Global spectral methods for BVPs
Part 1: an overview

We will transition from finite difference methods for BVPs to a new class of methods, called *spectral methods*. Here is the philosophical difference between these two categories of methods:

Philosophy behind spectral methods

Whereas finite difference methods are based on locally interpolating the differential equation, spectral methods minimize the least-squares error in the numerical solution.

Said differently, finite difference methods are analogous to interpolation of functions, and spectral methods are analogous to least squares approximation of functions.

As with least squares approximation of functions, there are both global and local variants. We will focus this week on global spectral methods, which use basis functions defined over the entire interval. Next week, we will consider local spectral methods, though these are more famously referred to as the *finite element method*.

As with finite difference methods, we will develop spectral methods for the 1D Poisson equation

$$\frac{d^2u}{dx^2} = f, \quad x \in [a,b] \tag{1}$$

$$u(a) = u_a,\ u(b) = u_b \tag{2}$$

Just as in our study of finite difference methods for BVPs, the use of the Poisson problem is for simplicity of presentation, but is not prescriptive. Straightforward changes can be incorporated to develop spectral methods for the more general BVP

$$\alpha\frac{d^2u}{dx^2} + \beta\frac{du}{dx} + \gamma u = f, \quad x \in [a,b] \tag{3}$$

Also note that we continue to close our BVP using Dirichlet boundary conditions. Other conditions can be accommodated, though this would require some detailed differences in the method.

In this class, we will focus on the specific case where $u_a = u_b = 0$. Nonzero boundary conditions can be accounted for in a relatively straightforward manner, but doing so would make our derivation more cumbersome and might make us lose the forest for the trees.

1 *The general formulation for spectral methods*

Since spectral methods minimize the least-squares error in the numerical solution, our aim is to find the $\hat{u}(x)$ that approximates the true solution $u(x)$ and satisfies the condition

$$\hat{u} = \min_{\tilde{u}\in\mathcal{V}} ||u - \tilde{u}|| \tag{4}$$

Remarkably, we will use *exactly* the same steps as in least-squares function approximation to approximate our solution to the 1D Poisson equation:

1. Pick a space, $\mathcal{V}$, on which to approximate the exact solution. Notice that we want our approximate solution $\hat{u}$ to satisfy the boundary conditions, so we must be sure to pick a space $\mathcal{V}$ that satisfies the zero Dirichlet boundary conditions.

We will give some example spaces below that satisfy the required boundary conditions, and will talk about appropriate bases for these example spaces.

2. Pick a basis for that space and represent the approximate solution as a linear combination of the basis functions (where the coefficients are unknown)

$$u(x) \approx \hat{u}(x) = \sum_{k=i_1}^{i_n} c_k \phi_k(x) \tag{5}$$

where i_1 and i_n are the starting and ending index, respectively, for our basis of choice; *e.g*, for the Lagrange polynomials $\{L_1, \ldots, L_{n+1}\}$, $i_1 = 1$ and $i_n = n + 1$.

3. Choose an inner product (and thus, a norm).

4. Use the fact that the minimizer $\hat{u}(x)$ of (4) satisfies the orthogonality condition $(u - \hat{u}, q) = 0$ for all $q \in \mathcal{V}$. In particular, since it holds for any $q \in \mathcal{V}$ it must hold each basis function $\phi_j(x) \in \mathcal{V}$:

$$(u - \hat{u}, \phi_j) = 0, \quad j = i_1, \ldots, i_n \tag{6}$$

Take a moment to appreciate this: because (4) is identical to the least squares formulation for approximating functions, we can use *exactly* the same steps to solve BVPs as in performing least squares approximation of functions!

5. Plug the expression (5) for $\hat{u}$ into (6) to solve for the coefficients $\{c_{i_1}, \ldots, c_{i_n}\}$

The question that remains is: what is the appropriate inner product to use?

2 *Choosing the right inner product*

The inner product that we will use is defined as

$$(f, g)_E = \int_a^b f'(x) g'(x) dx, \quad \forall f, g \in \mathcal{V} \tag{7}$$

Check that this is indeed an inner product by verifying that it satisfies the three properties of an inner product we defined in week 1.

The subscript E is used to denote the fact that this is referred to as the *energy inner product*. Why is this the case? Notice that the induced energy norm is

$$||g||_E = \sqrt{(g, g)_E} = \sqrt{\int_a^b (g'(x))^2 \, dx} \tag{8}$$

How is $||g||_E$ related to energy? Remember that the Poisson problem (1) is the steady-state heat equation. In this context, the derivative of a temperature field is the heat flux density (*i.e.*, the amount of energy that flows through an object per unit area per unit time). Thus, $||g||_E$ represents the integration of the energy density associated with a temperature field g across the entire domain.

Why are we using the energy inner product (and induced energy norm) to derive our spectral method? We will answer this question next.

3 *Using the energy inner product to derive our equations*

Plug the expression (5) for $\hat{u}$ into (6) and using the energy inner product gives

$$\left(u - \sum_{k=i_1}^{i_n} c_k \phi_k, \phi_j \right)_E = 0, \quad j = i_1, \ldots, i_n \tag{9}$$

$$\implies \quad \sum_{k=i_1}^{i_n} c_k \left(\phi_k, \phi_j \right)_E = \left(u, \phi_j \right)_E, \quad j = i_1, \ldots, i_n \tag{10}$$

Now here is where the energy inner product comes in handy. Let's probe the righthand side term:

$$\left(u, \phi_j \right)_E = \int_a^b u'(x) \phi_j'(x) dx \tag{11}$$

$$= \left[u'(x) \phi_j(x) \right]_a^b - \int_a^b u''(x) \phi_j(x) dx \quad \text{[Integrate by parts]} \tag{12}$$

$$= - \int_a^b u''(x) \phi_j(x) dx \quad \left[\phi_j \in \mathcal{V} \text{ so it satisfies the BCs} \right] \tag{13}$$

$$= - \int_a^b f(x) \phi_j(x) dx \quad \text{[Follows from (1)]} \tag{14}$$

Thus, we can write (10) as

$$\sum_{k=i_1}^{i_n} c_k \left(\phi_k, \phi_j \right)_E = - \left(f, \phi_j \right)_s, \quad j = i_1, \ldots, i_n \tag{15}$$

We can express (15) in matrix form as

$$\begin{bmatrix} (\phi_{i_1}, \phi_{i_1})_E & (\phi_{i_2}, \phi_{i_1})_E & \cdots & (\phi_{i_{n-1}}, \phi_{i_1})_E & (\phi_{i_n}, \phi_{i_1})_E \\ (\phi_{i_1}, \phi_{i_2})_E & (\phi_{i_2}, \phi_{i_2})_E & \cdots & (\phi_{i_{n-1}}, \phi_{i_2})_E & (\phi_{i_n}, \phi_{i_2})_E \\ \vdots & \vdots & \cdots & \vdots & \vdots \\ (\phi_{i_1}, \phi_{i_{n-1}})_E & (\phi_{i_2}, \phi_{i_{n-1}})_E & \cdots & (\phi_{i_{n-1}}, \phi_{i_{n-1}})_E & (\phi_{i_n}, \phi_{i_{n-1}})_E \\ (\phi_{i_1}, \phi_{i_n})_E & (\phi_{i_2}, \phi_{i_n})_E & \cdots & (\phi_{i_{n-1}}, \phi_{i_n})_E & (\phi_{i_n}, \phi_{i_n})_E \end{bmatrix} \begin{bmatrix} c_{i_1} \\ c_{i_2} \\ \vdots \\ c_{i_{n-1}} \\ c_{i_n} \end{bmatrix} = \begin{bmatrix} -(f, \phi_{i_1})_s \\ -(f, \phi_{i_2})_s \\ \vdots \\ -(f, \phi_{i_{n-1}})_s \\ -(f, \phi_{i_n})_s \end{bmatrix} \tag{17}$$

One important observation before we move on: where are the boundary conditions? You may recall from our lecture on finite difference methods for BVPs that the boundary conditions have to be incorporated into the matrix system. That is not true here: the boundary conditions are *already* built into $\mathcal{V}$, and thus into the basis functions $\{\phi_{i_1}, \ldots, \phi_{i_n}\}$. Because the boundary conditions are built into our approximation space, we do not need to modify the system (17) in any way.

We now have a general framework for developing spectral methods for the 1D Poisson equation! Next time, we will consider a few examples where we apply this formulation to approximate the BVP solution.

Notice the magic behind what we have done in this sequence of equations: we wrote the pesky (u, ϕ_j) term, which we know nothing about because we do not know the solution u, in terms of an inner product involving the source term f that we do know. This procedure is at the heart of spectral methods. The specific choice of energy product is problem dependent, but always revolves around this principle of enabling us to rewrite the (u, ϕ_j) term in terms of a quantity involving f.

Note that $(f, \phi_j)_s$ denotes use of the standard inner product defined as

$$(f, \phi_j)_s = \int_a^b f(x) \phi_j(x) dx \tag{16}$$