



Obrechhoff Versus Super-Implicit Methods for the Solution of First- and Second-Order Initial Value Problems

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Abstract—This paper discusses the numerical solution of first-order initial value problems and a special class of second-order ones (those not containing first derivative). Two classes of methods are discussed, super-implicit and Obrechhoff. We will show equivalence of super-implicit and Obrechhoff schemes. The advantage of Obrechhoff methods is that they are high-order one-step methods and thus will not require additional starting values. On the other hand, they will require higher derivatives of the right-hand side. In case the right-hand side is complex, we may prefer super-implicit methods. The disadvantage of super-implicit methods is that they, in general, have a larger error constant. To get the same error constant we require one or more extra future values. We can use these extra values to increase the order of the method instead of decreasing the error constant. One numerical example shows that the super-implicit methods are more accurate than the Obrechhoff schemes of the same order. © 2003 Elsevier Science Ltd. All rights reserved.

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1. INTRODUCTION

In this paper, we discuss the numerical solution of first-order initial value problems (IVPs)

$$y'(x) = f(x, y(x)), \quad y(0) = y_0, \quad (1)$$

and a special class (for which y' is missing) of second-order IVPs

$$y''(x) = f(x, y(x)), \quad y(0) = y_0, \quad y'(0) = y'_0. \quad (2)$$

There is a vast literature for the numerical solution of these problems as well as for the general second-order IVPs

$$y''(x) = f(x, y(x), y'(x)), \quad y(0) = y_0, \quad y'(0) = y'_0. \quad (3)$$

See, for example, the excellent book by Lambert [1]. Here, we are interested specifically in two classes of methods. The first class, called super implicit, was developed recently by the second

author [2] for the first-order IVPs (1) and for the special second-order IVPs (2). The general form of such methods for the second-order IVPs (2) is given by

$$y_{n+1} + \sum_{j=1}^k \alpha_j y_{n+1-j} = h^2 \sum_{j=0}^{\ell} \beta_j f_{n+1+m-j}, \quad \alpha_k \beta_0 \beta_{\ell} \neq 0. \tag{4}$$

For $m > 0$, the methods are called super implicit because they require the knowledge of functions not only at past and present but also at future time steps. Fukushima developed Cowell and Adams type super-implicit methods of arbitrary degree and auxiliary formulae to be used in the starting procedure. The first step is evaluating y_1 using the initial conditions and some future values

$$y_1 = y_0 + hy'_0 + h^2 \sum_{j=0}^{\ell} b_j^{(0)} f_j. \tag{5}$$

Next, obtain the additional value y_2, \dots, y_{m-1} , using

$$y_{n+1} = 2y_n - y_{n-1} + h^2 \sum_{j=0}^{\ell} b_j^{(n)} f_j, \quad n = 1, \dots, m. \tag{6}$$

Coefficients $b_j^{(n)}$ are given in [2]. In the case of the sixth-order method, we discussed here

$$y_1 = y_0 + hy'_0 + h^2 \left(\frac{367}{1440} f_0 + \frac{3}{8} f_1 - \frac{47}{240} f_2 + \frac{29}{360} f_3 - \frac{7}{480} f_4 \right), \tag{7}$$

$$y_2 = 2y_1 - y_0 + h^2 \left(\frac{19}{240} f_0 + \frac{17}{20} f_1 + \frac{7}{120} f_2 + \frac{1}{60} f_3 - \frac{1}{240} f_4 \right). \tag{8}$$

Thus, we have to solve a system of nonlinear equations. In order, to make the system smaller, one can subdivide the total interval of integration to subintervals. This will require special formulae to obtain the ending values. Symmetric Cowell type methods of order up to 12 are given along with starting and ending formulae. The integration error grows linearly with respect to time as in symmetric multistep methods.

The second one is due to Obrechhoff¹, see [3]. These methods for the solution of first-order IVPs (1) are given by (see, e.g., [1, pp. 199-204; 4-6])

$$\sum_{j=0}^k \alpha_j y_{n+j} = \sum_{i=1}^{\ell} h^i \sum_{j=0}^k \beta_{ij} y_{n+j}^{(i)}, \quad \alpha_k = 1. \tag{9}$$

According to [6], the error constant decreases more rapidly with increasing ℓ rather than the step k . It is difficult to satisfy the zero stability for large k . The weak stability interval appears to be small. The advantage of Obrechhoff methods is the fact that these are one-step high-order methods and as such do not require additional starting values. A list of Obrechhoff methods for $\ell = 1, 2, \dots, 5 - k$, $k = 1, 2, 3, 4$ is given in [6]. For example, for $k = 1$ and $\ell = 2$, we get an implicit method of order 4 with an error constant $C_5 = 1/720$, and the method is

$$y_{n+1} - y_n = \frac{h}{2} (y'_{n+1} + y'_n) - \frac{h^2}{12} (y''_{n+1} - y''_n). \tag{10}$$

For $k = 1$ and $\ell = 3$, we get an implicit method of order 6 with an error constant $C_7 = -1/100800$, and the method is

$$y_{n+1} - y_n = \frac{h}{2} (y'_{n+1} + y'_n) - \frac{h^2}{10} (y''_{n+1} - y''_n) + \frac{h^3}{120} (y'''_{n+1} + y'''_n). \tag{11}$$

¹Bulgarian mathematician Academician Nikola Obrechhoff (1896-1963, born in Varna) who did pioneering work in such diverse fields as analysis, algebra, number theory, numerical analysis, summation of divergent series, probability and statistics.

Obrechhoff methods for the solution of second-order IVPs (2) can be found in [7]. Here, P-Stable Obrechhoff methods with minimal phase-lag for periodic initial-value problems are discussed. Also Simos [8] presents P-stable Obrechhoff method. In [9], Obrechhoff methods for general second-order differential equations (3) are developed.

Before we continue, we need several definitions. For the multistep method to solve the first-order IVP

$$\sum_{i=0}^k a_i y_{n+i} = h \sum_{i=0}^k b_i f_{n+i}, \tag{12}$$

we define the characteristic polynomials (see, e.g., [1])

$$\rho(\omega) = \sum_{i=0}^k a_i \omega^i, \tag{13}$$

and

$$\sigma(\omega) = \sum_{i=0}^k b_i \omega^i. \tag{14}$$

The order of the method is defined to be p if for an adequately smooth arbitrary test function $\zeta(x)$,

$$\sum_{i=0}^k a_i \zeta(x + ih) - h \sum_{i=0}^k b_i \zeta'(x + ih) = C_{p+1} h^{p+1} \zeta^{(p+1)}(x) + O(h^{p+2}),$$

where C_{p+1} is the error constant. The method is assumed to satisfy the following:

- (1) $a_k = 1, |a_0| + |b_0| \neq 0$,
- (2) ρ and σ have no common factor (irreducibility),
- (3) $\rho(1) = 0, \rho'(1) = \sigma(1)$ (consistency),
- (4) the method is zero-stable (relates to the magnitude of the roots of ρ).

For the multistep method to solve the second-order IVP

$$\sum_{i=0}^k a_i y_{n+i} = h^2 \sum_{i=0}^k b_i f_{n+i}, \tag{15}$$

we define the characteristic polynomials ρ and σ as before.

The order of the method is defined to be p if for an adequately smooth arbitrary test function $\zeta(x)$,

$$\sum_{i=0}^k a_i \zeta(x + ih) - h^2 \sum_{i=0}^k b_i \zeta''(x + ih) = C_{p+2} h^{p+2} \zeta^{(p+2)}(x) + O(h^{p+3}),$$

where C_{p+2} is the error constant. The method is assumed to satisfy the following:

- (1) $a_k = 1, |a_0| + |b_0| \neq 0, \sum_{i=0}^k |b_i| \neq 0$,
- (2) ρ and σ have no common factor (irreducibility),
- (3) $\rho(1) = \rho'(1) = 0, \rho''(1) = 2\sigma(1)$ (consistency),
- (4) the method is zero-stable.

The method is called symmetric if

$$a_i = a_{k-i}, \quad b_i = b_{k-i}, \quad \text{for } i = 0, 1, \dots, k.$$

DEFINITION. (See [10].) The method described by the characteristic polynomials ρ, σ is said to have interval of periodicity $(0, H_0^2)$ if for all H^2 in the interval the roots of

$$V(\omega, H^2) = \rho(\omega) + H^2 \sigma(\omega) = 0, \quad H = \omega h,$$

satisfy

$$\omega_1 = e^{i\theta(H)}, \quad \omega_2 = e^{-i\theta(H)}, \quad |\omega_s| \leq 1, \quad s = 3, 4, \dots, k,$$

where $\theta(H)$ is a real function.

DEFINITION. (See [10].) The method described by the characteristic polynomials ρ, σ is said to be P -stable if its interval of periodicity is $(0, \infty)$.

Lambert and Watson proved that a method described by ρ, σ has a nonvanishing interval of periodicity only if it is symmetric and for P -stability the order cannot exceed 2. Fukushima [11] has proved that the condition is also sufficient. To be precise, we quote the result of [11].

THEOREM. Consider an irreducible, convergent, symmetric multistep method. Define a function

$$g(\theta) = -\frac{\rho(e^{i\theta})}{\sigma(e^{i\theta})}.$$

Then, the method has a nonvanishing interval of periodicity if and only if

- (1) $g(\theta)$ has no nonzero double roots in the interval $[0, \pi]$, or
- (2) $g''(\theta)$ is positive on all the nonzero double roots of $g(\theta)$ in the interval $[0, \pi]$.

However, higher-order P -stable methods were developed by introducing off-step points or higher derivatives of $f(x, y)$.

DEFINITION. (See [12].) Phase-lag is the leading coefficient in the expansion of $|(\theta(H) - H)/H|$.

Symmetric two-step Obrechhoff methods involving higher-order derivatives were developed by Ananthakrishnaiah [7].

2. FIRST-ORDER IVPS

To show the similarity between Obrechhoff and super-implicit methods, let us consider the method given by (10). Now, if we approximate the higher-order derivatives (in this case y'') by some finite differences, we get super-implicit methods (see [2]). Clearly, the approximation must be of high enough order so as to preserve the order of Obrechhoff method. If this is *not* done, we may get a super-implicit method of a lower order. For example, suppose we use centered differences for the second derivatives, then

$$y''_n = \frac{y'_{n+1} - y'_{n-1}}{2h}, \quad y''_{n+1} = \frac{y'_{n+2} - y'_n}{2h}. \tag{16}$$

Substituting these in (10), we get

$$y_{n+1} - y_n = \frac{h}{2} (y'_{n+1} + y'_n) - \frac{h^2}{12} \left(\frac{y'_{n+2} - y'_n}{2h} - \frac{y'_{n+1} - y'_{n-1}}{2h} \right).$$

Simplifying, one has a second-order approximation

$$y_{n+1} - y_n = -\frac{h}{24} y'_{n+2} + \frac{13h}{24} (y'_{n+1} + y'_n) - \frac{h}{24} y'_{n-1}. \tag{17}$$

Using MAPLE [13], we find that the truncation error is

$$\frac{11}{720} h^5 y^{(5)} + O(h^6),$$

so the method is actually fourth order. Notice that, the error constant is 11 times larger than the original Obrechhoff method (10). We had to pay a price for not requiring y'' and it comes in the form of larger error constant *and* requiring a future value (y_{n+2}).

If we take a forward approximation of order 3

$$\begin{aligned}
 y''_n &= \frac{1}{2h} (y'_{n+1} - y'_{n-1}) - \frac{1}{12h} (y'_{n+2} - 2y'_{n+1} + 2y'_{n-1} - y'_{n-2}), \\
 y''_{n+1} &= \frac{1}{2h} (y'_{n+2} - y'_n) - \frac{1}{12h} (y'_{n+3} - 2y'_{n+2} + 2y'_n - y'_{n-1}).
 \end{aligned}
 \tag{18}$$

Substituting these in (10), we get

$$\begin{aligned}
 y_{n+1} - y_n &= \frac{h}{2} (y'_{n+1} + y'_n) - \frac{h^2}{12} \left(\frac{1}{2h} (y'_{n+2} - y'_n) - \frac{1}{12h} (y'_{n+3} - 2y'_{n+2} + 2y'_n - y'_{n-1}) \right) \\
 &\quad + \frac{h^2}{12} \left(\frac{1}{2h} (y'_{n+1} - y'_{n-1}) - \frac{1}{12h} (y'_{n+2} - 2y'_{n+1} + 2y'_{n-1} - y'_{n-2}) \right).
 \end{aligned}$$

Simplifying

$$\begin{aligned}
 y_{n+1} - y_n &= \frac{h}{2} (y'_{n+1} + y'_n) - \frac{h}{24} (y'_{n+2} - y'_{n+1} - y'_n + y'_{n-1}) \\
 &\quad + \frac{h}{144} (y'_{n+3} - 3y'_{n+2} + 2y'_{n+1} + 2y'_n - 3y'_{n-1} + y'_{n-2}).
 \end{aligned}$$

After collecting like terms, we get a third-order approximation

$$y_{n+1} - y_n = \frac{h}{144} y'_{n+3} - \frac{h}{16} y'_{n+2} + \frac{5h}{9} y'_{n+1} + \frac{5h}{9} y'_n - \frac{h}{16} y'_{n-1} + \frac{h}{144} y'_{n-2}. \tag{19}$$

Again using MAPLE, we find that the truncation error is

$$\frac{1}{720} h^5 y^{(5)} + O(h^6),$$

so the method is actually fourth order. This time we have the same error constant as Obrechhoff method (10), but require more future values than before. One can use these extra values to get a higher-order method. The price now is two future values to get the same error constant. It does not seem to be worthwhile to get the same error constant if we can increase the order.

3. SECOND-ORDER IVPS

The numerical integration methods for (2) can be divided into two distinct classes,

- (a) problems for which the solution period is known (even approximately) in advance,
- (b) problems for which the period is not known [7].

For the first class, see [14,15] and references there. Here, we consider the second class only. In this section, we take the P-stable method of order 6 given by Ananthakrishnaiah [7]

$$\begin{aligned}
 y_{n+1} - 2y_n + y_{n-1} &= \frac{h^2}{20} (y''_{n+1} + 18y''_n + y''_{n-1}) - \frac{h^4}{600} (y^{(4)}_{n+1} - 22y^{(4)}_n + y^{(4)}_{n-1}) \\
 &\quad + \frac{h^6}{14400} (y^{(6)}_{n+1} + 2y^{(6)}_n + y^{(6)}_{n-1}),
 \end{aligned}
 \tag{20}$$

and show how to get a super-implicit method equivalent to it. This method has a truncation error

$$-\frac{1}{50400} h^8 y^{(8)} + O(h^{10}),$$

and it is of minimal phase-lag. In order, to get a super implicit, we expand $y^{(6)}_{n+1} + 18y^{(6)}_n + y^{(6)}_{n-1}$ in terms of y'' at n and neighboring points, i.e.,

$$y^{(6)}_{n+1} + 2y^{(6)}_n + y^{(6)}_{n-1} = Ay''_n + By''_{n+1} + Cy''_{n-1} + Dy''_{n+2} + Ey''_{n-2}, \tag{21}$$

where the undetermined coefficients can be found by comparing coefficients of the Taylor series expansion on both sides. The resulting system of equations is

$$\begin{aligned}
 A + B + C + D + E &= 0, \\
 B - C + 2(D - E) &= 0, \\
 B + C + 4(D + E) &= 0, \\
 B - C + 8(D - E) &= 0, \\
 B + C + 16(D + E) &= 4\frac{24}{h^4}, \\
 B - C + 32(D - E) &= 0.
 \end{aligned}
 \tag{22}$$

With five unknowns we can satisfy the first five equations, but it turns out that the symmetric property of the solution satisfies also the sixth automatically. It is easy to see that

$$A = \frac{24}{h^4}, \quad B = C = -\frac{16}{h^4}, \quad D = E = \frac{4}{h^4}.
 \tag{23}$$

Thus,

$$y_{n+1}^{(6)} + 2y_n^{(6)} + y_{n-1}^{(6)} = \frac{24y_n'' - 16(y_{n+1}'' + y_{n-1}'') + 4(y_{n+2}'' + y_{n-2}'')}{h^4}.
 \tag{24}$$

Now, we do the same for the fourth-order derivatives

$$y_{n+1}^{(4)} - 22y_n^{(4)} + y_{n-1}^{(4)} = ay_n'' + by_{n+1}'' + cy_{n-1}'' + dy_{n+2}'' + ey_{n-2}'',
 \tag{25}$$

where the undetermined coefficients can be found in a similar fashion. It is easy to see that

$$a = \frac{168}{3h^2}, \quad b = c = -\frac{92}{3h^2}, \quad d = e = \frac{8}{3h^2}.
 \tag{26}$$

Thus,

$$y_{n+1}^{(4)} - 22y_n^{(4)} + y_{n-1}^{(4)} = \frac{168y_n'' - 92(y_{n+1}'' + y_{n-1}'') + 8(y_{n+2}'' + y_{n-2}'')}{3h^2}.
 \tag{27}$$

Substituting (24) and (27) into (20), we have

$$\begin{aligned}
 y_{n+1} - 2y_n + y_{n-1} &= \frac{h^2}{20} (y_{n+1}'' + 18y_n'' + y_{n-1}'') \\
 &- \frac{h^4}{600} \left(\frac{168y_n'' - 92(y_{n+1}'' + y_{n-1}'') + 8(y_{n+2}'' + y_{n-2}'')}{3h^2} \right) \\
 &+ \frac{h^6}{14400} \left(\frac{24y_n'' - 16(y_{n+1}'' + y_{n-1}'') + 4(y_{n+2}'' + y_{n-2}'')}{h^4} \right).
 \end{aligned}$$

Collecting terms, we get

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left\{ \frac{97}{120}y_n'' + \frac{1}{10} (y_{n+1}'' + y_{n-1}'') - \frac{1}{240} (y_{n+2}'' + y_{n-2}'') \right\},
 \tag{28}$$

which is the sixth-order method given as equation (3) in [2]. The error constant of this sixth-order method is $C_8 = 31/60480$, which is larger than the error constant for the P-stable sixth-order method (20) of Ananthakrishnaiah by a factor of more than 25. Are super-implicit methods always giving larger error constant? In first-order IVPs, we showed that we can get the same error constant if we allow an extra future value (two instead of one). We now get a super-implicit

method of the same order *and* error constant. The price is an extra future value. It can be shown that

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left\{ \frac{1723}{2160} y''_n + \frac{311}{2880} (y''_{n+1} + y''_{n-1}) - \frac{53}{7200} (y''_{n+2} + y''_{n-2}) + \frac{23}{43200} (y''_{n+3} + y''_{n-3}) \right\}, \tag{29}$$

has an error constant of $C_8 = -1/50400$, exactly as (20). We try the eighth-order super implicit

$$y_{n+1} - 2y_n + y_{n-1} = h^2 \left\{ \frac{12067}{15120} y''_n + \frac{2171}{20160} (y''_{n+1} + y''_{n-1}) - \frac{73}{10080} (y''_{n+2} + y''_{n-2}) + \frac{31}{60480} (y''_{n+3} + y''_{n-3}) \right\}. \tag{30}$$

Again using MAPLE, we find the error constant $C_{10} = -289/3628800$. Compare this to the eighth-order Obrechhoff method of [7] with an error constant

$$C_{10} = -\frac{2}{7 \cdot 10!}.$$

The super implicit has an error constant more than 1012 times larger. We can create super-implicit method of the same error constant but requiring more future values than the ones in [2].

4. NUMERICAL EXPERIMENT

We consider the nonlinear undamped Duffing's equation

$$y'' + y + y^3 = B \cos \Omega t,$$

with $B = 0.002$ and $\Omega = 1.01$. The exact solution (see [16]) is given by

$$y(t) = A_1 \cos \Omega t + A_3 \cos 3\Omega t + A_5 \cos 5\Omega t + A_7 \cos 7\Omega t,$$

where

$$\begin{aligned} A_1 &= 0.200179477536, & A_3 &= 0.246946143(-03), \\ A_5 &= 0.304016(-06), & A_7 &= 0.374(-09). \end{aligned}$$

We give here the results of the sixth-order Obrechhoff method as given in [7] and the same order super-implicit method. Both are implicit methods and Picard iteration is used. The step size used is $h = \pi/5$. The absolute errors for $t = 2\pi(2\pi)10\pi$ are presented in the following two tables. The super-implicit methods give smaller absolute errors.

If we reduce the step size to $h = \pi/12$, we reduce the absolute errors by two orders of magnitude.

Table 1. Absolute errors in $y(t)$ with $h = \pi/5$.

| t | Obrechhoff | Super Implicit |
|------|------------|----------------|
| 1.00 | 1.88(-04) | 2.04(-05) |
| 2.00 | 7.46(-04) | 8.09(-05) |
| 3.00 | 1.63(-03) | 1.80(-04) |
| 4.00 | 2.78(-03) | 3.15(-04) |
| 5.00 | 4.11(-03) | 4.82(-04) |

Table 2. Absolute errors in $y(t)$ with $h = \pi/5$ and $h = \pi/12$.

| t | Super Implicit $\frac{\pi}{5}$ | Super Implicit $\frac{\pi}{12}$ |
|------|-----------------------------------|------------------------------------|
| 1.00 | 2.04(-05) | 2.53(-07) |
| 2.00 | 8.09(-05) | 1.01(-06) |
| 3.00 | 1.80(-04) | 2.25(-06) |
| 4.00 | 3.15(-04) | 3.95(-06) |
| 5.00 | 4.82(-04) | 6.05(-06) |

5. CONCLUSIONS

In this paper, we showed the equivalence of super-implicit and Obrechhoff methods. The advantage of Obrechhoff methods is that they are high-order one-step methods and thus will not require additional starting values. On the other hand, they will require higher derivatives of the right-hand side. In case the right-hand side is complex, we may prefer super-implicit methods. One can use super-implicit methods given by Fukushima. In general, these methods have larger error constants. We have found here that one can develop super-implicit method having the same error constants as Obrechhoff but requiring an extra future value. On the other hand, Fukushima showed that one can get a higher-order method for the additional future value. A numerical example shows that the super-implicit methods are more accurate than Obrechhoff schemes of the same order.

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