4 Orthogonality, generalized Fourier series

In the last two lectures we saw how various boundary conditions for the eigenvalues of the operator $A = -d^2/dx^2$ gave rise to the sine, cosine, and the full Fourier series. This corresponded to the Dirichlet, Neumann and periodic boundary conditions respectively. Today we would like to extend the procedure of obtaining Fourier series to more general boundary conditions, which in turn will allow one to solve a wider class of boundary value problems.

We will consider the ODE

$$-X'' = \lambda X, \tag{1}$$

on the interval $a < x < b$, along with the pair of boundary conditions

$$\begin{aligned} \alpha_1 X(a) + \beta_1 X(b) + \gamma_1 X'(a) + \delta_1 X'(b) = 0, \\ \alpha_2 X(a) + \beta_2 X(b) + \gamma_2 X'(a) + \delta_2 X'(b) = 0. \end{aligned} \tag{2}$$

Suppose X_n denotes the eigenfunction for the eigenvalue problem (1)-(2). We would like to find a way of expanding any reasonably nice function $\phi(x)$ in terms of these eigenfunctions, and to find the coefficients of the series

$$\phi(x) = \sum_n A_n X_n. \tag{3}$$

Recall that for the classical Fourier series we relied on the pairwise orthogonality of the eigenfunctions, which uniquely determined the coefficients in the expansion (3). This pairwise orthogonality was simple to verify for the trigonometric functions, however for the general boundary conditions (2), one cannot use explicit eigenfunctions. We thus need to find a condition for (2), that would guarantee the orthogonality of the set of eigenfunctions $\{X_n\}$.

To do this, let us assume that X_1 and X_2 are two eigenfunctions corresponding to the distinct eigenvalues λ_1, λ_2. That is,

$$\begin{aligned} -X_1'' = \lambda_1 X_1, \\ -X_2'' = \lambda_2 X_2. \end{aligned}$$

Taking the dot product of the first equation with X_2, and the second equation with X_1, and then subtracting the second equation from the first, and using commutativity of the dot product, we get

$$(\lambda_1 - \lambda_2)(X_1, X_2) = \int_a^b (-X_1'' X_2 + X_1 X_2'')\, dx.$$

But notice that

$$-X_1'' X_2 + X_1 X_2'' = (-X_1' X_2 + X_1 X_2')'.$$

Plugging this into the previous identity, and using the Fundamental Theorem of Calculus gives

$$(\lambda_1 - \lambda_2)(X_1, X_2) = \int_a^b (-X_1' X_2 + X_1 X_2')'\, dx = (-X_1' X_2 + X_1 X_2')\Big|_a^b.$$

Now, since the eigenvalues are distinct, and thus $\lambda_1 - \lambda_2 \neq 0$, we can deduce that the dot product of the eigenfunctions X_1, X_2 is zero, i.e. they are orthogonal, if the quantity on the right hand side is zero,

$$(-X_1' X_2 + X_1 X_2')\Big|_a^b = 0. \tag{4}$$

Notice that in the last identity all the terms are either the values of the functions X_1, X_2, or their derivatives at the endpoints of the interval (a, b). But these come from the boundary conditions (2), prompting the following definition.

Definition 4.1. We say that the boundary conditions (2) are *symmetric*, if for any two functions X_1 and X_2 satisfying these boundary conditions identity (4) holds.

It is easy to check that all the boundary conditions that we have encountered so far are symmetric. Indeed:

Dirichlet: $X_1(a) = X_1(b) = 0 = X_2(a) = X_2(b)$, and clearly (4) holds.

Neumann: $X_1'(a) = X_1'(b) = 0 = X_2'(a) = X_2'(b)$, and again (4) holds trivially.

Periodic: $X_1(a) = X_1(b)$, $X_1'(a) = X_1'(b)$; $X_2(a) = X_2(b)$, $X_2'(a) = X_2'(b)$. Then one also has that $(-X_1'X_2 + X_1X_2')(a) = (-X_1'X_2 + X_1X_2')(b)$, and thus (4) holds.

It is not hard to show that mixed Dirichlet-Neumann, as well as Robin conditions are also symmetric. It is then not surprising, that in all these cases the eigenvalues were found to be pairwise orthogonal. For the general boundary conditions (2), the above computation established the following.

Theorem 4.2. *If the boundary conditions* (2) *are symmetric, then the eigenfunctions corresponding to distinct eigenvalues of the eigenvalue problem* (1)-(2) *are orthogonal.*

Using this fact, we can compute the coefficients in the expansion (3) following the same strategy that we employed for the classical Fourier series. That is, to find a particular coefficient, we take the dot product of the expansion with the corresponding eigenvalue.

$$(\phi, X_m) = \int_a^b \phi(x)X_m(x)\,dx = \int_a^b \left(\sum_n A_nX_n, X_m\right)\,dx = \sum_n (A_nX_n, X_m) = A_m(X_m, X_m),$$

since due to the pairwise orthogonality only the term with $n = m$ survives. We can then solve for the coefficient, obtaining

$$A_m = \frac{(\phi, X_m)}{(X_m, X_m)}. \tag{5}$$

This is the coefficients formula for the generalized Fourier series (3). The procedure of finding the coefficients, of course, again resembles finding the components of a vector in terms of the orthogonal basis elements. The question of convergence of such expansions will be addressed later on.

We should remark that in proving pairwise orthogonality of the eigenfunctions we ignored the case of having more than one linearly independent eigenfunction corresponding to the same eigenvalue. In the above proof we relied on the fact that X_1 and X_2 corresponded to distinct eigenvalues. However, this is not always so, and the set $\{X_n\}$ may contain linearly independent eigenfunctions corresponding to the same eigenvalue. This was the case for the periodic boundary conditions, for which we had two linearly independent eigenfunctions corresponding to each of the eigenvalues $\lambda_n = (n\pi/l)^2$, namely, $\cos(n\pi x/l)$, and $\sin(n\pi x/l)$. These happened to be mutually orthogonal, as was shown explicitly, however, if we instead chose the pair of eigenfunctions $\sin(n\pi x/l)$ and $\sin(n\pi x/l) + \cos(n\pi x/l)$ for the same eigenvalue, we would not have the pairwise orthogonality required for the derivation of the coefficients formula (5).

We thus need a way of extracting pairwise orthogonal sets from the eigenfunctions corresponding to the same eigenvalue. And such a way out is provided by the Gram-Schmidt orthogonalization procedure. We demonstrate this on a set of two eigenfunctions, but it can be trivially generalized to any number of them. If X_1 and X_2 correspond to the same eigenvalue λ, then take the pair

$$X_1, \widetilde{X}_2 = X_2 - \frac{(X_1, X_2)}{(X_1, X_1)}X_1.$$

the new function $\widetilde{X}_2$ will be an eigenfunction corresponding to the eigenvalue λ, and it is essentially the projection of X_2 onto the "direction orthogonal to X_1". It is not hard to check that $(X_1, \widetilde{X}_2) = 0$, i.e. they are orthogonal.

4.1 Complex eigenvalues

So far we have completely ignored the question of complex eigenvalues and eigenfunctions, however the complex form of the full Fourier series discussed last time hints at the usefulness of considering such eigenfunctions. Notice that the complex valued function $e^{in\pi x/l} = \cos(n\pi x/l) + i\sin(n\pi x/l)$ is an eigenvalue corresponding to $\lambda_n = (n\pi/l)^2$ for the eigenvalue problem associated with the periodic boundary conditions. We thus would like to find all such eigenfunctions, for which we also need to consider the question of having complex eigenvalues associated with the general boundary conditions (2).

First, recall that for complex valued functions the dot product was defined to be

$$(f, g) = \int_a^b f(x)\overline{g(x)}\,dx,$$

where the upper bar denotes the complex conjugate. In this case one has $(f, g) = \overline{(g, f)}$, and two functions will be orthogonal if their dot product is zero. This is similar to how the dot product for complex vectors is defined. The reason for having the complex conjugation in the definition is to guarantee that the dot product of a function (vector) with itself is a real positive number.

We now consider the general boundary conditions (2) with real coefficients $\alpha_{1,2}, \beta_{1,2}, \gamma_{1,2}, \delta_{1,2}$. We say that the boundary conditions are *hermitian*, if for any two functions X_1, X_2 satisfying them the following identity holds

$$(-X_1'\overline{X}_2 + X_1\overline{X}_2')\Big|_a^b = 0. \tag{6}$$

Notice that for real functions X_1, X_2 this definition coincides with the definition of symmetric boundary conditions. Also, under this condition Theorem 4.2 is true for complex valued functions with no change. In addition, the hermitian symmetry of the boundary conditions guarantees that there are no complex eigenvalues.

Theorem 4.3. *If the boundary conditions* (2) *are hermitian, then all the eigenvalues of the eigenvalue problem* (1)-(2) *are real. Moreover, all the eigenfunctions can be chosen to be real valued.*

The proof of the above Theorem relies on the observation that, if X is an eigenfunction corresponding to the eigenvalue λ, then its complex conjugate $\overline{X}$ will be an eigenfunction corresponding to the eigenvalue $\overline{\lambda}$. Indeed, taking the complex conjugate of both sides of the equation $-X'' = \lambda X$ gives $-\overline{X}'' = \overline{\lambda X}$. The boundary conditions will be also satisfied, since the coefficients are real, and do not change under complex conjugation. But then taking the (complex) dot product of the first equation with X and the second equation with $\overline{X}$, and subtracting them using the facts that $\overline{\overline{X}} = X$ and $(X, X) = (\overline{X}, \overline{X})$, we have

$$(\lambda - \overline{\lambda})(X, X) = \int_a^b (-X''\overline{X} + X\overline{X}'')\,dx = (-X'\overline{X} + X\overline{X}')\Big|_a^b = 0,$$

by the hermitian property. So

$$(\lambda - \overline{\lambda})\int_a^b X\overline{X}\,dx = 0.$$

But $X\overline{X} = |X|^2 \geq 0$, and the function $X(x) \not\equiv 0$, so the above integral cannot be zero, and hence, $\lambda = \overline{\lambda}$, which means that λ is real.

Now, if X is a complex eigenfunction corresponding to the eigenvalue λ, then so is $\overline{X}$, since λ is real. But then any (complex) linear combination of these will be an eigenfunction as well, and will satisfy the same boundary conditions (2). Taking

$$Y(x) = \frac{1}{2}(X + \overline{X}), \quad \text{and} \quad Z(x) = \frac{1}{2i}(X - \overline{X}),$$

we will have two real eigenfunctions. These are, of course, the real and imaginary parts of $X(x)$, i.e. $X(x) = Y(x) + iZ(x)$.

4.2 Conclusion

In this lecture we explored the eigenvalue problem for the operator $-d^2/dx^2$ with the general boundary conditions (2), and showed that if the BC's are symmetric, then the eigenfunctions are pairwise orthogonal, and one can determine Fourier expansions in terms of these eigenfunctions. These generalized Fourier expansions are similar to the expansions in terms of a basis in linear algebra, where the basis is formed by the eigenvectors of a linear symmetric transformation given by a real symmetric matrix. So the operator $-d^2/dx^2$ acts on the set of functions satisfying the symmetric boundary conditions like a symmetric linear transformation. The difference, as we pointed out several times before, is in the fact that the space of functions is infinite dimensional, and the expansion takes the form of a series, rather than a finite linear combination.

We also showed that if the boundary conditions are hermitian, then all the eigenvalues are real and one can work exclusively with real eigenfunctions. In the coming lectures we will show that these eigenfunctions form a true basis, in the sense that any (L^2) function can be uniquely expanded into a series in terms of these functions.