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# Numerical methods and asymptotic error expansions for the Emden–Fowler equations

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## Abstract

In the present paper we analyse a numerical method for computing the solution of some boundary-value problems for the Emden–Fowler equations. The differential equations are discretized by a finite-difference method and we derive asymptotic expansions for the discretization error. Based on these asymptotic expansions, we use an extrapolation algorithm to accelerate the convergence of the numerical method.

*Keywords:* Boundary-value problem; Finite-difference method; Asymptotic error expansion; Extrapolation method

*AMS classification:* 65L12; 65B05

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## 1. Introduction

Recently, we have analysed in [6] the use of convergence acceleration techniques to improve the accuracy of finite-difference schemes. There we considered a boundary-value problem (BVP) for a second-order linear differential equation on the interval  $[0, 1]$ :

$$\frac{d}{dx} \left( k_1 \frac{du}{dx} \right) - k_2 u = f, \quad (1.1)$$

$$u(0) = u(1) = 0, \quad (1.2)$$

where the coefficients  $k_1$  and  $k_2$  are piecewise smooth functions in  $[0, 1]$  and the right-hand side  $f$  is a function that is smooth in  $]0, 1[$  but may be unbounded or have unbounded derivatives near the boundary. For the case when  $f(x) = x^\alpha(1-x)^\beta$ ,  $\alpha$  and  $\beta$  being real numbers, greater than  $-2$ , we have derived asymptotic expansions for the error of the usual finite-difference method and used the E-algorithm of Brezinski [1] to accelerate the convergence of the method. The performance of this scheme was illustrated by several numerical examples.

Although this method was not designed for any specific physical problem, it turns out that similar problems with singularities arise in many applications. For example, in [9, 10] numerical methods for the Thomas–Fermi problem and other related BVPs have been considered. As it is pointed out in these papers, the main trouble when solving numerically that equation results from the existence of a degeneracy at the endpoint 0. Although the scheme we developed in [6] for linear problems with singularities is not directly applicable to that problem (the Thomas–Fermi equation is nonlinear), it is clear that the nature of the mathematical problem is essentially the same.

The aim of the present work is to generalize the scheme, developed in [6], to the case of non-linear degenerate BVP. As an important case, we shall consider a generalization of the Emden–Fowler equation with the form:

$$\frac{d^2 y}{dx^2} + cx^p y^q = 0, \quad x \in ]0, 1[ , \quad (1.3)$$

where  $p$ ,  $q$  and  $c$  are real numbers,  $p < -2$ ,  $q > 1$ . We shall be concerned about the solution of (1.3) which satisfies the boundary conditions:

$$y(0) = 1; \quad y(1) = 0. \quad (1.4)$$

We are specially interested in the case when  $-2 < p < 0$ . In this case the equation is said to be degenerate. When  $q = \frac{3}{2}$ ,  $p = -\frac{1}{2}$ ,  $c = -1$ , (1.3) becomes the Thomas–Fermi equation, studied in [9, 10]. Using the definition given in [10], the order of the degeneracy of  $y(x)$  at  $x = 0$  depends on the limit

$$\lim_{x \rightarrow 0} \{y^{(R)}(x)x^S\},$$

where  $R$  is an integer and  $S$  is a rational number ( $0 < S \leq 1$ ). The degeneracy is said to be of order  $(r, s)$  if  $r$  is the minimal value of  $R$ , for which  $y^{(R)}(0)$  is infinite, and  $s$  is the smallest value of  $S$  for which the considered limit is finite (when  $R = r$ ). According to this definition, the order of the degeneracy for problem (1.3)–(1.4) is  $(2, -p)$ , if  $-1 < p < 0$ , and  $(1, -1 - p)$ , if  $-2 < p < -1$ . The numerical scheme, presented in [10], is not applicable to this last case, when the convergence of the usual numerical methods is particularly slow. Therefore, the use of convergence acceleration techniques seems to be the best way to obtain accurate numerical solutions in this case.

The present study may find application in the numerical solution of many problems, where the Emden–Fowler equation arises. Such problems are known, for example, in astrophysics, gas and fluid dynamics, nuclear physics and chemical reactions. A summary of the historical developments of the Emden–Fowler equation may be found in [14], where an excellent bibliography on its applications in mechanics and physics is also given. The problem about the existence and uniqueness of solution of different kinds of boundary-value problems for the Emden–Fowler equation has been studied by several authors; very interesting surveys on this theme are given in [5, 14].

As discussed in [10], the solution of the problem (1.3)–(1.4) may be numerically approximated by iterative processes, where each iterate is the solution of a linear BVP. One of the most frequently used iterative methods is the Picard method. In Section 2, we derive asymptotic expansions for the Picard iterates near the origin in the case  $p = -\frac{1}{2}$ ,  $p = -1$ ,  $p = -\frac{5}{4}$ . In Section 3 these results are used to obtain asymptotic expansions for the discretization error of the finite-differences method, when applied to the considered BVP. In Section 4, we use the E-algorithm of Brezinski to accelerate the convergence of the numerical solutions obtained by a finite-difference method, for the three cases

referred to above. The use of the E-algorithm is based on the asymptotic expansion, obtained in the previous section. The results for the case  $p = -\frac{1}{2}$  are compared with the ones obtained in [10].

## 2. Asymptotic expansions of the Picard iterates near the singularity

In order to approximate the solution of the nonlinear BVP (1.3)–(1.4), we shall use well-known iterative schemes, based on the Picard and the Newton methods [10]. This means that the solution of this problem is considered as the limit of a sequence of functions, each of them being the solution of a linear BVP. In the case of the Picard sequence, we start with an initial function,  $y_0(x) \equiv 0$  or  $y_0(x) = 1 - x$ , and define each subsequent iterate as the solution of the following BVP:

$$y_v''(x) + cqx^p y_v(x) = x^p (-c y_{v-1}(x)^q - q y_{v-1}(x)), \quad 0 < x < 1, \tag{2.1}$$

$$y_v(0) = 1, \quad y_v(1) = 0; \quad v = 1, 2, \dots \tag{2.2}$$

### 2.1. The homogeneous equation

We shall consider only the case of rational  $p$  and  $q$ , that is,  $p = -m/n$ ,  $q = m'/n$ , with  $m, n \in \mathbb{N}$ . Then, since  $p > -2$  and  $q > 1$ , we shall have  $m < 2n$ ,  $m' > n$ . In the present section we shall study the asymptotic behaviour of the solution of (2.1)–(2.2) near the singularity at  $x = 0$ . Therefore we shall begin by analysing the linear homogeneous equation, associated to (2.1):

$$y'' + cqx^p y = 0, \quad 0 < x < 1. \tag{2.3}$$

Introducing the new variable  $x = t^n$  and multiplying both sides of (2.3) by  $t^{2n}$  gives

$$\frac{1}{n^2} \left( t^2 \frac{d^2 y}{dt^2} + (1 - n)t \frac{dy}{dt} \right) + cqt^{2n-m} y = 0, \quad 0 < t < 1. \tag{2.4}$$

Eq. (2.4) has a regular singular point at  $t = 0$ . The asymptotic behaviour of its solutions near this point may be studied by well-known methods, discussed, for example, in [3, pp. 13–15; 11, Section 13.3]. Let us write the general solution of (2.4) in the form

$$y(t) = C_1 y_1(t) + C_2 y_2(t), \tag{2.5}$$

where  $y_1$  and  $y_2$  are particular solutions of (2.4), forming a linear independent system in  $[0, 1]$ . In order to obtain an asymptotic expansion for each of these solutions, we must solve the corresponding indicial equation

$$\rho(\rho - 1) + (1 - n)\rho = 0,$$

whose roots are  $\rho_1 = n$ ,  $\rho_2 = 0$ . Since these roots differ by an integer, the solutions  $y_1(t)$  and  $y_2(t)$  should be of the form

$$y_1(t) = t^n \phi_1(t), \tag{2.6}$$

$$y_2(t) = a y_1(t) \ln t + \phi_2(t), \tag{2.7}$$

where  $a$  is a real constant,  $\phi_1$  and  $\phi_2$  are analytical functions of  $t$ , allowing power series expansions in a neighbourhood of 0:

$$\phi_1(t) = \sum_{k=0}^{\infty} a_k t^k, \quad (2.8)$$

$$\phi_2(t) = \sum_{k=0}^{\infty} b_k t^k. \quad (2.9)$$

Substituting (2.6) in (2.4) yields a linear system of equations. This system gives us recursive formulae, from which we can obtain successively all the coefficients  $a_k$  ( $k = 1, 2, \dots$ ), after giving an arbitrary value to  $a_0$  (for example  $a_0 = 1$ ). This gives the particular solution  $y_1$ . The particular solution  $y_2$  can be obtained in the same way.

Substituting  $t = x^{1/n}$  into (2.6) and (2.7) and using (2.8) and (2.9), we may now obtain the particular solutions  $y_1$  and  $y_2$  in terms of the variable  $x$ :

$$y_1(x) = x \sum_{k=0}^{\infty} a_k x^{k/n}, \quad (2.10)$$

$$y_2(x) = a' y_1(x) \ln x + \sum_{k=0}^{\infty} b_k x^{k/n}, \quad (2.11)$$

where  $a' = a/(\ln n)$ .

Knowing  $y_1$  and  $y_2$ , we may obtain any solution of (2.3) as a linear combination of them. In particular, the solution satisfying the boundary conditions (2.2) can be obtained if we choose the constants  $C_1$  and  $C_2$  in (2.5) so that these conditions are satisfied.

Let us now consider particular cases.

*Case 1:*  $p = -\frac{1}{2}$  ( $m = 1, n = 2$ ). In this case the coefficients  $a_k$  in the right-hand side of (2.10) are given by the explicit formulae

$$\begin{aligned} a_k &= [-4cq/k(k+2)] a_{k-3}, \quad \text{if } k \text{ is a multiple of 3,} \\ a_k &= 0, \quad \text{if } k \text{ is not a multiple of 3.} \end{aligned} \quad (2.12)$$

The constant  $a'$  on the right-hand side of (2.11) may be shown to be 0 and the  $b_k$ 's may be obtained by

$$\begin{aligned} b_k &= [-4cq/k(k-2)] b_{k-3}, \quad \text{if } k \text{ is a multiple of 3,} \\ b_k &= 0, \quad \text{if } k \text{ is not a multiple of 3.} \end{aligned} \quad (2.13)$$

Therefore, (2.10) and (2.11) may be in this case rewritten as

$$y_1(x) = x \sum_{k=0}^{\infty} a_{3k} x^{(3k)/2}, \quad (2.14)$$

$$y_2(x) = \sum_{k=0}^{\infty} b_{3k} x^{(3k)/2}, \quad (2.15)$$

where  $a_{3k}$  and  $b_{3k}$  are given by (2.12) and (2.13), respectively.

Case 2:  $p = -1$ . In this case it follows from (2.10) and (2.11) that the general solution of (2.4) may be expressed as

$$y(x) = b_0 + \sum_{k=0}^{\infty} a_k x^{k+1} \ln x + \sum_{k=1}^{\infty} b_k x^k, \tag{2.16}$$

where  $b_0$  and  $b_1$  are arbitrary constants,  $a_0 = -cq b_0$  and the remaining coefficients satisfy the relations

$$a_k = \frac{-qc}{(k+1)k} a_{k-1}, \quad k = 1, 2, \dots, \tag{2.17}$$

$$b_k = \frac{-qcb_{k-1} - (2k-1)a_k}{k(k-1)} \quad k = 2, 3, \dots \tag{2.18}$$

In particular, when  $b_0 = 0, b_1 = 1$ , the solution (2.16) is of the form (2.10); if  $b_0 \neq 0$ , the solution becomes a function with an expansion of the form (2.11).

Case 3:  $p = -\frac{5}{4}$  ( $m = 5, n = 4$ ). In this case, the coefficients  $a_k$  in the right-hand side of (2.10) are given by

$$\begin{aligned} a_k &= [-16cq/k(k+4)] a_{k-3}, \quad \text{if } k \text{ is a multiple of } 3, \\ a_k &= 0, \quad \text{if } k \text{ is not a multiple of } 3. \end{aligned} \tag{2.19}$$

The constant  $a'$  in the right-hand side of (2.11) may be shown to be 0 and the coefficients  $b_k$  in the same formula are given by the recurrence relations:

$$\begin{aligned} b_k &= [-16cq/k(k-4)] b_{k-3}, \quad \text{if } k \text{ is a multiple of } 3, \\ b_k &= 0, \quad \text{if } k \text{ is not a multiple of } 3. \end{aligned} \tag{2.20}$$

Therefore, (2.10) and (2.11) may be in this case rewritten as

$$y_1(x) = x \sum_{k=0}^{\infty} a_{3k} x^{(3k)/4}, \tag{2.21}$$

$$y_2(x) = \sum_{k=0}^{\infty} b_{3k} x^{(3k)/4}, \tag{2.22}$$

with  $a_k$  and  $b_k$  given by (2.19) and (2.20).

### 2.2. The nonhomogeneous equation

When the Picard iterative scheme is used to approximate the solution of the nonlinear problem (1.3)–(1.4), starting with the initial approximation  $y_0(x) \equiv 0$ , the first iterate  $y_1(x)$  is obtained by solving the linear homogeneous equation (2.3), studied above, with the boundary conditions (2.2). The subsequent iterates  $y_v(x), v = 2, 3, \dots$ , are obtained by solving the nonhomogeneous equation (2.1). This equation must also be solved to obtain  $y_1(x)$ , if  $y_0(x)$  is not equal to 0 in  $[0, 1]$ . Therefore, to analyse the properties of the Picard iterates approximating the nonlinear problem (1.3)–(1.4) we must study a nonhomogeneous equation of the general form

$$y''(x) + cqx^p y(x) = f(x), \tag{2.23}$$

where  $f(x)$  is a given function (depending on the previous iterate and on  $q$ ). We shall look for the solution of (2.23) which satisfies the boundary conditions (2.2). This solution may be expressed in the form

$$y(x) = \int_0^1 G(x, x') f(x') dx' + \frac{\beta(x)}{\beta(0)}, \tag{2.24}$$

where  $G(x, x')$  is the Green function of the considered BVP, given by

$$G(x, \xi) = \begin{cases} \alpha(x)\beta(\xi)/\alpha(1), & \text{if } x \leq \xi, \\ \alpha(\xi)\beta(x)/\alpha(1), & \text{if } x > \xi, \end{cases} \tag{2.25}$$

$\alpha$  and  $\beta$  being the solutions of the homogeneous equation (2.3) which satisfy the conditions

$$\alpha(0) = 0, \quad \alpha'(0) = 1, \tag{2.26}$$

$$\beta(1) = 0, \quad \beta'(1) = -1. \tag{2.27}$$

If we substitute (2.25) into (2.24), we obtain

$$y(x) = \frac{\beta(x)}{\alpha(1)} \int_0^x \alpha(\xi) f(\xi) d\xi + \frac{\alpha(x)}{\alpha(1)} \int_x^1 \beta(\xi) f(\xi) d\xi + \frac{\beta(x)}{\beta(0)}. \tag{2.28}$$

The following lemma gives the asymptotic expansion for the solution of the nonhomogeneous equation (2.23), in the functions  $\alpha$ ,  $\beta$  and  $f$  satisfying certain conditions.

**Lemma 2.1.** *Let  $p$  and  $q$  be rational numbers,  $p = -m/n > -2$ ,  $q = m'/n > 1$ . Suppose that the solutions  $\alpha$  and  $\beta$  of the homogeneous equation (2.3) have representations of the form*

$$\alpha(x) = \sum_{k=n}^{\infty} \alpha_k x^{k/n}, \tag{2.29}$$

and

$$\beta(x) = \beta(0) + \sum_{k=2n-m}^{\infty} \beta_k x^{k/n} \quad (\text{if } m > n), \tag{2.30}$$

$$\beta(x) = \beta(0) + \beta_n x + \sum_{k=2n-m}^{\infty} \beta_k x^{k/n} \quad (\text{if } m < n). \tag{2.31}$$

Let  $f(x)$  be a function having an asymptotic expansion of the form

$$f(x) \sim \sum_{k=-m}^{\infty} f_k x^{k/n} \quad (\text{as } x \rightarrow 0). \tag{2.32}$$

Then the solution of equation (2.23) which satisfies the boundary conditions (2.2) may be expanded in a neighbourhood of  $x = 0$  as follows:

$$y(x) = 1 + \sum_{k=2n-m}^{\infty} y_k x^{k/n} \quad (\text{if } m > n), \tag{2.33}$$

or

$$y(x) = 1 + y_n x + \sum_{k=2n-m}^{\infty} y_k x^{k/n} \quad (\text{if } m < n). \tag{2.34}$$

**Proof.** From the conditions of the lemma, we have for the second integral on the right-hand side of (2.28) the following expansion:

$$\int_x^1 \beta(\xi) f(\xi) d\xi = \sum_{k=n-m}^{\infty} g_k x^{k/n} \quad \forall x \in ]0, 1], \tag{2.35}$$

where the  $g_k$  are real coefficients, independent of  $x$ ; therefore the following asymptotic expansion holds:

$$\alpha(x) \int_x^1 \beta(\xi) f(\xi) d\xi = \sum_{k=2n-m}^{\infty} \gamma_k x^{k/n} \quad \forall x \in [0, 1], \tag{2.36}$$

where the  $\gamma_k$  are coefficients, independent of  $h$ ; this last series is convergent  $\forall x \in [0, 1]$ .

Similarly we have

$$\int_0^x \alpha(\xi) f(\xi) d\xi = \sum_{k=2n-m}^{\infty} e_k x^{k/n}, \quad \text{as } x \rightarrow 0, \tag{2.37}$$

where the  $e_k$  are coefficients, independent of  $h$ ; the series is convergent  $\forall x \in [0, 1]$ . Thus we may assure that an asymptotic expansion of the following form holds:

$$\beta(x) \int_0^x \alpha(\xi) f(\xi) d\xi = \sum_{k=2n-m}^{\infty} \varepsilon_k x^{k/n}, \quad \text{as } x \rightarrow 0. \tag{2.38}$$

On the other hand, from (2.30) and (2.31) it follows that

$$\frac{\beta(x)}{\beta(0)} = 1 + \frac{1}{\beta(0)} \sum_{k=2n-m}^{\infty} \beta_k x^{k/n} \quad (\text{if } m > n); \tag{2.39}$$

$$\frac{\beta(x)}{\beta(0)} = 1 + \frac{\beta_n}{\beta(0)} x + \frac{1}{\beta(0)} \sum_{k=2n-m}^{\infty} \beta_k x^{k/n} \quad (\text{if } m < n). \tag{2.40}$$

The expansion (2.33) is obtained by substituting (2.36), (2.38) and (2.39) into (2.28); in the same way, (2.34) is obtained from (2.36), (2.38) and (2.40). This concludes the proof of Lemma 2.1.  $\square$

With the help of Lemma 2.1, we may obtain the general form of the asymptotic expansion of the Picard iterates which approximate the solution of the Emden–Fowler equation (1.3)–(1.4). This will be done in the next theorem.

**Theorem 2.2.** *Let  $y_v(x)$  be the  $v$ th Picard iterate, obtained as the solution of the nonhomogeneous equation (2.1) with the boundary conditions (2.2). Suppose that the conditions (2.29), (2.30) and (2.31) are satisfied by the solutions  $\alpha$  and  $\beta$  of the homogeneous equation and that  $p, q$  satisfy the*

conditions of Lemma 2.1. Let the initial approximation  $y_0(x)$  be either  $y_0(x) \equiv 0$  or  $y_0(x) = 1 - x$ . Then  $y_n(x)$  has an asymptotic expansion of the form:

$$y_1(x) = 1 + \sum_{k=2n-m}^{\infty} y_{k,v} x^{k/n} \quad (\text{if } m > n) \tag{2.41}$$

or

$$y_1(x) = 1 + y_{n,v} x + \sum_{k=2n-m}^{\infty} y_{k,v} x^{k/n} \quad (\text{if } m < n), \quad \text{as } x \rightarrow 0, \tag{2.42}$$

where the  $y_{k,v}$  are real coefficients independent of  $x$ .

**Proof.** We shall prove this theorem by induction. Let us show that the first iterate  $y_1(x)$  satisfies (2.41) or (2.42). We have assumed that the solutions  $\alpha$  and  $\beta$  satisfy the conditions of Lemma 2.1. Moreover, in the case of Eq. (2.1), with  $v = 1$ , the right-hand side has the form

$$f(x) = x^p ((-c y_0(x))^q - q y_0(x)). \tag{2.43}$$

Therefore if  $y_0(x) \equiv 0$ ,  $f(x) \equiv 0$  and  $y_1(x)$  is the solution of the homogeneous equation (2.3); thus  $y_1(x)$  has an asymptotic expansion of the form (2.41) or (2.42), according to the results obtained above for the homogeneous equation. Suppose now that  $y_0(x) = 1 - x$ ; then

$$f(x) = x^p (-c(1-x)^q - q(1-x)). \tag{2.44}$$

Since  $q > 1$  and  $p = -m/n > -2$ , by assumption,  $f$  may be expanded in a series with the form (2.32). Therefore, the conditions of Lemma 2.1 are satisfied by  $f(x)$ ; from this lemma it follows immediately that the first Picard iterate  $y_1$  satisfies (2.41) or (2.42).

Let us now assume, by induction, that the Picard iterate  $y_\mu$  satisfies (2.41) or (2.42), for a certain  $\mu \geq 1$ . We must verify that the same condition is satisfied by  $y_{\mu+1}$ . If  $y_\mu$  may be expanded in a series of the form (2.41) or (2.42), then  $(y_\mu)^q$  may be expanded in a series of the same form. Substituting this series into the expression of  $f$ , we verify that  $f$  has an asymptotic expansion of the form (2.32). Therefore we may apply Lemma 2.1, which assures that  $y_{\mu+1}$  will also satisfy (2.41) or (2.42).  $\square$

Let us now analyse how the Theorem 2.2 may be used to obtain asymptotic expansions of the Picard iterates in some particular cases.

*Case 1:*  $p = -\frac{1}{2}$ . From the initial conditions  $\alpha(0) = 0$ ,  $\alpha'(0) = 1$ , it follows that  $\alpha = 1/a_0 y_1$ , where  $y_1$  is the solution of the homogeneous equation, given by (2.14). Therefore, we may assure that  $\alpha$  has, in this case, an asymptotic expansion of the form

$$\alpha(x) = x + \frac{a_3}{a_0} x^{5/2} + \frac{a_6}{a_0} x^4 + \dots = \sum_{k=0}^{\infty} a_{3k+2} x^{(3k+2)/2}, \tag{2.45}$$

where the  $a_k$  are the coefficients defined by (2.12). On the other hand, the solution  $\beta$  may be expressed as a linear combination of  $y_1$  and  $y_2$ , given by (2.14) and (2.15); therefore, we may write

$$\beta(x) = \sum_{k=0}^{\infty} \beta_{3k} x^{(3k)/2} + x \sum_{k=0}^{\infty} \beta_{3k+2} x^{(3k)/2} = 1 + \beta_2 x + \beta_3 x^{3/2} + \beta_5 x^{5/2} + \dots, \tag{2.46}$$



where each coefficient  $\beta_k$  is a linear combination of  $a_k$  and  $b_k$ , given by (2.12) and (2.13),  $k = 0, 1, 2, \dots$ .

Therefore, all the conditions of Theorem 2.2 are satisfied in this case and, if we start with the Picard iterative scheme with  $y_0(x) \equiv 0$  or  $y_0(x) = 1 - x$ , all the iterates will have asymptotic expansions of the form

$$y_v(x) = 1 + y_{2,v}x + \sum_{k=3}^{\infty} y_{k,v}x^{k/2}, \quad \text{as } x \rightarrow 0, \quad v = 1, 2, \dots \tag{2.47}$$

*Case 2:  $p = -1$ .* In this case, we cannot apply Theorem 2.2 directly, because the asymptotic expansion of the general solution of the homogeneous equation, obtained in (2.16), contains terms with the form  $x^k \ln x$ ,  $k = 1, 2, \dots$ .

However, based on the initial conditions satisfied by  $\alpha$ , we can say that this particular solution has a power series expansion of the form

$$\alpha(x) = \sum_{k=1}^{\infty} b_k x^k, \tag{2.48}$$

where the  $b_k$  are the coefficients given by (2.19). The solution  $\beta$ , in this case, allows an asymptotic expansion with the form (2.16) (containing terms with  $x^k \ln x$ ).

Based on (2.16) and (2.48), we may derive the asymptotic expansion of the first Picard iterate  $y_1(x)$ , knowing that the right-hand side function of the corresponding nonhomogeneous equation, in this case, has the form:

$$f(x) = x^{-1} ((-cy_0(x))^q - qy_0(x)) \sim f_{-1}x^{-1} + f_0 + f_1x + \dots \tag{2.49}$$

From here, following the same method, as in the proof of Lemma 2.1, we may show that

$$y_1(x) = 1 + y_{1,1}x \ln x + \tilde{y}_{1,1}x + y_{2,1}x^2 \ln x + \tilde{y}_{2,1}x^2 + \dots \tag{2.50}$$

Further, using mathematical induction, as in the proof of Theorem 2.2, we may obtain the asymptotic expansion of the  $v$ th Picard iterate:

$$y_v(x) = 1 + y_{1,v}x \ln x + \tilde{y}_{1,v}x + P_{1,v}(\ln x)x^2 + \dots + P_{k-1,v}(\ln x)x^k + \dots, \tag{2.51}$$

where  $P_k(y)$  is a polynomial of degree not greater than  $k$ , with constant coefficients.

*Case 3:  $\gamma = -\frac{5}{4}$ .* In this case, we can use again the Theorem 2.2 to obtain the asymptotic expansion of the Picard iterates near the origin. Actually, from (2.21) and (2.22) it follows that all the solutions of the corresponding homogeneous equations have asymptotic expansions in powers of  $x^{1/4}$ . In particular,  $\alpha$  has the asymptotic expansion

$$\alpha(x) = x \sum_{k=0}^{\infty} \alpha_{3k+4} x^{3k/4} = \alpha_4 x + \alpha_7 x^{7/4} + \alpha_{10} x^{10/4} + \dots \tag{2.52}$$

and the asymptotic expansion of  $\beta(x)$  may be written as

$$\beta(x) = \sum_{k=0}^{\infty} \beta_{3k} x^{3k/4} + x \sum_{k=0}^{\infty} \beta_{3k+4} x^{3k/4} = \beta_0 + \beta_3 x^{3/4} + \beta_4 x + \beta_6 x^{6/4} + \beta_7 x^{7/4} + \dots \tag{2.53}$$

(since  $\beta(x)$  is a linear combination of  $y_1$  and  $y_2$ , given by (2.21) and (2.22)). Therefore, the conditions of Theorem 2.2 are satisfied in the case  $p = -\frac{5}{4}$  and, by this theorem, we obtain that the Picard iterates have asymptotic expansions of the form

$$y_v(x) = \sum_{k=0}^{\infty} y_{3k,v} x^{3k/4} + x \sum_{k=0}^{\infty} y_{3k+4,v} x^{3k/4} = 1 + y_{3,v} x^{3/4} + y_{4,v} x + \dots \tag{2.54}$$

Note that, in all the examples above, the form of the expansion does not depend on the value of  $q$ . However, the coefficients  $y_{v,k}$  will obviously depend on this value.

### 3. Asymptotic expansions for the discretization error

In the present section, we shall derive asymptotic expansions for the error of the approximate solution of the boundary-value problem (1.3)–(1.4). The approximation method combines the Picard method and a finite-difference scheme. In [13], Stetter proved a very general theorem that gives sufficient conditions for the existence of an asymptotic expansion of the error of discretization algorithms. However, this theorem may not be applied in our case, due to the existence of the singularity at the boundary. Mayers [8] developed a different method for obtaining asymptotic error expansions in a paper where he analyses the discretization of boundary-value problems with singularities. Our approach is based on this last method. The existence of asymptotic error expansions for the finite-difference method in the case of linear differential equations is studied in detail in [7].

Consider now the numerical solution of the boundary-value problem (1.3)–(1.4), using the Picard method (2.1) and (2.2), which we rewrite explicitly as

$$L y_v(x) = y_v''(x) + c q x^p y_v(x) = x^p (-c y_{v-1}(x)^q - q y_{v-1}(x)) , \quad 0 < x < 1, \tag{3.1}$$

$$y_v(0) = 1, \quad y_v(1) = 0; \quad v = 1, 2, \dots \tag{3.2}$$

We select a set of  $n$  equispaced points, denoted  $X_h = \{x_1, x_2, \dots, x_n\}$ , in the interval  $[0, 1]$ , and set  $h = 1/n$ . Using a central difference approximation, we replace (3.1) and (3.2) by

$$\frac{1}{h^2} \delta_h^2 \tilde{y}_v(x_i, h) + c q \tilde{y}_v(x_i, h) x_i^p = f(x_i, \tilde{y}_{v-1}(x_i, h)), \quad i = 1, 2, \dots, n - 1, \tag{3.3}$$

$$\tilde{y}_v(0, h) = 1 ; \quad \tilde{y}_v(0, 1) = 0, \tag{3.4}$$

where

$$f(x, y) = x^p (-c y^q - q y); \tag{3.5}$$

and  $\delta_h^2$  denotes the finite-difference operator defined by

$$\delta_h^2 v(x_i, h) = v(x_{i+1}, h) - 2v(x_i, h) + v(x_{i-1}, h); \tag{3.6}$$

here and throughout the text,  $v(x, h)$  will denote a grid function, i.e., a function defined at the points of the grid  $X_h$ . In particular, if  $v(x)$  is a function, defined on  $[0, 1]$ , then  $v(x, h)$  is the grid function resulting from the evaluation of  $v(x)$  at the points of grid  $X_h$ .

Let us denote the error as

$$\Phi_v(x, h) = \tilde{y}_v(x, h) - y_v(x). \tag{3.7}$$

Our aim is to obtain an asymptotic expansion of  $\Phi_v(x, h)$ , valid as  $h \rightarrow 0$ , for  $x \in ]0, 1]$ . From the linearity of Eq. (3.1) it follows that the error of the first approximation  $\Phi_1(x, h)$  satisfies

$$L^h \Phi_1(x, h) = -\varepsilon(x, h), \tag{3.8}$$

where  $L^h$  is the finite-difference operator on the left-hand side of (3.3) and  $\varepsilon(x, h)$  denotes the local discretization error of the finite-difference scheme:

$$\varepsilon(x, h) = \frac{1}{h^2} \delta_h^2 y(x, h) - y''(x). \tag{3.9}$$

From the boundary conditions (3.2) and (3.4) we obtain

$$\Phi_1(0, h) = 0, \tag{3.10a}$$

$$\Phi_1(1, h) = 0, \quad \forall h > 0. \tag{3.10b}$$

When  $y(x)$  is sufficiently smooth in the interval  $[0, 1]$ , the local discretization error has an asymptotic expansion of the form

$$\varepsilon(x, h) = \sum_{k=1}^{M-1} \frac{2y^{(2k+2)}(x)}{(2k+2)!} h^{2k} + O(h^{2M}), \quad \forall x \in [0, 1], \quad \text{as } h \rightarrow 0. \tag{3.11}$$

Moreover, if the problem (3.1)–(3.2) has a unique solution in  $C^{2M}([0, 1])$  and the finite-difference scheme (3.3)–(3.4) is stable, it is possible to show (see, for example, [7]) that the error  $\Phi_1(x, h)$  also has an asymptotic expansion of the form

$$\Phi_1(x, h) = \sum_{k=1}^{M-1} \phi_{2k}(x) h^{2k} + O(h^{2M}), \quad \forall x \in [0, 1], \quad \text{as } h \rightarrow 0, \tag{3.12}$$

where the  $\phi_{2k}$ ,  $k = 1, 2, \dots$  are smooth functions of  $x$ , which can be determined successively, by solving a sequence of boundary-value problems.

In the present case, however, this is not possible, because the solution is not differentiable at  $x = 0$  and therefore the asymptotic expansion (3.11) does not hold for any positive  $M$ . In spite of this, it is possible to obtain an asymptotic error expansion, with a form, different from (3.11), using a method, first used in [8]. The idea of this method is the following. Since the singularity of the solution is at the boundary, more precisely, at  $x = 0$ , we consider, instead of the interval  $[0, 1]$ , the interval  $[h, 1]$ , and formulate a new boundary-value problem for this interval, whose solution coincides with the solution of (3.8) on  $[h, 1]$ . Therefore, the boundary condition (3.10a), satisfied by  $\Phi_1(x, h)$ , when  $x = 0$ , must be replaced by a different condition, when  $x = h$ . We shall now derive such a boundary condition for our case. For this purpose, we shall begin by proving the following auxiliary lemma.

**Lemma 3.1.** *Let  $y(x)$  be a function represented by a series of the form*

$$y(x) = y_0 + x^{2+p} \sum_{k=0}^{\infty} y_k x^{k/n}, \quad \forall x \geq 0, \tag{3.13}$$

where  $p = -m/n > -2$ ,  $m, n \in \mathbb{N}$ . Then the following asymptotic expansion holds, for  $x_i = ih > 0$  and  $k_{ma} \in \mathbb{N}$ :

$$\varepsilon(x_i, h) = \frac{1}{h^2} \delta_h^2 y(x_i, h) - y''(x_i) = h^p \sum_{k=1}^{k_{m1}-1} \varepsilon_k(i) h^{k/n} + O(h^{p+k_{m1}/n}), \quad i = 1, 2, \dots, \tag{3.14}$$

where the coefficients  $\varepsilon_k$  ( $k = 1, 2, \dots$ ) do not depend on  $h$ .

**Proof.** From (3.13) it follows that

$$y^{(2j+2)}(x) = y_0^{(2j+2)} x^{p-2j} + y_1^{(2j+2)} x^{p-2j+1/n} + \dots = x^{p-2j} \sum_{k=0}^{\infty} y_k^{(2j+2)} x^{k/n} \tag{3.15}$$

for  $x > 0$ , where

$$y_k^{(2j+2)} = y_k \prod_{l=0}^{2j+1} \left( 2 + p + \frac{l}{n} - 1 \right).$$

Substituting (3.15) into (3.11) yields

$$\varepsilon(x_i, h) = \sum_{j=1}^m \frac{2}{(2j+2)!} \left( x_i^{p-2j} \sum_{k=0}^{k_{ma}} y_k^{(2j+2)} x_i^{k/n} \right) h^{2j} + O(h^{2m}), \quad x_i > 0. \tag{3.16}$$

As noted before, the coefficients of  $h^{2j}$  in the right-hand side of (3.15) are unbounded, as  $x_i \rightarrow 0$ . Thus we must write the terms of the series in a different way. Substituting  $x_i = ih$ , we obtain

$$\begin{aligned} \varepsilon(x_i, h) &= h^p \sum_{j=1}^{m-1} \sum_{k=0}^{k_{ma}} \frac{2}{(2j+2)!} y_k^{(2j+2)} i^{k/n+p-2j} h^{k/n} \\ &= h^p \sum_{k=0}^{k_{ma}} i^{p+k/n} \sum_{j=1}^{m-1} \frac{2}{(2j+2)!} y_k^{(2j+2)} i^{-2j} h^{k/n} = h^p \sum_{k=0}^{k_{ma}} \varepsilon_k(i) h^{k/n} + R(h), \end{aligned} \tag{3.17}$$

where

$$\varepsilon_k(i) = i^{p+k/n} \sum_{j=1}^{m-1} \frac{2}{(2j+2)!} y_k^{(2j+2)} i^{-2j}, \tag{3.18}$$

$$R(h) = O(h^{p+k_{ma}/n}).$$

For  $i \geq 1$ , the series on the right-hand side (3.18) converges, as  $m \rightarrow \infty$ .  $\square$

**Remark.** In [9, 10], Mooney analyses the particular case of the series (3.12) when  $k = 0$ . In these papers  $\varepsilon_0(i)$  is represented by  $\sum \alpha_{rm}$ . In [9], the sum of this series is given in an explicit form, for the case  $p = -\frac{1}{2}$  and, in [10], for the more general case  $p > -1$ . As pointed out in [9], the convergence of the series is very slow, when  $i = 1$ , and very fast, for large values of  $i$ .

Using Lemma 3.1 and the results of Section 2, we may obtain an asymptotic expansion of  $\Phi_1(x, h)$ . With this purpose, we introduce a new variable  $i = x/h$  and represent the error of the numerical solution as a function of  $i$  and  $h$ :

$$\Phi_1(x, h) = \phi(i)\gamma(h), \tag{3.19}$$

where  $\phi$  depends on  $i = x/h$ , and  $\gamma$  depends only on  $h$ . If we now consider  $i$  fixed, for example  $i = 1$ , we may obtain from (3.8) the equation satisfied by  $\gamma(h)$ :

$$\frac{d^2\gamma}{dh^2} + cq h^p \gamma = \frac{\varepsilon(x_1, h)}{\phi(1)}, \quad h > 0. \tag{3.20}$$

We may obtain an asymptotic expansion of the solution of this last equation, when  $j \rightarrow 0$ , using the results of Section 2. Actually, for many values of  $p$  (in particular, for  $p = -\frac{1}{2}$  and  $p = -\frac{5}{4}$ ), the associated homogeneous equation has two independent solutions, which we may represent as  $\alpha$  and  $\beta$  and have series expansions of the forms (2.30) and (2.31), respectively. Moreover, using Lemma 3.1, we may also represent the right-hand side of (3.20) as a series:

$$\frac{\varepsilon(x_1, h)}{\phi(1)} = \frac{h^p}{\phi(1)} \sum_{k=0}^{k_{mu}} \varepsilon_k(1)h^{k/n} + R(h). \tag{3.21}$$

Therefore, we may apply Lemma 2.1, which says that the general solution of (3.20) may be represented as a series of the form

$$\gamma(h) = \gamma_0 + \gamma_1 h + \gamma_2 h^{2+p} + \gamma_3 h^{2+p+1/n} + O(h^{2+p+2/n}) \quad (\text{if } p > -1) \tag{3.22}$$

or

$$\gamma(h) = \gamma_0 + \gamma_2 h^{2+p} + \gamma_3 h^{2+p+1/n} + O(h^{2+p+2/n}) \quad (\text{if } p < -1, \text{ as } h \rightarrow 0). \tag{3.23}$$

Since  $\lim_{h \rightarrow 0} \Phi_1(x, h) = 0, \forall x \in [0, 1]$ , and  $\phi(1) \neq 0$ ,  $\gamma$  must satisfy the boundary condition

$$\lim_{h \rightarrow 0} \gamma(h) = 0. \tag{3.24}$$

Therefore the term  $\gamma_0$  is equal to zero in (3.22) and (3.23). Moreover, when  $p > -1$ , the first derivative of  $\gamma$  is continuous and its limit is zero, when  $h \rightarrow 0$ ; hence,  $\gamma_1 = 0$  in (3.22).

Introducing these simplifications in (3.22) and (3.23), we obtain

$$\gamma(h) = \gamma_2 h^{2+p} + \gamma_3 h^{2+p+1/n} + O(h^{2+p+2/n}) \quad (\text{as } h \rightarrow 0). \tag{3.25}$$

Substituting (3.25) into (3.19) yields

$$\Phi(h, h) = \phi(1)\gamma(h) = \phi(1)(\gamma_2 h^{2+p} + \gamma_3 h^{2+p+1/n} + O(h^{2+p+2/n})). \tag{3.26}$$

This last equation gives a boundary condition that may be used (instead of (3.10a)) to determine  $\Phi_1(x, h)$ .

According to the usual method for solving a linear nonhomogeneous equation, we shall represent the general solution of (3.8) as

$$\Phi_1(x, h) = a(h)\alpha(x) + b(h)\beta(x) + \tilde{\Phi}_1(x, h), \tag{3.27}$$

where  $\alpha$  and  $\beta$ , as usual, denote two independent solutions of the associated homogeneous equation;  $a$  and  $b$  are coefficients, independent of  $x$ , and  $\tilde{\Phi}_1(x, h)$  is a particular solution of the nonhomogeneous equation. If we obtain this particular solution, in the form of a series, we can determine the expansion of  $\Phi_1(x, h)$ , by substituting (3.27) into the boundary conditions (3.26) and (3.10b) and then determining  $a(h)$  and  $b(h)$  from these conditions. We shall now apply this method to the cases  $p = -\frac{1}{2}$ ,  $p = -1$  and  $p = -\frac{5}{4}$ .

Case 1:  $p = -\frac{1}{2}$ . In this case, according to (3.25), we can expand  $\gamma$  into the form

$$\gamma(h) = \gamma_1 h^{3/2} + \gamma_2 h^2 + \gamma_3 h^{5/2} + O(h^3). \quad (3.28)$$

In order to find a particular solution of the nonhomogeneous equation (3.8), we shall expand the right-hand side of that equation according to (3.11). Moreover, since the solution of (3.8) is differentiable on the interval  $[h, 1]$  (for a fixed  $h$ ), we may rewrite (3.8) as

$$\begin{aligned} & (L + h^2 L_2 + h^4 L_4 + \dots + h^{2k-2} L_{2k-2}) \Phi_1(x, h) \\ &= - \left( \frac{2y^{(4)}}{4!} h^2 + \frac{2y^{(6)}}{6!} h^4 + \dots + \frac{2y^{(2k-2)}}{(2k-2)!} h^{2k-2} \right) + O(h^{2k}), \end{aligned} \quad (3.29)$$

where the  $L_{2k}$ ,  $k = 1, 2, \dots$ , denote the coefficients of the expansion of the finite-difference operator  $L_h$  into a power series in  $h$ . Hence, we may look for a particular solution  $\tilde{\Phi}_1(x, h)$  of (3.29) of the form (3.12) and determine the coefficients  $\phi_k$  in the following way. The equation from which the main term  $\phi_2$  is obtained may be derived by equating the terms in  $h^2$  in both sides of (3.29):

$$L\phi_2(x) = -2y^{(4)}(x)/2. \quad (3.30)$$

Using the results of the previous section, we may write the right-hand side of (3.30) into the form of a power series in  $x$  and look for a particular solution of this equation also under the form of a series:

$$\phi_2(x) = \phi_{2,1} x^{-1/2} + \phi_{2,2} + \phi_{2,3} x^{1/2} + o(x^{1/2}). \quad (3.31)$$

Analogously, the subsequent coefficients  $\phi_4, \phi_6, \dots$ , may be determined under the form of a series:

$$\phi_{2n}(x) = \phi_{2n,1} x^{(1-2n)/2} + \phi_{2n,2} x^{(2-2n)/2} + \phi_{2n,3} x^{3-2n/2} + o(x^{(3-2n)/2}). \quad (3.32)$$

Once the first  $n$  terms of (3.12) have been determined, we can obtain an approximation of  $\tilde{\Phi}_1(x, h)$ , for every  $x \in [h, 1]$ :

$$\tilde{\Phi}_1(x, h) = h^2 \phi_2(x) + h^4 \phi_4(x) + \dots + h^{2n} \phi_{2n}(x) + o(h^{2n}). \quad (3.33)$$

In particular, using (3.31) and (3.32), we obtain, for  $x = h$ :

$$\tilde{\Phi}_1(h, h) = h^{3/2} c_{2,1} + h^2 c_{3,1} + h^{5/2} c_{4,1} + o(h^{5/2}), \quad (3.34)$$

where  $c_{k,1} = \sum_{j=1}^{\infty} \phi_{2j,k}$ ,  $k = 2, 3, 4$ .

Writing (3.27) with  $x = 1$ , we obtain, according to (3.10b)

$$\Phi_1(1, h) = a(h)\alpha(1) + \tilde{\Phi}_1(1, h) = 0; \quad (3.35)$$

therefore, using (3.33),

$$a(h) = -\frac{\tilde{\Phi}_1(1, h)}{\alpha(1)} = Ch^2; \tag{3.36}$$

where  $C$  does not depend on  $h$ . Moreover, from (3.27) and (3.36), we obtain

$$b(h) = [\Phi_1(h, h) - Ch^2\alpha(h) - \tilde{\Phi}_1(h, h)]/\beta(h). \tag{3.37}$$

The expression on the right-hand side of (3.37) may be represented as a series, using (3.26), (3.34) and the expansions of  $\alpha$  and  $\beta$ , obtained in Section 2. The first terms of this series are

$$b(h) = \frac{\phi(1)\gamma_1 - c_{2,1}}{\beta(0)}h^{3/2} + \frac{\phi(1)\gamma_2 - c_{3,1}}{\beta(0)}h^2 + \frac{\phi(1)\gamma_3 - c_{4,1}}{\beta(0)}h^{5/2} + o(h^{5/2}). \tag{3.38}$$

Finally, substituting (3.34), (3.36) and (3.38) into (3.27), we obtain the needed asymptotic error expansion:

$$\Phi(x, h) = C_{1,1}(x)h^{3/2} + C_{2,1}(x)h^2 + C_{3,1}(x)h^{5/2} + o(h^{5/2}) \text{ (as } h \rightarrow 0). \tag{3.39}$$

*Case 2:  $p = -1$ .* In this case, based on the results of Section 2, we may expand  $\gamma(h)$  into a series of the form

$$\gamma(h) = \gamma_1 h \ln h + \gamma_2 h + \gamma_3 h^3 (\ln h)^2 + \gamma_4 h^2 \ln h + O(h^2). \tag{3.40}$$

From here, following the same steps as in previous case, we may conclude that the first terms of the error expansion are, in this case:

$$\Phi_1(x, h) = C_{1,1}(x, x)h \ln h + C_{2,1}(x)h + C_{3,1}(x)h^2 (\ln h)^2 + C_{4,1}(x)h^2 \ln h + O(h^2). \tag{3.41}$$

*Case 3:  $p = -\frac{5}{4}$ .* In the same way as above, we may obtain the expansion of  $\gamma(h)$ , which, in this case, has the form

$$\gamma(h) = \gamma_1 h^{3/4} + \gamma_2 h + \gamma_4 h^{3/2} + \gamma_5 h^{7/4} + O(h^2). \tag{3.42}$$

From (3.42) and from an analogous expansion of  $\tilde{\Phi}_1(x, h)$ , we may obtain the form of the first terms of the error expansion:

$$\tilde{\Phi}(x, h) = C_{1,1}(x)h^{3/4} + C_{2,1}(x)h + C_{3,1}(x)h^{3/2} + C_{4,1}(x)h^{7/4} + O(h^2) \text{ (as } h \rightarrow 0). \tag{3.43}$$

**Remark.** Here we have considered only the asymptotic error expansion for the boundary-value problem (3.1)–(3.2), in the case  $\nu = 1$ , which gives the first approximation of the solution of the Emden–Fowler equation, by the Picard method. However it is easy to verify that if a given term of the Picard sequence has an asymptotic error expansion of one of the forms considered, then all the subsequent terms of the sequence will have asymptotic error expansions of the same form. This explains why extrapolation algorithms, based on the expansions obtained, may be applied to the solution of the Emden–Fowler equation approximated by the Picard sequence. The numerical results, obtained in Section 4, confirm that the asymptotic error expansions (3.39), (3.41) and (3.43) form a good basis for applying the E-algorithm to the present problem.

#### 4. Numerical results

In this section we shall present some numerical results obtained by applying a well-known extrapolation method to the solutions of the finite-difference scheme (3.1)–(3.4). These solutions were computed with different stepsizes  $h$ , using double precision arithmetics. The successive iterates of the Picard sequence were computed for each  $h$ , forming a monotone sequence:

$$y_0(x, h) \leq y_1(x, h) \leq \dots \leq y_\nu(x, h) \quad (4.1)$$

or

$$y_0(x, h) \geq y_1(x, h) \geq \dots \geq y_\mu(x, h), \quad (4.2)$$

depending on the initial approximation. The monotonicity of the sequences (4.1) and (4.2) follows from well-known results [9, 10]. Moreover, for every  $\mu, \nu$  we have

$$y_\nu(x, h) \leq y(x, h) \leq y_\mu(x, h), \quad (4.3)$$

where  $y(x, h)$  is the limit of the sequences (4.1) and (4.2). Sequences (4.1) and (4.2) are computed for a sequence of different stepsizes  $h_k = h_0/2^k$ ,  $k = 1, 2, \dots, 8$ . For each value of  $h$ , the terms of the sequences (4.1) and (4.2) were computed until the condition

$$\|y_{\nu+1}(x, h) - y_\nu(x, h)\| \leq \varepsilon \quad (4.4)$$

was satisfied, for a given  $\varepsilon$ ; here  $\|\cdot\|$  denotes the norm

$$\|u\| = \left( \sum_{i=1}^n |u(x_i)|^2 \right)^{1/2}.$$

In our computation, since we used double precision arithmetics, we set  $\varepsilon = 10^{-14}$ . Then, we verified that the approximation obtained by the sequence (4.2) (upper bound of the exact solution) is the same as that obtained by the sequence (4.1) (lower bound), within the limits of rounding-off errors. Hence we have considered this value as the solution of the nonlinear problem.

Defining the value of  $\nu$  from (4.4), we may now consider, for each gridpoint  $x_i$ , a sequence

$$y_\nu(x_i, h_0), y_\nu(x_i, h_1), \dots, y_\nu(x_i, h_7). \quad (4.5)$$

In our computations, we have used the following stepsizes:

$$h_0 = \frac{1}{30}, \quad h_k = \frac{h_{k-1}}{2}, \quad k = 1, 2, \dots, 7. \quad (4.6)$$

The sequence (4.5) was used as the initial sequence of the extrapolation process. When applying an extrapolation algorithm we obtain, from the sequence (4.5), successive transforms that may converge to the same limit  $y_\nu(x)$ . If each transform converges with an order higher than the previous one, we say that the extrapolation algorithm accelerates the convergence of the original sequence.



In order to choose the adequate extrapolation algorithm, we must know the character of the convergence of the initial sequence. One of the most used extrapolation algorithms is the Richardson extrapolation (also called deferred approach to the limit) [12]. As it is known (see, for example, [7]), the Richardson extrapolation method accelerates the convergence of the sequence (4.5) if the asymptotic error expansion has the form

$$y_v(x, h) = \sum_{k=1}^n C_k(x)h^k + \rho_{n+1}(x, h), \tag{4.7}$$

where  $\|\rho_{n+1}\| = O(h^{n+1})$  and  $C_k$  do not depend on  $h$ . This is not our case, because the asymptotic error expansions (3.39), (3.41) and (3.43) contain terms that are not integral powers of  $h$ .

When an expansion of the error is known, such as those obtained in Section 3, a natural way to accelerate the convergence of the sequence (4.5) is to use the E-algorithm of [1, 4]. This is a very general algorithm designed under the assumption that we know the asymptotic error expansion for a given sequence  $(S_n)$ :

$$S_n = S + a_1g_1(n) + a_2g_2(n) + \dots + a_kg_k(n) + \dots, \quad n = 0, 1, 2, \dots, \tag{4.8}$$

where the  $\{g_i(n)\}$  are known sequences, which satisfy the condition  $g_{i+1}(n) = o(g_i(n))$ , when  $n \rightarrow \infty$ . If  $r + 1$  terms of the sequence  $S_n$  are known, we can compute  $S$  by solving the linear system

$$S_{n+i} = S + a_1g_1(n + i) + a_2g_2(n + i) + \dots + a_kg_k(n + i), \quad i = 0, 1, \dots, r. \tag{4.9}$$

Usually the terms of  $S_n$  do not satisfy (4.8) exactly (to obtain (4.9) we must ignore the remainder of the asymptotic error expansion). Therefore, the solution of (4.9) is only an approximation of  $S$  and depends on  $n$  and  $k$ . We shall denote this value by  $E_k^{(n)}$ . The E-algorithm is a recursive way to compute  $E_k^{(n)}$ . Note that the usual algorithms for solving linear systems (such as Gaussian elimination) are not recommendable to solve (4.9), because they are numerically unstable in this case. The computation of  $E_k^{(n)}$ , using the E-algorithm, starts with

$$E_0^{(n)} = S_n, \quad n = 0, 1, 2, \dots, n_{ma}, \tag{4.10}$$

$$g_{0,i}(n) = g_i(n), \quad i = 1, 2, \dots, n_{ma}, \quad n = 1, 2, \dots, n_{ma} - 1. \tag{4.11}$$

For  $k = 1, 2, \dots, n_{ma}$ , and  $n = 0, 1, \dots, n_{ma} - k$  the recursive formulae are [1]

$$E_k^{(n)} = E_{k-1}^{(n)} + g_{k-1,k}^{(n)} \frac{E_{k-1}^{(n)} - E_{k-1}^{(n+1)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}}, \tag{4.12}$$

$$g_{k,i}^{(n)} = g_{k-1,i}^{(n)} + g_{k-1,k}^{(n)} \frac{g_{k-1,i}^{(n)} - g_{k-1,i}^{(n+1)}}{g_{k-1,k}^{(n+1)} - g_{k-1,k}^{(n)}}, \quad i = k + 1, k + 2, \dots, n_{ma}. \tag{4.13}$$

Table 1

Approximate values of the solution in the case  $p = 0.5, q = 1.5$  (Thomas–Fermi problem) at the gridpoints  $x_i = 0.1, 0.2, \dots, N$  is the total number of gridpoints used for each approximation

$x_i$	$N = 60$	$N = 480$	$N = 3840$	EXTRA
0.1	0.8497892482	0.8494898911	0.8494750906	0.8494743810
0.2	0.7275141383	0.7272451707	0.7272324534	0.7272318523
0.3	0.6195388560	0.6193058204	0.6192950221	0.6192945151
0.4	0.5206216119	0.5204239737	0.5204149288	0.5204145060
0.5	0.4277212100	0.4275577758	0.4275503624	0.4275500169
0.6	0.3388225043	0.3386922878	0.3386864222	0.3386861495
0.7	0.2525003851	0.2524027674	0.2523983962	0.2523981933
0.8	0.1677173342	0.1676520630	0.1676491563	0.1676490216
0.9	0.0837211353	0.0836882891	0.0836868348	0.0836867675

Note: The last column contains the best approximation of the solution obtained by extrapolation using the E-algorithm.

Here the  $g_{k,i}^{(n)}$  are auxiliary sequences, which depend only on the terms  $g_i(n)$  of the asymptotic expansion (4.9) The values of  $E_k^{(n)}$  are usually displayed in a double-entry array, as follows

$$\begin{aligned}
 E_{\circ}^{(0)} &= S_0; \\
 E_{\circ}^{(1)} &= S_1, E_1^{(0)}; \\
 E_{\circ}^{(2)} &= S_2, E_1^{(1)}, E_2^{(0)}; \\
 E_{\circ}^{(3)} &= S_3, E_1^{(2)}, E_2^{(1)}, E_3^{(0)}; \\
 &\dots
 \end{aligned}
 \tag{4.14}$$

The first column of this array is the initial sequence (4.5), whose convergence we want to accelerate (in our case, the sequence  $y_v(x_i, h_k), k = 0, 1, 2, \dots$ . Each subsequent column contains a new transformed sequence. The performance of the E-algorithm as a convergence accelerator is evaluated by analysing the behaviour of the successive columns of the E-array.

In a recent paper [6], this algorithm was used with success to accelerate the convergence of sequences which have asymptotic error expansions of different forms. Some of these asymptotic expansions had a form similar to (3.39), (3.41) or (3.43) obtained in this paper. These results encouraged us to apply the E-algorithm to the present problem.

In the sequel we shall present some numerical results obtained for the boundary-value problem considered in the previous sections, and comment these results. As done in the previous sections, we shall present these results separately for different values of  $p := -0.5, p = -1, p = -1.25$ . These results were obtained using the program EXTRA01 [6], which incorporates several subroutines, written by C. Brezinski and Redivo-Zaglia [2], allowing to apply the most well-known extrapolation algorithms to a given sequence.

*Case 1:*  $p = -\frac{1}{2}$ . The first numerical results we present here for the problem (1.3)–(1.4) were obtained in the case  $p = -\frac{1}{2}, q = \frac{3}{2}, c = -1$ . In this case the BVP (1.3)–(1.4) is known as the Thomas–Fermi problem. The Picard approximation of the solution of this problem which satisfies (4.4) was obtained with  $v = 15$  (in the case  $y_0(x) \equiv 0$ ) or  $v = 14$  (if  $y_0(x) = 1 - x$ ). In Table 1 we give the values of  $y_{15}(x_i, h), x_i = i/10, i = 1, 2, \dots, 9$ , obtained by the present method with different

Table 2

The columns of the E-array corresponding to the extrapolation process for the computation of  $y(0.5)$  in the case  $p = -0.5, q = 1.5$

$k$	$E_0^{(k)} = y(0.5, h_k)$	$E_2^{(k)}$	$E_4^{(k)}$	$E_6^{(k)}$
1	0.42802495189			
2	0.42772120997			
3	0.42761128229	0.42754985179		
4	0.42757184844	0.42754998819		
5	0.42755777585	0.42755001193	0.42755001697	
6	0.42755276978	0.42755001607	0.42755001695	
7	0.42755099256	0.42755001678	0.42755001694	0.42755001693
8	0.42755036242	0.42755001687	0.42755001688	0.42755001687

Note: The first column contains the initial sequence obtained by the finite-differences scheme, and the subsequent columns contain its second, fourth and sixth transforms obtained by the E-algorithm.

stepsizes. In this table we give also the best approximations obtained by the extrapolation method, at each gridpoint. In this case, the extrapolation process was based on the asymptotic error expansion (3.39). This means that the sequences  $\{g_i(n)\}$ , in this case, have the form

$$g_1(n) = (h_n)^{3/2}, \quad g_2(n) = (h_n)^2, \quad g_3(n) = (h_n)^{5/2}, \dots \tag{4.15}$$

Comparing the columns of the E-array for each  $x_i$ , we observe that the values of the first column ( $E_0^{(n)}$ ) have 3 common decimal digits; the terms of the column  $E_2^{(n)}$  have 5 common digits; the number of common digits in the column  $E_4^{(n)}$  and in the subsequent columns is 10. Based on this fact, we have taken the common digits of  $E_4^{(n)}$  as the best approximations obtained by extrapolation. This process is illustrated in Table 2 where some columns of the E-array are displayed (in the case of the approximation of  $y(0.5)$ ). The values in the last column of Table 1 agree with the corresponding values presented in [10].

Case 2:  $p = -1$ . Next we have analysed the numerical results in the case  $p = -1, q = 2, c = -1$ .

If we start the Picard iteration process with  $y_0(x) \equiv 0$ , the approximation of the solution which satisfies (4.4) is obtained with  $v = 22$ ; if we start with  $y_0(x) = 1 - x$ , the approximation which satisfies (4.4) is obtained with  $v = 21$ . In Table 3 we present the values of  $y_{21}(x_i, h)$ ,  $x_i = i/10, i = 1, 2, \dots, 9$ , obtained by the present method with  $h = 1/60, h = 1/480$  and  $h = 1/3840$ . In this table we also give the results obtained by extrapolation. In this case the asymptotic error expansion of the finite-difference method is given by (3.41). This means that the sequences  $\{g_i(n)\}$ , in this case, have the form:

$$g_1(n) = h_n \ln(h_n), \quad g_2(n) = h_n, \quad g_3(n) = h_n^2 (\ln h_n)^2, \quad g_4(n) = h_n^2 \ln h_n, \quad g_5(n) = h_n^2, \dots \tag{4.16}$$

The best approximations obtained have apparently 9–10 digits depending on the gridpoints considered. In Table 4 we display some columns of the E-array, in the case of  $x_i = 0.5$ , starting from the sequence  $S_n$ , whose convergence is very slow (only three digits coincide), until the 6th transform (whose terms have 12 common digits).

Table 3

Approximate values of the solution in the case  $p = -1.0, q = 2.0$  at the gridpoints  $x_i = 0.1, 0.2, \dots, N$  is the total number of gridpoints used for each approximation

$x_i$	$N = 60$	$N = 480$	$N = 3840$	EXTRA
0.1	0.7856713601	0.7808375568	0.7802145946	0.780125259
0.2	0.6619833203	0.6580410620	0.6575404128	0.657468748
0.3	0.5620923700	0.5588211863	0.5584077292	0.55834858
0.4	0.4732135031	0.4704997105	0.4701574951	0.4701085515
0.5	0.3901168829	0.3878995908	0.3876203645	0.3875804363
0.6	0.3101516883	0.3083978723	0.3081772098	0.3081456595
0.7	0.2318377682	0.2305301570	0.2303657404	0.2303422339
0.8	0.1543208470	0.1534512950	0.1533420117	0.1533263885
0.9	0.0771207308	0.0766862143	0.0766316259	0.0766238223

Note: The last column contains the best approximation of the solution obtained by extrapolation using the E-algorithm.

Table 4

The columns of the E-array corresponding to the extrapolation process for the computation of  $y(0.5)$ , in the case  $p = -1.0, q = 2.0$

$k$	$E_0^{(k)} = S_k$	$E_2^{(k)}$	$E_4^{(k)}$	$E_6^{(k)}$
1	0.39261605886			
2	0.39011688292			
3	0.38885341739	0.387562197		
4	0.38821813479	0.387575752		
5	0.38789959078	0.387579241	0.387580176	
6	0.38774009045	0.387580133	0.387580394	
7	0.38766028278	0.387580360	0.387580429	0.3875804363192
8	0.38762036448	0.387580417	0.387580434	0.3875804363199

Note: The first column contains the initial sequence obtained by the finite-differences scheme, and the subsequent columns contain its second, fourth and sixth transforms obtained by the E-algorithm.

Case 3:  $p = -\frac{5}{4}$ . Finally we present the numerical results obtained in the case  $p = -\frac{5}{4}, q = \frac{9}{4}, c = -1$ .

In this case, the Picard iterates satisfy condition (4.4) beginning with  $v = 28$  or  $v = 27$ , if we start with  $y_0(x) \equiv 0$  or  $y_0(x) = 1 - x$ , respectively. In Table 5 we present the values of  $y_{27}(x_i, h)$ ,  $x_i = i/10, i = 1, 2, \dots, 9$ , obtained with different stepsizes, as in the previous examples. In this table we also give the results obtained by extrapolation. In this case the asymptotic error expansion of the finite-difference method is given by (3.43). This means that the  $g_i(n)$  sequences, in this case, have the form:

$$g_1(n) = (h_n)^{3/4}, \quad g_2(n) = h_n, \quad g_3(n) = (h_n)^{3/2}, \quad g_4(n) = (h_n)^{7/4}, \quad g_5(n) = (h_n)^2, \dots \quad (4.17)$$

The best approximations obtained have apparently 7–8 exact digits, depending on the gridpoints considered. In Table 6 we display some columns of the E-array, obtained in the case of  $x_i = 0.5$ , beginning from the sequence  $S_n$ , whose convergence is very slow (only three digits coincide in different terms) until the 6th transform (whose terms have 7 common digits).

Table 5

Approximate values of the solution in the case  $p = -1.25$ ,  $q = 2.25$  at the gridpoints  $x_i = 0.1, 0.2, \dots, N$  is the total number of gridpoints used for each approximation

$x_i$	$N = 60$	$N = 480$	$N = 3840$	EXTRA
0.1	0.7243310984	0.7086484640	0.7052930535	0.704396
0.2	0.6058343675	0.5934905863	0.5908652928	0.5901638
0.3	0.5145680324	0.5044204038	0.5022648263	0.5016888
0.4	0.4340467335	0.4256413499	0.4238566193	0.4233797
0.5	0.3585507266	0.3516769786	0.3502177754	0.3498278
0.6	0.2855147462	0.2800702786	0.2789146600	0.2786059
0.7	0.2136540855	0.2095903303	0.2087278747	0.20849740
0.8	0.1423038323	0.1395999025	0.1390260983	0.13887276
0.9	0.0711327953	0.0697815237	0.0694947898	0.06941817

Note: The last column contains the best approximation of the solution obtained by extrapolation using the E-algorithm.

Table 6

The columns of the E-array corresponding to the extrapolation process for the computation of  $y(0.5)$  in the case  $p = -1.25$ ,  $q = 2.25$

$k$	$E_0^{(k)}$	$E_2^{(k)}$	$E_4^{(k)}$	$E_6^{(k)}$
1	0.364426967829			
2	0.358550726625			
3	0.355033373389	0.3498169		
4	0.352931510161	0.3498229		
5	0.351676978608	0.3498252	0.34982652	
6	0.350928908619	0.3498265	0.34982746	
7	0.350483187072	0.3498272	0.34982773	0.34982784
8	0.350217775419	0.3498275	0.34982782	0.34982785

Note: The first column contains the initial sequence obtained by the finite-difference scheme, and the subsequent columns its second, fourth and sixth transforms obtained by the E-algorithm.

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