ON A NEW ALGORITHM FOR THE COMPUTATION OF ENCLOSURES FOR THE TITCHMARSH-WEYL $m$-FUNCTION *

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1 Introduction

Recently two of the present authors [1] reported on a method for computing safe bounds for the value of the Titchmarsh-Weyl $m$ function associated with the differential expression

$$M y \equiv \frac{1}{w}(-py')' + qy$$  \hfill (1. 1)

defined over $[a, \infty)$, $-\infty < a$, where $p, q, w$ are real-valued functions which satisfy $p^{-1}, q, w \in L^1_{loc}[a, \infty)$ and $w(x) > 0$ a.e. In the case that $w = 1$ Weyl [2] showed that the differential equation

$$M y = \lambda y, \quad \lambda \in C_+ \cup C_-$$  \hfill (1. 2)

has at least one solution that belongs to the set

$$L^2_w(a, \infty) \equiv \{ f : \int_a^\infty w | f |^2 \, dx < \infty \}.$$  

The proof of this result introduced the Titchmarsh-Weyl $m$ function to the mathematics literature. It was however Titchmarsh who investigated the properties of $m(\lambda)$ as an analytic function of $\lambda$ and established the connection between the location of its poles, of necessity on the real line, and the eigenvalues of the differential equation (1.2).

The analytic form of the $m$ function is determined by the form of the $L^2$ solutions of (1.2) and it is perhaps not suprising that there are few examples of $m$ known in closed form. For example if $a = 0$ and $p = w = 1$ then, when $q = \pm x^2$, the $m$ function is known as a rational function of gamma functions, while if $q = \pm x$ it may be written in terms of Bessel functions. For a detailed discussion of the $m$ function, together with examples, see [3].

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In [4] the central role of the $m$ function in the spectral theory of (1.1) is established. It is shown that the behaviour of the $m$ function near the real line classifies all points of the real line as belonging to the point spectrum, continuous spectrum, point-continuous spectrum or the resolvent set of the self-adjoint operator generated in $L^2_w(a,\infty)$ by (1.1) together with initial conditions. A further use for the $m$ function is in determining the best constant in Everitt’s HELP inequality. See [5] for further details.

In view of the central importance of the $m$ function and also in view of the difficulties in obtaining its values analytically, much effort has been expended in devising computational algorithms to estimate its value. These are reported on in a series of papers which include [6],[7],[8]. However these papers only contain estimates for the value of $m$ and do not seek to address the question of absolute bounds on the error in the computations.

In [1] we reported on an algorithm to compute rigorous bounds for the $m$ function. This algorithm worked well for examples $q = x^\alpha, \alpha \geq 2$ or $\alpha = 1$, but was shown to be computationally inefficient for examples $q = -x^\alpha, \alpha = 1, 2$, and the interval based algorithm needed in the computation in [1] did not cover the case $q = \pm x^\alpha, 0 < \alpha < 2, \alpha \neq 1$. The purpose of this paper is to present two new algorithms which overcome these difficulties and enable the $m$ function now to be enclosed for a much wider class of problems.

In section 2 we review the relevant extracts from the theory of the Titchmarsh-Weyl $m$ function that are needed to develop our algorithm. Section 3 is devoted to recalling certain asymptotic results that are central to our method as well as presenting an overview of an interval based algorithm that is fundamental to the implementation of our $m$ computation. Section 4 contains the results of the numerical experiments that we have performed, while section 5 deals with the extension of the algorithm to overcome the problems encountered with $q = \pm x^\alpha, 0 < \alpha < 2, \alpha \neq 1$.

## 2 Titchmarsh-Weyl limit-point, limit-circle classification

In the classical limit-point, limit-circle theory of (1.2) it is shown that, starting from a pair of solutions $\theta, \phi$ of (1.2) which for strictly complex $\lambda$ satisfy

\[
\begin{align*}
\theta(a,\lambda) &= 0 \quad (p\theta')(a,\lambda) = 1 \\
\phi(a,\lambda) &= -1 \quad (p\phi')(a,\lambda) = 0,
\end{align*}
\]

there exists a complex-valued function $m(\lambda)$ such that

\[
\psi_0(\cdot,\lambda) = \theta(\cdot,\lambda) + m(\lambda)\phi(\cdot,\lambda) \in L^2_w(a,\infty).
\]
When, up to constant multiples, there is precisely one solution of (1.2) in $L^2_{w}(a,\infty)$, we say (1.1) or (1.2) is limit-point at infinity. If all the solutions of (1.2) are in $L^2_{w}(a,\infty)$, we say that (1.1) or (1.2) is limit-circle at infinity. Further, the limit point, limit-circle classification is determined by $p, q, w$ and is independent of the strictly complex parameter $\lambda$. In this paper we shall be exclusively concerned with the limit-point case. The $m$ function is a Nevanlinna function, mapping the upper (lower) half-plane to itself, and as such has any singularities confined to the real line. From (2.1) and (2.2) it follows that

$$m(\lambda) = -\frac{\psi(a,\lambda)}{p(a)\psi'(a,\lambda)}$$

(2.3)

where $\psi$ is any (non-zero) constant multiple of $\psi_0$. The result (2.3) is the basis of our algorithm to compute $m(\lambda)$.

We choose a point $X > 0$ such that for $x \in [X,\infty)$ we may develop an asymptotic expansion for $\psi(x,\lambda)$, together with a precise estimate on the error committed. This expansion enables us to determine intervals in which $\psi(X,\lambda)$ and $\psi'(X,\lambda)$ lie, thus providing initial data to an interval based initial value solver that is used to compute complex intervals which enclose $\psi(a,\lambda)$ and $\psi'(a,\lambda)$. The result (2.3) yields an interval which encloses $m(\lambda)$. In section 3 we review the asymptotic method and interval ODE solver that is used to perform these tasks.

### 3 Overview of the components of the algorithm

#### 3.1 Asymptotic theory

The method that we use to obtain the asymptotic solution (1.2) as $x \to \infty$ is the repeated diagonalization method of Eastham which is fully explained in the book [3] and here we shall be brief. The method is concerned with estimating and improving error terms in the asymptotic solution of the linear differential system

$$Z'(x) = \rho(x)\{D + R(x)\}Z(x) \quad (a \leq x < \infty)$$

(3.1)

where $Z$ is an $n$–component vector, $\rho$ is a real or complex scalar factor, $D$ is a constant diagonal matrix

$$D = dg(d_1, d_2, ..., d_n)$$

with distinct $d_k$ and $R$ is a perturbation such that

$$R(x) = O(x^{-\delta}) \quad (x \to \infty)$$

(3.2)
for some $\delta > 0$.

If it is the case that $\rho R \in L(a, \infty)$, the Levinson asymptotic theorem can be applied to (3.1) to give solutions

$$Z_k(x) = \{e_k + \eta_k(x)\} \exp(d_k \int_a^x \rho(t) dt)$$  \hspace{1cm} (3.3)

where $e_k$ is the unit coordinate vector in the $k$–direction and $\eta_k(x) \to 0$ as $x \to \infty$. The size of the error term is related to the size of $R$ as $x \to \infty$, and therefore the accuracy of (3.3) can be improved if the perturbation $R$ can be reduced as $x \to \infty$. Under suitable conditions on $\rho$ and $R$ this improvement can be achieved by a sequence of repeated transformations which lead to a computational procedure to estimate the solution of (1.2) together with a bound on the associated error.

The sequence of transformations may be obtained either by an exact diagonalization or by an approximate diagonalization procedure. These methods are discussed in detail in [10]. The exact diagonalization method involves the explicit construction of an $n \times n$ matrix $T$ such that

$$T^{-1}(x)\{D + R(x)\}T(x) = D_1(x)$$

and this in turn requires the explicit eigenvectors of $D + R(x)$ which, although available for the second order system, are not generally known for the $n$–th order system. In this investigation we choose to work with the more generally applicable approximate diagonalization method which may be used for $n$–th order systems of differential equations. A discussion on the asymptotic method of exact diagonalization as applied to estimating the $m$ function can be found in [11].

3.1.1 Approximate diagonalization

We assume that $R$ is a differentiable $n \times n$ matrix satisfying (3.2), and we define an $n \times n$ matrix $P$ by

$$PD - DP = R - dgR$$

with diagonal entries $p_{ii} = 0$ and other entries

$$p_{ij} = r_{ij}/(d_j - d_i).$$  \hspace{1cm} (3.4)

We note that $P = O(R) = O(x^{-\delta})$ and the construction of the $P$ matrix cancels out the dominant terms in the following system (3.5). With $Z = (I + P)W$, (3.1) is transformed into the system

$$W' = \rho(\tilde{D} + S)W$$  \hspace{1cm} (3.5)
where we have written the \( n \times n \) matrices

\[
\tilde{D} = D + dgR
\]

\[
S = (I + P)^{-1}(RP - PdgR - \rho^{-1}P') = O(x^{-2\delta}) + O(\rho^{-1}x^{-\delta - 1})
\] (3. 6)

which is of smaller magnitude than \( R \). We write

\[
(I + P)^{-1} = I - P + P^2 + \ldots + (-1)^\nu P^\nu + (-1)^{\nu+1}(I + P)^{-1}P^{\nu+1}
\] (3. 7)

and specify an order of magnitude \( O(x^{-K}) \) which we wish to achieve as an error in the asymptotic solution of (3. 1). Substituting (3. 7) into (3. 6), we have

\[
S = V_2 + \ldots V_{M-1} + E
\] (3. 8)

where

\[
V_m = O(x^{-m\delta})
\]

\[
E = O(x^{-K})
\]

and \((M - 1)\delta < K \leq M\delta\). Thus \( \nu \) is chosen so that \( P^{\nu+1} \) in (3. 7) gives rise to terms which contribute to \( E \) by at most this order of magnitude, and will be estimated in the final stages of the algorithm.

This transformation procedure may be repeated for the \( W \) system (3. 5), but with a new \( P \) defined in terms of \( V_2 \) which replaces \( R \) in (3. 1). We continue to use the matrix \( D \) and not \( \tilde{D} \) to simplify the construction of an efficient computational algorithm. However this procedure introduces additional terms into the analysis which must be eliminated at subsequent iterations of the algorithm. A repetition of the above process leads to a new matrix \( S \) viz.

\[
S = V_3 + \ldots + V_{M-1} + E
\]

with new \( V \)'s and a new \( E \).

The above ideas may be used to form the basis of an iterative procedure, which can be implemented in the symbolic algebra system Mathematica, to compute the asymptotic solutions of (3. 1). Taking (3. 1) as a starting point with \( m = 1 \), we have at the \( m \)-th stage

\[
Z'_m = \rho(D_m + R_m)Z_m,
\]

\[
R_m = V_{1m} + V_{2m} + \ldots + V_{M-m,m} + E_m,
\]

\[
V_{jm} = O(x^{-(m+j-1)\delta}).
\]
\[ \begin{align*}
dg V_{1m} &= 0, \\
D_m &= D + \Delta_m, \\
Z_m &= (I + P_m)Z_{m+1}
\end{align*} \]

where \( P_m \) is defined explicitly in terms of \( V_{1m} \) and \( D \) as in (3.4). Thus \( V_{1m} \) is eliminated at this stage.

At the end of the process all the \( V \)'s are eliminated and this gives

\[ Z'_M = \rho(D_M + R_M)Z_M \]

where

\[ R_M = E_M = O(x^{-K}) \]

and \( M\delta \geq K \). The Levinson theorem then yields the solution of the \( Z_M \) system, and reversal of the \( M - 1 \) transformations gives

\[ Z = \{ \Pi^{M-1}_1(I + P_m)\}(e + \eta)\exp\left(\int_a^x \rho(...)dt\right) \]

with \( \eta = O(x^{-K}) \), (see [10] for further details).

### 3.2 Interval ODE solver

In this sub-section we introduce briefly the concepts of interval arithmetic that we need to give a short account of Lohner’s AWA algorithm. For an in-depth discussion of interval arithmetic, see [11], while Lohner’s AWA algorithm is discussed in [12] and [1].

Denoting any of the four basic arithmetic operations by \( \star \), we define, for real intervals \([a], [b], \]

\[ [a] \star [b] = \{ a \star b \mid a \in [a], b \in [b] \}. \]

Thus we can compute an enclosure for \([a] \star [b] \) by obtaining computable upper, and lower bound, for \([a] \star [b] \) which is derived from the lower and upper bounds of \([a], [b] \) respectively, by some directed rounding facilities. Any algorithm that is realised on a computer consists of finitely many operations \( \star \) and thus an enclosure for the results of arithmetic operations which constitute the algorithm may be computed. In practice this simple approach would soon lead to an explosion of the interval width but many sophisticated techniques are available to control this phenomenon [11].

Lohner’s approach to computing an enclosure of the solution of initial value problems is based on the well known Taylor method for solving initial value problems. Suppose that a solution of the
IVP

\[ u' = f(x, u), \quad u(0) = u_0, \quad (3.9) \]

where \( f : [0, \infty) \times \mathbb{R}^n \rightarrow \mathbb{R}^n \) is sufficiently smooth, is known at some point \( x_0 \). Then the solution at \( x_0 + h \) is

\[ u(x_0 + h) = u(x_0) + h\phi(x_0, h) + z_{x_0+h} \quad (3.10) \]

where \( u(x_0) + h\phi(x_0, h) \) is the \((r-1)\)-th degree Taylor polynomial of \( u \) expanded about \( x_0 \) and \( z_{x_0+h} \) is the associated local error. This method lends itself well to computation since the coefficients of the polynomial may be computed via an automatic differentiation package by differentiating the differential equation \((3.9)\). However the error term is not known exactly since the standard formulae give, for some unknown \( \tau \),

\[ z_{x_0+h} = u^{(r)}(\tau)h^r/r! \quad \tau \in [x_0, x_0 + h]. \quad (3.11) \]

In Lohner’s algorithm, \((3.11)\) is used to advance an enclosure \( [u(x_0)] \) for the solution \( u \) at \( x_0 \), to one for the solution \( u \) at \( x_0 + h \) which we denote by \( [u(x_0+h)] \). A suitable enclosure for the error \((3.11)\) is

\[ [z_{x_0+h}] = f^{(r)}([x_0, x_0 + h], [u])h^r/r! \]

provided that an enclosure \( [u] \) for \( \{u(x) : x_0 \leq x \leq x_0 + h\} \) can be computed. This is achieved by the following means. Choose some interval \( [u^0] \supset [u(x_0)] \) and try to prove that

\[ [u] = [u(x_0)] + [0, h] \cdot f([x_0, x_0 + h], [u^0]) \subset [u^0]. \]

If this is true then Banach’s fixed-point theorem implies that \( [u] \) is an enclosure for \( u(x) \) for all \( x \in (x_0, x_0 + h) \). In order to achieve efficient performance and tight bounds, the details of the algorithm are more complex than this short overview can show. We refer the reader to \([12]\) and \([1]\) for a complete discussion of the method.

4 Results for \( q = -x^\alpha, \quad \alpha = 1, 2 \)

In this section we discuss the computation of \( m \) when \( a = 0 \) and \( p = w = 1 \) and the potential \( q = -x^\alpha, \quad 0 \leq \alpha \leq 2 \). In terms of the asymptotic analysis presented in section 3 this means that we take \( \delta = \alpha/2 \). However, while the general algorithm is applicable to all \( \alpha \) in this range, the implementation of Lohner’s AWA interval ODE solver requires at least two derivatives of the function \( q \), see \([13]\), to be available at \( x = 0 \). Clearly this is not possible for \( 0 < \alpha < 2, \quad \alpha \neq 1, 2 \).
and for $\alpha$ in this range a revised algorithm is presented in section 5. Here we present an algorithm to compute $m$ when $q = -x$ or $q = -x^2$. We remark that the algorithm which we present here is also applicable to problems where $q = x^\alpha$, $2 \leq \alpha$ or $\alpha = 1$, while that in section 5 covers the case $0 < \alpha < 2$.

We first write (1.2) as the system

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ q - \lambda & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$$

and as in [4, chapter 2] introduce the transformation

$$T = \begin{pmatrix} 1 & 1 \\ \sqrt{q - \lambda} & -\sqrt{q - \lambda} \end{pmatrix}.$$ 

This enables us to write (1.2) in the form (3.1) with

$$\rho = \sqrt{q - \lambda}, \quad D = dg(1, -1)$$

and

$$R = \frac{q'}{4(q - \lambda)^{3/2}} \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}.$$ 

We next apply 6 iterations of the asymptotic algorithm of section 3.1 to obtain bounds on $\psi(x, \lambda)$ and $\psi'(x, \lambda)$ ($X \leq x < \infty$) the $L^2[a, \infty)$ solution obtained from the asymptotic algorithm. This gives intervals which enclose $\psi(X, \lambda)$ and $\psi'(X, \lambda)$ which are the initial data required by the AWA algorithm. The asymptotic analysis and estimation of the error is performed using purpose written Mathematica code, the detail of which is fully reported on in [10].

The C-XSC implementation of Lohner’s algorithm is used with purpose written shell script to interface the asymptotic results to the interval arithmetic code.

In all cases the enclosures that we obtain for $m(\lambda)$ are in agreement with the closed form of $m(\cdot)$ given in terms of either gamma functions or Bessel functions [13], and evaluated by numerical routines, (see [14] and [15] for further details). We further remark that the algorithm reported on in [14] could not perform the computation required to produce the above results.
$$\lambda \quad m(\lambda)$$

| $\lambda$          | $m(\lambda)$                                      |
|-------------------|--------------------------------------------------|
| $-1 + i$          | $0.7237897644403761 + 0.4287071190558884$        |
| $i$               | $0.5550505090709121 + 0.6653607324705136$        |
| $0.5 + i$         | $0.4240432899140527 + 0.7009461148568185$        |
| $0.1 + 0.1 i$     | $0.599793075913471 + 1.0966409756787717$        |
| $1 + i$           | $0.3127627739736355 + 0.6886661844509032$        |
| $10 + 10 i$       | $0.1017531391523634 + 0.2444418723660981$        |
| $1 + 0.5 i$       | $0.265973056163538 + 0.7947538755051292$        |
| $1 + 0.1 i$       | $0.1873568032104862 + 0.8857549186094842$        |
| $1 + 0.01 i$      | $0.16289085986685 + 0.9047935039573860$         |
| $1 + 0.001 i$     | $0.1602956820262119 + 0.90963145095583608$      |
| $1 + 0.0001 i$    | $0.1600085544702433 + 0.9068324622237933$      |

Table 1: $X = 10$ and $\alpha = 1$, where $e_6(10) = 1.09576673 \times 10^{-8}$.

$$\lambda \quad m(\lambda)$$

| $\lambda$          | $m(\lambda)$                                      |
|-------------------|--------------------------------------------------|
| $-1 + i$          | $0.7215463224447454 + 0.3676480842327160$        |
| $i$               | $0.6266507272135664 + 0.626657622008661$         |
| $0.5 + i$         | $0.4999306961394433 + 0.7052913470794993$        |
| $0.1 + 0.1 i$     | $0.8975088699388575 + 1.0328950653972185$        |
| $1 + i$           | $0.3676489849868459 + 0.7215463223138745$        |
| $10 + 10 i$       | $0.1020664354130717 + 0.2455420822914867$        |
| $1 + 0.5 i$       | $0.3372315718010399 + 0.8679537555127644$        |
| $1 + 0.1 i$       | $0.2561260389488290 + 1.0228215685241975$        |
| $1 + 0.01 i$      | $0.2252728850846718 + 1.061093701720598$         |
| $1 + 0.001 i$     | $0.2218527093136766 + 1.0649430729902692$        |
| $1 + 0.0001 i$    | $0.2210572705977203 + 1.065328561152201$         |
| $1 + 0.00001 i$   | $0.2214726824328328 + 1.0653666564746155$        |

Table 2: $X = 10$ and $\alpha = 2$, where $e_6(10) = 1.20325893 \times 10^{-9}$. 
Table 3: $X = 40$ and $\alpha = 1$, where $\epsilon_0(40) = 5.21570339 \times 10^{-15}$.

5 Results for $q = -x^\alpha, 0 < \alpha < 2$, $a = 0, p = w = 1$

As we mentioned at the beginning of section 4 we have to modify our algorithm to deal with values of $\alpha$ other than 1 and 2. We do this by choosing some number $\epsilon > 0$. Then, instead of solving (1.2) over the whole of $[0, X]$, we now solve the equation over the interval $[\epsilon, X]$. The following Theorem 5.1 enables us to obtain an enclosure for $y(0)$ and $y'(0)$ in terms of the enclosures for $y(\epsilon)$ and $y'(\epsilon)$.

**Theorem 5.1** Let $c(x) = q(x) - \lambda$ and, for some $\epsilon > 0$, let $f, g \in C[0, \epsilon]$ satisfy $f(\epsilon) = y(\epsilon)$, $g(\epsilon) = y'(\epsilon)$. In addition let

$$b = \epsilon \int_0^\epsilon |c| \, dt < 1.$$

Then

1. $|y(0) - f(0)| \leq \frac{1}{1 - b} \left[ \int_0^\epsilon |f' - g| \, dt + \epsilon \int_0^\epsilon |g' - cf| \, dt \right]$ \hspace{1cm} (5.1)

2. $|y'(0) - g(0)| \leq \frac{1}{1 - b} \left[ \int_0^\epsilon |c| \, dt \int_0^\epsilon |f' - g| \, dt + \int_0^\epsilon |g' - cf| \, dt \right]$ \hspace{1cm} (5.2)
Proof: Define

\[ u(x) = \begin{pmatrix} y(x) \\ y'(x) \end{pmatrix} - \begin{pmatrix} f(x) \\ g(x) \end{pmatrix}. \]

Then \( u(\epsilon) = 0 \) and

\[ u'(x) = \begin{pmatrix} y'(x) \\ c(x)y(x) \end{pmatrix} - \begin{pmatrix} f'(x) \\ g'(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ c(x) & 0 \end{pmatrix} u(x) - \tau(x), \]

where

\[ \tau = \begin{pmatrix} f' - g \\ g' - cf \end{pmatrix}. \]

Define

\[ T : (C[0, \epsilon])^2 \rightarrow (C[0, \epsilon])^2 \]

by

\[ (Tv)(x) := \int_\epsilon^x \begin{pmatrix} 0 & 1 \\ c(t) & 0 \end{pmatrix} v(t)dt - \int_\epsilon^x \tau(t)dt, \]

for \( x \in [0, \epsilon] \) and \( v \in (C[0, \epsilon])^2 \). Then it follows that

\[ u = Tu. \]

We shall prove that \( T \) has a globally unique fixed point in

\[ U := \{ v \in (C[0, \epsilon])^2 : |v_1(x)| \leq \alpha_1, |v_2(x)| \leq \alpha_2 \ (0 \leq x \leq \epsilon) \} \]

where \( \alpha_1 \) and \( \alpha_2 \) denote the right-hand sides of the inequalities (5.1) and (5.2), respectively. To show this we use the Banach fixed point theorem. This requires us to show

1. \( T \) is a contraction with respect to some suitable norm;

2. \( TU \subset U \).

In order to show (1) let

\[ \| v \| := \max_{x \in [0, \epsilon]} \{ \max \left( \frac{1}{\sqrt{\epsilon}}, \frac{1}{\sqrt{\int_0^\epsilon |c| dt}} \right) |v_1(x)|, \frac{1}{\sqrt{\int_0^\epsilon |c| dt}} |v_2(x)| \}. \]
Since for all $v, \tilde{v} \in (C[0,\epsilon])^2$ and $x \in [0,\epsilon]$,

\[
| (Tv - T\tilde{v})_1(x) | \leq \int_x^\epsilon | v_2(t) - \tilde{v}_2(t) | \, dt \leq \epsilon \| v - \tilde{v} \| \sqrt{\int_0^\epsilon | c | \, dt},
\]
\[
| (Tv - T\tilde{v})_2(x) | \leq \int_x^\epsilon | c(t) || v_1(t) - \tilde{v}_1(t) | \, dt \leq \sqrt{\epsilon} \| v - \tilde{v} \| \int_0^\epsilon | c | \, dt.
\]

we have

\[
\| Tv - T\tilde{v} \| \leq \sqrt{\epsilon \int_0^\epsilon | c | \, dt} \| v - \tilde{v} \|.
\]

Since

\[
\epsilon \int_0^\epsilon | c | \, dt < 1
\]

it follows that $T$ is a contraction.

In order to establish part 2 we take $v \in U$. Then

\[
| (Tv)_1(x) | \leq \int_x^\epsilon | v_2 | \, dt + \int_x^\epsilon | \tau_1 | \, dt
\]
\[
\leq \epsilon \alpha_2 + \int_0^\epsilon | \tau_1 | \, dt
\]
\[
= \alpha_1
\]

and

\[
| (Tv)_2(x) | \leq \int_x^\epsilon | c || v_1 | \, dt + \int_x^\epsilon | \tau_2 | \, dt
\]
\[
\leq \alpha_1 \int_0^\epsilon | c | \, dt + \int_0^\epsilon | \tau_2 | \, dt
\]
\[
= \alpha_2.
\]

Thus $T$ has a globally unique fixed point in $U$ which implies $u \in U$. In particular,

\[
| u_1(0) | \leq \alpha_1, \quad | u_2(0) | \leq \alpha_2
\]

which establishes the theorem.

\section{5.1 Numerical examples}

We now turn to two examples which illustrate the use of Theorem 5.1 to compute enclosures for $m$. These examples are: $p = w = 1$, and

1. $q(x) = -\sqrt{x}$;

2. $q(x) = -x^{3/2}$. 


In both these examples there is insufficient smoothness in the function $q$ for Lohner’s code to compute enclosures at $x = 0$. We therefore compute enclosures at $x = \epsilon$ and use the above theorem to obtain enclosures at $x = 0$.

In the first example we choose $f$ and $g$ to be the first-order Taylor polynomial approximations to $y$ and $y'$ expanded about $x = \epsilon$. Writing $A_0 = y(\epsilon)$ and $A_1 = y'(\epsilon)$ these are respectively

\[
  f(x) = A_0 + (x - \epsilon)A_1, \\
  g(x) = A_1 + (x - \epsilon)(-\sqrt{\epsilon} - \lambda)A_0.
\]

Since for this example

\[
  \int_0^\epsilon |c| \, dt \leq \frac{2}{3} \epsilon^{3/2} + |\lambda| \epsilon \\
  \int_0^\epsilon |c - c(\epsilon)| \, dt = \frac{1}{3} \epsilon^{3/2} \\
  \int_0^\epsilon |c| (\epsilon - t) \, dt \leq \frac{4}{15} \epsilon^{5/2} + \frac{1}{2} |\lambda| \epsilon^2,
\]

the inequalities (5.1) and (5.2) become

\[
  |y(0) - (A_0 - \epsilon A_1)| \leq \frac{\epsilon^2}{1 - \epsilon^2(\lambda - \frac{1}{2} \sqrt{\epsilon})} \times \\
  \left\{ \left( \frac{1}{2} |\lambda| + \frac{5}{6} \sqrt{\epsilon} \right) |A_0| + \epsilon \left( \frac{1}{2} |\lambda| + \frac{4}{15} \sqrt{\epsilon} \right) |A_1| \right\}
\]

\[
  |y'(0) - (A_1 + \epsilon (\lambda + \sqrt{\epsilon}) A_0)| \leq \frac{\epsilon^{3/2}}{1 - \epsilon^2(\lambda - \frac{1}{2} \sqrt{\epsilon})} \times \\
  \left\{ \frac{1}{2} \epsilon^{3/2}(|\lambda| + \sqrt{\epsilon})(|\lambda| + \frac{2}{3} \sqrt{\epsilon}) + \frac{1}{3} |A_0| + \sqrt{\epsilon}(\frac{1}{2} |\lambda| + \frac{4}{15} \sqrt{\epsilon}) |A_1| \right\}
\]

In the example that we report on, $\lambda = 1 + i$ and we have taken $\epsilon = 0.000015625$. However, since Lohner’s code uses a fixed step size algorithm, in order to achieve such a small value of $\epsilon$ we have integrated over $[10, 0.03125]$ with a step size of 0.03125, then reduced the step size to 0.000015625 to perform the integration over $[0.03125, 0.000015625]$. This yields an enclosure

\[
  m(1 + i) = 0.25936^{82}_{61} + 0.6719^{82}_{78}i.
\]

We have compared our result with the estimate of $m(1 + i)$ obtained from the Brown Kirby Pryce code [3]. That algorithm gives $m(1 + i) = 0.25937860 + 0.67196464i$ which is slightly outside our enclosures and reflects the lack of smoothness in $q$ experienced by the Runga-Kutta method they employ.
In the next example we take $q = -x^{3/2}$ and as before we take $f$ and $g$ to be the first-order Taylor approximations of $y$ and $y'$ respectively, expanded about $x = \epsilon$. This time we get

$$|y(0) - (A_0 - \epsilon A_1)| \leq \frac{\epsilon^2}{1 - \epsilon^2(|\lambda| + \frac{2}{5}\epsilon^{3/2})} \left\{ \left( \frac{1}{2} |\lambda| + \frac{11}{10}\epsilon^{3/2} \right) |A_0| + \epsilon \left( \frac{1}{2} |\lambda| + \frac{4}{35}\epsilon^{3/2} \right) |A_1| \right\}$$

$$|y'(0) - (A_1 + \epsilon(\lambda + \epsilon^{3/2})A_0)| \leq \frac{\epsilon^2}{1 - \epsilon^2(|\lambda| + \frac{2}{5}\epsilon^{3/2})} \left\{ \left( \frac{1}{2} \epsilon(|\lambda| + \epsilon^{3/2}) |\lambda| + \frac{2}{5}\epsilon^{3/2} + \frac{3}{5}\sqrt{\epsilon} \right) |A_0| + \epsilon \left( \frac{1}{2} |\lambda| + \frac{4}{35}\epsilon^{3/2} \right) |A_1| \right\}.$$

This gives an enclosure

$$m(1 + i) = 0.345229^{40}_1 + 0.705227^{85}_1i.$$

We have investigated the possibility of choosing $f$ and $g$ to be the second-order Taylor polynomials. However, for both the examples that we have considered there appears to be no improvement in the bound over that achieved by linear functions $f, g$.

References

[1] B. M. Brown, W. D. Evans, V. G. Kirby, and M. Plum. Safe numerical bounds for the Titchmarsh-Weyl $m(\lambda)$-function. Math. Proc. Camb. Phil. Soc., 113:583–599, 1993.

[2] H. Weyl. Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen. Math. Annln., 68:220–269, 1910.

[3] C. Bennewitz and W. N. Everitt. Some remarks on the Titchmarsh-Weyl $m$-coefficient. In A tribute to Ake Pleijel, Proc. Pleijel conference, Uppsala, pages 49–108. Department of Mathematics, University of Uppsala, 1980.

[4] J. Chaudhuri and W. N. Everitt. On the spectrum of ordinary second-order differential operators. Proc. Roy. Soc. Edin., A(68):95–119, 1968.

[5] W. N. Everitt. On an extension to an integro-differential inequality of Hardy, Littlewood and Polya. Proc. Roy. Soc. Edin., A:295–333., 1971/72.

[6] B. M. Brown, V. G. Kirby, and J. D. Pryce. Numerical determination of the Titchmarsh-Weyl $m$-coefficient and its application to HELP inequalities. Proc. Roy. Soc. Lond., (A)(380):167–188, 1989.

[7] B. M. Brown, V. G. Kirby, and J. D. Pryce. A numerical determination of the $m$-coefficient. Proc. Roy. Soc. Lond., 425(A):535–549, 1991.

[8] B. M. Brown, M. S. P. Eastham, W. D. Evans, and V. G. Kirby. Repeated diagonalization and the numerical computation of the Titchmarsh-Weyl $m(\lambda)$ function. Proc. Roy. Soc. Lond. A, 445:113–126, 1994.

[9] M. S. P. Eastham. The asymptotic solution of linear differential systems. London Math. Soc. Monographs 4. Clarendon Press, Oxford, 1989.
[10] B. M. Brown, M. S. P. Eastham, W. D. Evans, and D. K. R. McCormack. Approximate diagonalization in differential systems and an effective algorithm for the computation of the spectral matrix. *Math. Proc. Camb. Phil. Soc.*, 121:495–517, 1997.

[11] G. Alefeld and J. Herzberger. Introduction to interval computations. Academic Press, New York and London, 1983.

[12] R. Lohner. Einschliessung der Lörenlicher Anfangs- und Randwertaufgaben und Anwendungen. PhD thesis, Universität Karlsruhe, 1988.

[13] E. C. Titchmarsh. Eigenfunction expansions, Part I. (2nd ed.) Clarendon Press, Oxford, 1962.

[14] I. J. Thompson and A. R. Barnett. Modified Bessel functions $i_\nu(z)$ and $k_\nu(z)$ of real order and complex argument, to selected accuracy. *Comput. Phys. Comm.*, 47:245–257, 1987.

[15] H. Kuki. Complex gamma function with error control. *Comm ACM.*, 15:262–267, 1972.

[16] B. M. Brown, W. D. Evans, W. N. Everitt, and V. G. Kirby. *Two integral inequalities*. WSSIAA 3, World Scientific Publishing Company, 1994.

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