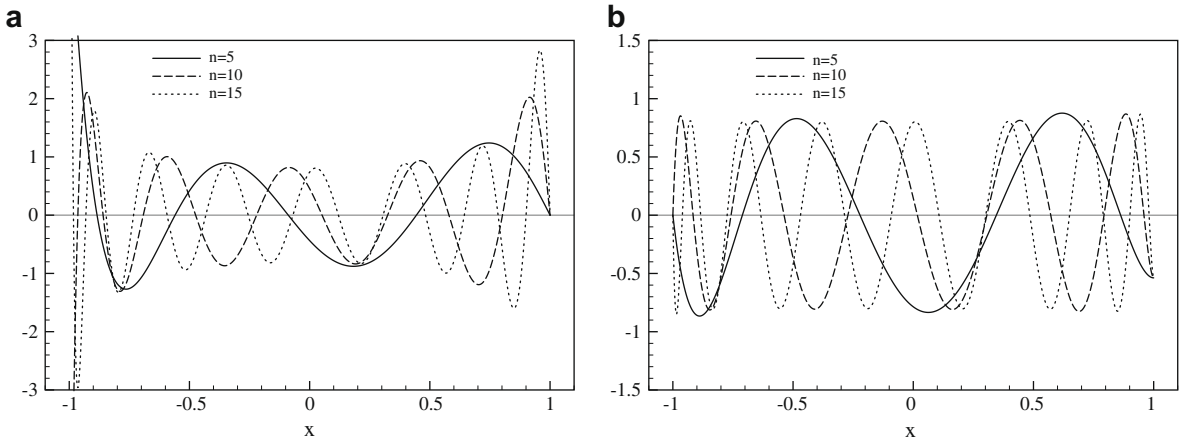

Fig. 1. Plots of basis functions for $n=5,10,15$. In (a), $\alpha=\beta=1/2$ and the functions satisfy the one-sided boundary condition $\Psi_n''(1)=\Psi_n(1)=0$. In (b), $\alpha=\beta=-1/2$ and the functions satisfy the two-sided boundary conditions $\Psi_n(-1)=\Psi_n'(1)=0$. Note the quasi-equal-area property of the functions in (a) and the quasi-equal-ripple property in (b). The functions are normalised by relation (11) in which, in (b), $\Psi_n(1)$ tends to a constant only for $n\to\infty$.

$$\int_{-1}^{1} \Psi_n(x)\Psi_m(x)(1-x)^{\alpha}(1+x)^{\beta}dx = \delta_{nm}. \tag{11}$$

For each of the above examples, more general (and much lengthier) expressions involving arbitrary (α, β) may be found in [13].

2.4. Numerical example

Here we demonstrate the asymptotic and exponential convergence properties of the basis functions in the specific case $\alpha = \beta = -1/2$ by considering the simple eigenvalue problem

$$y''(x) + \lambda^2 y(x) = 0 \tag{12}$$

with boundary conditions $y(-1) = y'(1) = 0$. The analytic solution is

$$y(x) = \cos(\lambda x) + \sin(\lambda x), \qquad \lambda = \frac{(2q+1)\pi}{4},$$

for any integer $q \geqslant 0$. We now test a variety of methods against the known solution with $q = 0$: (i) the Jacobi–Galerkin method (ii) a recombined Chebyshev–Galerkin scheme and (iii) a Chebyshev-tau method [2]. For method (i), the (normalised) basis functions are described above in Section 2.3; in method (ii), a (non-orthogonal) basis set is defined by recombining Chebyshev polynomials:

$$\Psi_n(x) = T_n(x) + AT_0(x) + BT_1(x),$$

where A and B are chosen to satisfy the two boundary conditions [3]. For the two Galerkin approaches, writing

$$y_N(x) = \sum_{i=1}^{N} v_i \Psi_i(x)$$

we obtain the discretised system for the spectral coefficients $\mathbf{v}$:

$$A\mathbf{v} + \lambda^2 B\mathbf{v} = 0,$$

where

$$A_{ij} = \int_{-1}^{1} \frac{d^2\Psi_j}{dx^2}\Psi_i w(x)dx, \qquad B_{ij} = \int_{-1}^{1} \Psi_j \Psi_i w(x)dx = \delta_{ij}.$$

The weight functions $w(x)$ appearing above are (i) $w(x) = (1-x^2)^{-1/2}$ and (ii) $w(x) = 1$; the latter being arbitrarily chosen as there is no natural choice. In case (i) B is the identity matrix and A is dense; in (ii) both A and B are dense. In either case, the matrix elements can be efficiently computed using Gaussian quadrature.

We now demonstrate the asymptotic properties of the Jacobi–Galerkin basis set. Using $N = 8$, the leftmost plot in Fig. 2 shows the pointwise error in representing the analytic solution (with $q = 0$, normalised to have unit rms over the interval) by

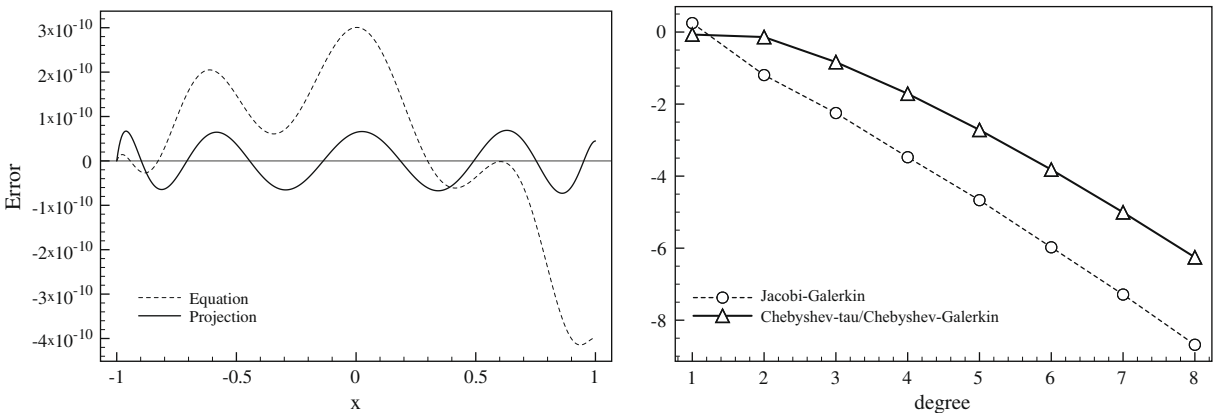

Fig. 2. A demonstration of the asymptotic properties and exponential convergence of the Galerkin method. (Left) The error between the analytic function with $q = 0$ and its (a) projection onto the first 8 Jacobi–Galerkin basis functions and (b) the eigenvector associated with the most positive eigenvalue of the matrix A of method (i). Note that the error of the projection is quasi-equal-ripple. (Right) The spectrum $(log_{10}|v_i|)$ of the eigenvector associated with the most positive eigenvalue of Eq. (12) as determined by the Jacobi–Galerkin, Chebyshev-tau and a recombined Chebyshev–Galerkin method (these latter two spectra over-plot). Note that all methods converge exponentially fast, but the Jacobi–Galerkin method is superior.

its projection onto the first eight basis functions $\{\Psi_1, \Psi_2, \ldots, \Psi_8\}$ (solid line). The error is quasi-equal-ripple as expected, producing a quasi-minimax fit. For comparison, the error between the analytic solution and the appropriately normalised eigenvector corresponding to the most positive eigenvalue of A (method (i)) is shown by the dashed line. Both errors are reassuringly small ($O(10^{-10})$ compared to the solutions which are $O(1)$).

The exponential convergence of all three methods is demonstrated in the rightmost plot of Fig. 2, which shows the spectrum for the approximation to the eigenvector corresponding to $q = 0$. Method (i) is shown by a dashed line with circles and methods (ii) and (iii), which over-plot, as solid lines with triangles. As expected, all methods converge exponentially fast but, although they have a similar slope, the Jacobi-Galerkin method is superior.

Lastly, we directly compare the two Galerkin schemes and comment briefly on their conditioning. In both cases, the (2-norm) condition number of the matrix $B^{-1}A$ can be well approximated by a polynomial in N, the truncation, that behaves as $O(N^4)$ (at least up to $N = 80$). This is an identical scaling as would be expected from a generic spectral method based on any type of Jacobi polynomials. However, despite having the same scaling, the two Galerkin methods do, in fact, achieve quite different accuracies in numerical computations for the eigenvalues λ. Fig. 3 shows the relative accuracy of the eigenvalues (in order of increasing distance from the origin) as computed using Matlab command *eig*. In method (ii), two lines are plotted corresponding to the two distinct ways of calculating the eigenvalues: (a) canonical eigenvalues of the matrix $B^{-1}A$ and (b) generalised eigenvalues of the system $A\mathbf{v} = \lambda B\mathbf{v}$. The Jacobi–Galerkin approach produces the first approximately 40 eigenvalues with a relative error of just $O(10^{-15})$. By comparison, the Chebyshev–Galerkin scheme only achieves an accuracy of $O(10^{-10})$ for eigenvalues with index between 10 and 40; the generalised eigenvalue problem is, in general, more accurate than its canonical formulation. At about index 40, both methods diverge from the true eigenvalues in a similar fashion.

2.5. Finding the Jacobi coefficients

Although Eqs. (4) or (8) give the general expression for an orthogonal basis in terms of a small number of Jacobi polynomials for prescribed (N, M), a mechanism for finding their coefficients c_i has not yet been provided. There are two levels on which we can now proceed. The simplest is to specify all the other quantities: the precise form of the boundary conditions and (α, β). Given the structure of each basis function in (4) or (8), we can then find the required c_i for specified n by simply imposing the boundary conditions and orthogonality to the first few basis functions. As an illustration, consider the first example shown in Section 2.3 where we construct a basis set satisfying $\Psi_n''(1) = \Psi_n(1) = 0$. First, we need to find Ψ_1, the lowest-degree polynomial that satisfies the boundary conditions: $\Psi_1(x) = 1 - x$. The four c_i are given, up to a normalisation, by the three constraints, namely the two boundary conditions and orthogonality to Ψ_1:

$$\sum_{i=1}^{4} c_i(n) \frac{d^2}{dx^2} P_{n+2-i}^{(5/2,-1/2)}(x)\bigg|_{x=1} = \sum_{i=1}^{4} c_i(n) P_{n+2-i}^{(5/2,-1/2)}(x)\bigg|_{x=1} = 0, \tag{13}$$

$$\sum_{i=1}^{4} c_i(n) \int_{-1}^{1} P_{n+2-i}^{(5/2,-1/2)}(x)(1-x)(1-x^2)^{-1/2} = 0, \tag{14}$$

where the factor $(1-x^2)^{-1/2}$ is the weight function $(1-x)^{\alpha}(1+x)^{\beta}$ with $\alpha = \beta = -1/2$. Having specified n in advance, we can form the explicit linear system for the c_i by using Eq. (A.6) to evaluate the Jacobi polynomials at $x = \pm 1$ and using computer algebra to calculate the weighted integral of the known polynomial appearing in (14). The system is then readily solved for the (unnormalised) c_i. It is worth pointing out that unlike a naive Gram-Schmidt procedure (as illustrated in (1)), we do not

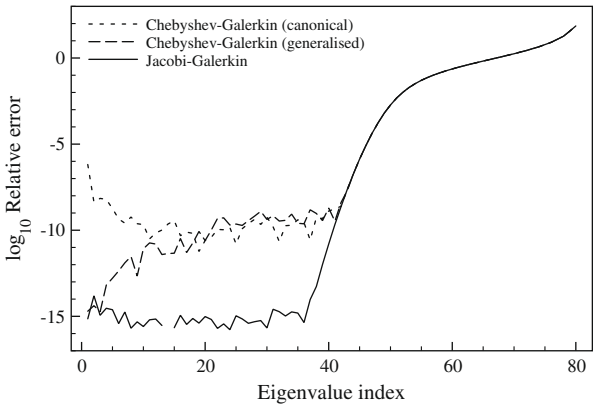

Fig. 3. A comparison of the relative error in the eigenvalues (ordered in increasing distance from the origin) for the two Galerkin methods as computed using the Matlab function *eig*. The Jacobi–Galerkin method achieves an accuracy of around $O(10^{-15})$ up to index of about 40. By contrast, the Chebyshev–Galerkin scheme only achieves an accuracy of $O(10^{-10})$. The two possible ways of computing its eigenvalues (either by a canonical or generalised formulation) are shown separately. Both Galerkin methods have condition numbers that scale as $O(N^4)$.

need to build the basis incrementally in n. The major downside of this approach, however, is that it does not generate an expression for arbitrary n, leaving open the question of the asymptotic behaviour.

A more difficult approach is to leave n and possibly other quantities (for instance, (α,β)) unspecified. In this case, the determination of the c_i is, in general, highly non-trivial and in order to spare the user from needing to do this, we have compiled a database of boundary conditions where the c_i are given explicitly in a large range of cases [13]. The complication arises from solving the linear system (13), (14) where the coefficients of c_i are not constant but functions of all the unknown parameters. Furthermore, although it is straightforward to evaluate (13), (14) is troublesome to evaluate in general, being the integral of a Jacobi polynomial $P_m^{(5/2,-1/2)}(x)$ with $(1-x)$ against a weight function which is not of the standard form $(1-x)^{5/2}(1+x)^{-1/2}$. In this simple example, a closed form expression can be obtained by using the formulae in [12] and it is immediate to solve the system to find c_i (up to a normalisation) as functions of n.

Computer algebra, making such a method practical, also holds this approach hostage by its own intrinsic limitations. In particular, the system of equations, although linear in c_i, will in general involve extremely lengthy expressions that depend on the unspecified parameters. Formally, although a solution exists, present-day computer algebra cannot provide it (and, in general, the software crashes in the attempt). Guided by the expectation that c_i are polynomials in n, an alternative method is simply to fit trial polynomials to expressions produced for specific n. For instance, consider trying to find c_2/c_1 which we anticipate to be a ratio of polynomials

$$\frac{c_2}{c_1}=\frac{\sum_{i=0}^{J}a_i n^i}{\sum_{i=0}^{K}b_i n^i},$$

where J and K are unknown in advance. Note that the coefficients a_i and b_i, although independent of n, may depend on (α,β) and other parameters appearing in the boundary conditions. We now proceed by empirical means by guessing K and J. Substituting $K+J+2$ values of c_2/c_1, derived from $K+J+2$ basis functions of any specified n, we may solve the system. To determine whether (K,J) are sufficiently high a further value of n can be tested with the resulting formulae for the c_i. Although more cumbersome, the fact that this method explicitly removes the dependence on n from the c_i means that other free parameters may be carried and maximally general expressions for the c_i obtained. Expressions for c_i depending on arbitrary n, α,β and boundary condition parameters are given in [13].

2.6. Other considerations

We have already remarked that the Galerkin basis functions become asymptotically similar to a single Jacobi polynomial as $n\to\infty$. This ability to 'forget' the boundary conditions, for large n, in fact only holds in the bulk of the domain and not in boundary layers. Indeed, it is within these boundary layers that the functions stray from the single Jacobi polynomial dependence to satisfy the required boundary conditions. To make this possible there is, in general, a rather delicate cancellation close to the boundary which is exacerbated by values of α and β greater than $-1/2$. This can be readily seen by considering the individual Jacobi polynomials, $P_n^{(\alpha,\beta)}(x)$ with $\alpha,\beta>-1/2$, making up any particular Galerkin function. These have extremely pronounced maxima at $x=\pm1$ yet must sum to produce much more modest behaviour (for example, quasi-equal-ripple when $\alpha=\beta=-1/2$), leading to loss of accuracy when using finite precision. We propose two remedies to evaluate the basis functions very close to the boundaries: (i) calculating a boundary layer expansion of the function near $x=\pm1$ or (ii) computing in very high precision (using, for instance, the software package Maple). A recurrence relation satisfied by these Galerkin basis functions, which would alleviate this problem, apparently does not exist.

A key use of these orthogonal basis functions is in the solution of the differential equation

$$\mathcal{D}f(x)=g(x),$$

where $g(x)$ is given and $\mathcal{D}$ is some differential operator. After expanding the unknown function $f(x)$ in our trial space of functions, a discretised system can either be formed by imposing that the residual, $\mathcal{D}f(x)-g(x)$, is identically zero at some set of collocation points or by imposing that it is orthogonal to the same (in the traditional Galerkin scheme) or different set of basis functions. In a collocation scheme, usually, the choice of grid is determined by its equivalence to the quadrature grid required by the standard Galerkin scheme [3]. We briefly consider whether such a collocation scheme is viable here, or in other words whether it is possible to represent an exact quadrature-based Galerkin scheme by a square matrix. In general, the first K basis functions are of degree higher than K and a standard Gauss-Legendre scheme with K abscissae will not be exact. The only chance of success is to tailor the scheme by encoding the information that the basis functions satisfy known boundary conditions. However, $\mathcal{D}\Psi_n$, and therefore the product $\mathcal{D}\Psi_n\Psi_m$ appearing in the integrated residual, satisfies no particular condition (barring the rather special case of, for example, $\Psi_n(1)=0$) and no general scheme can be constructed.

3. Extension to a polar geometry

In either 2D or 3D polar geometries, due to the singularity of the coordinate systems at the origin, a certain regularity condition applies to any function that is everywhere smooth. In the 3D case, a smooth function has a representation

$$\sum_{lm}Y_l^m(\theta,\phi)f_l^m(r),\qquad f_l^m(r)=r^l g_l^m(r^2),$$

where Y_l^m is a spherical harmonic of degree l and order m and g_l^m is smooth [3,14]. A similar result holds in the 2D polar case. In this section, it will be shown that the machinery developed for the one-sided Cartesian case carries over to the spherical geometry where, for each spherical harmonic component, the sole radial boundary condition is at $r = 1$. In applications, it is often expedient to define vector potentials depending on $f(r,\theta,\phi)\hat{\mathbf{r}}$ rather than $f(r,\theta,\phi)\mathbf{r}$, where f is a scalar function and $\mathbf{r} = r\hat{\mathbf{r}}$ the position vector. Since $\mathbf{r}$ is regular, this means that a slightly modified regularity condition must hold for the coefficients $f_l^m(r) = r^{l+1}g_l^m(r^2)$. In the proceeding sections, we present examples involving both types of regularity as motivated by physical problems which, for the most part, are trivially interchangeable by $l \leftrightarrow l+1$.

3.1. One sided Jacobi polynomials

For any given wavenumber l, an expedient basis in which to expand an unknown function of the form $r^{l+1}g(r^2)$ for some smooth function g is the so-called one-sided Jacobi polynomials [3,15,16]:

$$G_n(r;\alpha,\beta,l) = r^{l+1}P_n^{(\alpha,\beta)}(2r^2-1).$$

These are even, defined on $r \in [0,1]$, and satisfy the regularity conditions. Additionally, they are orthogonal,

$$\int_0^1 G_n G_m w(r)dr = \delta_{nm}h_n, \qquad w(r) = (1-r^2)^\alpha r^{2(\beta-l)-1},$$

for some h_n and converge exponentially fast to any function satisfying the same regularity condition [14]. In addition, there are two free parameters, (α,β), that we are free to choose. However, as pointed out in [14], it is often expedient to choose β in order that the weight function is independent of l, making the basis set much better conditioned for large l. Furthermore, restrictions on the asymptotic behaviour (for large n) will further constrain (α,β). For instance, suppose we wanted the basis functions to be quasi-equal-ripple, mimicking the Chebyshev polynomials and their associated optimal properties. By using Theorem 8.21.8 of [17] and the change of variable $\cos\theta = 2r^2-1$, we can write

$$r^{l+1}P_n^{(\alpha,\beta)}(2r^2-1) \sim K\left(\sin\frac{\theta}{2}\right)^{-\alpha-1/2}\left(\cos\frac{\theta}{2}\right)^{l+1-\beta-1/2}\cos(N\theta+\gamma), \tag{15}$$

where K, N and γ are independent of θ and N increases linearly with n. In order to obtain an asymptotically equal-ripple function, we need to choose $\alpha = -1/2$, $\beta = l+1/2$ in order to remove the first two trigonometric prefactors. To obtain quasi-equal-area polynomials, similar considerations lead to the choice $\alpha = 1/2, \beta = l+1/2$.

3.2. Auto orthogonal basis sets

We now show it is possible to construct an auto-orthogonal regular basis set from the one-sided Jacobi polynomials which, in essence, follows directly from the change of variable $x = 2r^2-1$ into the one-sided Cartesian case and absorbing the factors of r^{l+1} into the weight function. A more detailed demonstration is achieved by devising a companion problem in a one-sided Cartesian geometry, associated with any given polar case, for which there is an auto-orthogonal basis set. Let us fix $\beta = l+1/2$ and consider arbitrary $\alpha > -1$ along with M boundary conditions of degree $N-1$ at $r = 1$. We would like to show that the (normalised) basis functions defined by

$$\Psi_n(r) = r^{l+1}\sum_{i=1}^{N+1} c_i P_{n+M-i}^{(\alpha+N,l+1/2)}(2r^2-1) \tag{16}$$

form an auto-orthogonal set with

$$\int_0^1 \Psi_n\Psi_m(1-r^2)^\alpha dr = \delta_{nm}.$$

Note that the weight function, $(1-r^2)^\alpha$, is now independent of β. By using the change of variable, $x = 2r^2-1$, such orthogonality is equivalent to

$$\int_{-1}^1 (1+x)^{l+1/2}(1-x)^\alpha\left[\sum_{i=1}^{N+1} c_i P_{n+M-i}^{(\alpha+N,l+1/2)}(x)\right]\left[\sum_{i=1}^{N+1} c_i P_{m+M-i}^{(\alpha+N,l+1/2)}(x)\right]dx = \delta_{nm}k_n,$$

for some k_n. That is, the companion problem involves the functions

$$\chi_n(x) = \sum_{i=1}^{N+1} c_i P_{n+M-i}^{(\alpha+N,l+1/2)}(x),$$

which are orthogonal with respect to the weight function $(1-x)^\alpha(1+x)^{l+1/2}$. We know from Section 2.1 that such a set generate an auto-orthogonal basis for any set of M boundary conditions of degree at most $N-1$ at $x = 1$. The only question that remains is whether the M boundary conditions of degree at most $N-1$ at $r = 1$ translate to an equivalent set at $x = 1$. Since

$(1+x)^{l+1}\chi_n(x) = \Psi_n(r)$ and, using $\frac{d}{dr} = 4r\frac{d}{dx}$, we can translate any boundary condition at $r = 1$ into one involving derivatives of the same order at $x = 1$. It then follows immediately that the construction (16) is auto-orthogonal as well. Lastly, since the Cartesian-companion basis functions behave asymptotically like $P_n^{(\alpha,\beta)}(x)$, it follows that the same is true of Ψ_n:

$$\Psi_n(r) \sim r^{l+1} P_{n+M-1}^{(\alpha,l+1/2)}(x)$$

as $n \to \infty$. When $\alpha = -1/2$, the Ψ_n are quasi-equal-ripple, and when $\alpha = 1/2$, they are quasi-equal-area.

3.3. Examples

We will now explore two examples of auto-orthogonal basis sets in a polar geometry, both of which arise when considering the so-called poloidal and toroidal components of a magnetic field defined in $r \leqslant 1$ which is in contact with a perfect electrical conductor at $r = 1$ [18]. We shall take $\alpha = -1/2$ and $\alpha = +1/2$, respectively, to demonstrate the different asymptotic behaviour. Firstly, consider the toroidal boundary condition $\Psi_n'(1) = 0$ with $\alpha = -1/2$. The associated auto-orthogonal basis set is

$$\Psi_n(r) = \begin{cases} r^{l+1}(r^2 - l + lr^2 - 3), & n = 1, \\ r^{l+1}\sum_{i=1}^{3} c_i P_{n+1-i}^{(3/2,l+1/2)}(x), & n \geqslant 2. \end{cases} \tag{17}$$

Secondly, we consider the poloidal boundary condition $\Psi_n''(1) = \Psi_n(1) = 0$ with $\alpha = +1/2$. The basis set is

$$\Psi_n(r) = \begin{cases} 4r^{l+1}(r^2-1)(2lr^2 - 2l + 3r^2 - 7), & n = 1, \\ r^{l+1}\sum_{i=1}^{4} c_i P_{n+2-i}^{(5/2,l+1/2)}(x), & n \geqslant 2. \end{cases} \tag{18}$$

Both examples are illustrated in Fig. 4; in either case, c_i are multinomials in n and l whose lengthy expressions are available in [13].

4. Orthogonality with respect to derivative operators

Although constructing Galerkin basis sets whose elements are mutually orthogonal is helpful in many cases, it is sometimes useful to extend the notion of orthogonality to include derivatives such as in Sobolev-type norms [19]. As discussed below, such an extension admits the possibility of band-limited matrix discretisations of differential equations, clearly a computational advantage. For instance, as noted in [20], a basis set for a second-order differential equation for which the solution vanishes at $x = \pm 1$ is

$$\Psi_n = (1 - x^2)P_n^{(1,1)}(x). \tag{19}$$

Each basis function has symmetry (being either even or odd) and the matrices defined by

$$A_{ij} = \int_{-1}^{1} \Psi_j'' \Psi_i \, dx, \quad B_{ij} = \int_{-1}^{1} \Psi_j \Psi_i \, dx,$$

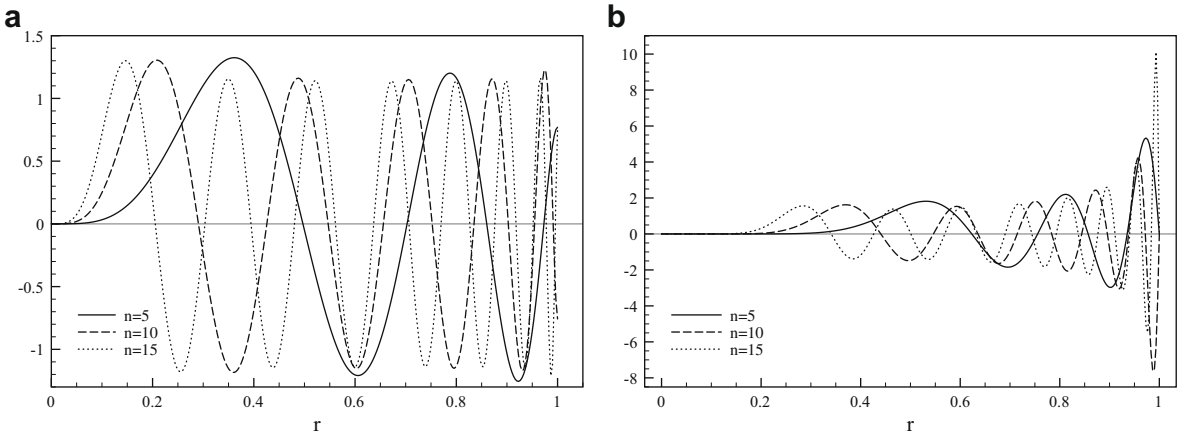

Fig. 4. Plots of the example orthogonal basis functions for $n = 5, 10, 15$ that behave as $O(r^{l+1})$ as $r \to 0$. In (a), $\alpha = -1/2, l = 3$ and the functions satisfy the boundary condition $\Psi_n'(1) = 0$. In (b), $\alpha = 1/2, l = 10$ and the functions satisfy the boundary conditions $\Psi_n''(1) = \Psi_n(1) = 0$. Note the quasi-equal-ripple property of the functions in (a) and the quasi-equal-area property in (b). The functions are normalised by relation (11).

are, within each symmetry class respectively, diagonal and tri-diagonal. That is, the basis functions are orthogonal as defined by a relation involving the second derivative. This approach can be extended to equations of arbitrary order where, in each case, the matrix B is band-limited. This sparse representation may be contrasted to the structure which occurs when the matrix B is diagonal (as in Section 2). In this case, the matrix A is dense and there is no sparse description of the differential operator.

Using such an approach expedites the analysis in many situations, for instance, the eigenvalue problem (12) where we need only find the eigenvalues of a tri-diagonal matrix. However, the construction (19) requires us to use rather special boundary conditions, namely that the function vanishes at either end of the interval. Note that on using (A.1) and (A.2) once, Ψ_n as defined above can be written

$$\Psi_n = \sum_{i=1}^{3} c_i P^{(0,0)}_{n+3-i}(x), \tag{20}$$

where c_i take the ratio $[1, 0, -1]$. By applying both (A.3) and (A.4) to $P_n^{(\alpha,\beta)}(x)$ we find that

$$P_n^{(\alpha,\beta)}(x) \sim P_n^{(\alpha+1,\beta+1)}(x) - P_{n-2}^{(\alpha+1,\beta+1)}(x)$$

and so $\Psi_n \sim P^{(-1,-1)}_{n+2}(x)$ as $n \to \infty$.

It is worth remarking here that, when α and β are non positive integers, there are two issues that concern $P_n^{(\alpha,\beta)}(x)$. First, the standard orthogonality relation between the Jacobi polynomials becomes invalid as the weight function is not integrable. However, there is no inconsistency here with the orthogonality of the basis functions themselves, for finite n, as the similarity to $P_n^{(-1,-1)}(x)$ only holds in the asymptotic limit and not within boundary layers. Second, the standard three-term recurrence relation [21] ostensibly breaks down, because the coefficient of P_{n+1}, expressed in terms of P_n and P_{n-1}, becomes zero. However, this problem is only superficial and in fact there is a remarkable cancellation leaving $P_n^{(-1,-1)}$ well-defined after all, as can be seen by computing $P_n^{(\alpha,\beta)}(x)$ for arbitrary α and β and then defining $\alpha = \beta = -1$.

4.1. Auto-orthogonality

We now generalise the above special case, restricted to functions that vanish at either end of the interval, to show that auto-orthogonality extends to the boundary conditions

$$\mu f'(1) + f(1) = 0, \qquad \nu f'(-1) + f(-1) = 0,$$

for any μ, ν. The basis set defined by

$$\Psi_n = \sum_{i=1}^{3} c_i P^{(0,0)}_{n+2-i}(x), \quad n \geqslant 1, \tag{21}$$

satisfies

$$\int_{-1}^{1} \Psi_n \frac{d^2\Psi_m}{dx^2} dx = \delta_{nm}, \tag{22}$$

where the (unnormalised) c_i are found to be

$$c_1 = \mu\nu n^4 - n^2\mu\nu - 2n^2\mu + 2n^2\nu - 4, \tag{23}$$
$$c_2 = 2(\nu + \mu)(2n + 1), \tag{24}$$
$$c_3 = -2\nu + 2\mu + 4 + (-2\mu\nu + 4\mu - 4\nu)n + (-5\mu\nu + 2\mu - 2\nu)n^2 - 4n^3\mu\nu - \mu\nu n^4. \tag{25}$$

Note that (20) is of the same form as (21) shifted in n by 1. It is of interest to note that the matrices defined by the elements

$$A_{ij} = \int_{-1}^{1} \Psi_i(x) \frac{d\Psi_j(x)}{dx} dx, \qquad B_{ij} = \int_{-1}^{1} \Psi_i(x)\Psi_j(x) dx, \tag{26}$$

are, respectively, upper triangular with a non-zero sub-diagonal and penta-diagonal.

Additionally, note that the coefficients c_i are proportional to [1, 0, −1] in the limit $n \to \infty$. As above, this means that

$$\Psi_n(x) \sim P^{(-1,-1)}_{n+1}(x)$$

as $n \to \infty$. These results are apparently only valid for $\alpha = \beta = 0$ and do not generalise, as in Section 2, to arbitrary (α, β). This point is discussed further in Section 5.

4.2. Extension to polar case

Lastly, of interest in a spherical geometry, is orthogonality involving

$$\mathcal{D} = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} - \frac{l(l+1)}{r^2},$$

the radial part of the Laplacian operator when looking for a separable solution using spherical harmonics in solid angle. There exists an orthonormal basis of polynomials with

$$\int_0^1 \mathcal{D}(\Psi_n)\Psi_m r^2 dr = \delta_{nm} \tag{27}$$

satisfying the boundary condition

$$\mu\frac{d\Psi}{dr}(1) + \Psi(1) = 0$$

for any (real) μ, where

$$\Psi_n = r^{l+1}\sum_{i=1}^{4} c_i P_{n+1-i}^{(2,l+1/2)}(2r^2-1),$$

and with coefficients c_i given in [13].

For this basis set, it is also of note that the matrix defined by

$$B_{ij} = \int_0^1 \Psi_i(r)\Psi_j(r) r^2 dr \tag{28}$$

is tri-diagonal.

Additionally, the coefficients c_i are proportional to $[1, -3, 3, -1]$ in the limit $n \to \infty$. By applying (A.3) thrice to $P_n^{(\alpha,\beta)}(x)$ we find that

$$P_n^{(\alpha,\beta)}(x) \sim P_n^{(\alpha+3,\beta)}(x) - 3P_{n-1}^{(\alpha+3,\beta)}(x) + 3P_{n-2}^{(\alpha+3,\beta)}(x) - P_{n-3}^{(\alpha+3,\beta)}(x).$$

Thus

$$\Psi_n(r) \sim r^{l+1}P_n^{(-1,l+1/2)}(x)$$

as $n \to \infty$. Note that Jacobi polynomials with $\alpha = -1$ are formally undefined (although this relation holds only in the asymptotic limit $n \to \infty$ and, for finite n, they are well defined.) However, since β is a positive half integer, the 3-term recurrence relation remains valid. As before, the structure of these basis functions is fixed: we have no latitude in being able to vary (α, β) and so their asymptotic behaviour. However, this shortcoming is outweighed by the utility of being able to discretise the Laplacian operator as the inverse of the tri-diagonal matrix, B^{-1}.

5. Discussion

In this paper, the construction of auto-orthogonal basis sets in a variety of geometries is described alongside many illustrative cases. Many more examples, including common physically motivated boundary conditions, can be found in [13]. We end with a discussion on what aspects of auto-orthogonality can be proven, and what is left to the interested reader as future research.

For a given set of M boundary conditions up to degree $N-1$, the proof of not only auto-orthogonality but the exponential convergence and asymptotic properties of the basis sets is given, in so far as what is currently possible, in [12]. The property of auto-orthogonality appears to rest on the rather complex algebraic structure of non-standard integrated products of Jacobi polynomials:

$$\int_{-1}^{1} P_n^{(\alpha+\mu,\beta+\nu)}(x)P_m^{(\alpha+\mu,\beta+\nu)}(x)(1+x)^{\beta}(1-x)^{\alpha}dx, \tag{29}$$

for arbitrary real $(\alpha, \beta) > -1$ and positive integers (ν, μ). For specified (N, M), the generalised construction as described in Sections 2 and 3 can be proved. What is yet unproven is the construction for unspecified (N, M), a much lower-level result which is presumably underpinned by a property much more fundamental than those currently understood. Furthermore, a general theory on which the results supplied in Section 4 (orthogonality relations involving derivatives) are based is also out of reach and it is therefore difficult to generalise the given examples. In contrast to the construction in Section 2, the values of (α, β) are apparently not free and are somehow intrinsically determined by the definition of the differential operator appearing inside the orthogonality integral.

In the first example in Section 4 we considered an orthogonality relation based on the second derivative operator. Note that

$$\frac{d^2}{dx^2}P_n^{(\alpha,\beta)}(x) = C(n,\alpha,\beta)P_{n-2}^{(\alpha+2,\beta+2)}(x)$$

for some C and thus the orthogonality relation (22), when $\alpha = \beta = 0$, involves integrated products of quantities of the form

$$\int_{-1}^{1} P_n^{(2,2)}(x) P_m^{(0,0)}(x) dx,$$

very similar, though distinct, to those of (29). It is unclear why auto-orthogonality does not extend to arbitrary (α, β).

Additionally, in the example of the orthogonality relation involving the (polar) Laplacian, we can gain insight by converting to a Cartesian geometry by the change of variable $x = 2r^2 - 1$. The system (27) is equivalent to the following

$$\widetilde{\mathcal{D}} = 2(1+x)\frac{d^2}{dx^2} + (3+2l)\frac{d}{dx}, \qquad \Psi_n = \sum_{i=1}^{4} c_i P_{n+1-i}^{(2,l+1/2)}(x),$$

with

$$\int_{-1}^{1} \widetilde{\mathcal{D}}(\Psi_n)\Psi_m (1+x)^{l+1/2} dx = \delta_{nm} k_n,$$

for some k_n and where a generalised first order boundary condition is imposed at $x = 1$. Note that

$$\widetilde{\mathcal{D}} P_n^{(\alpha,\beta)}(x) = C(\alpha, \beta, n, x) P_{n-1}^{(\alpha+2,\beta)}(x),$$

where C becomes independent of x, for each n, only when $\beta = l + 1/2$. This suggests that, for this choice of differential operator, we must choose $\beta = l + 1/2$ for auto-orthogonality, which is found to be the case. Furthermore, as above, the choice of α is not arbitrary and we must choose $\alpha = 2$ in order for the basis functions to become orthogonal (although it is not clear why).

These examples strongly suggest the following conjecture. Consider a differential operator $\mathcal{H}$ which acts as a raising (or lowering) operator on a Jacobi polynomial:

$$\mathcal{H}(P_n^{(\alpha,\beta)}(x)) = C(n, \alpha, \beta) P_{n-q}^{(\alpha+a,\beta+b)}(x)$$

for some C, non-negative integer q and integers (either positive or negative) (a, b). Then we can find an auto-orthogonal basis set for which

$$\int_{-1}^{1} \mathcal{H}(\Psi_n)\Psi_m (1-x)^{\alpha}(1+x)^{\beta} dx = \delta_{nm}.$$

The determination of (α, β), which depend on $\mathcal{H}$, remains an open question. Furthermore, guided by the examples above, we speculate that the matrix representing integrated products of such basis functions,

$$A_{nm} = \int_{-1}^{1} \Psi_n \Psi_m (1-x)^{\alpha}(1+x)^{\beta} dx,$$

is band-limited, meaning that the action of $\mathcal{H}$ on the basis set can be written succinctly as A^{-1}, the inverse of a band-limited matrix. Further research on auto-orthogonal schemes, particularly with regard to orthogonality relations involving derivatives, is clearly of great interest as such a general construction would allow a large subset of differential operators to be discretised in terms of such sparse matrices.

Acknowledgments

PL was supported by NSF Grant number DMS0724331 and would like to thank Professor Glenn Ierley for useful discussions throughout this work.

Appendix A

We make use of the following identities satisfied by Jacobi polynomials (see [22, p. 276])

$$(2n+\alpha+\beta+2)(1-x)P_n^{(\alpha+1,\beta)} = 2(n+\alpha+1)P_n^{(\alpha,\beta)} - 2(n+1)P_{n+1}^{(\alpha,\beta)}, \tag{A.1}$$

$$(2n+\alpha+\beta+2)(1+x)P_n^{(\alpha,\beta+1)} = 2(n+\beta+1)P_n^{(\alpha,\beta)} + 2(n+1)P_{n+1}^{(\alpha,\beta)}, \tag{A.2}$$

$$(2n+\alpha+\beta)P_n^{(\alpha-1,\beta)} = (n+\alpha+\beta)P_n^{(\alpha,\beta)} - (n+\beta)P_{n-1}^{(\alpha,\beta)}, \tag{A.3}$$

$$(2n+\alpha+\beta)P_n^{(\alpha,\beta-1)} = (n+\alpha+\beta)P_n^{(\alpha,\beta)} + (n+\alpha)P_{n-1}^{(\alpha,\beta)}, \tag{A.4}$$

$$\frac{d^k}{dx^k}P_n^{(\alpha,\beta)}(x) = \frac{\Gamma(\alpha+\beta+n+1+k)}{2^k\Gamma(\alpha+\beta+n+1)}P_{n-k}^{(\alpha+k,\beta+k)}(x). \tag{A.5}$$

For imposing boundary conditions, we make use of the following:

$$\frac{d^k}{dx^k}P_n^{(\alpha,\beta)}(\pm 1) = (\pm 1)^{n+k}\frac{2^{-k}\Gamma(n+k+\alpha+\beta+1)\Gamma(n+\alpha+1)}{\Gamma(n+\alpha+\beta+1)\Gamma(k+\alpha+1)\Gamma(n-k+1)}. \tag{A.6}$$

References

[1] C. Canuto, M.Y. Hussaini, A. Quarteroni, T.A. Zang, Spectral Methods: Fundamentals in Single Domains, Springer, 2006.
[2] B. Fornberg, A Practical Guide to Pseudospectral Methods, CUP, 1998.
[3] J.P. Boyd, Chebyshev and Fourier Spectral Methods, Dover, 2001.
[4] J.C. Mason, D.C. Handscomb, Chebyshev Polynomials, Chapman & Hall, 2003.
[5] L. Fox, I.B. Parker, Chebyshev Polynomials in Numerical Analysis, Oxford University Press, London, 1968.
[6] W.H. Press, S.A. Teukolsky, W.T. Vetterling, B.P. Flannery, Numerical Recipes in Fortran 77, second ed., CUP, 1992.
[7] J. Shen, Efficient spectral-Galerkin methods II: Direct solvers of second- and fourth-order equations using Chebyshev polynomials, SIAM J. Sci. Comput. 16 (1) (1995) 74–87.
[8] G. Dumas, A. Leonard, A divergence-free spectral expansions method for three-dimensional flows in spherical-gap geometries, J. Comput. Phys. 111 (1994) 204–219.
[9] O.C. Zienkiewicz, R.L. Taylor, J.K. Zhu, The Finite Element Method: Its Basis and Fundamentals, sixth ed., vol. 1, Elsevier, 2005.
[10] P.W. Livermore, A. Jackson, On magnetic energy instability in spherical stationary flows, Proc. R. Soc. A 460 (2004) 1453–1476.
[11] E.H. Doha, H. Bhrawy, A, Efficient spectral-Galerkin algorithms for direct solution for second-order differential equations using Jacobi polynomials, Numer. Alg. 42 (2) (2006) 137–164.
[12] P. Livermore, G. Ierley, Quasi-L^p norm orthogonal expansions in sums of Jacobi polynomials, Numer. Alg., submitted for publication, doi:10.1007/s11075-009-9353-5.
[13] P. Livermore, A Compendium of Galerkin Orthogonal Polynomials, Tech. rep., Scripps Institute of Oceanography. <http://escholarship.org/uc/item/9vk1c6cm> (2009).
[14] P. Livermore, C.A. Jones, S. Worland, Spectral radial basis functions for full sphere computations, J. Comput. Phys. 227 (2007) 1209–1224.
[15] W.T.M. Verkley, A spectral model for two-dimensional incompressible fluid flow in a circular basin, J. Comput. Phys. 136 (1997) 100–114.
[16] T. Matsushima, P.S. Marcus, A spectral method for polar coordinates, J. Comput. Phys. 120 (1995) 365–374.
[17] G. Szegö, Orthogonal Polynomials, fourth ed., vol. 1, American Mathematical Society, 1975.
[18] G.A. Glatzmaier, Numerical simulations of stellar convective dynamos. I. The model and method, J. Comput. Phys. 55 (1984) 461–484.
[19] F. Marcellan, A. Ronveaux, On a class of polynomials orthogonal with respect to a discrete Sobolev inner product, Indagat. Math., N.S. 1 (4).
[20] G. Ierley, A class of sparse spectral operators for inversion of powers of the Laplacian in n dimensions, J. Sci. Comput. 12 (1) (1997) 57–73.
[21] M. Abramowitz, I.A. Stegun, Pocketbook of Mathematical Functions, Verlag Harri Deutsch, 1984.
[22] Y. Luke, The Special Functions and their Approximations, vol. 1, Academic Press, 1969.