Garrett Birkhoff and Robert E. Lynch

Numerical Solution of Elliptic Problems

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Preface

The science of solving elliptic problems has been revolutionized in the last 35 years. Today's large-scale, high-speed computers can solve most two-dimensional boundary value problems at moderate cost *accurately*, by a variety of numerical methods. The aim of this monograph is to provide a reasonably well-rounded and up-to-date survey of these methods.

Like its predecessor (Birkhoff [69]), written at an earlier stage in the Computer Revolution, our book emphasizes problems which have important scientific and/or engineering applications, and which are solvable at moderate cost on current computing machines. Because of this emphasis, it devotes much space to the two-dimensional 'linear source problem'

$$-\nabla \cdot [p(x,y)\nabla u] + q(x,y)u = f(x,y), \quad p > 0, \quad q \ge 0.$$

We make no claim to completeness. Indeed, our main concern is with *linear* boundary value problems, and we say little about eigenproblems. Readers seeking additional information should consult the carefully selected references cited in our many footnotes.

Chapters 1 and 2 are preliminary in nature, and are included to make our book largely self-contained. The first chapter explains the physical origins of several typical, relatively simple elliptic problems, indicating their practical importance. The second chapter reviews some of the most helpful and easily appreciated relevant theorems of classical analysis. It is the properties stated in these theorems (e.g., the smoothness of solutions), that give to elliptic problems their special mathematical flavor. Classical analysis also provides known exact solutions to many 'model problems', which can be used to test the accuracy of numerical methods.

Our analysis of numerical methods begins in Chapter 3. Some of the best known and most successful difference approximations to elliptic problems are reviewed, with emphasis on their simplicity and accuracy. Examples are given to show how their accuracy depends on the problem being solved, as well as on roundoff, Richardson extrapolation, etc.

We then devote two chapters to effective algorithms for solving numerically the very large systems of linear algebraic equations (involving

200-5000 or more unknowns) to which such difference approximations give rise. After briefly sketching several direct 'sparse matrix' methods in the first part of Chapter 4, we concentrate on *iterative* and semi-iterative methods. The latter are not only advantageous for treating very large problems and essential for solving nonlinear problems, but they seem destined to play a crucial role in solving the three-dimensional elliptic problems whose solution will, we hope, become routine during the next decade.

Chapters 6 and 7 return to approximation methods, especially the finite element methods (FEM) that have been adopted so widely during the past two decades. In analyzing these FEM, we emphasize techniques for piecewise polynomial approximations having higher-order accuracy, and simple estimates of their errors. Though our discussion is much less general than that in Philippe Ciarlet's admirable book The Finite Element Method for Elliptic Problems, we hope that our sharp error estimates for the most widely used piecewise polynomial approximations will be adequate for many practical purposes.

Chapter 8 gives a brief review of integral equation methods. Although far less versatile and less widely used than difference or FEM methods, these give extremely accurate results with little computation in some important special cases. Moreover, their theoretical analysis is mathematically interesting for its own sake, involving considerations that help to round out and complete Chapter 2.

Our book concludes with a short description of ELLPACK, a powerful new system designed to solve elliptic boundary value problems. The relevant tasks, such as placing a grid on a domain, discretizing the differential equation and the boundary conditions, sequencing the resulting linear algebraic equations, solving the system, and producing printed or plotted output, are all done automatically by ELLPACK. ELLPACK uses the approximation schemes explained in Chapters 3, 6, 7 and 8; it solves the linear system by one of the methods we discuss in Chapters 3, 4, and 5. ELLPACK can also be used to solve nonlinear equations, by methods discussed at the end of Chapter 6. Users' programs are written in a high-level, user-oriented language, which makes it easy to define a problem and to specify a solution method and various kinds of output.

Much of the research whose fruits are summarized here was supported by the Office of Naval Research, to which we are greatly indebted. Purdue University, Carnegie-Mellon University, and the Fairchild Foundation of the California Institute of Technology gave additional support for our work. We also thank William Ames, Donald Anderson, Ronald Boisvert, John Brophy, Wayne Dyksen, Vincent Ervin, Bengt Fornberg, E. C. Gartland, Alan George, Charles Goldstein, Louis Hageman, Elias Houstis, Lois Mansfield, Douglas McCarthy, John Nohel,

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But above all, we wish to acknowledge the patient and generous advice given us by Richard Varga and David Young. As an expression of our gratitude for this advice, and of our admiration for their many basic contributions to the numerical solution of elliptic problems, we dedicate this monograph to them.

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Garrett Birkhoff
Robert E. Lynch

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Chapter 1

Typical Elliptic Problems

1. Introduction. The aim of this monograph is twofold: first, to describe a variety of powerful numerical techniques for computing approximate solutions of elliptic boundary value problems and eigenproblems on high speed computers, and second, to explain the reasons why these techniques are effective.

In boundary value problems, one is given a partial differential equation (DE), such as the Poisson equation $u_{xx} + u_{yy} = f(x,y)$, to be satisfied in the interior of a region Ω , and also boundary conditions to be satisfied by the solution on the boundary $\Gamma = \partial \Omega$ of Ω . Such boundary value problems involving elliptic DE's arise naturally as descriptions of equilibrium states, in many physical and engineering contexts. In contrast, partial DE's of parabolic or of hyperbolic type (like the heat equation $u_t = u_{xx}$ or the wave equation $u_{tt} = u_{xx}$) arise naturally from time-dependent initial value problems, in which the DE to be satisfied is supplemented by appropriate initial conditions, to be satisfied (for example) at time t = 0.

For two independent variables, a general second-order linear differential equation has the form

$$(1.1) Au_{xy} + 2Bu_{yy} + Cu_{yy} + Du_{y} + Eu_{y} + Fu = G,$$

where $A = A(x,y), \dots, G = G(x,y)$. Such a DE is called *elliptic* when $AC > B^2$; this implies that A and C are nonzero and have the same sign. The DE (1.1) is called *self-adjoint* when B = 0, $D = A_x$, and $E = C_y$.

We will emphasize the two-dimensional case n=2, because numerical techniques have been most thoroughly tested in this case. Computations involving unknown functions of three or more variables are usually costly. We will also emphasize second-order linear problems, for other problems, see §§7–9. For most second-order DE's the following characterization of ellipticity is adequate.

A subscripted letter signifies the derivative with respect to the indicated variable.

DEFINITION. A semi-linear second-order DE, of the form²

(1.2)
$$\sum_{i=1}^{n} \sum_{j=1}^{n} a_{i,j}(\mathbf{x}) \frac{\partial^{2} u}{\partial x_{i} \partial x_{j}} = f(\mathbf{x}, u, \nabla u),$$

where $\mathbf{x} = (x_1, \dots, x_n)$ and $\nabla u = \operatorname{grad} u = (\partial u/\partial x_1, \dots, \partial u/\partial x_n)$, is called *elliptic* when the matrix $\mathbf{A}(\mathbf{x}) = ||a_{i,j}(\mathbf{x}')||$ is positive definite (or negative definite) identically, for all \mathbf{x} in the domain Ω of interest. This means that, for nonzero $\mathbf{q} = (q_1, \dots, q_n)$, the quadratic form $\sum a_{i,j}(\mathbf{x}) q_i q_j$ has constant sign. It is *linear* when

$$f(\mathbf{x}, u, \nabla u) = \sum_{j=1}^{n} b_{j}(\mathbf{x}) \frac{\partial u}{\partial x_{j}} + c(\mathbf{x}) u + g(\mathbf{x}).$$

Note that, since $\partial^2 u/\partial x_i \partial x_j = \partial^2 u/\partial x_j \partial x_i$, the matrix A = A(x) can be assumed to be symmetric without loss of generality. Moreover, off-diagonal terms can be combined as in (1.1), whose (symmetric) matrix is

$$A = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} A & B \\ B & C \end{bmatrix},$$

when n = 2. Finally, our definition is equivalent to the condition that $\sum a_{i,j}(\mathbf{x}) q_i q_j = 0$ implies $\mathbf{q} = \mathbf{0}$.

Likewise, the fourth-order linear operator

$$L[u] = \sum_{k=0}^{4} a_k(\mathbf{x}) \frac{\partial^4 u}{\partial x^{4-k} \partial y^k} + \text{lower-order terms}$$

is called *elliptic* at \mathbf{x} when $\sum a_k(\mathbf{x})\xi^{4-k}\eta^k$ has constant sign for $(\xi,\eta) \neq (0,0)$. The definition of ellipticity in the general case is similar (see Bers-John-Schechter [64, p. 135]).³

The remainder of this chapter is devoted to reviewing some physical and engineering problems to which numerical techniques are often applied. We do this for two reasons. First, the most familiar elliptic problems originated in the attempts of nineteenth-century mathematicians like Fourier to develop a science of mathematical physics. Second, scientists and engineers who solve elliptic problems today usually want to describe son especific physical phenomenon or engineering artifact.

Since these problems are rooted in physics and other sciences, physical intuition often helps one to decide: (a) how to approximate them

² Differential equations like (1.2), which are linear in the highest derivatives, are called *semi-linear*; if the $a_{i,j}$ depend also on u and ∇u , they are called *quasi-linear*.

Numbers in square brackets abbreviate a year (e.g., [64] for 1964) and refer to an item in the bibliography, letters in square brackets, such as [K], refer to the list of general references given at the beginning of the bibliography.

accurately, (b) which parameters are most important over which ranges, and (c) whether erratic numerical results are due to physical or to numerical instability. For these reasons, we describe the intuitive physical background of some of the most commonly studied elliptic partial DE's of mathematical physics. We include examples which illustrate various specific features of problems that influence the method of numerical solution. Some of these examples may be familiar to the reader, but we hope their inclusion will help to make our mathematical (and numerical) analysis more meaningful. The others are included to indicate the enormous variety of elliptic problems that arise in engineering and physics.

2. Dirichlet and related problems. The most deeply studied elliptic boundary value problem is the *Dirichlet problem*. Mathematically, this consists in finding a function that satisfies the *n*-dimensional *Laplace equation*

(2.1)
$$\nabla^2 u = \sum_{i=1}^n \frac{\partial^2 u}{\partial x_i^2} = 0 \quad \text{in } \Omega, \quad \Omega \subset \mathbb{R}^n,$$

in some bounded region $\Omega \subset \mathbb{R}^n$, assumes specified values g(y) for all y on the boundary Γ of Ω , and is continuous in the closed domain $\overline{\Omega} = \Omega \cup \Gamma$. The boundary conditions assumed,

(2.1a)
$$u(y) = g(y)$$
 on Γ ,

are called Dirichlet boundary conditions.

Physically, $n \le 3$, and u(x) = u(x,y,z) describes the equilibrium temperature in a homogeneous solid occupying Ω , whose boundary Γ is maintained at a temperature g(y). The Laplace equation can be derived by assuming (with Fourier) the Law of Conservation of (thermal) Energy, and that the flow ('flux') of heat energy at any point is proportional to the temperature gradient ∇u there.

The Laplace equation (2.1) arises in a variety of other physical contexts, often in combination with other kinds of boundary conditions. In general, a function which satisfies (2.1) is called *harmonic* (in Ω); the study of harmonic functions (see Chapter 2) is called *potential theory*. Many problems of potential theory are described in Bergman-Schiffer [53], and in Morse-Feshbach [53].

Exterior problem. The Laplace equation (2.1) is satisfied in empty regions of space by gravitational, electrostatic, and magnetostatic potentials (e.g., see [K]). Thus the electrostatic potential due to a charged conductor occupying a closed domain $\overline{\Omega} = \Omega \cup \Gamma$ satisfies (2.1) in the exterior Ω' of $\overline{\Omega}$ and, in suitable units,

(2.1b)
$$u = 1$$
 on Γ , and $u \to 0$ as $r \to \infty$,

where r is equal to the length of x. The problem of solving (2.1) and (2.1b) is called the *conductor* problem. It can be shown that as r tends to infinity, $u \sim C/r$ (here and elsewhere, $f(x) \sim g(x)$ means that $f(x)/g(x) \rightarrow 1$ as $x \rightarrow \infty$). In solving this problem, one must also determine the *capacity* C which is the total charge that the conductor can 'hold' when at a unit potential or voltage. The capacity of a sphere of radius a is clearly a, since u = a/r is harmonic and satisfies (2.1b).

Likewise, the irrotational flows of an incompressible fluid studied in classical hydrodynamics (see Lamb [32, Chaps. IV-VI]) have a 'velocity potential' which satisfies (2.1); see §6. For liquids of (nearly) constant density, this remains true under the action of gravity. Moreover, (2.1) is also applicable to some problems of petroleum reservoir mechanics in a homogeneous medium (soil); 4 see §3.

Neumann problem. However, the boundary conditions which are appropriate for hydrodynamical applications are usually quite different from those of (2.1a) or (2.1b). Thus, when $u = \phi$ is the 'velocity potential', they are often of the form⁵

(2.1e)
$$\partial \phi / \partial n = h(y)$$
 on Γ .

We will discuss some such applications in §6.

The problem of finding a harmonic function with given normal derivative on the boundary is called the *Neumann problem*; boundary conditions of the form (2.1c) are called *Neumann boundary conditions*. In Neumann problems for heat flow, the normal derivative of u is proportional to the thermal energy flux and h(y) specifies this flux at each point of the boundary.

Mixed boundary conditions. More generally, in the theory of heat conduction, it is often assumed that a solid loses heat to the surrounding air at a rate roughly proportional to its excess surface temperature u (Newton's 'Law of Cooling'). For k the constant of proportionality, this leads one to solve (2.1) for the boundary conditions

(2.1d)
$$\partial u/\partial n + ku = g(y)$$
 on Γ , $k > 0$,

where g(y) is the rate of absorption of radiant energy. Boundary conditions such as (2.1d), of the general form

(2.1e)
$$\alpha(\mathbf{y})u + \beta(\mathbf{y})\partial u/\partial n = g(\mathbf{y}), \quad \alpha^2(\mathbf{y}) + \beta^2(\mathbf{y}) \neq 0,$$

⁴ See Muskat [37]; also P. Ya. Polubarinova-Kochina, Advances in Applied Mechanics 2, Academic Press, 1951, 153–221; A. E. Scheidegger, Physics of Flow through Porous Media, Macmillan, 1957; and D. W. Peaceman, Fundamentals of Numerical Reservoir Simulation, Elsevier, 1977.

⁵ Here and below $\partial/\partial n$ denotes the exterior normal derivative.

are called *mixed boundary conditions*. (If the solid is cut out of sheet metal, and so is essentially two-dimensional, the temperature can be assumed to satisfy (2.1a) and the *modified Helmholtz equation* $u_{xx} + u_{yy} = \lambda u$, $\lambda > 0$, inside the solid, instead of (2.1).)

3. Membranes; source problems. Potential theory is concerned not only with harmonic functions, but also with solutions of the *Poisson* equation

$$(3.1) -\nabla^2 u = f(\mathbf{x}),$$

in free space and in bounded domains, subject to various boundary conditions such as (2.1a)-(2.1d). In the case $\mathbf{x}=(x_1,x_2)$ of two independent variables, the DE (3.1) is satisfied approximately⁶ by the vertical deflection, $z=u(x,y)=u(x_1,x_2)$, of a nearly horizontal membrane (or 'drumhead') under uniform lateral tension T, which supports a load $Tf(\mathbf{x})$ per unit area. If such a membrane spans a rigid frame whose height above Γ in the (x_1,x_2) -plane is given by a function $g(\mathbf{y})$, $\mathbf{y} \in \Gamma$, the appropriate Dirichlet boundary condition is

$$(3.1') u = g(y) on F.$$

The special case $g(\mathbf{y}) \equiv 0$ of (3.1') arises naturally in fluid dynamics. The velocity field $\mathbf{u}(x,y) = (u(x,y),v(x,y))$ of any plane flow of an incompressible fluid is determined by a stream function $\psi(x,y)$. Specifically, we have $u = \partial \psi/\partial y$ and $v = -\partial \psi/\partial x$, and consequently div $\mathbf{u} = \psi_{xy} - \psi_{yx} = 0$; moreover, the vorticity $\zeta = \partial v/\partial x - \partial u/\partial y$ satisfies $-\nabla^2 \psi = \zeta$, the Poisson equation. If the fluid is in a stationary simply connected container with boundary Γ , then Γ is necessarily a streamline, and so we can assume $\psi = 0$ on Γ . Hence the vorticity $\zeta(x,y)$ determines the stream function $\psi(x,y)$ as the solution of the Poisson equation $-\nabla^2 \psi = \zeta$ with $\psi \equiv 0$ on Γ .

In our studies of numerical methods in later chapters, we will study repeatedly the following even more special case.

Example 1. The 'Model Problem' [Y, §1.1] defined by the Poisson DE $-\nabla^2 u = f(\mathbf{x})$ in the unit square S: 0 < x, y < 1, with the boundary condition $u \equiv 0$ on $\Gamma = \partial S$, has many physical interpretations.

For example, with f(x,y) = 4, u(x,y) gives the deflection of a taut elastic membrane held in a square frame, due to a small difference in air pressure on the two sides. It also expresses the velocity profile associated with viscous flow through a square tube parallel to the z-axis. Finally,

⁶ In the 'linearized approximation', obtained by replacing $\sin \alpha = \alpha - \alpha^3/3! + \alpha^5/5! - \cdots$ with α .

⁷ See Synge [57, p. 130], for fuller discussions of these interpretations.

 $u(x,y) + (x^2 + y^2)$ represents the 'warping function' of a long straight bar with square cross-section under pure torsion.

For other domains Ω with boundary Γ , the DE $-\nabla^2 u = f(\mathbf{x})$ in Ω

with $u \equiv 0$ on Γ has analogous physical interpretations.

When n = 3, the DE (3.1) with $f(\mathbf{x}) = 4\pi\rho(\mathbf{x})$ is satisfied by the gravitational potential of a continuous distribution of mass with density $\rho(\mathbf{x})$ (mass per unit volume). Likewise, it is satisfied by the electrostatic potential of a continuous charge distribution having this density.

A more general elliptic DE is

(3.2)
$$L[u] = -\nabla \cdot [p(\mathbf{x})\nabla u] + q(\mathbf{x})u = f(\mathbf{x}), \quad p > 0 \text{ and } q \ge 0.$$

Whereas the Laplace operator in (2.1) has constant coefficients, the linear differential operator L[u] in (3.2) has variable coefficients. Moreover, the Laplace DE itself leads to second-order linear elliptic problems with variable coefficients when spherical, ellipsoidal, or other coordinate systems are used.

The DE (3.2) is satisfied approximately by the temperature distribution $u(\mathbf{x})$ in a solid having space-dependent thermal conductivity $p(\mathbf{x})$, in which heat is being produced at the rate $f(\mathbf{x})$ (energy per unit volume and time); $q(\mathbf{x})u$ gives the absorption. Since one may think of $f(\mathbf{x})$ as representing a source of heat, the DE (3.2) for specified boundary conditions such as (2.1a)-(2.1d) is often said to be a source problem. Such source problems arise, typically, in the analysis of diffusion phenomena.

Similar elliptic problems having variable coefficients arise also in the study of electrostatic, magnetostatic, and gravitational potentials, in which the materials involved have physical properties (e.g., dielectric constants or magnetic permeabilities) that depend on position. Moreover, a related elliptic DE also arises from Darcy's Law, in petroleum reservoirs occupying soils (or sands) of variable 'permeability' k(x,y,z). As is explained in Muskat [37, p. 242], the pressure p in such a reservoir satisfies

$$(3.3) -\nabla \cdot [k\nabla p] = \rho g \, \partial k / \partial z.$$

In practice, k(x) is known only very roughly, and (like thermal and electrical conductivity) it can vary by orders of magnitude.

4. Two-endpoint problems. The problems described in §§2-3 have counterparts which involve functions of one space variable, and hence lead to ordinary DE's. Since the boundary of a one-dimensional domain (interval) consists of two points, such problems are often called two-endpoint problems. The numerical techniques which are most effective for solving such two-endpoint problems are very different from those used in two or more dimensions. However, we have devoted this section to them

because they illustrate so simply various kinds of boundary conditions and other basic ideas.

Example 2. The simplest two-endpoint problem concerns a transversely loaded string, in the small deflection or linear approximation. (For some nonlinear elliptic problems, see §9.) If the string (assumed nearly horizontal) is under a constant tension T, then the deflection y induced by a load exerting a vertical force f(x) per unit length satisfies the ordinary DE

$$(4.1) -y'' = f(x)/T.$$

If the endpoints of the string of length a are fixed, then the deflection also satisfies the two-endpoint conditions

$$(4.1') y(0) = y(a) = 0.$$

The differential operator $L[u] = -d^2/dx^2$ on the left side of (4.1) is a linear differential operator with constant coefficients; it is linear because for any constants α, β and functions⁸ $y, z \in C^2[0,a]$, clearly

$$L[\alpha y + \beta z] = \alpha L[y] + \beta L[z].$$

The differential equation (4.1) is *inhomogeneous* since its right side is nonzero. On the other hand, the boundary conditions (4.1') are linear and *homogeneous*.

To solve (4.1)-(4.1'), first note that for any continuous f(x), the function

$$g(x) = -\frac{1}{T} \int_0^x (x-t) f(t) dt$$

is a solution of (4.1) satisfying the initial conditions g(0) = g'(0) = 0.9The general solution of (4.1) is $g(x) + \alpha + \beta x$, where α and β are arbitrary constants. To construct the solution satisfying (4.1'), set $\alpha = 0$ and

$$\beta = \frac{1}{aT} \int_0^a (a-t) f(t) dt.$$

The problem of a vertical loaded spring is similar. If p(x) is the (variable) stiffness of the spring and f(x) is the load per unit length, then the appropriate DE for vertical (longitudinal) displacement u(x) is

$$(4.2) -[p(x)u']' = f(x), p(x) > 0.$$

⁸ The symbol $C^k[0,a]$ denotes the set of functions on the interval [0,a] whose k-th derivative exists and is continuous.

⁹ In other words, G(x;t) = (x-t) is the *Green's function* for the operator L for x > 0 and the initial data g(0) = g'(0) = 0 (Birkhoff-Rota [78, Chap. 2, §8]).

Here the linear differential operator L[u] = -[p(x)u']' has variable coefficients. If the spring is held fixed at x = 0 and the other end is free, then one has the boundary conditions

$$(4.2') u(0) = 0, u'(a) = 0.$$

If a mass m is attached to the bottom of the spring, then the second condition in (4.2') is replaced with u'(a) = mg/p(a), where g is the acceleration due to gravity.

Sturm-Liouville systems. As a third example, we consider Sturm-Liouville systems. These typically arise from separating out the time variable from simple harmonic solutions of time-dependent problems such as that of a vibrating string $\rho(x)u_{tt} = [p(x)u_x]_x$ with variable density $\rho(x)$ and tension p(x). With $u(x,t) = y(x)\cos kt$, one gets homogeneous linear DE's for y of the form $[p(x)y']' + k^2\rho(x)y = 0$, or, more generally,

(4.3)
$$[p(x)y']' + [\lambda \rho(x) - q(x)]y = 0, \quad p > 0, \quad \rho > 0,$$

in which $\lambda = k^2$ is a parameter, and homogeneous linear boundary conditions of the form (4.1'). More generally, Sturm-Liouville systems can involve *separated* boundary conditions of the form

(4.3')
$$\alpha_0 y(0) + \beta_0 y'(0) = \alpha_1 y(a) + \beta_1 y'(a) = 0, \quad \alpha_i^2 + \beta_i^2 > 0.$$

Problems like (4.3)-(4.3') which involve the solution of a homogeneous linear (elliptic) DE for homogeneous boundary conditions and unknown values of a parameter λ are called eigenproblems. The values of the parameter for which nontrivial solutions 10 exist are called eigenvalues, and the solutions themselves are called eigenfunctions. It is well known that any Sturm-Liouville system (4.3) with separated boundary conditions admits an infinite sequence of real eigenfunctions $\phi_j(x)$ with real eigenvalues $\lambda_1 < \lambda_2 < \lambda_3 < \cdots$, where $\lambda_j \longrightarrow \infty$.

Other endpoint conditions. Many kinds of 'endpoint conditions' can be prescribed for Sturm-Liouville systems. Thus, for the trigonometric DE $y'' + \lambda y = 0$, the Mathieu equation

(4.4)
$$y'' + (\lambda + \mu \cos x)y = 0$$
,

and other second-order DE's with periodic coefficients, one typically wants solutions which satisfy *periodic* boundary conditions such as

$$(4.4') y(0) = y(2\pi), y'(0) = y'(2\pi).$$

The 'trivial' solution is $y \equiv 0$. For a fuller discussion of Sturm-Liouville problems and the endpoint conditions which are appropriate for them, see Birkhoff-Rota [78, Chap. 10].