Note

A Slightly Modified Prüfer Transformation Useful for Calculating Sturm–Liouville Eigenvalues*

INTRODUCTION

Among the methods suggested for solving Sturm–Liouville eigenvalue problems

$$(p\Psi')' + (q + \lambda r)\Psi = 0 \qquad \text{on } (a, b),$$

$$A_1\Psi(a) + A_2 p(a) \, \Psi'(a) = 0,$$

$$B_1\Psi(b) + B_2 p(b) \, \Psi'(b) = 0,$$

there are several [1–3] which employ either the standard Prüfer transformation [4; 5, pp. 209–213]

$$\Psi(x) = \rho(x) \sin \theta(x),$$

$$p(x) \, \Psi'(x) = \rho(x) \cos \theta(x) \tag{1}$$

or the modified [6–8] (when $p(x) \equiv 1$)

$$\Psi(x) = \rho(x) \sin \theta(x),$$

$$\Psi'(x) = [\lambda r + q]^{1/2} \, \rho(x) \cos \theta(x) \tag{2}$$

to convert the given problem in terms of a second-order linear differential equation for Ψ into an equivalent one involving a first-order nonlinear equation for θ.

There are some fairly obvious reasons for being attracted to the modified form, especially when the eigenvalue is relatively large. At the same time it is also obvious, because of the possible vanishing of $q + \lambda r$ that the modified form can be comparatively complicated to use.

The purpose of this note is to point out that much of the advantage of the modified Prüfer transformation can be had with only a very slight change in the standard form, and correspondingly only an insignificant increase in complexity.

The Modification

The change we have in mind is simply to insert a positive constant, z, into the transformation. Thus in place of θ and ρ defined by (1) we have found that considerable improvement can often be had by defining σ and φ by

$$
\begin{aligned}
\Psi(x) &= \sigma(x) \sin \varphi(x), \\
p(x)\,\Psi'(x) &= z\sigma(x) \cos \varphi(x).
\end{aligned} \tag{3}
$$

Plainly φ and θ are related by

$$
\tan \varphi = z \tan \theta. \tag{4}
$$

In particular, φ and θ agree exactly whenever either is a multiple of $\pi/2$.

To see why this almost trivial change could be so beneficial, consider the differential equation for θ

$$
\theta' = 1/p \cos^2 \theta + (q + \lambda r) \sin^2 \theta \tag{5}
$$

along with that for φ

$$
\varphi' = \frac{z}{p} \cos^2 \varphi + \left(\frac{q}{z} + \lambda \frac{r}{z}\right) \sin^2 \varphi, \tag{6}
$$

when the problem is such that λ is large. Take, for example, the case

$$
p = 1, \quad q = -x^2, \quad r = 1, \quad A_2 = 0, \quad B_2 = 0
$$

on the interval $(0, 1)$ considered by Hargrave [8]. The eigenvalues of this problem get large fairly fast, the 10th and 20th being

$$
\lambda_{10} = 987.29, \quad \lambda_{20} = 3948.2.
$$

Now looking at (5) it is easy to see that the right-hand side fluctuates in value from 1 (when $\theta(x)$ is a multiple of π) to about λ (when $\theta(x)$ is an odd multiple of $\pi/2$). But if z in (6) is chosen to be about the size of $\lambda^{1/2}$, then the right-hand side of (6) is never very far from the value $\lambda^{1/2}$. This means $\varphi'(x)$ is pretty nearly a constant, and so the numerical integration of (6) is very much easier than (5). Of course the difference in ease of computation becomes even more dramatic for the higher eigenvalues.

While it is true that to be able to take advantage of this "slightly modified" Prüfer transformation one must be able to choose a suitable value for z, it is not necessary to be able to pick the actual optimum value. Most of the improvement will be obtained even if z is only *about* the right size, at least in the case of the higher eigenvalues.

Since the choice of z is dictated by a desire to minimize both the magnitude of the right-hand side of (6) and the magnitude of its fluctuations, probably the best that can be done is to choose z so that, in some average sense,

$$
z \doteq (p \mid q + \lambda r \mid)^{1/2}.
$$

The places where $q + \lambda r$ is positive will, of course, be the most important when choosing z.

TYPICAL NUMERICAL RESULTS

To give some idea of the potential savings from this simple idea we counted the number of function evaluations needed by one of the standard numerical integrators when applied to a number of representative eigenvalue problems. The table below lists the number, N, of evaluations required when $z = 1$ (the standard Prüfer transformation) and when z was chosen by the simple rule

$$z = n\pi/U,$$

where n is the eigenvalue index and U is approximately the length of interval on which $\lambda r + q$ is positive. (No attempt was made to optimize the choice of z.) This rule of thumb results from observing that the eigenfunction Ψ_n has $n - 1$ zeros.

Of course most problems do not show as much savings as the first two examples, but many do show a substantial savings, and none we have so far tried showed a significant loss.

1. Weber's equation. $p = 1, r = 1, q = -x^2, a = 0, b = 1$:

$$\lambda_1 = 10.15 \qquad \begin{cases} z = 1.0 & N = 143 \\ z = 3.133 & N = 74 \end{cases}$$

$$\lambda_{10} = 987.29 \qquad \begin{cases} z = 1.0 & N = 3074 \\ z = 31.416 & N = 110 \end{cases}$$

$$\lambda_{100} = 98696.5 \qquad \begin{cases} z = 1.0 & N = 51409 \\ z = 314.16 & N = 110. \end{cases}$$

2. Mathieu's equation. $p = 1, r = 1, q = -2\cos 2x, a = 0, b = \pi/2$:

$$\lambda_1 = 4 \qquad \begin{cases} z = 1.0 & N = 120 \\ z = 2.004 & N = 92 \end{cases}$$

$$\lambda_5 = 100 \qquad \begin{cases} z = 1.0 & N = 1084 \\ z = 10.0 & N = 128 \end{cases}$$

$$\lambda_{10} = 400 \qquad \begin{cases} z = 1.0 & N = 2812 \\ z = 20.0 & N = 146 \end{cases}$$

$$\lambda_{100} = 40,000 \qquad \begin{cases} z = 1.0 & N = 48719 \\ z = 200.0 & N = 128. \end{cases}$$

3. Harmonic oscillator. $p = 1$, $r = 1$, $q = -x^2$, $a = -\infty$, $b = +\infty$:

$$\lambda_1 = 1.0 \qquad \begin{cases} z = 1.0 & N = 210 \\ z = 1.076 & N = 215 \end{cases}$$

$$\lambda_{10} = 19 \qquad \begin{cases} z = 1.0 & N = 2377 \\ z = 3.51 & N = 1159. \end{cases}$$

4. Hydrogen atom. $p = 1$, $r = 1$, $q = 1/x - 2/x^2$, $a = 0$, $b = +\infty$:

$$\lambda_1 = -0.0625 \qquad \begin{cases} z = 1.0 & N = 382 \\ z = 0.142 & N = 269 \end{cases}$$

$$\lambda_{10} = -0.002066 \qquad \begin{cases} z = 1.0 & N = 2773 \\ z = 0.12 & N = 1349. \end{cases}$$

5. Airy differential equation. $p = 1$, $r = 1$, $q = -x$, $a = 0$, $b = +\infty$:

$$\lambda_1 = 2.338 \qquad \begin{cases} z = 1.0 & N = 233 \\ z = 1.11 & N = 228 \end{cases}$$

$$\lambda_{10} = 12.829 \qquad \begin{cases} z = 1.0 & N = 1903 \\ z = 2.54 & N = 1128. \end{cases}$$

6. Bessel equation ($\nu = 2$). $p = x$, $r = x$, $q = -4/x$, $a = 0$, $b = 1$:

$$\lambda_1 = 26.37 \qquad \begin{cases} z = 1.0 & N = 192 \\ z = 4.22 & N = 138 \end{cases}$$

$$\lambda_{10} = 1136.8 \qquad \begin{cases} z = 1.0 & N = 2532 \\ z = 31.45 & N = 961. \end{cases}$$

7. Bessel equation ($\nu = \frac{1}{4}$). $p = x$, $r = x$, $q = -0.0625/x$, $a = 0$, $b = 3$:

$$\lambda_1 = 0.8593 \qquad \begin{cases} z = 1.0 & N = 120 \\ z = 0.70 & N = 92 \end{cases}$$

$$\lambda_4 = 16.49 \qquad \begin{cases} z = 1.0 & N = 699 \\ z = 3.8 & N = 368. \end{cases}$$

8. Legendre's equation. $p = 1 - x^2$, $r = 1$, $q = 0$, $a = -1$, $b = 1$:

$$\lambda_2 = 2.0 \qquad \begin{cases} z = 1.0 & N = 74 \\ z = 1.57 & N = 74 \end{cases}$$

$$\lambda_{10} = 90.0 \qquad \begin{cases} z = 1.0 & N = 1951 \\ z = 14.14 & N = 878. \end{cases}$$

9. Rotation Morse oscillator. $p = 1$, $r = 1$, $q = 2000(2E - E^2) - 2/x^2$, $E = \exp(-1.7(x - 1.3))$, $a = 0$, $b = +\infty$:

$$\lambda_1 = -1923.5 \qquad \begin{cases} z = 1.0 & N = 2943 \\ z = 10.67 & N = 2535 \end{cases}$$

$$\lambda_{10} = -815.5 \qquad \begin{cases} z = 1.0 & N = 4900 \\ z = 27.1 & N = 2131. \end{cases}$$

REFERENCES

1. P. B. BAILEY, Sturm–Liouville eigenvalues via a phase function, *SIAM J. Appl. Math.* **14** (1966), 242–249.
2. M. GODART, An iterative method for the solution of eigenvalue problems, *Math. Comp.* **20** (1966), 399–406.
3. D. O. BANKS AND G. J. KUROWSKI, Computation of eigenvalues of singular Sturm–Liouville systems, *Math. Comp.* **22** (1968), 304–310.
4. H. PRÜFER, Neue Herleitung der Sturm–Liouvilleschen Reihenentwicklung stetiger Functionen, *Math. Ann.* **95** (1926), 499–518.
5. E. A. CODDINGTON AND N. LEVINSON, "Theory of Ordinary Differential Equations," McGraw-Hill, New York, 1955.
6. G. FIX, Asymptotic eigenvalues of Sturm–Liouville systems, *J. Math. Anal. Appl.* **19** (1967), 519–525.
7. D. J. KAUP, A modification of the variable phase method for optimum calculation of phase shifts, *J. Computational Phys.* **9** (1972), 254–272.
8. B. A. HARGRAVE, Numerical approximation of eigenvalues of Sturm–Liouville systems, *J. Computational Phys.* **20** (1976), 381–396.

PAUL B. BAILEY

Sandia Laboratories,
Albuquerque, New Mexico 87115