THE SLEIGN2 STURM-LIOUVILLE CODE

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Dedicated to the inheritance from C. Sturm and J. Liouville

Abstract. The SLEIGN2 code is based on the ideas and methods of the original SLEIGN code of 1979.

The main purpose of the SLEIGN2 code is to compute eigenvalues and eigenfunctions of regular and singular self-adjoint Sturm-Liouville problems, with both separated and coupled boundary conditions, and to approximate the continuous spectrum in the singular case. The code uses some new algorithms, which we describe, and has a driver program that offers a user-friendly interface.

In this paper the algorithms and their implementation are discussed, and the class of problems to which each algorithm applies is identified.

Contents

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1. General introduction

The ideas for the original SLEIGN code, for Sturm-Liouville problems, were conceived by Bailey, then at Sandia National Laboratory, USA, see [1], and subsequently developed by Bailey, Gordon and Shampine, see [11] and [12]. For the certification of the SLEIGN code see the paper [27] of Marletta, which reports on the degree of success in the numerical computation of eigenvalues and eigenfunctions, for a wide range of problems.

Work on the successor code SLEIGN2 was started by Bailey, Everitt and Zettl at the University of Birmingham, England, UK in 1988 under SRC funding; thereafter the code was essentially developed, under NSF funding, at Northern Illinois University, USA; see [6], [7] and [8]. Additional analytical results for establishing the validity of the approximation to singular problems by regular problems, were obtained in collaboration with Weidmann [5], and with Möller [19] and [20]. This code has now been developed to work with all forms of self-adjoint, separated or coupled boundary conditions, and with nearly all cases involving the classification of the endpoints of the interval of the differential equation, to give both quantitative and qualitative information about the properties of self-adjoint Sturm-Liouville problems. The code has a user-friendly interface to help with the input of the, at times unavoidably complicated, information required for the general form of Sturm-Liouville problems. A clear indication of the scope and effectiveness of the code is to be seen in the list of 32 prepared examples given in the file xamples.tex (a constituent part of the SLEIGN2 code files); in particular attention is drawn to a number of these examples which are, in part, reproduced in Section 9 below. There are default entries of the problem data in the case when the user decides to avoid the full generality of the capabilities of the code.

SLEIGN2 is a Fortran77 sub-routine for the computation of eigenvalues and eigenfunctions of regular and singular Sturm-Liouville boundary value problems. These problems include:

(1) The classical, regular problems consisting of the differential equation

$$-(py')' + qy = \lambda wy \text{ on } [a, b] \tag{1.1}$$

with separated, regular boundary conditions

$$A_1 y(a) + A_2 (py')(a) = 0 \tag{1.2}$$

$$B_1 y(b) + B_2 (py')(b) = 0. \tag{1.3}$$

(2) The classical, regular problems consisting of the differential equation (1.1) with coupled boundary conditions such as the periodic conditions

$$y(a) = y(b) \quad \text{and} \quad (py')(a) = (py')(b), \tag{1.4}$$

and the semi-periodic conditions

$$y(a) = -y(b) \quad \text{and} \quad (py')(a) = -(py')(b). \tag{1.5}$$

Singular analogues of all these regular boundary value problems also fall within the capabilities of the code.

In fact SLEIGN2 can be used for all classes of self-adjoint Sturm-Liouville problems with positive leading coefficient p and positive weight function w, with one exception: the class of problems with a limit-point endpoint and a spectrum which is discrete and unbounded both above and below.

For other problems with a limit-point endpoint and a more complicated spectrum (*e.g.* when the spectrum is or contains a Cantor-like set) the success of applying the code may be limited but, in principle, SLEIGN2 when used together with appropriate theoretical results, can provide some information about the spectrum. For example, the starting point of the continuous spectrum, the number and numerical value of the eigenvalues below the continuous spectrum, and an approximation of the first few spectral bands and gaps.

The SLEIGN2 "package" and a number of related papers can be downloaded from the Web at

http://www.math.niu.edu/~zettl/SL2

This package contains a built-in driver; the user can then identify the problem by answering questions interactively from the keyboard. There is also a built-in tutorial (HELP) containing basic information which can be accessed at every point where a keyboard entry is requested.

As mentioned above a number of examples is also provided in the package. These examples include many of the celebrated Sturm-Liouville differential equations of special functions and applied mathematics, *e.g.* the equations known by the names of Bessel, Hermite, Jacobi, Laguerre, Legendre, Mathieu, Meissner, Whittaker, and the hydrogen, harmonic oscillator and Morse oscillator equations. Information about these examples is contained in the file xamples.tex as part of the package.

SLEIGN2 has a number of features which, to the best of our knowledge, are not available in any other general Sturm-Liouville code, *e.g*:

(1) The SLEIGN code developed by Bailey, Gordon and Shampine, see [12].
(2) The NAG code developed by Pryce, see [31] and [30].
(3) The SLEDGE code developed by Fulton and Pruess, see [21].
(4) The earlier, but less comprehensive, copy of SLEIGN2 now contained in the test package [32] developed by Pryce.

Among these new and radical features are the capabilities to compute eigenvalues and eigenfunctions of boundary value problems with:

(1) All coupled self-adjoint regular boundary conditions.
(2) All separated self-adjoint singular boundary conditions.
(3) All coupled self-adjoint singular boundary conditions.

There is also a numerical capability for initial value problems at regular and limit-circle endpoints.

The numerical implementation of several of the algorithms used by the SLEIGN2 code has a number of novel features; some of these features are discussed in Part II of this paper.

The contents of the paper are as follows:

(1) **Part I** is concerned with the analytical background of Sturm-Liouville problems; there is a general introduction in Section 2; in Section 3 there is information on intervals and notations; endpoint classification is discussed in Section 4, boundary conditions in Section 5 and initial value problems in Section 6; self-adjoint Sturm-Liouville problems and spectrum properties are discussed in Sections 7 and 8.
(2) **Part II** is concerned with the computational methods involved with the SLEIGN2 code: Section 9 and its subsections is concerned with the implementation of the code for separated boundary conditions, and Section 10 and its subsections for coupled boundary conditions; there is a number of important general remarks in Section 11.

Part I: The analytical background

2. Introduction

Sturm-Liouville problems are concerned with solutions of the linear, homogeneous, ordinary differential equation

$$-(p(x)y'(x))' + q(x)y(x) = \lambda w(x)y(x) \quad (x \in (a,b)) \tag{2.1}$$

where (a,b) is an open interval of the real line $\mathbb{R}$, $\{p,q,w\}$ are real-valued coefficients defined on (a,b), and λ is a spectral parameter.

To specify a Sturm-Liouville problem, to this differential equation (2.1) is added at most two linearly independent, self-adjoint, homogeneous boundary conditions; the required number and form of these conditions depends upon the interval (a,b) and the properties of the coefficients $\{p,q,w\}$ at the endpoints a and b; additional information in this respect, including the *classification* of the endpoints a and b as *regular, limit-point* or *limit-circle*, is given in subsequent sections. In the so-called *regular* case, the boundary conditions can be *separated*, for example,

$$y(a) = 0 \quad y(b) = 0, \tag{2.2}$$

or *coupled*, for example

$$y(a) = y(b) \quad (py')(a) = (py')(b). \tag{2.3}$$

A self-adjoint Sturm-Liouville problem is determined by the differential equation (2.1), and boundary conditions, similar to (2.2) or (2.3) or of a more general form. The *spectrum* of such problems is then known to consist of only real values of the spectral parameter λ; an eigen-solution to the problem is a pair (λ,ψ), where λ is the *eigenvalue* and for which the differential equation has a non-null solution ψ, the *eigenfunction*, which satisfies the boundary conditions. If the problem has only eigenvalues then the spectrum of the problem is called *discrete*; this is always the case for regular problems. In the more general case of

singular problems the spectrum may be rather complicated and contain not only eigenvalues but *essential* spectrum consisting of bands of *continuous* spectrum; see [35].

For the general theory of self-adjoint boundary value problems see the references [15], [29], [33], [34] and [37].

3. Notations

Intervals Let $\mathbb{R}$ represent the real line; then

$$\left\{\begin{array}{lll}(i) & \text{Open} & (a,b)=\{x\in\mathbb{R}:-\infty\le a<x<b\le+\infty\}\\ (ii) & \text{Compact} & [a,b]=\{x\in\mathbb{R}:-\infty<a\le x\le b<+\infty\}.\end{array}\right. \tag{3.1}$$

Continuity
Let I be any interval of $\mathbb{R}$ and let $n\in\{0,1,2,\cdots\}$; then

$$\left\{\begin{array}{lll}(i) & C_p(I) & \{f:I\to\mathbb{C}:f \text{ is piece-wise continuous on } I\}\\ (ii) & C^{(n)}(I) & \{f:I\to\mathbb{C}:f^{(r)} \text{ is continuous on } I \text{ for } r=0,1,2,\cdots,n\}\\ (iii) & AC_{\mathrm{loc}}(I) & \{f:I\to\mathbb{C}:f \text{ is absolutely continuous on all } [\alpha,\beta]\subseteq I\}.\end{array}\right. \tag{3.2}$$

Integrability
Let I be any interval of $\mathbb{R}$ and let $w(x)\ge 0$ for all $x\in I$; then

$$\left\{\begin{array}{lll}(i) & L^1(I) & \{f:I\to\mathbb{C}:\int_I|f|\equiv\int_I|f(x)|\,dx<+\infty\}\\ (ii) & L^1_{\mathrm{loc}}(I) & \{f:I\to\mathbb{C}:\int_\alpha^\beta|f(x)|\,dx<+\infty \text{ for all } [\alpha,\beta]\subset I\}\\ (iii) & L^2(I:w) & \{f:I\to\mathbb{C}:\int_I w(x)\,|f(x)|^2\,dx<+\infty\}.\end{array}\right. \tag{3.3}$$

Coefficient conditions
Let the open interval (a,b) be given and let $\{p,q,w\}:(a,b)\to\mathbb{R}$; then

$$\left\{\begin{array}{llll}(i) & \text{Minimal} & p^{-1},q,w\in L^1_{\mathrm{loc}}(a,b) & p(x),w(x)>0 \text{ for almost all } x\in(a,b)\\ (ii) & \text{Smooth} & p,p',q,w\in C(a,b) & p(x),w(x)>0 \text{ for all } x\in(a,b).\end{array}\right. \tag{3.4}$$

Remarks

(1) The interval (3.1), continuity (3.2) and integrability (3.3) notations are now standard in the literature of Sturm-Liouville theory; see the paper [36] and the text of Zettl [37].
(2) The minimal conditions of (3.4) allow for the definition of the fundamental linear, differential operators of the Sturm-Liouville theory, in the Hilbert function space $L^2(I:w)$ and thereby the full implementation of endpoint classification and boundary conditions; see Sections 4 and 5 below.
(3) Under either of the coefficient conditions (3.4) the initial value problem for the differential equation (2.1) can be solved for any point $c\in(a,b)$, *i.e.* given two complex numbers $\xi,\eta\in\mathbb{C}$ and any complex value of the parameter $\lambda\in\mathbb{C}$, there exists a unique solution of the differential equation, say $y(\cdot,\lambda):(a,b)\to\mathbb{C}$, with the properties

$$\left\{\begin{array}{ll}(i) & y(\cdot,\lambda) \text{ and } (py')(\cdot,\lambda)\in AC_{\mathrm{loc}}(a,b)\\ (ii) & y(c,\lambda)=\xi \text{ and } (py')(c,\lambda)=\eta.\end{array}\right. \tag{3.5}$$

(4) Although the conditions (3.4) require the coefficient w to be positive on the interval (a, b) it is possible to consider spectral and eigenvalue problems when w changes sign on the interval; see [9]. This remark holds also for the case when w is zero on sub-intervals of (a, b); see [18].

4. Endpoint classification

Suppose given the interval (a, b) and the set of coefficients $\{p, q, w\}$.

We now give the classification of the endpoints a and b of the differential equation (2.1), valid under the coefficient conditions (3.4); details are given for the endpoint a but there is a similar classification scheme for the endpoint b.

Throughout this classification scheme let $c \in (a, b)$; however the classification that emerges is independent of the choice of the point c.

Additionally the scheme involves a choice of λ but again the classification can be shown to be independent of this spectral parameter.

Regular

The endpoint a is *regular* (notation R) if

$$\begin{cases} (i) & a \in \mathbb{R}, \textit{i.e. } a > -\infty, \text{ and} \\ (ii) & p^{-1}, q, w \in L^1(a, c]. \end{cases} \tag{4.1}$$

Singular

The endpoint a is *singular* (notation S) if it is not R, *i.e.*

$$\begin{cases} (i) & \text{either } a = -\infty \\ (ii) & \text{or } a \in \mathbb{R} \text{ but } \int_a^c \{(p(x))^{-1} + |q(x)| + w(x)\}\, dx = +\infty. \end{cases} \tag{4.2}$$

If a is S then there are two main classification sub-cases as follows:

Limit-point

The endpoint a is *limit-point* (notation LP) if a is S and for some $\lambda \in \mathbb{C}$ there exists at least one solution $y(\cdot, \lambda)$ of the differential equation (2.1) such that

$$\int_a^c w(x) \left|y(x, \lambda)\right|^2 dx = +\infty. \tag{4.3}$$

Limit-circle

The endpoint a is *limit-circle* (notation LC) if a is S and for some $\lambda \in \mathbb{C}$ any solution $y(\cdot, \lambda)$ of the differential equation (2.1) satisfies

$$\int_a^c w(x) \left|y(x, \lambda)\right|^2 dx < +\infty. \tag{4.4}$$

The LC classification has two sub-cases:

(1) **Limit-circle non-oscillatory**

The endpoint a is *limit-circle non-oscillatory* (notation LCNO) if there exists a point $d \in (a, c)$, a real value $\lambda \in \mathbb{R}$ and a solution $y(\cdot, \lambda)$ with the property

$$y(x, \lambda) > 0 \text{ for all } x \in (a, d). \tag{4.5}$$

(2) **Limit-circle oscillatory**

The endpoint a is *limit-circle oscillatory* (notation LCO) if

$$\text{(4.6)} \qquad \begin{cases} (i) & \text{for any real } \lambda \in \mathbb{R} \text{ and any non-null solution } y(\cdot,\lambda), \\ (ii) & \text{for any } d \in (a,c], \\ (iii) & \text{there exists a point } \xi \in (a,d] \text{ such that } y(\xi,\lambda)=0. \end{cases}$$

Remarks

(1) We stress the point made above that although the spectral parameter λ is involved in the endpoint classification it can be shown that this classification is independent of λ and depends only on the interval (a,b) and the set of coefficients $\{p,q,w\}$.

(2) When a is R the initial value problem, as detailed in (3.5), can be solved at the endpoint a to give a unique solution on the interval $[a,b)$.

(3) The classification a is R can be considered as a special case of the LCNO classification at a.

(4) When a is R or LCNO the differential equation (2.1), for any *real* value $\lambda \in \mathbb{R}$, has two linearly independent solutions $u(\cdot,\lambda), v(\cdot,\lambda) : (a,b) \to \mathbb{R}$, such that for some $c \in (a,b)$

$$\text{(4.7)} \qquad \begin{cases} (i) & u(x,\lambda)>0 \text{ and } v(x,\lambda)>0 \text{ for all } x \in (a,c), \\ (ii) & \lim_{x\to a+} u(x,\lambda)/v(x,\lambda)=0, \\ (iii) & \int_a^c \{p(x)u(x,\lambda)^2\}^{-1}dx=+\infty \text{ and } \int_a^c \{p(x)v(x,\lambda)^2\}^{-1}dx<+\infty. \end{cases}$$

The solution $u(\cdot,\lambda)$ is unique, up to scalar multiples, and is called the *principal* solution of the differential equation for this value of the parameter λ. The solution $v(\cdot,\lambda)$ is called a *non-principal* solution, noting that this solution is not unique.

In particular when a is R, a principal solution $u(\cdot,\lambda)$ is determined by the initial conditions

$$u(a,\lambda)=0 \quad \text{and} \quad (pu')(a) \neq 0.$$

(5) When a is LCO then for any real $\lambda \in \mathbb{R}$ all solutions of the differential equation (2.1) have infinitely many zeros in any right-neighbourhood (a,d) of a.

(6) All the above remarks apply equally well, with change of notation, to the classification cases of endpoint b; note that the classification of a and of b are independent of each other.

(7) When b is R or LCNO the principal solution, for $\lambda \in \mathbb{R}$, is denoted by $U(\cdot,\lambda)$ and any non-principal solution by $V(\cdot,\lambda)$.

In particular when b is R a principal solution $U(\cdot,\lambda)$ is determined by the initial conditions

$$U(b,\lambda)=0 \quad \text{and} \quad (pU')(b,\lambda) \neq 0.$$

(8) The original differential equation (2.1) can be considered for transformation to Liouville normal form; for details see [13, Chapter 10, Section 9] and [17].

If the original coefficients $\{p,q,w\}$ are sufficiently differentiable on (a,b) the transformation gives the Liouville normal form as

$$\text{(4.8)} \qquad -Y''(X)+Q(X)Y(X)=\lambda Y(X) \quad \text{for} \quad X \in (A,B)$$

where now all the properties of the original equation can be associated with the properties of the coefficient $Q(\cdot)$ on the transformed interval (A, B). In this form the properties of the original differential equation may be easier to consider, for both analytical and numerical purposes.

In particular the endpoint classification at a, b of (2.1) as R, LP, LCNO, LCO in $L^2((a, b) : w)$ is invariant under the Liouville transformation and is identical with the endpoint classification at A, B of (4.8) in $L^2(A, B)$, except that the cases R and LCNO may interchange.

See also Remark 8, Section 11 below.

5. Boundary conditions

The number and form of boundary conditions is essential to the understanding of the structure of self-adjoint Sturm-Liouville problems.

Given the interval (a, b) and the coefficients $\{p, q, w\}$ satisfying the minimal conditions of (3.4), define the maximal domain Δ, a linear manifold that is dense in $L^2(I : w)$, by

$$\Delta := \{f : (a, b) \to \mathbb{C} : f, pf' \in AC_{\text{loc}}(a, b) \text{ and } f, w^{-1}(-(pf')' + qf) \in L^2(I : w)\}. \tag{5.1}$$

The Green's formula is given by

$$\int_\alpha^\beta \{\overline{g}(-(pf')' + qf) - f(-(p\overline{g}')' + q\overline{g}\} = [f, g](\beta) - [f, g](\alpha) \tag{5.2}$$

valid for all compact intervals $[\alpha, \beta] \subset (a, b)$ and all $f, g \in \Delta$, where the skew-symmetric, sesquilinear form $[\cdot, \cdot]$ is defined by

$$[f, g](x) := f(x)(p\overline{g}')(x) - (pf')(x)\overline{g}(x) \tag{5.3}$$

for all $x \in (a, b)$. It may be seen, from (5.1) and (5.2) that the two limits

$$[f, g](a) := \lim_{x \to a+} [f, g](x) \quad \text{and} \quad [f, g](b) := \lim_{x \to b-} [f, g](x) \tag{5.4}$$

both exist in $\mathbb{C}$ and are finite, for all $f, g \in \Delta$.

There is an important connection between the limits (5.4) and the endpoint classification of a:

$$a \text{ is LP if and only if } [f, g](a) = 0 \text{ for all } f, g \in \Delta. \tag{5.5}$$

Similarly

$$b \text{ is LP if and only if } [f, g](b) = 0 \text{ for all } f, g \in \Delta. \tag{5.6}$$

Note also that if a is LC and $y(\cdot)$ is any solution of the differential equation (2.1) then, again from (5.2),

$$[y, g](a) := \lim_{x \to a+} [y, g](x) \tag{5.7}$$

exists and is finite for all $g \in \Delta$. There is a similar result if b is LC for the limit

$$[y, g](b) := \lim_{x \to b-} [y, g](x). \tag{5.8}$$

The form and number of boundary conditions depends upon the classification of the endpoints a and b.

Separated boundary conditions

(1) Let a or b be R; then separated boundary conditions take the form, for a solution y,

$$A_1 y(a) + A_2(py')(a) = 0 \tag{5.9}$$

$$B_1 y(b) + B_2(py')(b) = 0 \tag{5.10}$$

where $A_1, A_2, B_1, B_2 \in \mathbb{R}$ and $A_1^2 + A_2^2 > 0$ and $B_1^2 + B_2^2 > 0$.

(2) Let a be LC; choose $u, v \in \Delta$ with the properties:

$$\begin{cases} (i) & u, v : (a, b) \to \mathbb{R} \\ (ii) & [u, v](a) \neq 0. \end{cases} \tag{5.11}$$

Such a choice is always possible; if $\lambda \in \mathbb{R}$ then take $u(\cdot) = u(\cdot, \lambda)$ and $v(\cdot) = v(\cdot, \lambda)$ on (a, b), where $\{u(\cdot, \lambda), v(\cdot, \lambda)\}$ is a real, linearly independent basis of solutions of the differential equation (2.1); however other choices are possible by direct construction. Then a separated boundary condition at a for a solution y takes the form, using (5.7),

$$A_1[y, u](a) + A_2[y, v](a) = 0 \tag{5.12}$$

with $A_1, A_2 \in \mathbb{R}$ and $A_1^2 + A_2^2 > 0$.

If b is LC then there is a similar form to a separated boundary condition but the notation adopted here is to take $U, V \in \Delta$ with the properties

$$\begin{cases} (i) & U, V : (a, b) \to \mathbb{R} \\ (ii) & [U, V](b) \neq 0. \end{cases} \tag{5.13}$$

and separated boundary condition for the solution y, using (5.8),

$$B_1[y, U](b) + B_2[y, V](b) = 0 \tag{5.14}$$

with $B_1, B_2 \in \mathbb{R}$ and $B_1^2 + B_2^2 > 0$.

(3) Let a be LP, then no separated boundary condition at a is required nor allowed; similarly if b is LP.

Remarks

(1) The separated LC boundary conditions (5.12) and (5.14) can also be applied in the R case. If, say, for some $\lambda \in \mathbb{R}$ the initial value data

$$\begin{cases} u(a, \lambda) = 0 & v(a, \lambda) = -1 \\ (pu')(a, \lambda) = 1 & (pv')(a, \lambda) = 0 \end{cases} \tag{5.15}$$

is used to construct solutions $u(\cdot, \lambda)$ and $v(\cdot, \lambda)$, then a calculation shows that $[u, v](a) = 1$ and, for a solution y,

$$[y, u](a) = y(a) \quad \text{and} \quad [y, v](a) = (py')(a);$$

thus the singular boundary condition (5.12) reduces, in this case, to the classical boundary condition (5.9).

Similarly for the solutions $U(\cdot, \lambda)$ and $V(\cdot, \lambda)$

$$\begin{cases} U(b, \lambda) = 0 & V(b, \lambda) = -1 \\ (pU')(b, \lambda) = 1 & (pV')(b, \lambda) = 0 \end{cases} \tag{5.16}$$

and the boundary conditions (5.10) and (5.14) at the endpoint b.

(2) In the case when a is R or LCNO the principal solution $u(\cdot,\lambda)$, given $\lambda \in \mathbb{R}$, and any non-principal solution $v(\cdot,\lambda)$ always satisfy the condition $[u(\cdot,\lambda), v(\cdot,\lambda)](a) \neq 0$; similarly $[U(\cdot,\lambda), V(\cdot,\lambda)](b) \neq 0$ at the endpoint b.

Coupled boundary conditions

Coupled, self-adjoint boundary conditions for the differential equation (2.1), see for example (2.3), can only be chosen when neither a nor b is in the LP endpoint classification. The general theory of coupled, self-adjoint Sturm-Liouville boundary conditions is given in [7].

Let a be R or LC and, independently, let b be R or LC. Note then that, for all $\lambda \in \mathbb{C}$, all solutions of the equation (2.1) are in the space $L^2((a,b) : w)$; indeed all solutions are in the maximal domain Δ, as defined by (5.1).

Choose $\{\theta, \varphi\}$ and $\{\Theta, \Phi\}$ such that

$$\theta, \varphi, \Theta, \Phi : (a,b) \to \mathbb{R} \text{ and } \theta, \varphi, \Theta, \Phi \in \Delta \tag{5.17}$$

and

$$[\theta, \varphi](a) = 1 \quad \text{and} \quad [\Theta, \Phi](b) = 1; \tag{5.18}$$

this can always be achieved through the properties of real-valued solutions of the equation (2.1) for some real value of the parameter λ. Then it is shown in [7] that the most general coupled, self-adjoint boundary conditions are given by, in matrix form,

$$\begin{bmatrix} [y,\Theta](b) \\ [y,\Phi](b) \end{bmatrix} = \exp(i\alpha)\mathbf{K} \begin{bmatrix} [y,\theta](a) \\ [y,\varphi](a) \end{bmatrix} \tag{5.19}$$

where the parameters α and the matrix $\mathbf{K}$ satisfy

$$\begin{cases} (i) & \alpha \in (-\pi, \pi] \\ (ii) & \mathbf{K} = [k_{rs}] \text{ with } k_{rs} \in \mathbb{R} \ (r,s = 1,2) \\ (iii) & \det(\mathbf{K}) = 1. \end{cases} \tag{5.20}$$

It is to be noted that the normalisations (5.18) and (iii) of (5.20) are critical to the determination of the self-adjoint property of the boundary condition (5.19).

To link the singular boundary condition with well known conditions in the literature the following three cases of (5.19) are named as shown, where $\mathbf{I}$ is the 2×2 unit matrix,

$$\begin{cases} \textbf{Periodic} & \alpha = 0 \text{ and } \mathbf{K} = \mathbf{I} \\ \textbf{Semi-periodic} & \alpha = 0 \text{ and } \mathbf{K} = -\mathbf{I} \end{cases} \tag{5.21}$$

and

$$\textbf{General periodic} \quad \alpha = 0 \text{ and } \mathbf{K} = \begin{bmatrix} m & 0 \\ 0 & m^{-1} \end{bmatrix} \text{ for some } m \in \mathbb{R} \text{ with } m \neq 0. \tag{5.22}$$

However it is important to note that this use of the terms **periodic, semi-periodic and general periodic** is applied with respect to the choice of the functions $\{\theta, \varphi\}$ and $\{\Theta, \Phi\}$ with the properties (5.17) and (5.18); a different choice of such functions will yield different coupled boundary conditions under one or more of these terms.

The reason for this terminology is that if the equation is regular on $[a,b]$ and if $\{\theta, \varphi\}$ satisfy the same initial conditions at a as $\{u, v\}$ in (5.15), and if $\{\Theta, \Phi\}$ satisfy the same

initial conditions at b as $\{U, V\}$ in (5.16) then (5.19) reduces to

$$\begin{bmatrix} y(b) \\ (py')(b) \end{bmatrix} = \exp(i\alpha)\mathbf{K} \begin{bmatrix} y(a) \\ (py')(a) \end{bmatrix}. \tag{5.23}$$

In this case then the three named conditions in (5.21) and (5.22) become, respectively,

$$\begin{array}{ll} (i) & y(b) = y(a) \text{ and } (py')(b) = (py')(a) \\ (ii) & y(b) = -y(a) \text{ and } (py')(b) = -(py')(a) \\ (iii) & y(b) = my(a) \text{ and } (py')(b) = m^{-1}(py')(a). \end{array} \tag{5.24}$$

These are the established uses of the terms periodic, semi-periodic and general periodic for coupled boundary conditions but are used also in the wider context of the general coupled boundary conditions (5.19), for singular endpoints.

In general coupled boundary conditions are considered in four cases:

(1) **Periodic**

For example: $y(b) = y(a)$ and $(py')(b) = (py')(a)$

(2) **Semi-periodic**

For example: $y(b) = -y(a)$ and $(py')(b) = -(py')(a)$

(3) **General periodic**

For example: $y(b) = my(a)$ and $(py')(b) = m^{-1}(py')(a)$ for some $m \neq 0$

(4) **General coupled**

For example: $\begin{bmatrix} y(b) \\ (py')(b) \end{bmatrix} = \exp(i\alpha)\mathbf{K} \begin{bmatrix} y(a) \\ (py')(a) \end{bmatrix}$.

For the four entries (1), (2), (3) and (4) if the endpoint a is R then the base functions $\{\theta, \varphi\}$ used are determined by the initial conditions

$$\begin{array}{ll} \theta(a) = 0 & \varphi(a) = -1 \\ (p\theta')(a) = 1 & (p\varphi')(a) = 0. \end{array} \tag{5.25}$$

Likewise for all four cases if the endpoint b is R then the base functions $\{\Theta, \Phi\}$ used are determined by the initial conditions

$$\begin{array}{ll} \Theta(b) = 0 & \Phi(b) = -1 \\ (p\Theta')(b) = 1 & (p\Phi')(b) = 0. \end{array} \tag{5.26}$$

In all four of these cases (1) to (4) if a is LC the coupled boundary conditions are based on the general form (5.19). To this end the functions $\{\theta, \varphi\}$ in (5.19) are defined by, where c is a point of the open interval (a, b) and $\{u, v\}$ satisfy (5.11),

$$\theta(x) := \frac{n}{d}u(x) \text{ and } \varphi(x) := \frac{1}{d}v(x) \text{ for all } x \in (a, c], \tag{5.27}$$

with $d := |[u, v](a)|^{1/2} > 0$ and $n := \text{sign}\{[u, v](a)\} = \pm 1$.

Similarly if b is LC the functions $\{\Theta, \Phi\}$ in (5.19) are defined by, where $\{U, V\}$ satisfy (5.13),

$$\Theta(x) := \frac{N}{D}U(x) \text{ and } \Phi(x) := \frac{1}{D}V(x) \text{ for all } x \in [c, b) \tag{5.28}$$

with $D := |[U,V](b)|^{1/2} > 0$ and $N := \text{sign}\{[U,V](b)\} = \pm 1$.

The definition of the functions $\{\theta, \varphi\}$ and $\{\Theta, \Phi\}$ in $[c,b)$ and $(a,c]$, respectively, is then completed to ensure that (5.17) is satisfied; this extension can be made on using the so-called Naimark "patching" lemma given in [29, Section 17.3, Lemma 2].

With these definitions a calculation then shows that the additional condition (5.18) is satisfied so that, for any $\alpha \in (-\pi, \pi]$ and for any $\mathbf{K}$, satisfying (ii) and (iii) of (5.20), the coupled boundary conditions (5.19) for this choice of the functions $\{\theta, \varphi\}$ and $\{\Theta, \Phi\}$, do provide self-adjoint conditions for the differential equation (2.1).

Remark

In the general coupled case it should be noted that the functions $\{\theta, \varphi\}$ and $\{\Theta, \Phi\}$ are determined from the arbitrarily chosen functions $\{u, v\}$ and $\{U, V\}$. Once this choice has been made all possible self-adjoint coupled conditions can then be obtained by appropriate choices of the two parameters α and $\mathbf{K}$.

6. Initial value problems

The initial value problem at any regular point c of the differential equation (2.1) can be solved; for details see the result given by (3.5).

In general it is impossible to solve initial value problems at a LP endpoint a or b.

However it is possible to solve a generalised initial value problem at any LC endpoint, say a. Let the set $\{u, v\}$ satisfy the properties given in (5.11), *i.e.*

$$\begin{cases} (i) & u, v : (a,b) \to \mathbb{R} \\ (ii) & u, v \in \Delta \\ (iii) & [u,v](a) \neq 0. \end{cases}$$

Then given two complex numbers $\xi, \eta \in \mathbb{C}$ and any complex value of the parameter $\lambda \in \mathbb{C}$, there exists a unique solution of the differential equation (2.1), say $y(\cdot, \lambda) : (a,b) \to \mathbb{C}$ with the properties

$$\begin{cases} (i) & y(\cdot,\lambda) \text{ and } (py')(\cdot,\lambda) \in AC_{\text{loc}}(a,b) \\ (ii) & [y(\cdot,\lambda), u(\cdot)](a) = \xi \text{ and } [y(\cdot,\lambda), v(\cdot)](a) = \eta. \end{cases} \tag{6.1}$$

For a proof of this result see [7, Section 2].

This result has an important application for the determination of eigenvalues for the general coupled boundary value problem with boundary conditions (5.19) and (5.20). Namely, let a, b be, independently, R or LC and choose the sets $\{\theta, \varphi\}$ and $\{\Theta, \Phi\}$ so that the conditions (5.17) and (5.18) are both satisfied.

Using the above initial value result determine two linearly independent solutions $\{y_1(\cdot,\lambda), y_2(\cdot,\lambda)\}$ of the differential equation (2.1) so that the generalised initial conditions are satisfied, for all $\lambda \in \mathbb{C}$,

$$\begin{matrix} [y_1(,\lambda), \theta(\cdot)](a) = 0 & [y_1(,\lambda), \varphi(\cdot)](a) = 1 \\ [y_2(,\lambda), \theta(\cdot)](a) = 1 & [y_2(,\lambda), \varphi(\cdot)](a) = 0. \end{matrix} \tag{6.2}$$

Given the matrix $\mathbf{K}$ from (5.20) define the function $D(\mathbf{K},\cdot):\mathbb{C}\to\mathbb{C}$ by, for all $\lambda\in\mathbb{C}$,

$$\begin{aligned} D(\mathbf{K},\lambda) := k_{11}[y_1(\cdot,\lambda),\Phi(\cdot)](b) + k_{22}[y_2(\cdot,\lambda),\Theta(\cdot)](b) \\ - k_{12}[y_2(\cdot,\lambda),\Phi(\cdot)](b) - k_{21}[y_1(\cdot,\lambda),\Theta(\cdot)](b). \end{aligned} \tag{6.3}$$

Then λ is an eigenvalue of the coupled boundary value problem determined by (5.19) and (5.20) if and only if

$$D(\mathbf{K},\lambda) = 2\cos(\alpha). \tag{6.4}$$

For details of this result see [7, Section 2].

The role of the endpoints a and b in (6.2) and (6.3) can be interchanged. Determine two linearly independent solutions Y_1, Y_2 of the equation (2.1) by the generalized initial conditions (6.1) but now with a replaced by b. Then (6.2) holds with a replaced by b and with y_j replaced by Y_j, $j=1,2$. Thus we obtain analogues of (6.3), (6.4) with b replaced by a, y_j by Y_j, $j=1,2$ and Θ,Φ by θ,ϕ. Next we observe that, instead of anchoring $D(\mathbf{K},\lambda)$ at a and evaluating at b or vice versa, we can get a symmetric form of $D(\mathbf{K},\lambda)$ as follows:

$$\begin{aligned} D(\mathbf{K},\lambda) := k_{11}[Y_2(\cdot,\lambda),y_1(\cdot,\lambda)] + k_{22}[y_2(\cdot,\lambda),Y_1(\cdot),\lambda] \\ + k_{12}[y_2(\cdot,\lambda),Y_2(\cdot,\lambda)] + k_{21}[Y_1(\cdot,\lambda),y_1(\cdot,\lambda)]. \end{aligned} \tag{6.5}$$

Note that all the sesquilinear forms $[\cdot,\cdot]$ in (6.5) are constant on the closed interval $[a,b]$. The equivalence of (6.5) and (6.3) can be seen from the Plücker identity, see [7, Lemma 6.2].

7. Self-adjoint problems

Given the differential equation, under any one of the coefficient conditions (3.4),

$$-(py')' + qy = \lambda wy \text{ on } (a,b) \tag{7.1}$$

we now list, under the endpoint classifications, the set of all self-adjoint boundary value problems together with the number and form of the boundary conditions:

(1) Let a be R or LC and, independently, let b be R or LC; then two linearly independent boundary conditions are required; **either** both conditions are separated **or** both are coupled.
(2) Let a be LP and b be R or LC; then no boundary condition is required nor allowed at a and there has to be one separated boundary condition at b; there is a corresponding situation if a is R or LC and b is LP.
(3) Let both a and b be LP; then no boundary conditions are required nor allowed at either endpoint.

8. Spectrum properties

Let $\mathbb{N}_0 = \{0,1,2,\cdots\}$ and $\mathbb{Z} = \{\cdots,-2,-1,0,1,2,\cdots\}$.

With the positive sign conditions on the coefficients $\{p,w\}$ given in (3.4) the spectrum, necessarily real, for any one of the self-adjoint boundary value problems for the differential equation (2.1), is unbounded above; the spectrum may or may not be bounded below.

(1) Let both endpoints a and b be, independently, R or LC; then:
   (a) The spectrum is always *discrete*, *i.e.* consists only of eigenvalues.
   (b) If the boundary conditions are separated then the spectrum is *simple*, *i.e.* all eigenvalues have multiplicity one.
   (c) If the boundary conditions are coupled then the spectrum may have multiplicity two, *i.e.* one or more eigenvalues may be *double*; a necessary, but not sufficient, condition for this property to occur is that the parameter $\alpha = 0$ or $\alpha = \pi$.
   (d) If neither endpoint a, b is LCO then the spectrum is bounded below and the eigenvalues are indexed as $\{\lambda_n : n \in \mathbb{N}_0\}$, with $\lambda_n \leq \lambda_{n+1}$ for all $n \in \mathbb{N}_0$ and $\lim_{n\to\infty} \lambda_n = +\infty$; if the spectrum is simple then $\lambda_n < \lambda_{n+1}$ for all $n \in \mathbb{N}_0$.
   (e) If either a or b, or both, is LCO then the spectrum is unbounded below, *i.e.* $\{\lambda_n : n \in \mathbb{Z}\}$ with $\lambda_n \leq \lambda_{n+1}$ for all $n \in \mathbb{Z}$ and $\lim_{n\to\pm\infty} \lambda_n = \pm\infty$; in this case the eigenvalues are indexed so that $\cdots \lambda_{-2} \leq \lambda_{-1} < 0 \leq \lambda_0 \leq \lambda_1 \cdots$.

(2) Let one or both endpoints a, b be LP; then:
   (a) The spectrum is always simple but may or may not be discrete, and may or may not be bounded below.
   (b) If the spectrum is discrete and bounded below then the eigenvalues are indexed as $\{\lambda_n : n \in \mathbb{N}_0\}$ with $\lambda_n < \lambda_{n+1}$ for all $n \in \mathbb{N}_0$ and $\lim_{n\to+\infty} \lambda_n = +\infty$; the nth eigenfunction has exactly n zeros in the open interval (a, b).
   (c) If the continuous (essential) spectrum is bounded below, say by σ, then:
      (i) there may be no eigenvalues below σ
      (ii) there may be a finite number of eigenvalues below σ, indexed as $\{\lambda_n : n = 0, 1, \cdots, N\}$, with $N \geq 0$, and $\lambda_n < \lambda_{n+1} \leq \sigma$ for $n = 0, 1, \cdots, N-1$; every eigenfunction belonging to λ_n has exactly n zeros in the open interval (a, b)
      (iii) there may be a countable infinity of eigenvalues below σ, indexed as $\{\lambda_n : n \in \mathbb{N}_0\}$ with $\lambda_n < \lambda_{n+1} < \sigma$ and $\lim_{n\to\infty} \lambda_n = \sigma$; every eigenfunction belonging to λ_n has exactly n zeros in the open interval (a, b)
      (iv) there may be a countable infinity of eigenvalues below σ such that the spectrum is unbounded below.
   (d) There are examples when a is R and b is LP for which the spectrum is discrete but unbounded above and below, say $\{\lambda_n : n \in \mathbb{Z}\}$ with $\lambda_n < \lambda_{n+1}$ for all $n \in \mathbb{Z}$, and $\lim_{n\to\pm\infty} \lambda_n = \pm\infty$; in such cases all eigenfunctions have infinitely many zeros; for some such examples see [26] and [28].

Remark The spectrum of all these Sturm-Liouville boundary value problems is invariant under the Liouville transformation discussed in Remark 8, Section 4 above.

9. Examples

To illustrate the scope and capabilities of the SLEIGN2 code we give here some details of a selected number of examples, taken from the collection of the 32 examples contained in the code file xamples.f, and from the information in the examples commentary file xamples.tex. The example numbers in the commentary are given below following the name of the example.

(1) **The Fourier equation** (example number 21)

$$-y''(x) = \lambda y(x) \text{ for all } x \in (-\infty, +\infty)$$

Endpoint classification in $L^2(-\infty,+\infty)$:

Endpoint	Classification
$-\infty$	LP
$+\infty$	LP

This is a simple constant coefficient equation whose eigenvalues, for any self-adjoint boundary condition, can be characterized in terms of a transcendental equation involving only trigonometric functions.

On the compact interval $[0,2\pi]$ the equation is R at the endpoints 0 and 2π; if the coupled boundary conditions

$$y(0) = y(2\pi) \quad \text{and} \quad y'(0) = y'(2\pi)$$

are chosen then the spectrum is discrete $\{\lambda_n = n^2 : n \in \mathbb{N}_0\}$; the eigenvalue $\lambda_0 = 0$ is simple with eigenfunction 1; the eigenvalues $\{\lambda_n = n^2 : n \in \mathbb{N}\}$ are all double with eigenfunctions $\{\cos(nx)$ and $\sin(nx) : n \in \mathbb{N}\}$; the code computes these eigenvalues, and reports on the one simple and all the other double eigenvalues.

On the interval $[0,\infty)$ the equation is LP at $+\infty$; there is no boundary condition required at $+\infty$ and if the separated boundary condition at 0 is chosen to be

$$y(0) + y'(0) = 0,$$

then there is an isolated eigenvalue $\lambda_0 = -1$, with eigenfunction $\exp(-x)$, and a continuous spectrum on $[0,\infty) \subset \mathbb{C}$. If the code is requested to compute the first two eigenvalues λ_0, λ_1 then it reports that $\lambda_0 = -1$, that there are no more eigenvalues and that there is a continuous spectrum on the half-line $[0,\infty)$.

As an example of complex coupled boundary conditions we have, in matrix form,

$$\begin{bmatrix} y(2\pi) \\ y'(2\pi) \end{bmatrix} = \exp(i) \begin{bmatrix} 2 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} y(0) \\ y'(0) \end{bmatrix};$$

this boundary value problem has two negative eigenvalues, and all other eigenvalues are positive; these numerical results indicate that the spectrum of the problem is simple.

(2) **Classical Legendre equation** (example number 1)

$$-\left(\left(1-x^2\right)y'(x)\right)' + \frac{1}{4}y(x) = \lambda y(x) \text{ for all } x \in (-1,+1).$$

Endpoint classification in $L^2(-1,+1)$:

Endpoint	Classification
-1	LCNO
$+1$	LCNO

For both endpoints the boundary condition functions u, v are given by (note that u and v are solutions of the Legendre equation for $\lambda = 1/4$)

$$u(x) = 1 \qquad v(x) = \frac{1}{2}\ln\left(\frac{1+x}{1-x}\right) \text{ for all } x \in (-1,+1).$$

(i) The Legendre polynomials are obtained by taking the principal (Friedrichs) boundary condition at both endpoints ± 1 : enter $A1 = 1, A2 = 0,\ B1 = 1, B2 = 0$; *i.e.* take the boundary condition function u at ± 1; eigenvalues: $\lambda_n = (n + 1/2)^2$; $n = 0, 1, 2, \cdots$; eigenfunctions: Legendre polynomials $P_n(x)$.

(ii) Enter $A1 = 0,\ A2 = 1,\ B1 = 0,\ B2 = 1$, *i.e.* use the boundary condition function v at ± 1; eigenvalues: μ_n; $n = 0, 1, 2, \cdots$ but no explicit formula is available; eigenfunctions are logarithmically unbounded at ± 1.

(iii) Observe that $\mu_n < \lambda_n < \mu_{n+1}$; $n = 0, 1, 2 \cdots$.

The code successfully computes the eigenvalues in both the cases (i) and (ii) and reports, by default, that all eigenvalues are not double.

(3) **The harmonic oscillator equation** (example number 15)

$$-y''(x) + x^2 y(x) = \lambda y(x) \text{ for all } x \in (-\infty, +\infty).$$

Endpoint classification in $L^2(-\infty, +\infty)$:

Endpoint	Classification
$-\infty$	LP
$+\infty$	LP

This is another classical equation; it is also the Liouville normal form of the differential equation for the Hermite orthogonal polynomials. On the whole real line the boundary value problem requires no boundary conditions at the endpoints of $\pm\infty$. Thus there is a unique self-adjoint extension with discrete spectrum given by :

$$\{\lambda_n = 2n + 1;\ n = 0, 1, 2, ...\}.$$

In this example, when entered into the code, no boundary conditions are required since both endpoints are LP; the code computes these eigenvalues and reports, by default, that they are not double.

(4) **Weakly regular** (example number 10)

The endpoint classification *weakly regular* (notation WR) is introduced for numerical analytic purposes, see Section 15 below, and is concerned with R endpoints for which coefficients p, q, w at endpoint a, say, are continuous on $[a, b]$ but have a *numerical* singularity caused by $p(a) = 0$ and/or $|q(a)| = +\infty$ and/or $w(a) = +\infty$; as an example we have

$$-(x^{1/2} y'(x))' = \lambda x^{-1/2} y(x) \text{ for all } x \in (0, +\infty).$$

Endpoint classification in $L^2((0, \infty); x^{-1/2})$:

Endpoint	Classification
0	WR
$+\infty$	LP

This is a devised example to illustrate the computational difficulties of weakly regular problems.

The differential equation gives $p(0) = 0$ and $w(0) = +\infty$ but nevertheless 0 is a regular endpoint in the Lebesgue integral sense; however 0 has to be classified as weakly regular in the computational sense.

The Liouville normal form of this equation is the Fourier equation, see Example 21 above; thus numerical results for this WR problem can be checked against numerical results from (i) a R problem, (ii) the roots of trigonometrical equations, and (iii) a LCNO problem (see below); the code performs effectively using both methods (i) and (iii).

There are explicit solutions of this equation given by

$$\cos(2x^{1/2}\sqrt{\lambda}) \ ; \ \sin(2x^{1/2}\sqrt{\lambda})/\sqrt{\lambda}.$$

If 0 is treated as a LCNO endpoint then $u,\ v$ boundary condition functions are

$$u(x) = 2x^{1/2} \qquad v(x) = 1.$$

The regular Dirichlet condition $y(0) = 0$ is equivalent to the singular condition $[y, u](0) = 0$. Similarly the regular Neumann condition $(py')(0) = 0$ is equivalent to the singular condition $[y,\ v](0) = 0$.

The following indicated boundary value problems have the given explicit formulae for the eigenvalues:

$$y(0) = 0 \text{ or } [y,\ u](0) = 0, \text{ and } y(1) = 0 \text{ gives}$$
$$\lambda_n = ((n+1)\pi)^2/4 \ (n = 0, 1, ...)$$

$$(py')(0) = 0 \text{ or } [y, v](0) = 0, \text{ and } (py')(1) = 0 \text{ gives}$$
$$\lambda_n = \left((n+\tfrac{1}{2})\pi\right)^2/4 \ (n = 0, 1, ...).$$

(5) **The Laguerre/Liouville equation** (example number 23)

$$-y''(x) + \left(\frac{\alpha^2 - 1/4}{x^2} - \frac{\alpha+1}{2} + \frac{x^2}{16}\right) y(x) = \lambda y(x) \text{ for all } x \in (0, +\infty)$$

where the parameter $\alpha \in (-\infty, +\infty)$.

Endpoint classification in the space $L^2(0, +\infty)$:

Endpoint	Parameter	Classification
0	$\alpha \le -1$	LP
0	$-1 < \alpha < 1$, but $\alpha^2 \ne 1/4$	LCNO
0	$\alpha^2 = 1/4$	R
0	$1 \le \alpha$	LP
$+\infty$	$\alpha \in (-\infty, +\infty)$	LP

For these WR/LCNO cases the boundary condition functions u, v are given by:

Endpoint	Parameter	u	v
0	$-1 < \alpha < 0$ but $\alpha \ne -1/2$	$x^{\frac{1}{2}-\alpha}$	$x^{\frac{1}{2}+\alpha}$
0	$\alpha = -1/2$	x	1
0	$\alpha = 0$	$x^{1/2}$	$x^{1/2}\ln(x)$
0	$0 < \alpha < 1$ but $\alpha \ne 1/2$	$x^{\frac{1}{2}+\alpha}$	$x^{\frac{1}{2}-\alpha}$
0	$\alpha = 1/2$	x	1

This is the Liouville normal form of the classical Laguerre equation.

The Laguerre polynomials are produced as eigenfunctions only when $\alpha > -1$. For $\alpha \geq 1$ the LP condition holds at 0. For $0 \leq \alpha < 1$ the appropriate boundary condition is the Friedrichs condition: $[y, u](0) = 0$; for $-1 < \alpha < 0$ use the non-Friedrichs condition: $[y,\ v](0) = 0$. In all these cases $\lambda_n = n$ for $n = 0, 1, 2, ...$ and the code works effectively except near to those values of the parameter α when the endpoint classification switches form one form to another.

(6) **The Krall equation** (example number 20)

$$-y''(x) + (1 - (k^2 + 1/4)x^{-2})y(x) = \lambda y(x) \text{ for all } x \in (0, +\infty)$$

where the parameter $k \in (0, +\infty)$.

Endpoint classification in the space $L^2(0, +\infty)$:

Endpoint	Classification
0	LCO
$+\infty$	LP

This example is a special case of the classical Bessel equation; solutions can be obtained in terms of the modified Bessel functions.

To help with the computations for this example the spectrum is translated by a term +1; this simple devise is used for numerical convenience.

For problems with a separated boundary conditions at endpoint 0 there is a continuous spectrum on $[1, \infty)$ with a discrete (and simple) spectrum on $(-\infty, 1)$. This discrete spectrum has cluster points at both $-\infty$ and 1.

For the LCO endpoint at 0 the boundary condition functions are given by

$$u(x) = x^{1/2}\cos(k\ln(x)) \qquad v(x) = x^{1/2}\sin(k\ln(x)).$$

For the boundary value problem with boundary condition $[y, u](0) = 0$ the eigenvalues are given explicitly by:

(i) suppose $\Gamma(1 + i) = \alpha + i\beta$ and $\mu > 0$ satisfies $\tan\left(\ln(\frac{1}{2}\mu)\right) = -\alpha/\beta$

(ii) $\theta = \mathrm{Im}(\log(\Gamma(1 + i)))$

(iii) $\ln(\frac{1}{2}\mu) = \frac{1}{2}\pi + \theta + s\pi$ for $\ s = 0, \pm1, \pm2, ...$

(iv) $\mu_s^2 = \left(2\exp(\theta + \frac{1}{2}\pi)\right)^2 \exp(2s\pi)\ \ s = 0, \pm1, \pm2, ...$

then the eigenvalues are $\lambda_n = -\mu^2_{-(n+1)} + 1$ $(n = 0, \pm1, \pm2, ...)$.

SLEIGN2 can compute only six of these eigenvalues, even in double precision, λ_{-3} to λ_2; other eigenvalues are, numerically, too close to 1 or too close to $-\infty$. Here we list these SLEIGN2 computed eigenvalues in double precision and compare them with the same eigenvalues computed from the transcendental equation; for the problem on $(0, \infty)$ with $k = 1$ and $A1 = 1.0,\ A2 = 0.0$.

NUMEIG	eig from SLEIGN2	eig from trans. equ.
-3	$-276,562.5$	$-14,519,130$
-2	$-27,114.48$	$-27,114.67$
-1	-49.62697	-49.63318
0	0.9054452	0.9054454
1	0.9998234	0.9998234
2	0.9999997	0.9999997

.

(7) **The Mathieu equation** (example number 12)

$$-y''(x) + 2k\cos(2x)y(x) = \lambda y(x) \text{ for all } x \in (-\infty, +\infty)$$

where the parameter $k \in (-\infty, 0) \cup (0, +\infty)$.

Endpoint classification in $L^2(-\infty, +\infty)$:

Endpoint	Classification
$-\infty$	LP
$+\infty$	LP

The classical Mathieu equation has a celebrated history and voluminous literature. There are no eigenvalues for this problem on $(-\infty, +\infty)$. There may be one negative eigenvalue of the problem on $[0, \infty)$ depending on the boundary condition at the endpoint 0. The continuous (essential) spectrum is the same for the whole line or half-line problems and consists of an infinite number of disjoint closed intervals. The endpoints of these - and thus the spectrum of the problem - can be characterized in terms of periodic and semi-periodic eigenvalues of Sturm-Liouville problems on the compact interval $[0, 2\pi]$; these can be computed with SLEIGN2.

Of special interest is the starting point of the continuous spectrum - this is also the oscillation number of the equation. For another Mathieu equation given by $p = 1, q = \cos(x), w = 1$, on both the whole line and the half line it is approximately -0.378; this result may be obtained by using the code to compute the first eigenvalue λ_0 of the periodic problem on the interval $[0, 2\pi]$.

For detailed information on the qualitative (and quantitative) use of the SLEIGN2 code in the study of the spectral properties of this Mathieu differential equation, see the discussion, and the diagrammatic illustrations, in the paper [35].

(8) **The Jörgens equation** (example number 27)

$$-y''(x) + (\exp(2x)/4 - k\exp(x))y(x) = \lambda y(x) \text{ for all } x \in (-\infty, +\infty)$$

where the parameter $k \in (-\infty, +\infty)$.

Endpoint classification in the space $L^2(-\infty, +\infty)$, for all $k \in (-\infty, +\infty)$:

Endpoint	Classification
$-\infty$	LP
$+\infty$	LP

This is a remarkable example from Jörgens and SLEIGN2 obtains excellent results. For all $k \in (-\infty, +\infty)$ the boundary value problem on the interval $(-\infty, +\infty)$ has a continuous spectrum on $[0, +\infty)$; for $k \leq 1/2$ there are no eigenvalues; for $h = 0, 1, 2, 3, \ldots$ and then k chosen by $h < k - 1/2 \leq h + 1$, there are exactly $h + 1$ eigenvalues and these are all below the continuous spectrum; these eigenvalues are given explicitly by

$$\lambda_n = -(k - 1/2 - n)^2, \quad n = 0, 1, 2, 3, \ldots, h.$$

(9) **The Marletta equation** (example number 14)

$$-y''(x) + \frac{3(x-31)}{4(x+1)(x+4)^2}y(x) = \lambda y(x) \text{ for all } x \in [0, +\infty).$$

Endpoint classification in $L^2(0,+\infty)$:

Endpoint	Classification
0	R
$+\infty$	LP

Since $q(x) \to 0$ as $x \to \infty$ the continuous spectrum consists of $[0,\infty)$ and every negative number is an eigenvalue for some boundary condition at 0.

For the boundary condition

$$5y(0) + 8y'(0) = 0$$

there is a negative eigenvalue λ_0 near -1.185. However the equation with $\lambda = 0$ has a solution

$$y(x) = \frac{1-x^2}{(1+x/4)^{5/2}} \text{ for all } x \in [0,\infty)$$

that satisfies this boundary condition which is NOT in $L^2(0,\infty)$ but is "nearly" in this space; this solution deceives SLEIGN and SLEIGN2 in single precision, and SLEDGE in double precision into reporting $\lambda = 0$ as a second eigenvalue; in double precision SLEIGN and SLEIGN2 correctly report that λ_0 is the only eigenvalue, and SLEIGN2 reports the start of the continuous spectrum at 0.

Part II: The computational methods

10. Introduction

Many numerical methods have been developed for the computation of eigenvalues and eigenfunctions of Sturm-Liouville boundary value problems. These techniques include the important finite difference [23], variational [14] and shooting [22] methods. However the accuracy of both variational and finite difference methods falls off rapidly with the increasing index of the eigenvalue. This is true also for many of the shooting methods when applied directly to the Sturm-Liouville differential equation.

Another drawback of many of these methods is that they cannot proceed directly to the computation of a particular eigenvalue, but necessarily require the prior computation of all the preceding eigenvalues.

The use of the Prüfer transformation, see [1] and Section 12 below, allows of the computation of a particular eigenvalue of given index, without the prior computation of all the preceding eigenvalues, and also makes it possible to obtain reasonable numerical accuracy for eigenvalues of higher index order.

The method used in SLEIGN2 for regular boundary value problems; *i.e.* when the coefficients $\{p, q, w\}$ satisfy the conditions (ii) of (3.4) on a compact interval $[a, b]$, are essentially the same conditions as required in the original SLEIGN code. However the situation when the same conditions hold on a bounded open interval (a, b) together with the integrability conditions $p^{-1}, q, w \in L^1(a, b)$ is considerably weaker since it permits coefficient functions that are unbounded near the endpoints of (a, b); these "weakly regular" (notation WR) endpoints require special numerical treatment.

In addition, boundary value problems with general coupled boundary conditions, see Section 5 above, require new numerical methods, given in SLEIGN2 but not available in any other codes for Sturm-Liouville problems. These coupled boundary condition methods apply not only to regular problems, but to any problems for which the endpoints a and b of the interval (a, b) are, independently, classified as R or LCNO or LCO on using the notation of Section 4 above.

11. Initial estimate of the eigenvalue

As a matter of programming convenience the original independent variable $x \in (a, b)$ is internally transformed in the code to a new variable $t \in (-1, 1)$. The transformation used is the appropriate bilinear, or homographic, change of variables; this transformation leaves invariant the spectrum of the self-adjoint Sturm-Liouville boundary value problem.

Before any significant computations are started in SLEIGN2 the given coefficient functions $\{p, q, w\}$ are evaluated at about 100 points in the interval (a, b) and the values stored for subsequent reference. This step provides data for some of the ensuing stages during the computation; this procedure makes it possible to form an estimate of the desired eigenvalue, thus relieving the user of having to provide an initial numerical guess. Iterative numerical methods generally require an initial guess, and it is not uncommon for a poor guess to lead to failure of the whole numerical scheme.

Essentially the initial estimate method solves the following equation for λ, on given the eigenvalue index n,

$$\int \sqrt{\frac{\lambda w(x) - q(x)}{p(x)}}\, dx = (n+1)\pi, \tag{11.1}$$

where the integration is taken over only that part of (a, b) for which the integrand is real. In the interests of numerical economy the integral is approximated by the trapezoidal rule and use is made of only the stored values of the coefficients $\{p, q, w\}$. (It is of interest to note that the equation (11.1) is similar to the well-known WKBJ formula of mathematical physics.) This formula sometimes fails, *e.g.* the integral may be infinite for some coefficients with singularities in (a, b), in which case a simple "ballpark" estimate is used; however, in general this method provides a good estimate of the eigenvalue. In particular, in most cases the method does prevent the insertion of really bad estimates, *e.g.* the use of a positive number when only negative eigenvalues are in the spectrum of the boundary value problem.

12. The Prüfer transformation

This transformation of the second order Sturm-Liouville linear differential equation (2.1), with dependent variable y, yields an equivalent first order non-linear system with dependent variables ρ and θ; these are the so-called Prüfer amplitude and phase variables. This transformation is effected by writing, for all $x \in (a, b)$,

$$y(x) = \rho(x) \sin(\theta(x)) \tag{12.1}$$

$$(py')(x) = \rho(x) \cos(\theta(x)). \tag{12.2}$$

The differential equations satisfied by ρ and θ, obtained by substituting (12.1) and (12.2) in (1.1), are for all $x \in (a,b)$,

$$\theta'(x) = p(x)^{-1}\cos^2(\theta(x)) + (\lambda w(x) - q(x))\sin^2(\theta(x)) \tag{12.3}$$

$$\rho'(x)/\rho(x) = \big(p(x)^{-1} - \lambda w(x) + q(x)\big)\sin(\theta(x))\cos(\theta(x)). \tag{12.4}$$

Boundary conditions to determine θ are inherited from (1.2) and (1.3), in the regular case, yielding

$$\alpha := \theta(a) = -\arctan(A_2/A_1) \quad \text{with } \alpha \in [0,\pi) \tag{12.5}$$

$$\beta := \theta(b) - n\pi = -\arctan(B_2/B_1) \quad \text{with } \beta \in (0,\pi], \tag{12.6}$$

where $n \in \mathbb{N}_0$ is the index of the required eigenvalue.

13. The regular eigenvalue problem

Suppose given the boundary value problem (1.1) and (1.2), (1.3), the latter with boundary condition parameters A_1, A_2, B_1, B_2.

The eigenvalue problem now consists of finding the value λ_n of the parameter λ, and the corresponding solution θ of (12.3), such that both boundary conditions (12.5) and (12.6) are satisfied. Basically, this requirement is accomplished by integrating the equation (12.3), with initial condition (12.5), from the endpoint a to some interior point x_{mid}, thereby obtaining a solution θ_{left}; then integrating (12.3), with initial condition (12.6), from endpoint b to x_{mid}, thereby obtaining a solution θ_{right}; both these integrations are made in (12.3) using the estimated value of λ, as discussed in Section 11 above. Theoretically, which interior point is chosen for x_{mid} is immaterial, but in practice it is best to avoid particularly poor choices for x_{mid}.

The difference function,

$$\text{dtheta}(\lambda) := \theta_{\text{left}}(x_{\text{mid}}) - \theta_{\text{right}}(x_{\text{mid}}) \tag{13.1}$$

is zero if and only if the used value λ of the spectral parameter satisfies $\lambda = \lambda_n$, the required eigenvalue. Thus the procedure for finding the numerical value of the eigenvalue λ_n, consists in evaluating the function dtheta(λ), numerically, and then through a finite series of iterations finding the value of λ such that dtheta(λ) $= 0$ to the required degree of approximation. Recall that, given $n \in \mathbb{N}_0$, this solution is unique in view of the form of the right hand initial condition (12.6).

Besides the differential equation (12.3) for the phase θ - which is all that is required for finding the numerical value of the eigenvalue - it is useful also to integrate the equation (12.4) for the amplitude ρ, if the numerical values for the eigenfunction are required. For reasons of stability in the numerical procedures, the differential equation actually integrated is

$$F'(x) = f(x) \text{ for all } x \in (a,b)$$

where the function f is defined by the right hand side of (12.4) *i.e.*

$$f(x) := \big(p(x)^{-1} - \lambda w(x) + q(x)\big)\sin(\theta(x))\cos(\theta(x)) \text{ for all } x \in (a,b). \tag{13.2}$$

Clearly then the amplitude function ρ is given by

$$\rho(x) = \rho(a)\exp(F(x)) \text{ for all } x \in (a,b)$$

or

$$\rho(x) = \rho(b)\exp(F(x)) \text{ for all } x \in (a,b),$$

according to making the choice $F(a) = 0$ or $F(b) = 0$, respectively.

Also, because it is useful to be able to use Newton iteration whilst searching for the zero of dtheta, the differential equation for the function dthde defined by

$$\text{dthde}(x) := \frac{d\theta(x,\lambda)}{d\lambda}$$

is also integrated at the same time; namely, see (13.2) above,

$$\text{dthde}'(x) = -2f(x) + w(x)\sin^2(\theta(x)). \tag{13.3}$$

14. Singular eigenvalue problems

Essentially the same procedure outlined in the previous section for regular problems, is also used for singular boundary value problems. As for the regular case the differential equation (12.3) for the Prüfer angle θ is integrated from the left to some interior point x_{mid} of the interval (a,b), using an appropriate initial condition; similarly the equation (12.3) is integrated from the right to x_{mid}, using an appropriate initial condition. As in the previous section, these integrations are carried out with some estimated value of λ, giving two solutions θ_{left} and θ_{right}, which then define the function dtheta(λ) as in (13.1). The numerical value of the requested eigenvalue is then obtained by iteration of the value of the parameter λ, as described in the previous section.

The main difference between the procedure for regular and singular problems (with separated boundary conditions) lies in the methods to solve the initial value problem for the Prüfer angle θ at a singular (or even a WR) endpoint.

At a WR endpoint the initial value problem that has to be solved to obtain θ_{left} or θ_{right} is of the same form as at a R endpoint, but because of the difficulty in numerically integrating such problems, special methods have to be employed as described in Section 15 below.

At a LC endpoint, since the form of limit circle boundary conditions is different from regular boundary conditions, the appropriate initial conditions to determine θ also require special methods; details for the cases LCNO and LCO are given in Sections 16 and 17 respectively.

Finally, at a LP endpoint, where no boundary condition is required, solutions for θ_{left} and θ_{right} are still required; this problem again requires a different method and details are given in Section 18 below.

15. Weakly regular initial value problems

The coefficient conditions of (i) of (3.4) for a regular endpoint are weak enough to include some coefficient functions of (12.3) which are unbounded, in particular at the endpoints a and b. Thus it may not be possible to integrate numerically the initial value problems (12.3) and either (12.5) or (12.6), by direct means, *i.e.* without first making some kind of alteration to enable the integrator to make a start on the integration process.

For example, consider the differential equation (12.3) in the case when

$$p(x) = \sqrt{x}, \quad q(x) = 0, \quad w(x) = 1/\sqrt{x} \quad \text{for all } x \in (0,1).$$

The initial value problem for θ is of the form

$$\theta'(x) = \frac{\cos^2(\theta(x))}{\sqrt{x}} + \lambda \frac{\sin^2(\theta(x))}{\sqrt{x}} \quad \text{for all } x \in (0,1) \tag{15.1}$$

and

$$\theta(0) = \alpha \tag{15.2}$$

which is a regular problem in the analytic sense. However, numerically, without taking suitable precautions - perhaps a change of variable - this initial value problem cannot be integrated by standard numerical integration.

On the other hand such initial value problems have unique analytic solutions, from standard existence theorems, which are continuous; in particular the unique solution of the problem (15.1) and (15.2) is continuous on the closed interval $[0,1]$.

In order to refer conveniently to an endpoint, which is regular in the analytic sense but for which one or more of the coefficients p^{-1}, q, w may not be evaluated numerically, it is called a *weakly regular* endpoint, with notation WR. Note that this is not an analytic classification of the endpoint, as covered in Section 4 above, but it is a useful and important numerical term and is so employed in this paper.

Consider then the initial value problem

$$\begin{aligned} y'(x) &= f(x, y(x)) \quad \text{for all } x \in [a,b] \\ y(a) &= A \end{aligned}$$

but for which the value $f(a, A)$ is not defined, including the possibility when $f(, A) = +\infty$, as for the special case of (15.1) and (15.2); then (without some kind of special treatment) numerical integrators cannot obtain a solution. If the dependent and independent variables are interchanged, so that

$$\begin{aligned} x'(y) &= \frac{1}{f(x,y)} \quad \text{for } y \in [A,B] \\ x(A) &= a \end{aligned}$$

then $x'(A) = 0$; but even so standard numerical integrators are not able to obtain a solution.

Since, unfortunately, there seems not to be any numerical integrator which can be used directly for WR problems, a brief description is given here of a general but somewhat "devious" device that can be used for such problems.

There is a "correction formula" that is sometimes used in the process of numerically integrating a differential equation - usually applied at the start of the process, say after only 4 or 5 integration steps have been taken using some "predictor" formulae. This correction can be obtained by integrating the Newton backward difference formula, and is written in the form

$$\begin{aligned} dx(0) = \; & h\{q(4) - (7/2)dq(3) + (53/12)d2q(2) - (55/24)d3q(1) \\ & + (251/720)d4q(0) \pm \ldots\}. \end{aligned}$$

Here $dx(0) = x(1) - x(0), dq(1) = q(2) - q(1), d2q(2) = dq(2) - dq(1)$, *etc.* and the $q(i)$ terms are the derivatives of the function x at the equally spaced points of the variable y. The error in using this formula is usually taken to be of the size of $(h/3)d5q(-1)$.

When the numerical integration for x has reached $y(4)$ and there is some uncertainty about the earlier value of $x(1)$ at $y(1)$, this formula can be used to effect a correction. Thus given the problem

$$x'(y) = 1/f(x,y) \quad \text{with } x(y(0)) = x(0)$$

let $y(i), i = 1,2,3,4$ be equally spaced points with $y(i+1) - y(i) = h$. Let $x(1)$ be an initial "guess" for the value of the solution at $y(1)$, and integrate the differential equation for the variable x from $y(1)$ to $y(4)$. Let $q(i), i = 1,2,3,4$ be the values of the derivative function for x at the points $y(i)$. Then, according to the above correction formula, a "corrected" value of the initial guess of $x(1)$ is

$$\begin{aligned} x(1) = \; x(0) + h\,\{q(4) - (7/2)dq(3) + (53/12)d2q(2) - (55/24)d3q(1) \\ +(251/720)d4q(0) \pm \ldots\}\,. \end{aligned}$$

Now repeat the process using the new value of $x(1)$ as the "guess". If the first guess for $x(1)$ is close enough to the correct value, then there is reason to expect that the iteration is convergent.

When the dependent and independent variables are interchanged to avoid an infinite derivative at the endpoint, after the iteration has been completed and $x(1)$ has been determined, the original differential equation is finally integrated from the point $(x(1), y(1))$.

In practice the process works reasonably well for many WR problems but a more direct integration for such problems would be valuable.

16. Limit circle non-oscillatory initial value problems

The initial value problem at a LC endpoint differs substantially from the R or WR cases. For, in one respect, a separated boundary condition at a LC endpoint a is of the form (5.12) *i.e.*

$$A_1[y,u](a) + A_2[y,v](a) = 0, \tag{16.1}$$

where $u, v \in \Delta$ are maximal domain functions, see (5.1), chosen by the user, in comparison with the separated boundary condition (5.9), *i.e.*

$$A_1 y(a) + A_2(py')(a) = 0,$$

at a R endpoint.

Note that in (16.1) the sesquilinear terms $[y,u](a)$ and $[y,v](a)$ are defined by limits, such as $\lim_{x \to a^-}[y,u](x)$, which always exist in the LC case, although in general the separate terms within the sesquilinear form, see (5.3), do not have finite limits at the endpoint a^+.

16.1. **Regularization.** To overcome the above change in the analytic form of the boundary conditions for LC endpoints the code introduces a "regularization" for use in the numerical process; for this purpose the code makes use of the maximal domain functions $u, v \in \Delta$, as used above.

This regularization is best considered in two steps:

(1) Set, for all $x \in (a,b)$

$$y(x) = z_1(x)u(x) + z_2(x)v(x)$$

and

$$(py')(x) = z_1(x)(pu')(x) + z_2(x)(pv')(x)$$

thus defining two new variables z_1 and z_2 in place of y and py' in the original differential equation (2.1). After substitution and simplification we obtain a first order system for z_1 and z_2 on the interval (a, b), as follows:

$$[u, v]z_1' = \lambda wv(z_1u + z_2v) - v(z_1Hu + z_2Hv) \tag{16.2}$$

$$[u, v]z_2' = -\lambda wu(z_1u + z_2v) + u(z_1Hu + z_2Hv), \tag{16.3}$$

where the differential expression H is defined by

$$Hu := -(pu')' + qu \text{ on } (a, b)$$

using the original coefficients p and q. This system for $\{z_1, z_2\}$ can be shown to be regular, in a generalized sense, even if the interval (a, b) is unbounded; from this result it follows that the functions $\{z_1, z_2\}$ both have finite limits at the endpoints a and b, which we write as $z_1(a)$ and $z_2(a)$ at the endpoint a, and similarly at the endpoint b. In fact, in terms of the original dependent and independent variables y and x, z_1 and z_2 have the representation

$$z_1(x) = \frac{[y, v](x)}{[u, v]} \quad \text{and} \quad z_2(x) = -\frac{[y, u](x)}{[u, v]} \text{ for all } x \in (a, b),$$

where $[u, v]$ represents the constant value of $[u, v](x)$ for all $x \in (a, b)$.

Under this transformation the boundary condition (16.1) is equivalent to the condition

$$A_1z_2(a) - A_2z_1(a) = 0.$$

(2) Now introduce a new variable φ, defined for all $x \in (a, b)$, by

$$\tan(\varphi(x)) := \frac{z_2(x)}{z_1(x)} \text{ for all } x \in (a, b).$$

On substitution in the system (16.2) and (16.3) we obtain the following differential equation for φ

$$[u, v]\varphi' = (u\cos(\varphi) + v\sin(\varphi))((Hu - \lambda wu)\cos(\varphi) + (Hv - \lambda wv)\sin(\varphi)) \tag{16.4}$$

with initial condition

$$\tan(\varphi(a)) = \frac{A_2}{A_1}. \tag{16.5}$$

This differential equation may be seen to have the equivalent of a WR condition at the endpoint a and can be integrated from this point by the method described in Section 14 above, for such initial value problems.

Once the integration for φ has progressed far enough away from the LC endpoint, so that the singularity ceases to be a problem for the numerical process, the solution φ is translated back to the Prüfer angle θ. (As mentioned above, it is not sufficient in this process to be an arbitrary small distance away from the LC endpoint; it is essential to be far enough away before it is safe to return to the original variables.)

In practice, it is useful to have available not only the variable θ but also the variables dthde and F, where $F := \ln(\rho)$, besides φ. We also define the comparable functions

$$\sigma := \sqrt{z_1^2 + z_2^2} \quad \text{and} \quad \text{dphide} := \frac{d\varphi}{d\lambda}.$$

Thus the system under integration for φ is of the 3rd order, as for the system for θ.

The relationship between θ and φ is just

$$\tan(\theta) = \frac{u\cos(\varphi) + v\sin(\varphi)}{pu'\cos(\varphi) + pv'\sin(\varphi)}. \tag{16.6}$$

Thus if the system for φ can be integrated numerically from the endpoint a to some intermediate point, then the results can be translated to the equivalent system for θ, and the integration then continued in terms of θ.

17. Limit circle oscillatory initial value problems

These problems differ from the LCNO case considered in the previous section in two important ways. First, the differential equation for φ, on the interval (a, b),

$$[u, v]\varphi' = (u\cos(\varphi) + v\sin(\varphi))((Hu - \lambda wu)\cos(\varphi) + (Hv - \lambda wv)\sin(\varphi)) \tag{17.1}$$

has oscillatory coefficients (it is known that in this LCO case the maximal domain functions u and v are infinitely oscillatory near the endpoint) and this makes it highly unlikely that a numerical integration scheme that attempts to approximate the solution by polynomials, will succeed. Second, because of the indexing problem for the eigenvalues, recall that all eigenfunctions have infinitely many zeros, it is necessary to "calibrate" the solutions for any particular λ with a solution obtained when $\lambda = 0$. Since the code has been determined so as to index the first non-negative eigenvalue as λ_0, then the eigenfunction corresponding to λ_1 is seen to have one more zero then the eigenfunction corresponding to λ_0; as both eigenfunctions have infinitely many zeros this statement only makes sense, in practice, since the computations are taking place on a compact subinterval of (a, b).

This last remark is enhanced by the fact that it is not possible to integrate the differential equation (17.1) starting with initial data at the endpoint a, it is necessary to truncate the interval so that numerical integration begins at some point near to a; this is the procedure within the code.

18. Limit point initial value problems

Although an arbitrary initial value problem cannot be specified at a LP endpoint, for numerical purposes it is necessary for the code to determine a suitable initial value for the solution of the differential equation (12.3) called θ_{left} (or θ_{right}). Of the several possible kinds of LP endpoints, only those endpoints are considered for which the differential equation (1.1) has an integrable square (with respect to the weight w) solution, that has a Prüfer angle θ tending to a finite limit. In this case there are several distinct possibilities:

(α) The coefficient p satisfies $p(a) \neq 0$, but at least one of the coefficients $\{q, w\}$ is infinite at a, in which case the limit $\lim_{x \to a} \theta(x)$ is a multiple of π; or

(β) The coefficient p satisfies $p(a) = 0$ and both of $\{q, w\}$ are finite at a, in which case $\lim_{x \to a} \theta(x)$ is an odd multiple of $\pi/2$; or

(γ) The coefficient p satisfies $p(a) = 0$ and at least one of $\{q, w\}$ is infinite at a, in which case $\lim_{x \to a} \theta(x)$ is congruent to

$$\lim_{x \to a} \arctan\left((p(x)q(x) - \lambda w(x))^{-1/2}\right).$$

Moreover λ may have to be restricted in order that the term

$$p(x)q(x) - \lambda w(x)$$

is non-negative near the LP endpoint a, which implies that the eigenvalues of the boundary value problem are bounded above; this can occur if there is only a finite number of eigenvalues, and/or there is a continuous spectrum extending to $+\infty$.

In any case, if it happens that λ must be restricted to being less than some upper bound C, and if, for some given index n, in trying to compute the eigenvalue λ_n it is found that the function dtheta is negative when $\lambda = C$ then there can be no eigenvalue of this index n. Moreover, if dtheta $< -\pi$ then there can be no eigenvalue with index $n - 1$. In general, there can be no eigenvalue with index greater than $n - 1 -$ integer part of (dtheta/π).

This case of LP endpoints presents computational difficulties for SLEIGN2, and indeed for all codes designed for Sturm-Liouville problems; in particular when the coefficient q is oscillatory near the LP endpoint such codes may not even be able to start with the computational process. Examples are Mathieu's equation (see Example 12 in the file xamples.tex)

$$-y''(x) + 2k\cos(2x)y(x) = \lambda y(x) \text{ for all } x \in [0, \infty) \text{ or } (-\infty, \infty)$$

which is LP at $\pm\infty$, and the Littlewood-McLeod differential equation (see Example 30 in the file xamples.tex)

$$-y''(x) + x\sin(x)y(x) = \lambda y(x) \text{ for all } x \in [0, \infty)$$

which is LP at $+\infty$.

19. Coupled boundary conditions

Sturm-Liouville problems with coupled boundary conditions, see Section 5 above, differ in several ways from problems with separated boundary conditions; in particular coupled conditions may lead to self-adjoint differential operators with spectra of multiplicity two and so to double eigenvalues.

In the first place, there are no convenient functions comparable to

$$\text{thetal}(\lambda) \quad \text{and} \quad \text{thetar}(\lambda),$$

which can be defined in terms of the separated boundary conditions at the endpoints, and which lead to the function

$$\text{dtheta}(\lambda) = \text{thetal}(\lambda) - \text{thetar}(\lambda)$$

whose zero determines the required eigenvalue.

In the second place, the function that can be defined, whose zeros determine the required eigenvalues, may have not one but infinitely many zeros; in fact all eigenvalues are determined by zeros of a single function. Moreover, it frequently occurs that these zeros may be either

simple or double. This leads to a complicated procedure to determine the index of the eigenvalues.

As an example of these differences between separated and coupled boundary condition problems consider regular coupled boundary conditions of the form, for the compact interval $[a, b]$,

$$y(b) = k_{11}y(a) + k_{12}(py')(a) \tag{19.1}$$

$$(py')(b) = k_{21}y(a) + k_{22}(py')(a), \tag{19.2}$$

where the parameters $k_{rs} \in \mathbb{R}$ for $r, s = 1, 2$ and the self-adjoint condition to be satisfied is

$$k_{11}k_{22} - k_{12}k_{21} = 1.$$

(These boundary conditions are a special case of the conditions (5.19) and (5.20) when the endpoints are both R and the parameter $\alpha = 0$.)

To define the function $D(\lambda)$, it is necessary to define a system of solutions of the differential equation (2.1); namely, as in Section 6 above but with the restriction to regular endpoints, define

$$y_1(a, \lambda; x) \quad \text{and} \quad y_2(a, \lambda; x) \quad \text{for all } x \in [a, b] \tag{19.3}$$

as solutions of (2.1) satisfying the initial conditions at a

$$\begin{cases} y_1(a, \lambda; a) = 0 & (py_1')(a, \lambda; a) = 1 \\ y_2(a, \lambda; a) = 1 & (py_2')(a, \lambda; a) = 0 \end{cases}. \tag{19.4}$$

Also define the solutions

$$Y_1(b, \lambda; x) \quad \text{and} \quad Y_2(b, \lambda; x) \quad \text{for all } x \in [a, b] \tag{19.5}$$

by the initial conditions

$$\begin{cases} Y_1(b, \lambda; b) = 0 & (pY_1')(b, \lambda; b) = 1 \\ Y_2(b, \lambda; b) = 1 & (pY_2')(b, \lambda; b) = 0 \end{cases}. \tag{19.6}$$

Then, as in (6.5), define the function $D(\lambda)$ by, for all $x \in [a, b]$,

$$D(\lambda) \equiv D(\lambda; x) := -k_{11}[y_1, Y_2](x) + k_{12}[y_2, Y_2](x) - k_{21}[y_1, Y_1](x) + k_{22}[y_2, Y_1](x), \tag{19.7}$$

noting that the right hand side is independent of the variable $x \in [a, b]$, for each of the sesquilinear forms is independent of x since the entries are all solutions of the differential equation (1.1) for the same value of λ.

The eigenvalues of the coupled boundary value problem are determined by the zeros, all real, of the function $D(\lambda) - 2$. This function has infinitely many zeros and this leads to serious complications for the numerical process. In particular, it is necessary to "bracket" a required zero in order to separate it from the neighboring zeros above and below on the real line. However, recent results of Eastham, Kong, Wu and Zettl [16] have shown that the required brackets can be determined analytically by the eigenvalues of two specially chosen Sturm-Liouville problems, for the same differential equation, with separated boundary conditions; these separated conditions are determined by the four real numbers $\{k_{rs} : r, s = 1, 2\}$ in the coupled boundary conditions (19.1) and (19.2), *i.e.* by the matrix $\mathbf{K}$ in the general coupled

form (5.19). These two special boundary conditions are determined by, recall the standard form for separated regular boundary conditions given by (5.9) and (5.10),

$$\begin{array}{llllll} (i) & A_1 = 0 & A_2 = 1 & B_1 = k_{21} & B_2 = -k_{11} \\ (ii) & A_1 = 1 & A_2 = 0 & B_1 = k_{22} & B_2 = -k_{12}. \end{array}$$

It is shown in [16], in the regular case, that two consecutive eigenvalues, necessarily simple, of the separated boundary value problem determined by the choice (i), together with the successive eigenvalues of the same indexes from the choice (ii), provide a bracket for exactly one eigenvalue of the coupled boundary value problem determined by a zero of the function $D(\lambda)-2$. (In some cases the lowest eigenvalue is bracketed by $-\infty$ and one of the eigenvalues from the problems (i) and (ii).)

The fact that the zeros of the function $D(\lambda) - 2$ may be either simple or double provides a serious complication for constructing the code. Even when the designated zero is isolated from the other zeros of $D(\lambda) - 2$ it has to be accepted that this real valued function, when considered for real values of λ, may not change sign at the zero.

20. Estimating errors

The numerical integrator used in SLEIGN2 is the same integrator provided for the original SLEIGN code, namely GERK; there are two reasons for making this decision. First, it has a built in "global error" estimator which means, in standard terminology for numerical analysis, that besides the solution vector $Y(i), i = 1, 2, 3$ it also provides error estimates $ERR(i), i = 1, 2, 3$, *i.e.* ERR estimates the error $(Y - TRUE\ SOLUTION)$. When trying to locate a zero of dtheta(λ), for example, it is helpful to know when the estimated errors in the values of $\theta(x_{\text{mid}})$ are as large as the values of the difference, dtheta(λ).

Second, while it is true that sometimes the system of differential equations is fairly "stiff", and GERK can be very inefficient on stiff equations, when compared with stiff ODE solvers GERK works very efficiently on most Sturm-Liouville problems. In addition, with a stiff ODE solver additional time is required to obtain useful error estimates.

In the regular case, when Newton iteration is being used, the size of the next step in the iteration is compared with the error tolerance requested by the user, in order to determine when the number of iterations is large enough. However, the error estimates for both of the functions dtheta(x) and dthde(x) are first checked to determine that they appear to have at least one significant digit.

For regular problems, passing the convergence test is the end of the numerical procedure. However, in some singular problems it is found to be necessary to approximate to the original problem by considering an inherited problem on a truncated compact subinterval $[\alpha, \beta]$ of (a, b). Again, in such a case it is necessary to estimate the error in the computed eigenvalue λ, where the error is associated with the truncation process. To estimate this particular error, use can be made of the function $d\theta(x)/d\alpha$, where $\theta(x)$ is considered to be a function of the truncation endpoint α. This function satisfies the differential equation (the variational equation)

$$\left(\frac{d\theta}{d\alpha}\right)' = -2f\frac{d\theta}{d\alpha},$$

and hence is just a scalar multiple of the function $\exp(-2F(x))$, where $F(x)$ is the function defined in Section 13 above, as $\ln(\rho(x))$ and which is available for the numerical procedure. (This is one of the reasons for computing F along with θ and dthde, even when only the eigenvalue is required.)

There is also the problem of keeping track of any integration errors when switching from the variable $\varphi(x)$, used in the "regularization" near a LC endpoint, to the customary Prüfer angle $\theta(x)$, before continuing the integration to the midpoint x_{mid}. For this purpose we use the relationship (16.6), above, between θ and φ. Differentiating both sides of this relationship gives

$$d\theta = FAC d\varphi$$

where

$$FAC = -\frac{[u,v]\cos^2(\theta)}{((pu')\cos(\varphi) + (pv')\sin(\varphi))^2}.$$

Thus if the errors in the system for $\varphi, \text{dphide}, \ln(\sigma)$ are estimated by GERK to be $ERZ(i), i = 1, 2, 3$ then the corresponding errors for $\theta, \text{dthde}, \ln(\sigma)$ would be estimated by

$$ERR(i) = FAC.ERZ(i), i = 1, 2, 3.$$

21. Modified Prüfer transformation

There are many Sturm-Liouville problems for which it is helpful to use a "modified" Prüfer angle, instead of the original angle defined in Section 12 above; see [3].

This modification is of particular importance when, for some part of the interval (a, b), one of the two functions $1/p(x)$ and $\lambda w(x) - q(x)$ is much greater in modulus than the other, then the integrator of the differential equation for the angle θ finds that the derivative θ', is oscillating between small and large values.

The modification amounts to inserting a number z into the definition of the angle θ. Namely, write, for all $x \in (a, b)$

$$y(x) = \rho_z(x)\sin(\theta_z(x))$$
$$(py')(x) = z\rho_z(x)\cos(\theta_z(x))$$

and choose a value for z which tends to minimize the fluctuations in the modulus of

$$\theta_z'(x) = \frac{z}{p(x)}\cos^2(\theta_z(x)) + \frac{(\lambda w(x) - q(x))\sin^2(\theta_z(x))}{z}.$$

Choosing a suitable value for this number z is done at the start of the numerical process, during the stage when an initial estimate of the eigenvalue is made; see Section 11 above. In practice, the code chooses a number of different values for z for different subintervals of the interval (a, b).

The simple relationship between θ and θ_z, *i.e.*

$$z\tan(\theta) = \tan(\theta_z)$$

makes it straightforward to change from the one angle to the other, but keeping track of the integration errors is more involved.

Suppose, for example, that at some point x_1 in the integrations, the estimated errors in the functions $\theta, \text{dthde}, \ln(\rho)$ are $ERR(i), i = 1, 2, 3$. Then from x_1 to x_2 the integration is

continued using $\theta_z, \mathrm{dthzde}, \ln(\rho_z)$ with associated estimated errors $ERRZ(i)$ over the range x_1 to x_2 at which point θ_z, *etc.* are switched back to θ, *etc.*

In addition to converting the values for $\theta_z(x_2)$, *etc.* to corresponding values for $\theta(x_2)$, *etc.*, and converting the integration errors in θ_z, *etc.* to errors in θ, we must also estimate the errors at x_2 due to the fact that there were errors in $\theta(x_1)$, *etc.* These errors, which must be added to the integration errors over the interval (x_1, x_2), are estimated as

$$(ERR(i) \text{ at } x_1)\exp(-2((F \text{ at } x_2) - (F \text{ at } x_1))), i = 1, 2, 3.$$

22. Errors for problems with coupled boundary conditions

Due to the complexity of the process used for finding eigenvalues of coupled boundary condition problems, trying to estimate the error in the eigenvalue by keeping track of all the errors that could have occurred in the whole process seems dubious. Note also that while searching for a zero of the function $D(\lambda) - 2$ we do not have a simple method to obtain information about the derivative of this function with respect to λ. Even if this information is available there is always the possibility that the eigenvalue is double which situation presents additional complications in assessing the accumulated errors.

For these coupled problems the code examines the computed values of the function $D(\lambda) - 2$ in the neighborhood of the computed eigenvalue, at 5 equally spaced points of λ; for example, values spaced a distance $h = 0.0001$ apart. If the table of values and their first and second differences are consistent with the computed eigenvalue being either a simple zero or a maximum (a double zero), and if the second differences are nearly constant, then it is concluded that the five values are not overly contaminated with errors. Otherwise the different values at the spacing of $h = 0.0001$ are considered slightly untrustworthy, and a coarser spacing, say $h = 0.001$, would be checked.

Incidentally, this process gives a reasonably reliable method of deciding whether or not a particular computed eigenvalue is a double. It is known [7] that an eigenvalue is double if and only if

$$[y_2, Y_1] = k_{11},\ [y_2, Y_2] = -k_{21},\ [y_1, Y_1] = k_{12},\ [y_1, Y_2] = -k_{22}.$$

However, in numerical terms these conditions can be expected to hold only approximately, and it is difficult to decide where to draw the line.

23. The eigenfunction

We give here some information on the numerical computation for the eigenfunctions following the computation of the eigenvalue.

23.1. **The case of separated boundary conditions.** Once an eigenvalue has been computed, the numerical data for the corresponding eigenfunction can be obtained by integrating again the differential equations for θ and $F = \ln(\rho)$. Up to this position the function F is obtained with initial value, at both a and b, of zero; thus $\rho(a) = \rho(b) = \exp(F(a)) = \exp(F(b)) = 0$.

In order for the eigenfunction to be given by

$$y(x) = \rho(x)\sin(\theta(x)) \text{ for all } x \in (a, b) \tag{23.1}$$

and the quasi-derivative by

$$(py')(x) = \rho(x)\cos(\theta(x)) \text{ for all } x \in (a,b), \tag{23.2}$$

it is necessary to alter the values of ρ at the endpoints a and b so that both y and py' are continuous at the point x_{mid}. Also, since the eigenfunction is unique only up to multiplication by a scalar, it can be determined by requiring that the norm in $L^2((a,b);w)$ satisfy

$$\int_a^b y(x)^2 w(x)\,dx = 1; \tag{23.3}$$

this requirement determines ρ in (23.1) and (23.2).

Now let the function S be determined by $S' = y^2 w$, or equivalently, $S' = \exp(2F)\sin^2(\theta)w$, and the make the substitution $S = U\exp(2F)$; it then follows that U satisfies the differential equation (13.3) above for the function dthde. It follows that the only difference between the functions U and dthde lies in the initial conditions to determine the solution of the same differential equation. Thus we can write

$$U_l = (\text{dthde}(x_{\text{mid}}) - \text{dthde}(a))\exp(-2F_l)$$
$$U_r = (\text{dthde}(x_{\text{mid}}) - \text{dthde}(a))\exp(-2F_r)$$

where U_l, F_l are the values of U, F at x_{mid} obtained by integrating from a, and U_r, F_r are the values obtained by integrating from b

It is straightforward to check that the requirements of continuity and the L^2-normalization (23.3) are satisfied if

$$F(a) = -F_l - \frac{\ln(U_l - U_r)}{2}$$
$$F(b) = -F_r - \frac{\ln(U_l - U_r)}{2}$$

instead of $F(a) = 0 = F(b)$.

There are two methods for computing eigenfunctions. If it is required to have values of the eigenfunction computed at a selected set of points $\{x_i : i = 1, 2, \ldots, M\}$, then these points can be placed in an array and the code returns with the points replaced by the corresponding values $\{y(x_i) : i = 1, 2, \ldots, M\}$ of the eigenfunction. All that is required is to effect one more integration from each endpoint a and b, recording the values obtained at each of the points $\{x_i : i = 1, 2, \ldots, M\}$ as they are encountered on the way to x_{mid}.

The other method, probably more suitable if the eigenfunction is required for use in further calculations (such as in inner products, for example), is to provide the now known initial conditions $\theta(a), F(a), \theta(b), F(b)$ and x_{mid}, so that the eigenfunctions can be generated by simply integrating the differential equations for θ and F.

23.2. **The case of coupled boundary conditions.** In this case the eigenfunction cannot be obtained by simply integrating the differential equations for θ and F as in the case of separated boundary conditions above, because the appropriate initial conditions for θ and F at the two endpoints a and b are not known.

On the other hand we have available means of computing the functions y_1, y_2 and Y_1, Y_2 defined in terms of (19.3) to (19.6) above; in terms of these functions, with λ now set equal to the known eigenvalue, the eigenfunction y can be written as

$$y = c_1 y_1 + c_2 y_2 = C_1 Y_1 + c_2 Y_2$$

for suitable numbers c_1, c_2, C_1, C_2. Assuming the boundary condition parameter $\alpha = 0$ for simplicity here, the boundary conditions (5.19) require

$$C_1 = k_{21} c_2 + k_{22} c_1 \tag{23.4}$$

$$C_2 = k_{11} c_2 + k_{12} c_1 \tag{23.5}$$

whilst continuity at x_{mid} requires

$$c_1 y_1 + c_2 y_2 = C_1 Y_1 + C_2 Y_2$$
$$c_1 y_1' + c_2 y_2' = C_1 Y_1' + C_2 Y_2'.$$

(If $\alpha \neq 0$ then the eigenfunction is complex valued and the code does not attempt to compute the eigenfunction values.) Substituting for C_1 and C_2 in the previous two equations gives

$$c_1(y_1 - k_{22} Y_1 - k_{12} Y_2) + c_2(y_2 - k_{21} Y_1 - k_{11} Y_2) = 0$$
$$c_1(y_1' - k_{22} Y_1' - k_{12} Y_2') + c_2(y_2' - k_{21} Y_1' - k_{11} Y_2') = 0,$$

where each of the functions is evaluated at the same point x_{mid}, say. Note that the determinant formed from the coefficients c_1, c_2 must vanish and this yields the result $D(\lambda) - 2 = 0$; but these equations also provide the ratio $c_1{:}c_2$ (twice).

In principle, it is now possible to compute the values of the eigenfunction y at any set of points $\{x_i : i = 1, 2, \ldots, M\}$, by evaluating the basis functions y_1, y_2 or Y_1, Y_2 at these points and setting, for $i = 1, 2, \ldots, M$,

$$y(x_i) = c_1 y_1(x_i) + c_2 y_2(x_i) \tag{23.6}$$

or

$$y(x_i) = c_1 Y_1(x_i) + c_2 Y_2(x_i) \tag{23.7}$$

The trouble with this method is that often the above equations determining the ratio $c_1{:}\,c_2$, gives very poor accuracy. For this reason the code tries to determine numerically the best ratio $c_1{:}\,c_2$ for continuity whilst maintaining the relations (23.4), (23.5) between c_1, c_2 and C_1, C_2.

In other words, the basis functions y_1, y_2 and Y_1, Y_2 are evaluated at all the selected points $\{x_i : i = 1, 2, \ldots, M\}$, then the best ratio $c_1{:}\,c_2$ is determined, and then y_1, y_2 obtained from (23.6) and /or (23.7).

24. SLEIGN, SLEDGE AND SLEIGN2

Of the three general purpose codes for computing the eigenvalues and eigenfunctions of Sturm-Liouville boundary value problems, SLEIGN is the oldest, see [1], [2], [3] and [4]. This code can treat regular problems where the coefficients are continuous, with p and w positive, on the compact interval $[a, b]$; all other problems are considered to be singular. Both LP and LC endpoints can be considered but there is no possibility of imposing arbitrary boundary

conditions at singular endpoints. In the case of the LCNO endpoint the code selects a boundary condition, which is generally the Friedrich's condition.

Unlike SLEIGN, which is based on the use of the Prüfer transformation, SLEDGE, see [21], is based on the idea of approximating the coefficients of the Sturm-Liouville differential equation by step functions, and then solving the resulting differential equation analytically in terms of trigonometric and exponential functions. In addition to R endpoints, including WR endpoints, this code can treat LP and LCNO endpoints; however, as in SLEIGN, there is no method to impose arbitrary boundary conditions at LCNO endpoints. Additionally, SLEDGE can treat boundary value problems when the eigenvalue parameter appears in the boundary conditions at one R endpoint. For some problems with a continuous spectrum, SLEDGE can approximate numerically to the spectral density function.

SLEIGN2 represents a very considerable extension of the capabilities of both the original SLEIGN and the SLEDGE codes. It is now possible to treat all problems with any combination of R or LCNO or LCO endpoints with either separated or coupled arbitrary boundary conditions; this set of endpoint cases allows for all the classical periodic and semi-periodic boundary conditions. All cases when the endpoints are R or LCNO or LCO or LP, in some combination, can be treated provided that in any LP case the spectrum is bounded below.

25. Comparative examples

In this section we give six examples of Sturm-Liouville boundary value problems for which we compare the numerical results on entering these problems separately into the three codes SLEIGN, SLEDGE and SLEIGN2, and three examples that can only be processed by the code SLEIGN2. All examples are taken from those entered in the file xamples.f; additional information on each example is to be found in the file xamples.tex.

For each example the name and number from xamples.f are given; information is given on the boundary conditions used; the numerical results for each code used are displayed along with the index of the computed eigenvalue.

All numerical results given below are computed in double precision.

(1) **The hydrogen atom equation** (Example number 13)

$$-y''(x) + (-x^{-1} + 2x^{-2})y(x) = \lambda y(x) \text{ for all } x \in (0, +\infty)$$

This differential equation is LP at 0 and $+\infty$ so that no boundary conditions are required; the spectrum is discrete below zero and continuous above zero.

Index	SLEIGN	SLEDGE	SLEIGN2
0	−0.062500	−0.062500	−0.062500
1	−0.027778	−0.027778	−0.027778
2	−0.015625	−0.015625	−0.015625

(2) **A weakly regular differential equation** (Example number 10)

$$-\left(x^{1/2}y'(x)\right)' = \lambda x^{-1/2}y(x) \text{ for all } x \in (0, 1]$$

This differential equation is WR at 0 and R at 1; separated boundary conditions are given; the spectrum is discrete.

$$A_1 = 1 \quad A_2 = 0 \quad B_1 = 1 \quad B_2 = 0$$

Index	SLEDGE	SLEIGN2
0	2.467401	2.467424
1	9.869605	9.869696
2	22.206610	22.206815

$A_1 = 0 \quad A_2 = 1 \quad B_1 = 1 \quad B_2 = 0$

Index	SLEDGE	SLEIGN2
0	0.616850	0.616856
1	5.551653	5.551704
2	15.421257	15.421399

Note that for this particular WR equation, with $p(0) = 0$ and $w(0) = +\infty$, the code SLEIGN cannot find the eigenvalues for these two boundary value problems; this is the explanation for the absence of the SLEIGN column for these problems.

(3) **The Legendre equation** (Example number 1)

$$-\left(\left(1-x^2\right)y'(x)\right)' + \tfrac{1}{4}y(x) = \lambda y(x) \text{ for all } x \in (-1,+1)$$

This differential equation is LCNO at -1 and $+1$; separated boundary conditions are given (for details of the boundary condition functions see xamples.tex); the spectrum is discrete and simple.

$A_1 = 1 \quad A_2 = 0 \quad B_1 = 1 \quad B_2 = 0$

Index	SLEIGN	SLEDGE	SLEIGN2
0	0.250000	0.250000	0.250000
1	2.250000	2.250000	2.250000
2	6.250000	6.250000	6.250000

$A_1 = 0 \quad A_2 = 1 \quad B_1 = 1 \quad B_2 = 0$

Index	SLEIGN	SLEDGE	SLEIGN2
0	0.250000	0.250000	-0.406453
1	2.250000	2.250000	1.298673
2	6.250000	6.250000	4.974116

Note that for this LCNO equation the code SLEIGN and SLEDGE can only enter the Friedrich's boundary condition at both ± 1, *i.e.* $A_1 = 1, A_2 = 0, B_1 = 1, B_2 = 0$; this is the explanation for the repeated SLEIGN and SLEDGE columns for the second problem.

(4) **The Morse equation** (Example number 31)

$$-y''(x) + (9\exp(-2x) - 18\exp(-x))y(x) = \lambda y(x) \text{ for all } x \in (-\infty,+\infty)$$

This differential equation is LP at $-\infty$ and $+\infty$ so that no boundary conditions are required; the spectrum has exactly three negative, simple eigenvalues, and a continuous spectrum on $[0,\infty)$; the eigenvalues are given explicitly by

$$\lambda_n = -(n-2.5)^2 \text{ for } n = 0,1,2.$$

Index	SLEIGN	SLEDGE	SLEIGN2
0	−6.249998	−6.250003	−6.250000
1	−2.249998	−9.000005	−2.250000
2	−0.250008	−0.250000	−0.250000

(5) **The Lohner equation** (Example number 26)

$$-y''(x) - 1000xy(x) = \lambda y(x) \text{ for all } x \in (0,1)$$

This differential equation is R at both 0 and 1; Lohner computed the Dirichlet eigenvalues using interval arithmetic and obtained rigorous bounds; in double precision SLEIGN2 computed eigenvalues in good agreement with these guaranteed bounds.

$$A_1 = 1 \quad A_2 = 0 \quad B_1 = 1 \quad B_2 = 0$$

Index	SLEIGN	SLEDGE	SLEIGN2	LOHNER
0	−766.1893	−766.1893	−766.1893	$-766.1892589\frac{39}{41}$
9	508.108022	508.10800748	508.10800738	$508.108007\frac{5}{3}$
49	24174.8549	24174.8549	24174.8549	$24174.85\frac{6}{4}$

(6) **The Marletta equation** (Example number 14)

$$-y''(x) + \frac{3(x-31)}{4(x+1)(x+4)^2}y(x) = \lambda y(x) \text{ for all } x \in [0,+\infty)$$

This differential equation is R at 0 and LP at $+\infty$; a separated boundary condition is required at 0; the spectrum is discrete below zero, with at most one negative eigenvalue, and continuous above zero; for the boundary condition $A_1 = 5, A_2 = 8$ there is the negative eigenvalue λ_0 near -1.185; the equation with $\lambda = 0$ has a solution, not in $L^2(0,+\infty)$,

$$y(x) = \frac{1-x^2}{(1+x/4)^{5/2}} \text{ for all } x \in [0,\infty);$$

which also satisfies the boundary condition $A_1 = 5, A_2 = 8$; this solution deceives SLEIGN and SLEIGN2 in single precision, and SLEDGE in double precision into reporting $\lambda = 0$ as a second eigenvalue; in double precision SLEIGN and SLEIGN2 correctly report that λ_0 is the only eigenvalue, and SLEIGN2 reports the start of the continuous spectrum at 0.

$$A_1 = 5 \quad A_2 = 8$$

Index	SLEIGN	SLEDGE	SLEIGN2
0	−1.185214	−1.185214	−1.185214

(7) **The BEZ equation** (Example number 7)

$$-(xy'(x))' - x^{-1}y(x) = \lambda y(x) \text{ for all } x \in (0,1]$$

This differential equation is LCO at 0 and LP at $+\infty$ (for details of the boundary condition functions for the LCO endpoint see xamples.tex).

$$A_1 = 1 \quad A_2 = 0 \quad B_1 = 1 \quad B_2 = 0$$

Index	SLEIGN2
-1	-5.426966
0	4.397838
1	18.120688

$$\alpha = 0 \quad k_{11} = 1 \; k_{12} = 0 \; k_{21} = 0 \; k_{22} = 1$$

Index	SLEIGN2
-1	-1.752741
0	14.574609
1	21.874933
2	55.573586

Note that the coupled boundary conditions for this last case are equivalent to generalized periodic boundary conditions; see (5.21) and the associated comments.

(8) **The Fourier equation** (Example number 21)

$$-y''(x) = \lambda y(x) \text{ for all } x \in (-\pi, +\pi)$$

This differential equation is R at both the endpoints $\pm\pi$.

$$\alpha = 0 \quad k_{11} = 1 \; k_{12} = 0 \; k_{21} = 0 \; k_{22} = 1$$

Index	SLEIGN2
0	0.000000
1	1.000000
2	1.000020
3	4.000000
4	4.000000

Note that this last case is the classical periodic boundary value problem with $y(-\pi) = y(\pi)$ and $y'(-\pi) = y'(\pi)$; for this problem all eigenvalues, except $\lambda_0 = 0$, are double and the code so reports on this property.

$$\alpha = \pi/4 \quad k_{11} = 2 \; k_{12} = 1 \; k_{21} = 1 \; k_{22} = 1$$

Index	SLEIGN2
0	-6.854103
1	-0.096053
2	0.392084
3	1.846735
4	3.014691

This is a case of complex coupled boundary conditions.

(9) **The Legendre equation** (Example number 1)

$$-\left(\left(1 - x^2\right) y'(x)\right)' + \tfrac{1}{4} y(x) = \lambda y(x) \text{ for all } x \in (-1, +1)$$

This differential equation is LCNO at -1 and $+1$; coupled boundary conditions are given (for details of the boundary condition functions see xamples.tex); the spectrum is discrete but may have multiplicity 2.

$$\alpha = 0 \quad k_{11} = 1 \; k_{12} = 0 \; k_{21} = 0 \; k_{22} = 1$$

Index	SLEIGN2
0	−0.627768
1	2.250000
2	3.710687

$$\alpha = 0 \quad k_{11} = -1 \; k_{12} = 0 \; k_{21} = 0 \; k_{22} = -1$$

Index	SLEIGN2
0	0.250000
1	0.250000
2	6.250000

Note that the coupled boundary conditions for the first case are equivalent to generalized periodic boundary conditions; for the second case they are equivalent to generalized semi-periodic boundary conditions; see (5.21) and the associated comments.

26. The SLEIGN2 package

This package contains the eleven files as follows:

(*i*) Two ASCII files: autoinput.txt readme.txt
(*ii*) Six Fortran files: coupdr.f drive.f makepqw.f sepdr.f sleign2.f xamples.f
(*iii*) Three AMS-LaTeX files: help.tex intro.tex xamples.tex

The .tex files can be compiled in UNIX or other LaTeX compilers and then printed out in hard copy.

The file sleign2.f consists of a number of subroutines, most notably SUBROUTINE SLEIGN (not to be confused with the older SLEIGN code), which is called for eigenvalue/eigenfunction problems with separated boundary conditions, and SUBROUTINE SLCOUP for problems with coupled boundary conditions.

The file makepqw.f requires the user to enter, using Fortran function subroutines, the data for:

(*i*) The coefficient functions p, q, w of the chosen Sturm-Liouville differential equation.
(*ii*) If required, the boundary conditions functions u, v and U, V (this step requires a knowledge of the endpoint classification).

The most convenient way to use the code SLEIGN2 is by means of the program drive.f, which acts as a driver for the code. This driver is best used in an "interactive" mode, but may also be used in shorter "automatic" mode.

In the interactive mode drive.f prompts the user to enter, via the keyboard, the required data such as:

(*i*) The interval (a, b) of the real line.
(*ii*) The classification of each endpoint as R, WR, LCNO, LCO, LP

(*iii*) The separated or coupled boundary conditions, as required.
(*iv*) The index or the indices of the required eigenvalues.
(*v*) The index of any eigenfunction for which numerical data is required.

To use the automatic mode - which is faster since it avoids the necessary "question and answer" format of the interactive mode - the relevant data is placed in a short text file which drive.f then uses to run the program. However, this mode is only recommended for the experienced user of the code; the interactive mode is more helpful to gain initial experience. For complete details see the file autoinput.txt.

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