The Liouville-Neumann approximation of the regular solutions of the standard, the confluent and the biconfluent Heun’s differential equations

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Resumen

In this work, we apply the Liouville-Neumann expansion at a regular singular point [2] to approximate the regular solution at the origin of the standard, the confluent and the biconfluent Heun’s differential equations. We design a sequence of elementary functions that converges uniformly over compacts containing the origin to the given Heun’s function. This sequence (Liouville-Neumann expansion) is defined by means of an integral recurrence. Several numerical experiments show that the convergence of the Liouville-Neumann expansion is extraordinarily fast.

1. Introduction

The standard canonical natural form of the Heun’s equation reads [[1], Chap. 3, eq. (3.1.1)]

\[
x(x-1)(x-s)y'' + [c(x-1)(x-s) + dx(x-s)]y' + (abx - \lambda)y = 0,
\]

where, for simplicity in the exposition we consider $a$, $b$, $c$, $d$, $s$ and $\lambda$ to be real parameters. This equation has two fixed regular singular points at $x = 0$, $x = 1$, a movable regular singular point at $x = s$ and an irregular singular point at $x = \infty$.

By means of different confluence processes of singular points we can obtain several confluent equations from the general Heun equation (1). We consider here two of them, the singly confluent Heun’s equation [[1], Chap. 3, eq. (3.1.3)]

\[
x(x-1)y'' + [dx - sx(x-1) + c(x-1)]y' + (\lambda - sax)y = 0,
\]
and the biconfluent Heun’s equation \([1], \text{Chap. 3, eq. (3.1.11)}\]

\[
xy'' + (c - x^2 - sx)y' + (\lambda - ax)y = 0.
\]  
\(3\)

(2) is obtained from (1) by a confluence process of the singular points at \(x = s\) and \(x = \infty\). After this confluence process the number of parameters is reduced to five. (3) is obtained from (2) by a confluence process of the singular points at \(x = 1\) and \(x = \infty\). After this confluence process the number of parameters is reduced to four.

These kind of differential equations appear in several problems of quantum mechanics. After separating the Schrödinger equation in angular and radial variables, the radial differential equation may be related to one of the Heun’s differential equations for several potentials like for example the \(x^4\) or \(x^6\) harmonic oscillators, the confluent potential \(Ax^2 + Bx - Cx^{-1}\), or other potentials with other combinations of Coulomb and centrifugal terms, rotating oscillators, scattering problems on paraboloids, etc.

In [2] we have proposed a new Liouville-Neumann algorithm to approximate the regular solution at \(x = 0\) of linear second order differential equations having a regular singular point at \(x = 0\). As it is shown in [2], this kind of approximation gives more uniform approximations of the solution than the Frobenius method. In this paper we apply the method introduced in [2] to the three equations (1), (2) and (3) to obtain sequences of functions that converge uniformly over compacts to the regular solutions at the origin (Heun’s functions) of these equations.

2. The Liouville-Neumann expansion at a regular singular point

Consider the initial value problem:

\[
\begin{cases}
  x\varphi(x)y'' + f(x)y' + g(x)y = 0, \\
  y(0) = y^0,
\end{cases}
\]  
\(4\)

where \(y^0 \in \mathbb{R}; \varphi''(x), f'(x), g(x) \in C[0,X]; X > 0\) and \(\varphi(x) > 0\) in \([0,X]\). Define the function

\[
\phi(x) := \frac{[f(0) - \varphi(0)]y^0}{\varphi(x)}
\]  
\(5\)

and the operator \(T : C[0,X] \rightarrow C^{(1)}[0,X]\) by means of the formula

\[
(Ty)(x) = \int_0^1 k(x,t)y(xt)dt,
\]

\[
k(x,t) := \frac{1}{\varphi(x)} \left\{ 2\varphi(xt) + 2(xt)\varphi'(x) - f(xt) + x(1-t)[f'(xt) - g(xt) - 2\varphi'(xt) - (xt)\varphi''(xt)] \right\}.
\]  
\(6\)

We have the following theorem proved in \([2], \text{Theorem 2}\),

**Theorem 1.** Assume \(\varphi(0) < f(0) < 3\varphi(0)\) and \(x \in [0,X]\). Then:

(i) The recurrence

\[
y_0(x) \quad \text{any continuous function on } [0,X],
\]

\[
y_n(x) = \phi(x) + (Ty_{n-1})(x), \quad n = 1, 2, 3, \ldots
\]  
\(7\)
converges uniformly on \([0, X]\) to the unique solution of (4).

(ii) If \(0 < f(0) < 4\phi(0)\), then the recurrence (7) converges uniformly on \([0, X]\) to the unique solution of (4) if we chose the initial seed \(y_0(x)\) satisfying \(y_0(0) = y^0\).

The convergence window (1, 3) or (0, 4) for \(f(0)/\phi(0)\) given in this theorem may be opened by choosing the initial seed \(y_0(x)\) close enough to the unique solution \(y(x)\) of (4): when we choose the initial seed \(y_0(x)\) to be the Taylor polynomial of \(y(x)\) at \(x = 0\). This is shown in [[2], Theorem 3]:

**Theorem 2.** Consider the recurrence (7) with \(y_0(x) = p_m(x), \ p_m(x)\) being the Taylor polynomial of degree \(m - 1\) at \(x = 0\) of the solution \(y(x)\) of (4):

\[
\begin{align*}
y_0(x) &= p_m(x), \\
y_n(x) &= \phi(x) + (T y_{n-1})(x), \quad n = 1, 2, 3, \ldots,
\end{align*}
\]

Then, the recursion (8) converges uniformly on \([0, X]\) to the unique solution of (4) if \((1 - m)\phi(0) < f(0) < (2 + m)\phi(0)\).

### 3. The Liouville-Neumann expansions of the Heun functions

In this section we use Theorem 1(ii) to obtain sequences of functions that converge uniformly on compacts to the regular solution at \(x = 0\) of equations (1), (2) and (3). An explicit representation of any of these functions is not known and then, it is not possible to compare the approximations supplied by Theorem 1 with an evaluation of that explicit representation. Instead, we compare those approximations with (i) the Taylor approximation supplied by the Frobenius methods and (ii) a numerical solution supplied by the following scheme in differences:

\[
\begin{cases}
x_i \phi(x_i) \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} + f(x_i) \frac{y_{i+1} - y_i}{h} + g(x_i)y_i = 0, \\
y_0 = y(0) = 1, \\
y_{-1} = y(0) - hy'(0) = 1 + h \frac{g(0)}{\phi'(0)}, \quad |h| << 1,
\end{cases}
\]

designed for initial value problems of the form (4).

#### 3.1. The standard Heun’s equation

The initial value problem obtained from (1) when we add the initial condition \(y(0) = 1\) is of the form (4) with \(\phi(x) = (x - 1)(x - s), \ f(x) = c(x - 1)(x - s) + dx(x - s) + (a + b + 1 - c - d)x(x - 1)\) and \(g(x) = abx - \lambda\). From Theorem 1(ii) with \(y_0(x) = y(0) = 1\) we find that the recurrence (8) reads

\[
\begin{align*}
y_0(a, b, c, d, s, \lambda; x) &= 1, \\
y_n(a, b, c, d, s, \lambda; x) &= \frac{s(c-1)x}{(x-1)(x-s)} + \\
&\quad \int_0^1 \frac{1}{(s-x)(x-t)} \left\{ s(-2 + (-2 + d + 6t - 2dt)x + c(1 + x - 2tx)) + \\
&\quad + x \left[ -1 - d - \lambda + 4t + 2dt + \lambda t + 6tx - 11t^2x + b (1 + 3\lambda^2x - 2tx + 1) + \\
&\quad a (1 - (b - 3)x + t (-2 + (b - 2)x)) \right] \right\} y_{n-1}(x)dt,
\end{align*}
\]

\[(10)\]
This sequence of functions \( y_n(a, b, c, d, s, \lambda; x) \) converges to the unique solution of initial value problem obtained from (1), the Heun’s function \( y_H(a, b, c, d, s, \lambda; x) \), for \( 0 < c < 4 \) uniformly in \( x \) on compacts of \( \mathbb{R} \) located on the left of \( \text{Min}\{s, 1\} \) if \( s > 0 \) or located between \( s \) and 1 if \( s < 0 \). We can see from the above recurrence that \( y_n(a, b, c, d, s, \lambda; x) \) are linear combinations of rational functions and polylogarithms. For example \( y_1(a, b, c, d, s, \lambda; x) \) reads

\[
y_1(a, b, c, d, s, \lambda; x) = \frac{6s(x-1) + x(6 - 3\lambda - 4x + abx)}{6(s-x)(x-1)}.
\]

In Figure 1 we compare the Taylor approximation, the numerical solution supplied by (9) and the Liouville-Neumann approximation.

Figura 1: The approximation to the Heun’s function given by the difference method (9) (green) with \( h = 0.005 \), and \( a = 1, b = 1.5, c = 2, d = 3, s = 4, \lambda = 5 \), the Taylor approximation \( y_H^{(5)}(1,1,5,2,3,4,5;x) \) (blue) and the Liouville approximation \( y_2(1,1,5,2,3,4,5;x) \) (red)

**3.2. The confluent Heun’s equation**

The initial value problem obtained from (2) when we add the initial condition \( y(0) = 1 \) is of the form (4) with \( \varphi(x) = x - 1, f(x) = sx(1-x) + c(x-1) + dx \) and \( g(x) = \lambda - axs \). From Theorem 1(ii) with \( y_0(x) = y(0) = 1 \) we find that the recurrence (8) reads

\[
\begin{align*}
y_0(a, c, d, s, \lambda; x) &= 1, \\
y_n(a, c, d, s, \lambda; x) &= \frac{c-1}{1-x} + \int_0^1 \frac{1}{1-x} \left\{ 2 - 4xt - sx^2t^2 + sxt + cxt - c + dx \right. \\
&\quad \left. + (1-t)(-sx + 2sx^2t - cx - dx + \lambda x - sax^2t + 2x) \right\} y_{n-1}(xt) dt,
\end{align*}
\]

\( n = 1, 2, 3, \ldots \). This sequence of functions \( y_n(a, c, d, s, \lambda; x) \) converges to the unique solution of initial value problem obtained from (2), the confluent Heun’s function \( y_C(a, b, c, d, s, \lambda; x) \),
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for $0 < c < 4$ uniformly in $x$ on compacts of $\mathbb{R}$ located on the left of $x = 1$. We can see from the above recurrence that $y_n(x)$ are linear combinations of rational functions and polylogarithms. For example $y_1(a, c, d, s, \lambda; x)$ and $y_2(a, c, d, s, \lambda; x)$ read

$$y_1(a, c, d, s, \lambda; x) = 1 + \frac{3\lambda x - asx^2}{6(1-x)}$$

$$y_2(a, c, d, s, \lambda; x) = \frac{c - 1}{4} + \frac{1}{2(x-1)} \left\{ -144 + 48as - 24ads + 12as^2 - 12a^2s^2 \\ + 18\lambda^2(x - 2) + 72x - 6as^2x + 6a^2s^2x + 24asx^2 - 2adsx^2 - 2as^2x^2 + 2a^2s^2x^2 \\ + as^2x^3 + a^2s^2x^3 + 2c \left[ 36 + 18\lambda - as(6 - 3x + x^2) \right] + 2\lambda \left[ 36d - 36(2 + x) \\ - s(-9(-2 + x) + 4a(-6 + 3x + x^2)) \right] + \frac{12}{\pi} (3\lambda - as) \\ \times (-4 + c - \lambda - s + as - d(-2 + x) + 2x - cx + \lambda x + sx - asx) \log(1 - x) \right\}. \quad (12)$$

In Figure 2 we compare (i) the Taylor approximation supplied by the first $n$ terms, the numerical solution supplied by (9) and the Liouville-Neumann approximation supplied by (12).

![Figura 2](image)

Figura 2: The approximation to the confluent Heun’s function given by the difference method (9) (green) with $h = 0.005$, and $a = 1$, $c = 2$, $d = 3$, $s = 4$, $\lambda = 5$, the Taylor approximation $y_C^5(1, 2, 3, 4, 5; x)$ (blue) and the Liouville approximation $y_3(1, 2, 3, 4, 5; x)$ (red)

### 3.3. The biconfluent Heun’s equation

The initial value problem obtained from (3) when we add the initial condition $y(0) = 1$ is of the form (4) with $\varphi(x) = 1$, $f(x) = c - x^2 - sx$ and $g(x) = \lambda - ax$. From Theorem 1(ii) with $y_0(x) = y(0) = 1$ we find that the recurrence (8) reads

$$\begin{cases} 
 y_0(a, c, s, \lambda; x) = 1, \\
 y_n(a, c, s, \lambda; x) = c - 1 + f_0^1 \left\{ 2 + (xt)^2 + sx - c \\ + (1 - t)x [(a - 2)xt - s - \lambda] \right\} y_{n-1}(xt) dt, \end{cases} \quad (13)$$
This sequence of functions $y_n(a, c, s, \lambda; x)$ converges for $0 < c < 4$ uniformly in $x$ on compacts of $\mathbb{R}$. It is easy to show by induction over $n$ that $y_n(a, c, s, \lambda; x)$ are polynomials in $x$ of degree $2n$:

$$y_n(a, c, s, \lambda; x) = \sum_{k=0}^{2n} a_k^{(n)} x^k,$$

where, for $n = 1, 2, 3, \ldots$,

$$a_0^{(n)} = 1, \quad a_{2n}^{(n)} = \frac{2^n}{(2n+1)!} \left( \frac{n}{2} \right)_n$$

and

$$a_k^{(n)} = \frac{2-c}{k+1} a_k^{(n-1)} + \frac{s(k-1)-\lambda}{k(k+1)} a_{k-1}^{(n-1)} + \frac{k-2+a}{k(k+1)} a_{k-2}^{(n-1)}$$

for $k = 1, 2, 3, \ldots, 2n - 1$.

In Figure 3 we compare the Taylor approximation, the numerical solution supplied by 9 and the Liouville-Neumann approximation supplied by 14.

![Figure 3: The approximation to the biconfluent Heun’s function given by the difference method 9 (green) with $h = 0.005$, and $a = 2$, $c = 1.5$, $s = 1.5$, $\lambda = 0.5$, the Taylor approximation $y_B^{(10)}(2, 1.5, 1.5, 0.5; x)$ (blue) and the Liouville approximation $y_{10}(2, 1.5, 1.5, 0.5; x)$](image)

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**References**
