

INTRODUCTION TO SLEIGN2

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The main purpose of this code is to compute eigenvalues and eigenfunctions of regular and singular self-adjoint Sturm-Liouville problems (SLP) and to approximate the continuous spectrum in the singular case. For a general description of the analytical and numerical properties of the SLEIGN2 code see [1] and [3].

These problems consist of a second order linear differential equation

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

together with boundary conditions (BC). The nature of the BC depends on the regular or singular classification of the end points a and b . For both cases the BC fall into two major classes: separated and coupled. The former are two separate conditions, one at each endpoint; the latter are two coupled conditions linking the values of the solution y and its quasi-derivative (py') near the two endpoints, e.g. periodic and semi-periodic boundary conditions. SLEIGN2 seems to be the only general purpose code available for arbitrary self-adjoint BC, separated or coupled, and for both regular and singular problems.

A number λ for which there is a nontrivial solution satisfying the BC is called an eigenvalue and such a solution is a (corresponding) eigenfunction. If one or both endpoints are LP (see below or section 4 of HELP for a definition) there may be points λ in the spectrum in addition to eigenvalues i.e. there may be continuous spectrum.

In the theory of SLP the coefficients $1/p$ and q and the weight function w are assumed to be real-valued and locally Lebesgue integrable on (a, b) .

To meet the needs of numerical computing techniques we make the stronger assumptions:

- (i) The interval (a, b) of \mathbb{R} may be bounded or unbounded
- (ii) p, q and w are real-valued functions on (a, b)
- (iii) p, q and w are piecewise continuous on (a, b)
- (iv) p and w are strictly positive on (a, b) .

For better error analysis in the numerical procedures, condition (iii) above is replaced with (iii)' p, q and w are four times continuously differentiable on (a, b) .

To study a SLP using operator theory one associates a self-adjoint operator in the weighted Hilbert space of square-integrable functions, with respect to the weight w , on (a, b) , with each SLP in such a way that the spectrum of the problem is the spectrum of the operator. In the case of a regular problem the spectrum consists entirely of eigenvalues and these are bounded below (when $p > 0$ and $w > 0$). This is still so for the case when each endpoint is either regular (R) or singular limit-circle nonoscillatory (LCNO). In case one endpoint is limit-circle oscillatory (LCO) and the other is not limit-point (LP) then there are still only eigenvalues in the spectrum but these are not bounded below. (The spectrum is never bounded above.)

If one or both endpoints is LP the spectrum may be extremely complicated. There may be no eigenvalues, finitely many, or infinitely many. Some may be embedded in the continuous

spectrum. For $p = 1, w = 1, q(x) = \sin(x)$ on $(-\infty, +\infty)$ there are no eigenvalues and the continuous spectrum consists of the union of an infinite number of disjoint compact intervals. (SLEIGN2 can be used to approximate this spectrum - see example 12 in the file `xamples.tex` and the references quoted there.)

See the HELP file `help.tex` for a definition of the terms regular (R), limit-circle (LC), limit-circle non-oscillatory (LCNO), limit-circle oscillatory (LCO), limit-point (LP).

SLP problems are classified into various classes based on the classification of the endpoints and on whether the boundary conditions are separated (S) or coupled (C). We have the following categories:

1. R/R, S
2. R/R, C
3. R/LCNO or LCNO/R, S
4. R/LCNO or LCNO/R, C
5. R/LCO or LCO/R, S
6. R/LCO or LCO/R, C
7. LCNO/LCO or LCO/LCNO or LCO/LCO, S
8. LCNO/LCO or LCO/LCNO or LCO/LCO, C
9. LP/R or LP/LCNO or LP/LCO or R/LP or LCNO/LP or LCO/LP
10. LP/LP

For 9 there is only a separated condition at the non-LP endpoint and for 10 there are no boundary conditions at either end.

There are only two other major general purpose codes for computing eigenvalues and eigenfunctions of Sturm-Liouville problems : SLEDGE (Fulton and Pruess) and the earlier code SLEIGN (Bailey *et al*). (There was another code, written by Pryce and Marletta, available from the NAG library but the current NAG library no longer includes such a code.)

SLEDGE uses a method based on piecewise constant approximations of the coefficients of the differential equation; SLEIGN and SLEIGN2 both use the Prüfer transformation.

Both SLEIGN and SLEDGE are designed for separated regular boundary conditions and both have a mechanism to automatically handle endpoints which are either regular or singular but non-oscillatory. In the latter case if an endpoint is LCNO the Friedrichs condition is usually, but not always, the one chosen by the code. SLEDGE can also determine the LP/LC classification but only in a restricted number of cases (the method requires that the coefficients p, q and w are analytic on (a, b) and depends on the Frobenius method for series solutions at regular singular endpoints); SLEIGN and SLEIGN2 do not have such a facility but, for the sake of generality, rely on the user input of this information.

SLEIGN2 is the only general purpose code in existence which can, in principle, handle arbitrary self-adjoint, separated or coupled, regular or singular, boundary conditions, see the HELP file `help.tex` and [3]. Problems with coupled boundary conditions, see[2], at singular endpoints are difficult to handle numerically, especially if one or both of the endpoints is LCO.

In addition to the above mentioned capabilities to compute eigenvalues and eigenfunctions SLEIGN2 also computes the solution of an initial value problem with the users choice of λ and either a regular or singular initial condition.

When combined with the algorithm established in [4], SLEIGN2 can be used to approximate the continuous spectrum.

An important feature of the SLEIGN2 program is its user friendly interface contained in `makepqw.f` and `drive.f`. Users who want to bypass this interface and use their own driver may wish to look at a sample driver; two such drivers are provided, see (7) and (8) below.

The whole package consists of the following files:

1. A brief “readme” file `readme.txt` with basic information on how to run the code.
2. This introduction file `intro.tex`.
3. `makepqw.f` - This is an interactive Fortran file to input the coefficient functions p, q, w and, if necessary, the functions u, v which define the singular boundary conditions
4. `drive.f` - This is an interactive Fortran file containing the driver, a HELP file `help.tex`, and a “user friendly” interface.
5. `sleign2.f` - The main code for the computation of eigenvalues and eigenfunctions.
6. `xamples.f` - A Fortran file with 32 examples ready to run. These examples were chosen to illustrate various features of the code.
7. `seprdr.f` - A sample driver for separated regular or singular boundary conditions.
8. `coupdr.f` - A sample driver for coupled regular or singular boundary conditions.
9. `xamples.tex` - A LaTeX file containing information about the 32 examples.
10. `help.tex` - A LaTeX file with information about endpoint classifications, boundary conditions etc. It is a separate text file and it can also be accessed from both `makepqw.f` and `drive.f`.
11. `autoinput.txt` - A file describing an “automatic” method for using SLEIGN2 which avoids the user friendly “question and answer” format; this is recommended for experienced users only.

When an eigenfunction has been computed it is stored. If it is real-valued, it can be examined:

- (i) by printing out the numerical data
- (ii) by using the discrete graph plotter in the program
- (iii) by using a local graph plotter.

Full details are given in HELP; see the file `help.tex`.

All six of the Fortran files in the SLEIGN2 package are in single precision.

REFERENCES

- [1] P.B. Bailey, W.N. Everitt and A. Zettl, *Computing eigenvalues of singular Sturm-Liouville problems*, Results in Mathematics, **20** (1991), 391-423.
- [2] P.B. Bailey, W.N. Everitt and A. Zettl, *Regular and singular Sturm-Liouville problems with coupled boundary conditions*, Proc. Royal Soc. Edinburgh (A) **126** (1996), 505-514.
- [3] P.B. Bailey, W.N. Everitt and A. Zettl, *The SLEIGN2 Sturm-Liouville code.*, ACM TOMS, ACM Trans. Math. Software 21, (2001), 143-192.
- [4] P.B. Bailey, W.N. Everitt, J. Weidmann and A. Zettl, *Regular approximation of singular Sturm-Liouville problems*. Results in Mathematics **23** (1993), 3-22.

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