Boundary Value Problems and Finite Differences

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The sophomore-level ordinary differential equations course at our institution focuses primarily on initial value problems, but the last few weeks does include a short unit on boundary value problems. The solution theory for boundary value problems is rather different from, and somewhat less intuitive than, the theory for initial value problems, as is illustrated by the following example.

Example. Consider the boundary value problem

$$u''(x) + \lambda u(x) = \sin(\pi x), \qquad x \in (0,1) \tag{1a}$$

$$u(0) = 0, \qquad u(1) = 0, \tag{1b}$$

where $\lambda > 0$ is some parameter. It is straightforward to find the general solution to (1a), from which we see that if $\lambda = \pi$ then (1) has a unique solution, while if $\lambda = \pi^2$ then there does not exist any solutions. Finally, if $\lambda = 4\pi^2$ then (1) has an infinite number of solutions.

This example illustrates that seemingly similar problems can have vastly different solvability properties, and thus raises the following question: How to make sense of a solution theory which *prima facie* differs greatly from the broad existence and uniqueness theorems applicable to the initial value problems that make up the bulk of an introductory course?

In this note we present an exploration of the solution theory for boundary value problems via finite difference approximations. This approach has three pedagogical advantages. The first is that it is rather 'low-tech,' requiring only material from single-variable calculus and a first course in linear algebra.

Second, an analogous approach can be used to discuss initial value problems; indeed Peano's existence theorem relies on constructing a sequence of approximate solutions via finite difference methods; see, for example, the proof in [6].

The final advantage lies in the fact that finite difference approximation yields a system of linear equations, the solvability of which can be analyzed by studying the associated linear transformation. Similarly, the existence theory for linear boundary value problems such as (1) can be obtained from analyzing the mapping properties of differential operators. While introductory treatments (e.g. [2]) often mention the parallels between boundary value problems and linear systems, the exploration here makes the connection much richer, and much more concrete, as the linear systems are themselves approximations of the differential equations problem.

1 Finite difference approximations

For simplicity, let us focus our attention on problems of the form

$$u''(x) + \lambda u(x) = f(x), \qquad x \in (0,1) \tag{2a}$$

$$u(0) = 0, \qquad u(1) = 0, \tag{2b}$$

where f is some prescribed function and $\lambda > 0$.

We first construct discrete approximations of a function. Dividing the interval $[0,1]$ into subintervals of size $\Delta x = \frac{1}{n+1}$, we set $x_k = k\,\Delta x$. A function $u : [0,1] \to \mathbb{R}$ satisfying the boundary conditions (2b) is approximated by vector $\mathbf{u} = (u_1, u_2, \ldots, u_n)^t \in \mathbb{R}^n$ with $u_k = u(x_k)$. We emphasize that the points x_k are all in the interior of $[0,1]$; thus the approximation of function u by vector $\mathbf{u}$ has the boundary conditions 'built in.'

Example. With $n = 3$, the function $f(x) = \sin(\pi x)$ in (1a) is represented by $\mathbf{f} = (\frac{1}{\sqrt{2}}, 1, \frac{1}{\sqrt{2}})^t$.

In order to approximate derivatives of a function, we make use of the Taylor expansions

$$u(x_k \pm \Delta x) = u(x_k) \pm u'(x_k)\,\Delta x + \frac{1}{2}u''(x_k)\,(\Delta x)^2 \pm \frac{1}{6}u'''(x_k)\,(\Delta x)^3 + \mathcal{O}\left((\Delta x)^4\right). \tag{3}$$

Adding both expansions yields

$$u''(x_k) = \frac{1}{(\Delta x)^2}\left[u_{k-1} - 2u_k + u_{k+1}\right] + \mathcal{O}\left((\Delta x)^2\right). \tag{4}$$

Thus we may approximate (2a) by the equations

$$\frac{1}{(\Delta x)^2}\left[u_{k-1} - 2u_k + u_{k+1}\right] + \lambda u_k = f_k, \quad k = 1, \ldots, n. \tag{5}$$

When $k = 1$ or n, we make use of the boundary condition (2b), which may be interpreted as setting $u_0 = 0$ and $u_{n+1} = 0$. The result is a linear system of n equations for n unknowns, which we write as

$$\mathbf{M}\mathbf{u} = (\Delta x)^2\,\mathbf{f}, \tag{6}$$

with

$$\mathbf{M} = \begin{bmatrix} \alpha & 1 & & & \\ 1 & \alpha & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & \alpha & 1 \\ & & & 1 & \alpha \end{bmatrix} \tag{7}$$

and $\alpha = -2 + \lambda(\Delta x)^2$. We emphasize that (6) is a finite difference approximation of the entire boundary value problem (2), as both the approximation of the differential equation (2a) and the boundary conditions (2b) are incorporated.

Example. With $n = 3$, the finite difference approximation of (1) is

$$\begin{bmatrix} -2+\frac{1}{16}\lambda & 1 & 0 \\ 1 & -2+\frac{1}{16}\lambda & 1 \\ 0 & 1 & -2+\frac{1}{16}\lambda \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \frac{1}{16} \begin{pmatrix} \frac{1}{\sqrt{2}} \\ 1 \\ \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{8}$$

2 Some linear algebra

Having constructed the approximate problem (6), we now recall the following result from linear algebra.

Proposition 1. *For linear transformation $\mathcal{L} : \mathbb{R}^n \to \mathbb{R}^n$, the solvability of the equation*

$$\mathcal{L}u = \mathbf{f} \tag{9}$$

is described as follows:

1. *If $\ker(\mathcal{L}) = \{\mathbf{0}\}$, then (9) has a unique solution for all $\mathbf{f} \in \mathbb{R}^n$.*
2. *If $\ker(\mathcal{L}) \neq \{\mathbf{0}\}$, then either*
   (a) $\mathbf{f} \in \ker(\mathcal{L}^*)^\perp$, in which case (9) has multiple solutions, or
   (b) $\mathbf{f} \notin \ker(\mathcal{L}^*)^\perp$, in which case (9) does not have a solution.

Here $\mathcal{L}^*$ is the adjoint transformation of $\mathcal{L}$, defined by $(\mathcal{L}^*\mathbf{u}) \cdot \mathbf{v} = \mathbf{u} \cdot (\mathcal{L}\mathbf{v})$ for all $\mathbf{v}$; if $\mathcal{L}$ is given by matrix $\mathbf{A}$, then $\mathcal{L}^*$ is given by the transpose $\mathbf{A}^t$.

Remark. First, the non-uniqueness of solutions when $\ker(\mathcal{L}) \neq \{\mathbf{0}\}$ is easy to see: If $\mathbf{u}$ is a solution to (9) and $\mathbf{v} \in \ker(\mathcal{L})$, then $\mathbf{u} + \mathbf{v}$ is also a solution.

Second, the necessity of condition $\mathbf{f} \in \ker(\mathcal{L}^*)^\perp$ is straightforward as well. If $\mathbf{u}$ is a solution to (9) and $\mathbf{v} \in \ker(\mathcal{L}^*)$, then $\mathbf{f} \cdot \mathbf{v} = (\mathcal{L}\mathbf{u}) \cdot \mathbf{v} = \mathbf{u} \cdot (\mathcal{L}^*\mathbf{v}) = 0$.

In view of Proposition 1, understanding the solvability of the approximate problem (6) is reduced to understanding the null space of the matrix $\mathbf{M}$ in (7); note that $\mathbf{M} = \mathbf{M}^t$.

Example. The determinant of the matrix in (8) is

$$\left(\frac{\lambda}{16} - 2\right)\left(\frac{\lambda}{16} - 2 + \sqrt{2}\right)\left(\frac{\lambda}{16} - 2 - \sqrt{2}\right). \tag{10}$$

Thus the approximate problem has a unique solution for all but three values of λ.

If $\lambda = 32$, then the matrix $\mathbf{M}$ has a null space spanned by $\mathbf{v} = (1, 0, -1)^t$. Since $\mathbf{v} \cdot \mathbf{f} = 0$, the approximate problem has multiple solutions. There are also multiple solutions if $\lambda = 32 + 16\sqrt{2}$.

If, however, $\lambda = 32 - 16\sqrt{2}$, then the null space of the matrix is spanned by $\mathbf{v} = (1, \sqrt{2}, 1)^t$. In this case $\mathbf{v} \cdot \mathbf{f} \neq 0$ and the approximate problem admits no solution.

3 Solvability of the approximate problem

In the above analysis of (8) we found that the approximate problem had a unique solution for all but a small number of 'exceptional' values for the parameter λ. This is generally the case, as the determinant of the matrix $\mathbf{M}$ is a polynomial of degree n in λ. In fact, we can explicitly find the values λ for which $\mathbf{M}$ is not invertible.

Let d_n be the determinant of the $n \times n$ matrix $\mathbf{M}$ in (7). Expanding about the first row, we see that d_n satisfies the linear recursion relation

$$\begin{aligned} &d_n = \alpha d_{n-1} - d_{n-2}, \\ &d_1 = \alpha, \qquad d_2 = \alpha^2 - 1. \end{aligned} \tag{11}$$

When $\alpha^2 \neq 4$, the solution to (11) is

$$d_n = \frac{1}{\sqrt{\alpha^2 - 4}} \left[(z_+)^{n+1} - (z_-)^{n+1} \right], \tag{12}$$

where

$$z_\pm = \frac{\alpha}{2} \pm \sqrt{\left(\frac{\alpha}{2}\right)^2 - 1} \tag{13}$$

are the roots of the characteristic equation $z^2 - \alpha z + 1 = 0$. When $\alpha^2 = 4$, the characteristic equation has repeated roots and the determinant is instead given by $d_n = (1+n)\left(\frac{\alpha}{2}\right)^n$.

Our goal is to determine for which values of α (and hence λ) the determinant d_n vanishes. As $d_n \neq 0$ when $\alpha^2 = 4$, we examine the expression in (12), which vanishes when the ratio z_+/z_- is an $(n+1)^{\text{st}}$ root of unity:

$$\frac{z_+}{z_-} = e^{i\frac{2\pi l}{n+1}}, \quad l = 1, 2, \ldots, n. \tag{14}$$

Using (13) and $\alpha = -2 + \frac{\lambda}{(n+1)^2}$ we find that the determinant of $\mathbf{M}$ vanishes when

$$\lambda = 2(n+1)^2 \left[1 - \cos\left(\frac{\pi l}{n+1}\right) \right], \quad l = 1, 2, \ldots, n. \tag{15}$$

Notice that this formula agrees with (10).

When λ is one of the values in (15), we can understand the null space of $\mathbf{M}$ via the following observations. Set $\mathbf{M}_0$ to be the symmetric matrix obtained from replacing α by -2 in (7). If $\mathbf{v}$ is in the null space of $\mathbf{M}$, then $\mathbf{M}_0\mathbf{v} = -\lambda(\Delta x)^2\mathbf{v}$. Thus the values $-\lambda(\Delta x)^2$, with λ given by (15), are eigenvalues of $\mathbf{M}_0$, and the corresponding eigenspace is the null space of $\mathbf{M}$ with that choice of λ. Therefore, since (15) gives n distinct eigenvalues for $n \times n$ matrix $\mathbf{M}_0$, each eigenspace is one-dimensional and is spanned by vector $\mathbf{v} = (v_1, \ldots, v_n)^t$ whose entries satisfy the recursion relation

$$\begin{aligned} &v_k + \alpha v_{k-1} + v_{k-2} = 0, \\ &v_2 = -\alpha v_1; \end{aligned} \tag{16}$$

here v_1 may be freely chosen, representing the freedom to rescale eigenvectors. For convenience we choose $v_1 = \sin\left(\frac{\pi l}{n+1}\right)$; the corresponding solution to (16) is

$$v_k = \sin\left(\frac{\pi l k}{n+1}\right) = \sin(\pi l x_k). \tag{17}$$

We summarize the above discussion in the following proposition.

Proposition 2. *Consider the finite difference approximation* (6) *of boundary value problem* (2).

1. *If λ is not one of the values given in* (15)*, then the null space of $\mathbf{M}$ is trivial and the approximate problem* (6) *has a unique solution for each vector $\mathbf{f}$.*
2. *If λ is one of the values in* (15)*, then the null space of $\mathbf{M}$ is non-trivial and is spanned by $\mathbf{v}$, as determined by* (17)*. Furthermore,*
   (a) *if $\mathbf{v} \cdot \mathbf{f} = 0$ the approximate problem has multiple solutions, while*
   (b) *if $\mathbf{v} \cdot \mathbf{f} \neq 0$ the approximate problem does not admit any solutions.*

In particular, for most values of λ the approximate problem has a unique solution, but there exists a collection of exceptional values for which either existence or uniqueness fails; note that this is consistent with the example above.

4 Solvability of boundary value problems

We now return to the boundary value problems for differential equations, keeping in mind the lessons learned whilst studying the approximate problem.

First is our expectation that, aside from when λ is one of a collection of exceptional values, there is a unique solution to (2) for all f. In fact, we can even use (15) to predict what these exceptional values might be. Using the Taylor expansion of cosine, we see that for fixed l we have

$$\lambda = 2(n+1)^2 \left[1 - \left\{1 - \frac{1}{2}\left(\frac{\pi l}{n+1}\right)^2 + \mathcal{O}\left(n^{-4}\right)\right\}\right] = (\pi l)^2 + \mathcal{O}\left(n^{-2}\right) \tag{18}$$

as $n \to \infty$. Thus we expect existence and uniqueness of solutions to (2), except when $\lambda = (l\pi)^2$ for integer l. Indeed this is consistent with our discussion of (1), where existence failed for $\lambda = \pi^2$ and uniqueness failed with $\lambda = (2\pi)^2$.

A second, and more fundamental, lesson we can learn from studying the finite difference approximation is that it is helpful to frame the boundary value problem (2) using linear mappings of inner-product spaces. In many senses, this is the 'right language' for describing the solvability of such problems.

To frame the problem (2) in this language, let us review the main features of the theory used to address the approximate problem (6). Three aspects of the approximate problem are important: the vector space structure of $\mathbb{R}^n$, the linearity of the equation, and the inner-product structure (namely, the dot product) on $\mathbb{R}^n$.

The vector space $\mathbb{R}^n$ is the set in which we seek solution $\mathbf{u}$; recall that the boundary conditions are 'built-in' to this set. The fact that the equation was linear allows us to interpret (6) as a question about the linear mapping $\mathcal{L}$ given by the matrix $\mathbf{M}$. Finally, the solvability of the equation (6) is described in terms of the kernel of linear mappings $\mathcal{L}$ and $\mathcal{L}^*$, using the notions of orthogonality and adjoint we obtain from the dot product.

A parallel approach is possible for the boundary value problem (2), we only need to specify the corresponding three key elements. First, set V to be the vector space of smooth functions $[0,1] \to \mathbb{R}$; let V_0 be the vector space of those functions satisfying the boundary conditions (2b).

We now consider $\frac{d^2}{dx^2} + \lambda$ as a linear mapping $V_0 \to V$. As with the approximate problem, issues of existence and uniqueness of solutions to (2) now become questions about this linear mapping.

In order to discuss these questions using the concepts of orthogonality and adjoint mappings, we introduce a natural inner product for functions

$$\langle u, v \rangle = \int_0^1 u(x)\, v(x)\, dx. \tag{19}$$

This inner product allows us to define the adjoint $\mathcal{L}^*$ of a linear map $\mathcal{L} : V_0 \to V$ as the map which satisfies the identity $\langle \mathcal{L}^* u, v \rangle = \langle u, \mathcal{L} v \rangle$. Notice that $\mathcal{L} = \frac{d^2}{dx^2} + \lambda : V_0 \to V$ is self-adjoint, meaning $\mathcal{L} = \mathcal{L}^*$; this can be observed using integration by parts. The inner product also allows us to discuss orthogonality of functions.

In order to state the theorem analogous to Proposition 1, we must introduce one technical condition. We say that a second-order, linear, ordinary differential operator $\mathcal{L} = a(x)\frac{d^2}{dx^2} + b(x)\frac{d}{dx} + c(x)$ is *non-degenerate* if the function a never vanishes on $[0,1]$. This condition is analogous to the fact that the matrix $\mathbf{M}_0$, discussed above, is invertible. With this in mind, we now state a theorem governing the solvability of boundary value problems.

Main Theorem. *For non-degenerate, second-order, linear, ordinary differential operator $\mathcal{L} : V_0 \to V$ with smooth coefficients, the solvability of the equation*

$$\mathcal{L} u = f \tag{20}$$

is described as follows:

1. *If $\ker(\mathcal{L})$ contains only the zero function, then (20) has a unique solution for all f.*

2. *If $\ker(\mathcal{L})$ contains a non-zero function, then either*

   (a) *$f \in \ker(\mathcal{L}^*)^\perp$, in which case (20) has multiple solutions, or*

   (b) *$f \notin \ker(\mathcal{L}^*)^\perp$, in which case (20) has no solution.*

The theorem above is a greatly simplified instance of the *Fredholm alternative*, an important result in functional analysis (see, for example, [3]). The 'alternative' is the dichotomy between the existence of a unique solution to the inhomogeneous problem in case 1 and the existence, in case 2, of non-zero solutions to the homogeneous problem, described in the theorem as elements of $\ker(\mathcal{L})$. In the latter situation, we also have a criterion by which we know whether uniqueness or existence will fail.

We emphasize the following: Not only is the form of the Main Theorem analogous to that of Proposition 1, but each part of the approximate problem (6), to which Proposition 1 is applied (the result being Proposition 2), corresponds to some part of the differential equations problem (2). This correspondence is what allows us to make sense of the seemingly complicated theory for boundary value problems, as each of the features corresponds to a feature of the approximate problem.

In order to make this correspondence concrete, and to advertise other features of this correspondence, we return to (2). Note that, as anticipated above, it is precisely when $\lambda = (l\pi)^2$ for integer l that the kernel of $\mathcal{L} = \frac{d^2}{dx^2} + \lambda$ contains a non-zero function, namely $\sin(\pi l x)$. From the Main Theorem we can conclude that for such values either existence or uniqueness of solutions to (1) fail, while for all other values there exists a unique solution.

As in the discussion following (15), we may interpret $-\lambda = -(l\pi)^2$ as the eigenvalues of the operator $\mathcal{L}_0 = \frac{d^2}{dx^2}$, and $\sin(\pi l x)$ as the corresponding eigenfunctions, which span the one-dimensional eigenspaces. In fact, we see that the eigenvectors given by (17), are precisely the discrete approximations of these eigenfunctions.

For the approximate problem, the eigenvectors of $\mathbf{M}_0$, which is symmetric and has trivial kernel, constitute an orthogonal eigenbasis of $\mathbb{R}^n$. A similar fact holds for the differential operator $\mathcal{L}_0$, which is self-adjoint and also has trivial kernel: The eigenfunctions $\sin(\pi l x)$ are mutually orthogonal, and complete in the sense that any function in V_0 can be expressed as a series $\sum_{l=1}^{\infty} a_l \sin(\pi l x)$. That this is generally the case for self-adjoint operators with trivial kernel is the content of Sturm-Liouville theory; see [1] for an excellent and accessible introduction.

Finally, we record a version of the Main Theorem for (2), which should be compared to Proposition 2.

Proposition 3.

1. *If $\lambda \neq (l\pi)^2$ for all integers l, then* (2) *has a unique solution for each smooth function f.*
2. *If $\lambda = (l\pi)^2$ for some integer l, then there exists a non-zero homogeneous solution to* (2)*, namely $v(x) = \sin(\pi l x)$. Furthermore,*
   (a) *if $\int_0^1 f(x)\sin(\pi l x)\,dx = 0$, then* (2) *admits multiple solutions, while*
   (b) *if $\int_0^1 f(x)\sin(\pi l x)\,dx \neq 0$, then* (2) *does not admit any solutions.*

While Proposition 3 follows direcly from the Main Theorem, it is instructive to present an independent argument making use of the orthogonality and completeness of the eigenfunctions.

Supposing $f(x) = \sum_{k=0}^{\infty} b_k \sin(\pi k x)$, we seek a solution to (2) of the form $u(x) = \sum_{k=0}^{\infty} a_k \sin(\pi k x)$. Inserting these in to (2a), we find that we must have $a_k[\lambda - (k\pi)^2] = b_k$ for each k. If $\lambda \neq (k\pi)^2$ for all k, then we easily obtain an expression for the coefficients a_k. If, however, $\lambda = (l\pi)^2$ for some integer l, then in order to obtain a solution we must have $b_l = 0$, in which case f is orthogonal to $\sin(\pi l x)$ and any choice of a_l yields a solution.

5 Further directions

The many technical aspects of Fredholm theory present a significant barrier for the typical sophomore student interested in learning more about the beautiful theory behind the Main Theorem. However, we can nevertheless suggest several activities for pursuing further the ideas in this note.

1. In place of the Dirichlet boundary condition (2b), one can consider the Neumann boundary condition $u'(0) = 0$, $u'(1) = 0$; another natural choice is the periodic boundary condition $u(0) = u(1)$, $u'(0) = u'(1)$. An excellent exercise is to construct the finite difference approximations of (1a) with these boundary conditions and analyze their solvability. Then solve the differential equations problem and compare.

   Finally, consider the mixed boundary conditions $a_0 u(0) + b_0 u'(0) = 0$, $a_1 u(1) + b_1 u'(1) = 0$. For what constants a_i, b_i does the boundary value problem have a unique solution? Analyze first the approximate problem before turning to the differential equation itself.

2. Finite difference approximations are useful for constructing numerical approximations of solutions to boundary-value problems. The linear system (6) can be solved very efficiently, due to the tridiagonal structure of the matrix $\mathbf{M}$; even the novice programmer is encouraged to construct the algorithm.

   A natural problem to consider next is the two-dimensional Poisson equation $\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = f$. The matrix appearing in the finite difference approximation is no longer tri-diagonal, but is still sparse (and banded). We encourage the reader to consider, independently, how one might construct an algorithm for solving such a linear system. We have found [4] to be a good resource.

3. The problem (2) is a simple example of a nonhomogeneous boundary value problem, described, for example, in Chapter 11 of [2]. There, solutions are constructed via a series of eigenfunctions.

   This procedure can also be carried out at the level of the approximate problem: Start with a self-adjoint, non-degenerate, second-order, linear ordinary differential operator $\mathcal{L}$.

Construct the finite difference approximation and find the eigenvectors of the corresponding matrix. Then express the solution to an approximate inhomogeneous problem in this eigenbasis. It is instructive to approximate an inhomogeneous problem for which you know the solution. How does your approximate solution compare to the known solution?

For the finite difference approximations, the procedure above works because invertible symmetric matrices have real eigenvalues, and give rise to bases of eigenvectors; the corresponding theory for differential operators is the content of Sturm-Liouville theory. For those who wish to pursue this further we find [1] to be an excellent resource.

For the more advanced student, and interested instructor, we mention that many of the technical difficulties surrounding Fredholm theory are related to notions of completeness, and thus are accessible to students who have taken a semester of advanced calculus. In addition to [1], which is appropriate for strong undergraduates, we have found helpful the monographs [5], [3].

Abstract

The solvability of boundary value problems differs greatly from that of initial value problems, and can be somewhat difficult to make sense of in the context of a sophomore-level differential equations course. We present an approach which uses finite difference approximations to motivate, and understand, the theory governing the existence and uniqueness of boundary value problems at an elementary level.

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