Scripps Institution of Oceanography Technical Report

A Compendium of Galerkin Orthogonal Polynomials

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1 Overview

This online resource concerns the construction of a polynomial Galerkin basis $\{\Psi_n(x)\}$, each member of which satisfies two key conditions: (i) any given set of M homogeneous linear boundary conditions up to degree $N-1$ and (ii) orthogonality to all other basis functions. The main bulk of the material is contained within the accompanying webpage, at present, archived in .zip format. The 'homepage' that should be opened in a web-browser is `Galerkin.html`; the rest of the files contained within the archive are supplementary images and other files which are required by the website. When the webpage is opened, the left hand frame lists a range of boundary conditions for (a) orthogonality in Cartesian coordinates, (b) orthogonality in polar geometries and (c) more general orthogonality relations involving derivatives. Common and physically motivated boundary conditions are given explicitly, followed by more general boundary conditions as far as the extent of computer algebra allows. As will quickly become apparent, the formulae for the expressions are extremely lengthly, particularly for the most general cases considered. The user simply needs to copy and paste the expressions given in plain text into either a symbolic package such as Maple or Mathematica, or equally into a high-level language such as Matlab, C or Fortran. Clearly if the boundary conditions or α and β are generalised (i.e. unspecified), simply substitute your particular preference.

A brief overview of Galerkin methods is presented below, although this is largely the same as the material contained in the introduction section of the website.

1.1 Galerkin methods

Adopting a spectral method, or equivalently expanding an unknown function in terms a given basis $\{\Psi_n\}$

$$f(x) = \sum_{n=1}^{N} a_n \, \Psi_n(x)$$

can be very helpful in solving, amongst others, partial differential equations, eigenvalue and variational problems. If each Ψ_n satisfies a prescribed set of linear and homogeneous boundary conditions, it follows simply that these same conditions are satisfied by $f(x)$. If the expansion converges at a spectral or super-algebraic rate [1], then a severely truncated expansion may represent the function extremely well. In addition, the method of solution involves only finding the coefficients a_n; of particular note is that, for all intents and purposes, the boundary conditions may be ignored since they are already hard-wired into the numerical scheme.

One method of constructing a polynomial Galerkin basis set is the recombination of standard orthogonal polynomials [1]. However, such a basis set may be not only ill-conditioned, but in general will not inherit any of the optimal properties of the polynomials from which it was constructed. For instance,

$$\Psi_n(x) = T_n(x) - n^2 \, T_1(x),$$

where T_n is a Chebyshev polynomial of the first kind, is a basis set suitable for representing all functions f for which $f\,'(1) = 0$. However, $\{\Psi_n(x)\}$ is not orthogonal (by any useful definition) and has no optimal fitting properties (such as minimising the L^∞ norm of the error as the Chebyshev polynomials themselves do). Furthermore, this basis set is very ill-conditioned as, when normalised, $\Psi_n(x) \to -x$ as $n \to \infty$ and so, for large n, all basis functions look the same.

A more general approach, in order to enforce orthogonality, is to adopt a Gram-Schmidt process. In the case of finding a set of polynomials that satisfy $f\,'(1) = 0$, we can write

$$\Psi_n(x) = \sum_{i=0}^{n} d_i\, x^i, \qquad n \geq 1.$$

Each coefficient d_i is determined by (i) the boundary condition $\Psi_n\,'(1) = 0$, (ii) orthogonality (by some definition) to each Ψ_j, $j < n$ and (iii) a normalisation condition. However, this procedure has two major shortcomings. Firstly, in general, it requires symbolic calculation to determine the d_i. Adopting an integral measure of orthogonality, such as

$$\int_{-1}^{1} \Psi_n(x)\, \Psi_m(x)\, w(x)\, dx = 0, \qquad n \neq m$$

leads to d_i that, in general, grow extremely rapidly with n. This is an immediate consequence of the parsimonious representation of such a basis set in Jacobi polynomials whose monomial coefficients grow rapidly with n (see the discussion below). The only practical (and accurate) way of computing Ψ_n is by using computer algebra. Second, and most importantly, there is no way of knowing in advance what properties the basis functions, derived via the "black-box" Gram-Schmidt procedure, will have.

If the boundary conditions are sufficiently simple, for instance, $f\,(1) = 0$, we can write down an orthogonal basis set by exploiting properties of Jacobi polynomials. It may be written

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

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

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

for some constants h_n. For more complex boundary conditions, such as $f\,''(1) = 0$ this approach is not possible.

1.2 An example of auto orthogonality

Perhaps the simplest case with which to illustrate the concept of auto-orthogonality is the above basis

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

that satisfies $f\,(1) = 0$. Using the standard index recurrence relations

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

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

$$(2n+\alpha+\beta)P_n^{(\alpha-1,\beta)} = (n+\alpha+\beta)P_n^{(\alpha,\beta)} - (n+\beta)P_{n-1}^{(\alpha,\beta)}\,, \tag{5}$$

$$(2n+\alpha+\beta)P_n^{(\alpha,\beta-1)} = (n+\alpha+\beta)P_n^{(\alpha,\beta)} + (n+\alpha)P_{n-1}^{(\alpha,\beta)}\,, \tag{6}$$

we can write

$$\Psi_n(x) = c_1(n)P_n^{(\alpha+2,\beta)} + c_2(n)P_{n-1}^{(\alpha+2,\beta)} + c_3(n)P_{n-2}^{(\alpha+2,\beta)}, \qquad n \geq 2 \tag{7}$$

for coefficients $c_i(n)$, which take the (unnormalized) form

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

for $n \geq 2$ and $\Psi_1(x) = 1 - x$. Suppose we now consider constructing a basis set of the form

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

where $\Psi_1(x) = 1 - x$ and the c_i are found using the three condition

- orthogonality to $\Psi_1(x)$,

$$\int_{-1}^{1} \Psi_n(x)\,\Psi_1(x)\,w(x)\,dx = 0, \qquad n > 1$$

  where $w(x) = (1-x)^\alpha\,(1+x)^\beta$.

- $\Psi_n(1) = 0$

- A normalisation condition.

It must be that this new basis is the same that we have already found, namely $\Psi_n(x) = (1-x)\,P_{n-1}^{(\alpha+2,\beta)}$. It follows that the Ψ_n form an orthogonal set, even though we have only explicitly imposed that each is orthogonal to Ψ_1. This property we term **auto-orthogonality** [3].

Note also that the c_i take on the ratio $[1, -2, 1]$ as $n \to \infty$, a property that has great significance since the same asymptotic behavior arises from writing $P_n^{(\alpha,\beta)}(x)$ in the form of (7) by applying (5) twice. It follows that

$$\Psi_n(x) \sim P_n^{(\alpha,\beta)}(x)$$

for large n.

This construction can be extended to the boundary condition $f\,'(1) = 0$. A basis set is

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

for any $\alpha > -1$, $\beta > -1$ and where $P_n^{(\alpha,\beta)}(x)$ is a Jacobi polynomial. The function $\Psi_1(x) = 1$ is the lowest degree polynomial that satisfies the boundary condition. The three coefficients c_i are determined by imposing

- orthogonality only to $\Psi_1(x)$,

$$\int_{-1}^{1} \Psi_n(x)\,\Psi_1(x)\,w(x)\,dx = 0, \qquad n \geq 2$$

  where $w(x) = (1-x)^\alpha\,(1+x)^\beta$.

- $\Psi_n'(1) = 0$

- A normalisation condition.

Remarkably, the $\{\Psi_n\}$ are themselves orthogonal (auto-orthogonality)

$$\int_{-1}^{1} \Psi_n(x)\,\Psi_m(x)\,w(x)\,dx = 0, \qquad n \neq m$$

The coefficients c_i are (taking $\beta = \alpha$)

$$
\begin{aligned}
c_1 &= 8\alpha^2 + 8n^3\alpha^3 - 12n^2\alpha - 9n^3\alpha + 5n^4\alpha^2 + 12n^3\alpha^2 - 14n\alpha^3 - 27n^2\alpha^2 + 2n\alpha^2 - 4n^2\alpha^3 + n^5\alpha \\
&\quad + 10n^4\alpha + 2n^5 + 4n^2\alpha^4 - 8n\alpha^4 + 10\alpha^3 + 4\alpha^4 + 8n\alpha + 2n - 4n^3 + 2\alpha \\
c_2 &= -(2\alpha^4 + 6n\alpha^3 + 9\alpha^3 + 6n^2\alpha^2 + 20n\alpha^2 + 14\alpha^2 + 2n^3\alpha + 15n^2\alpha + 19n\alpha + 5\alpha + 4n^3 + 6n^2 + 2n) \\
&\quad \times (-1 + n^2 - 2\alpha + 2n\alpha) \\
c_3 &= -4n - \alpha - 6n^2 + 2n^3 + 6n^4 - \alpha^2 + \alpha^3 + 2n^5 + \alpha^4 + 11n\alpha^3 + 2\alpha^5 n + 8n\alpha^4 + 25n^2\alpha^3 + 28n^3\alpha^2 \\
&\quad + 13n^4\alpha + 9n^3\alpha^3 + 5n^4\alpha^2 + 26n^2\alpha^2 - 11n\alpha - 2n\alpha^2 + 22n^3\alpha + 7n^2\alpha^4 + n^5\alpha
\end{aligned}
$$

The details of how these are computed are given in [2].

Additional features of these auto-orthogonal sets are

- Exponential convergence to any function f that satisfies the boundary conditions.
- They behave asymptotically like a single Jacobi polynomial

$$\Psi_n(x) \sim P_n^{(\alpha,\beta)}(x) \qquad \text{as } n \to \infty$$

  For instance, if $\alpha = \beta = -1/2$, the $\{\Psi_n\}$ behave like Chebyshev polynomials for large n and thus inherit their optimal characteristics.

1.3 Auto orthogonality: one-sided

We consider here a one-dimensional Cartesian domain (or one in which no further constraints are imposed on the functions apart from boundary conditions and smoothness). We will impose a given set of M homogeneous linear boundary conditions involving derivatives up to degree $N-1$ at $x = 1$ *only* (hence the name "one-sided"). A basis set can be written

$$\Psi_n(x) = \sum_{i=1}^{N+1} c_i \, P_{n+M-i}^{(\alpha+N,\beta)}(x), \qquad n \geq N - M + 1$$

where the c_i are found using

- $N - M$ orthogonality conditions
- M boundary conditions
- One normalisation condition.

and Ψ_n, $n = 1, 2, \ldots, N - M$ are computed using a Gram-Schmidt orthogonalisation procedure.

This basis set has the properties

1. $$\int_{-1}^{1} \Psi_n \, \Psi_m(x) \, w(x) \, dx = 0 \qquad n \neq m$$
2. $\Psi_n(x) \sim P_n^{(\alpha,\beta)}(x)$ as $n \to \infty$.

The imposition of boundary conditions at $x = -1$ (only) requires a basis set of the form

$$\Psi_n(x) = \sum_{i=1}^{N+1} c_i \, P_{n+M-i}^{(\alpha,\beta+N)}(x) \,, \qquad n \geq N - M + 1$$

where the c_i are found as before.

1.4 Auto orthogonality: two-sided

In the Cartesian domain $[-1, 1]$ we consider a basis set that satisfies any given set of M homogeneous linear boundary conditions up to degree $N-1$ imposed at $x=-1$ or $x=1$ (or both). It may be written

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

where the c_i are found using

- $2N - M$ orthogonality conditions
- M boundary conditions
- One normalisation condition.

and Ψ_n, $n = 1, 2, \ldots, 2N - M$ are computed using a Gram-Schmidt orthogonalisation procedure.

The basis sets are found in various specific cases of the boundary conditions in section 3 of the website.

As in the one-sided case,

$$\Psi_n(x) \sim P_n^{(\alpha,\beta)}(x)$$

as $n \to \infty$.

1.5 Auto orthogonality: polar geometry

In polar geometries, due to the singularity of the coordinate system at the origin, expansions in radius (r) often require a regularity condition. This restricts the class of scalar functions within which the solution must lie to one of the form

$$f(r) = r^{l+1} \, p(r^2)$$

for some integer l and a function p. We assume this to be the case in what follows. In such a situation, we require a basis set that is of the above form and, in addition, satisfies M boundary conditions of maximum degree $N-1$ at $r=1$. It follows from the one-sided Cartesian case that such a basis can be written

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

As before, the first few Ψ_n are determined using a Gram-Schmidt procedure. These satisfy the auto-orthogonality

$$\int_0^1 \Psi_n(r) \, \Psi_m(r) \, (1-r^2)^\alpha \, dr = 0 \qquad n \neq m$$

and

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

as $n \to \infty$.

There are two things of note. Firstly, the argument of the Jacobi polynomials is $2r^2 - 1$, mapping $[0, 1] \to [-1, 1]$ and rendering the Jacobi polynomial contribution an even function. Secondly, β is no longer free, being set to $l + 1/2$. This ensures that the limiting behaviour of $P_n^{(\alpha,l+1/2)}(2r^2-1)$ takes on the equal-ripple or equal-area property of the Chebyshev polynomials of the first and second kinds when $\alpha = -1/2$ or $\alpha = 1/2$ respectively. However, other choices of β are possible [4].

The basis sets are found in various specific cases of the boundary conditions in section 4 of the website.

1.6 Auto orthogonality with respect to derivatives

Making the functions orthogonal, as we have done, is transparently helpful for expansions of many kinds. But this is not always the best way to approach solutions of a differential equation as the resulting matrices may be full and poorly conditioned.

Given the developments so far, it is natural to ask if our algorithm can be extended, so that we impose orthogonality between, say, $(d/dx)^k\,\Psi_n(x)$ and $(d/dx)^k\,\Psi_m(x)$, or $(d/dx)^k\,\Psi_n(x)$ and $\Psi_m(x)$, in place of that between Ψ_n and Ψ_m. For instance, if we were to solve the differential equation

$$y''(x) = \lambda\, y(x)$$

for an eigenvalue λ, this could be represented by the matrix problem

$$\big(A - \lambda\ B\big)\mathbf{q} = \mathbf{0}$$

where we have written $y(x) = \sum_i\ q_i\,\Psi_i(x)$ and

$$A_{ij} = \int_{-1}^{1} \Psi_i\,\Psi_j{}''\,w(x)\,dx, \qquad B_{ij} = \int_{-1}^{1} \Psi_i\,\Psi_j\,w(x)\,dx$$

and $\mathbf{q}$ is a vector of the unknown spectral coefficients. If, for some choice of Ψ and weight function $w(x)$, A and B could be made band-limited, then the numerical solution would be obtained expediently. In section 5 of the website, we will give examples where A is diagonal. In general, the matrix B turns out to have significant structure, for instance, becoming either penta-diagonal or tri-diagonal.

References

[1] Boyd, J. P., 2001. *Chebyshev and Fourier Spectral Methods*, Dover.

[2] Livermore, P., 2009. Generalized orthogonal polynomials, *J. Comp. Phys.*, p. submitted.

[3] Livermore, P. & Ierley, G., 2009. Quasi-L^p norm orthogonal expansions in sums of Jacobi polynomials, *Num. Alg.*, p. submitted.

[4] Livermore, P., Jones, C. A., & Worland, S., 2007. Spectral radial basis functions for full sphere computations, *J. Comp. Phys.*, **227**, 1209–1224.