

Computing Eigenvalues of Regular Sturm-Liouville Problems *

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Abstract

An algorithm is presented for computing eigenvalues of regular self-adjoint Sturm-Liouville problems with matrix coefficients and arbitrary coupled boundary conditions.

Introduction

SLEDGE [8], SLEIGN [3],[2] (see also [6]) and the NAG library code [9] are all highly effective, state of the art *general purpose* codes for computing eigenvalues of regular scalar Sturm-Liouville (SL) problems with *separated* boundary conditions. Although there are special purpose codes (e.g. [7]) for computing eigenvalues of regular scalar SL problems with periodic boundary conditions there seems to be no general purpose algorithm available for general coupled self-adjoint boundary conditions, even in the scalar case.

The purpose of this paper is to present such an algorithm not only for the scalar case but also for SL problems with matrix coefficients and general self-adjoint coupled boundary conditions. Our method is based on a construction which, given an SL problem with a coupled boundary condition, constructs a higher dimensional problem with separated conditions which has exactly the same eigenvalues as the given coupled problem. The general purpose code for SL problems of arbitrary dimension with separated boundary conditions developed by Dwyer in [4] can then be used to compute these eigenvalues. The eigenfunctions of the original problem can also be recovered from the eigenfunctions of the constructed higher dimensional problem.

It is worth noting that the eigenvalues and eigenfunctions of the new problem with separated conditions are *not* simply approximations for those of the original problem; the correspondence is exact. This may have theoretical implications as well as numerical ones.

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Problems and Theorems

A Sturm-Liouville (SL) problem consists of the second order linear ordinary differential equation

$$-(py')' + qy = \lambda wy \text{ on } (a, b) \quad (1)$$

together with boundary conditions. For the case when both endpoints a, b are regular, these have the form

$$C \begin{pmatrix} y(a) \\ (py')(a) \end{pmatrix} + D \begin{pmatrix} y(b) \\ (py')(b) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}. \quad (2)$$

Theorem 1 *Let p, q, w be complex $m \times m$ matrix functions defined on the interval $[a, b]$, $-\infty < a < b < \infty$, satisfying the following conditions:*

1. *The matrix $p(t)$ is invertible for almost all $t \in (a, b)$.*
2. *Each component of p^{-1}, q, w is in $L^1(a, b)$.*
3. *The matrices $p(t), q(t), w(t)$ are hermitian for almost all $t \in (a, b)$.*
4. *The matrices $p(t)$ and $w(t)$ are positive definite for almost all $t \in (a, b)$.*

Assume that the complex constant $2m \times 2m$ matrices C and D satisfy:

5. *The $2m \times 4m$ matrix $(C|D)$ has full rank.*
6. *$CJC^* = DJD^*$, where $J = \left(\begin{array}{c|c} 0 & I_m \\ -I_m & 0 \end{array} \right)$ and I_m denotes the $m \times m$ identity matrix.*

Then the boundary value problem, (1),(2) is self-adjoint; its eigenvalues are all real, there are countably many of them $\{\lambda_n : n \in N_0 = \{0, 1, 2, \dots\}\}$, and they can be ordered to satisfy

$$-\infty < \lambda_0 \leq \lambda_1 \leq \lambda_2 \leq \dots, \text{ with } \lambda_n \rightarrow \infty \text{ as } n \rightarrow \infty.$$

Proof: See Möller and Zettl [5]. \square

It is convenient to partition the two matrices C and D into four $2m \times m$ matrices

$$C = (C_2 \mid -C_1), \quad D = (-D_2 \mid D_1). \quad (3)$$

Using these, the boundary condition (2) may be rewritten in a form which closely resembles the Lagrange sesquilinear form

$$(D_1(py')(b) - D_2y(b)) - (C_1(py')(a) - C_2y(a)) = 0. \quad (4)$$

Below we consider the question: How can the eigenvalues λ_n be computed numerically? The codes SLEDGE, and SLEIGN, as well as the codes in the

NAG library, address this question only for the special case when $m = 1$ and the boundary conditions 2 are separated, i.e., can be reduced to the form

$$A_1y(a) + A_2(py')(a) = 0, \quad B_1y(b) + B_2(py')(b) = 0. \quad (5)$$

The algorithms used by SLEIGN and the NAG routine are based on the Prüfer transformation, while SLEDGE is based on a piece-wise constant approximation of the coefficient functions. (We understand that the NAG library routine has been updated to incorporate some features of SLEDGE.) The methods underlying these codes do not seem to be susceptible to an extension to the cases when $m > 1$ and probably also not to the case $m = 1$ when the boundary conditions are coupled.

Our method consists in constructing a new problem of dimension $2m$ (i.e., $m \rightarrow 2m$) which has exactly the same eigenvalues and *separated* boundary conditions. On this new problem, the method due to Atkinson, Krall, Leaf, and Zettl [1] as extended and refined by Dwyer [4] can then be applied.

Construction of an Equivalent Separated Problem

We begin with an m -dimensional self-adjoint problem, (1), (2) satisfying the conditions of Theorem 1.

Definition

1. Let $P(x) = \left(\begin{array}{c|c} p(x) & 0 \\ \hline 0 & p((a+b)-x) \end{array} \right)$ for all $x \in [a, b]$
2. Let $Q(x) = \left(\begin{array}{c|c} q(x) & 0 \\ \hline 0 & q((a+b)-x) \end{array} \right)$ for all $x \in [a, b]$
3. Let $W(x) = \left(\begin{array}{c|c} w(x) & 0 \\ \hline 0 & w((a+b)-x) \end{array} \right)$ for all $x \in [a, b]$
4. Let $A_1 = \left(\begin{array}{c|c} I & -I \\ \hline 0 & 0 \end{array} \right)$, $A_2 = \left(\begin{array}{c|c} 0 & 0 \\ \hline I & I \end{array} \right)$
5. Let $B_1 = (-D_2 \mid C_2)$, $B_2 = (D_1 \mid C_1)$.

Consider the problem on the interval $[c, b]$, where $c = (a+b)/2$, given by

$$-(PY')'(x) + Q(x)Y(x) = \lambda W(x)Y(x) \quad (6)$$

subject to:

$$A_1Y(c) + A_2(PY')(c) = 0 \quad (7)$$

$$B_1Y(b) + B_2(PY')(b) = 0. \quad (8)$$

Theorem 2 *Let m be a positive integer, and let Problem 1 be a boundary value problem of dimension m defined by equations (1), (2) which satisfies the conditions of Theorem 1. Let Problem 2 be the boundary value problem defined by (6),(7),and (8). Then Problem 2 is a regular self-adjoint Sturm-Liouville problem of dimension $2m$ on the compact interval $[c, b]$, with separated boundary conditions, and the following statements are true:*

1. *A real value λ is an eigenvalue of Problem 1 if, and only if, λ is an eigenvalue of Problem 2.*
2. *The multiplicity of λ as an eigenvalue of Problem 1 is equal to the multiplicity of λ as an eigenvalue of Problem 2.*
3. *Let λ be an eigenvalue of Problem 1, and hence also of Problem 2. A function y is an eigenfunction of Problem 1 if, and only if, the function Y defined by*

$$Y(x) = \begin{pmatrix} y(x) \\ y((a+b)-x) \end{pmatrix} \quad (9)$$

is an eigenfunction of Problem 2.

4. *Let λ be an eigenvalue of multiplicity k for Problem 1, and hence also for Problem 2, and let y_1, \dots, y_k be linearly independent eigenfunctions of λ for Problem 1.*

Let Y_1, \dots, Y_k be defined according to equation (9) using y_1, \dots, y_k respectively. Then $\{y_1, \dots, y_k\}$ is an orthonormal set in the Hilbert space $L_w^2(a, b)$ if, and only if, the set $\{Y_1, \dots, Y_k\}$ is an orthonormal set in the Hilbert space $L_W^2(c, b)$.

Proof: To verify that Problem 2 is a regular, self-adjoint problem, simply verify that all of the constraints are met. We then have:

1. Suppose that λ is an eigenvalue of Problem 1. Then there is a nontrivial solution $y(x)$ defined on the interval $[a, b]$ such that

$$(a) \quad -(py)'(x) + q(x)y(x) = \lambda w(x)y(x) \text{ for all } x \in [a, b]$$

$$(b) \quad C_2y(a) - C_1(py')(a) - D_2y(b) + D_1(py')(b) = 0.$$

Since the interval is $[a, b]$, the differential equation also holds at $(a+b)-x$; for all $x \in [a, b]$:

$$-(py)'((a+b)-x) + q((a+b)-x)y((a+b)-x) = \lambda w((a+b)-x)y((a+b)-x).$$

For $x \in [c, b]$, define

$$Y(x) = \begin{pmatrix} y(x) \\ y((a+b)-x) \end{pmatrix}.$$

Clearly Y is nontrivial, and Y and PY' are absolutely continuous, since y is a nontrivial solution.

The differential equation of Problem 2 is satisfied by the function Y . At the left endpoint we have

$$\begin{aligned} & A_1Y(c) + A_2(PY')(c) \\ &= \begin{pmatrix} I & -I \\ 0 & 0 \end{pmatrix} \begin{pmatrix} y(c) \\ y(c) \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ I & I \end{pmatrix} \begin{pmatrix} (py')(c) \\ -(py')(c) \end{pmatrix} \\ &= \begin{pmatrix} y(c) - y(c) \\ (py')(c) - (py')(c) \end{pmatrix} = 0. \end{aligned}$$

At the right endpoint we have

$$\begin{aligned} & B_1Y(b) + B_2(PY')(b) \\ &= \begin{pmatrix} -D_2 & C_2 \end{pmatrix} \begin{pmatrix} y(b) \\ y(a) \end{pmatrix} + \begin{pmatrix} D_1 & C_1 \end{pmatrix} \begin{pmatrix} (py')(b) \\ -(py')(a) \end{pmatrix} \\ &= -D_2y(b) + C_2y(a) + D_1(py')(b) - C_1(py')(a) = 0. \end{aligned}$$

Thus the boundary conditions are satisfied, so Y is an eigenfunction for Problem 2 corresponding to the eigenvalue λ . The proof of the converse is similar.

2. The first part of the proof establishes a correspondence between eigenfunctions of Problem 1 and eigenfunctions of Problem 2. Clearly, a set of eigenfunctions $\{y_1, \dots, y_k\}$ is linearly independent if, and only if, the corresponding set of functions $\{Y_1, \dots, Y_k\}$ is linearly independent. Thus the number of linearly independent eigenfunctions for Problem 1 is equal to the number for Problem 2; the multiplicities for the eigenvalue λ are equal.
3. The first part of the proof establishes the relationship between the eigenfunctions.
4. Consider two eigenfunctions of Problem 1, y_j and y_k , and the corresponding functions for Problem 2, Y_j and Y_k . The inner product of y_j and y_k in the Hilbert space $L_w^2(a, b)$ is

$$\langle y_j, y_k \rangle_w = \int_a^b y_j^*(t)w(t)y_k(t) dt.$$

The inner product of Y_j and Y_k in the space $L_W^2(c, b)$ is

$$\langle Y_j, Y_k \rangle_W = \int_c^b Y_j^*(t)W(t)Y_k(t) dt$$

$$\begin{aligned}
&= \int_c^b \left(\begin{array}{c} y_j(t) \\ y_j((a+b)-t) \end{array} \right)^* \left(\begin{array}{c|c} w(t) & 0 \\ \hline 0 & w((a+b)-t) \end{array} \right) \times \\
&\quad \left(\begin{array}{c} y_k(t) \\ y_k((a+b)-t) \end{array} \right) dt \\
&= \int_c^b y_j^*(t)w(t)y_k(t) + y_j^*((a+b)-t)w((a+b)-t)y_k((a+b)-t) dt \\
&= \int_c^b y_j^*(t)w(t)y_k(t) dt + \int_a^c y_j^*(t)w(t)y_k(t) dt \\
&= \int_a^b y_j^*(t)w(t)y_k(t) dt = \langle y_j, y_k \rangle_w .
\end{aligned}$$

Since the corresponding inner products are equal, we see that if either set of eigenfunctions is orthonormal, then the other set will be also. \square

Examples

Two examples will be presented. In the first, a comparison is made with results obtained by a technique which is quite different from the one described here.

In the second, a problem will be transformed into three distinct problems, sharing the same set of eigenvalues. All three problems produce comparable results, providing evidence that the technique is working as expected. The method used to solve the separated problems produces an interval estimate for the desired eigenvalue. In a recent paper [7] Plum, using an algorithm based on a homotopy, computes eigenvalues of a scalar periodic problem, Problem a. This method is in no way similar to the algorithm developed here which transforms Problem a into a separated problem, Problem A.

Problem a On the interval $[0, \pi]$,

$$-y'' + 100(\cos x)^2 y = \lambda y$$

subject to the periodic boundary conditions

$$y(0) = y(\pi) , \quad y'(0) = y'(\pi).$$

In the notation we have been using, we have

$$p(x) = 1 , \quad q(x) = 100(\cos x)^2 , \quad w(x) = 1$$

with boundary conditions defined by four 2×1 matrices

$$C_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad C_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} , \quad D_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \quad D_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

Problem A On the interval $[\frac{\pi}{2}, \pi]$,

$$P(x) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, W(x) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$Q(x) = \begin{pmatrix} 100(\cos x)^2 & 0 \\ 0 & 100(\cos(\pi - x))^2 \end{pmatrix}$$

with the boundary conditions constants given by

$$A_1 = \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix}, A_2 = \begin{pmatrix} 0 & 0 \\ 1 & 1 \end{pmatrix}, B_1 = \begin{pmatrix} 0 & 0 \\ -1 & 1 \end{pmatrix}, B_2 = \begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}.$$

The results given by Plum are quite comparable to those computed by solving Problem A, as shown in Table 1. The subscripts and superscripts at the end of the numbers in Table 1 and Table 2 below specify the interval in which the given eigenvalue is located; i.e. the superscript gives an upper bound and the subscript gives a lower bound for the eigenvalue.

n	Plum	Problem A
1	9.7432204 ₀ ⁶	9.7432 ₁₄ ²³
2	28.6851 ₃₈ ⁴¹	28.6851 ₃₁ ⁴¹
3	46.47783 ₄ ⁷	46.4778 ₁₄ ²³
4	62.9864 ₈₆ ⁹³	62.9864 ₈₈ ⁹⁸
5	77.8052 ₃₇ ⁴⁴	77.8050 ₆₁ ⁷¹
6	91.80 ₀₇ ¹¹	91.801 ₀₇₁ ¹⁴⁷
7	98.975 ₄ ⁸	98.975 ₃₇₂ ⁴⁴⁹

Table 1: Comparison of Results

The next example begins with a scalar problem, Problem b, with a general, coupled boundary condition, with a non-constant, non-periodic coefficient. The second problem, Problem c, is constructed from the first by “folding” the interval in thirds, producing a dimension 3 problem with the same eigenvalues. The third problem, Problem d, is constructed from the first by a change of variable: $x \mapsto \sqrt{1+x}$. Each problem is solved using the technique described above, involving two problems of dimension 2, and a problem of dimension 6.

Problem b On the interval $[0, 3]$, with coefficients

$$p(x) = 2, q(x) = 1 + x^2, w(x) = 1$$

subject to the boundary conditions

$$\begin{pmatrix} 1 & 2 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} y \\ py' \end{pmatrix} (0) + \begin{pmatrix} 1.5 & 0 \\ 4 & 2 \end{pmatrix} \begin{pmatrix} y \\ py' \end{pmatrix} (3) = 0.$$

Problem c On the interval $[0, 1]$, with coefficients

$$p(x) = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad w(x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$q(x) = \begin{pmatrix} 1+x^2 & 0 & 0 \\ 0 & 1+(x-2)^2 & 0 \\ 0 & 0 & 1+(x+2)^2 \end{pmatrix}$$

subject to the boundary conditions

$$\begin{pmatrix} 1 & 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix} \begin{pmatrix} y \\ py' \end{pmatrix} (0)$$

$$+ \begin{pmatrix} 0 & 0 & 1.5 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 & 2 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} y \\ py' \end{pmatrix} (1) = 0.$$

Problem d On the interval $[1, 2]$, with coefficients

$$p(x) = \frac{1}{x}, \quad q(x) = 2x(x^4 - 2x^2 + 2), \quad w(x) = 2x$$

subject to the boundary conditions

$$\begin{pmatrix} 1 & 2 \\ 0 & 3 \end{pmatrix} \begin{pmatrix} y \\ py' \end{pmatrix} (1) + \begin{pmatrix} 1.5 & 0 \\ 4 & 2 \end{pmatrix} \begin{pmatrix} y \\ py' \end{pmatrix} (2) = 0.$$

The corresponding separated problems, Problem B, Problem C, and Problem D were solved; the bisection process was continued in each case until the width of the interval estimate was less than 0.00001. The bisection process began with intervals with integer endpoints in all cases. The results are shown in Table 2. All of the separated problems were solved using a multi-step numerical integration method. To control run times, the integrator uses a relatively coarse mesh, which we believe is the source of the disagreements between some of these results.

n	Problem B	Problem C	Problem D
1	1.6359 ⁷⁹ ₇₁	1.6359 ⁷⁹ ₇₁	1.6359 ⁷⁹ ₇₁
2	7.9569 ⁷⁰ ₆₃	7.9569 ⁷⁰ ₆₃	7.9569 ⁷⁰ ₆₃
3	12.8206 ⁴¹ ₃₃	12.8206 ⁴¹ ₃₃	12.8206 ⁴¹ ₃₃
4	25.2577 ⁶⁷ ₅₉	25.2577 ⁶⁷ ₅₉	25.2577 ⁶⁷ ₅₉
5	38.4839 ²⁵ ₁₇	38.4839 ³² ₂₅	38.4839 ²⁵ ₁₇
6	60.1740 ⁶⁵ ₅₇	60.1740 ⁵⁷ ₄₉	60.1740 ²⁶ ₁₉
7	82.2650 ¹⁵ ₀₇	82.2653 ⁸¹ ₇₃	82.2652 ⁵¹ ₄₄
8	112.7659 ⁴⁵ ₃₈	112.7656 ⁹⁴ ₈₆	112.7644 ⁷³ ₆₅

Table 2: Results

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Addendum

January 10, 1996. A remark and a FORTRAN code for the main algorithm of this article have been placed as an appendix. See files “appendix.tex” and “Dwyer.fort” in the directory *EJDE/Volumes/1994/06-Dwyer-Zettl*. See also the article

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