stichting
mathematisch
centrum

MC

AFDELING NUMERIEKE WISKUNDE NW 9/74 FEBRUARY

P.W. HEMKER

A METHOD OF WEIGHTED ONE-SIDED DIFFERENCES FOR STIFF BOUNDARY VALUE PROBLEMS WITH TURNING POINTS

2e boerhaavestraat 49 amsterdam

Printed at the Mathematical Centre, 49, 2e Boerhaavestraat, Amsterdam.

The Mathematical Centre, founded the 11-th of February 1946, is a non-profit institution aiming at the promotion of pure mathematics and its applications. It is sponsored by the Netherlands Government through the Netherlands Organization for the Advancement of Pure Research (Z.W.O), by the Municipality of Amsterdam, by the University of Amsterdam, by the Free University at Amsterdam, and by industries.

AMS (MOS) subject classification scheme (1970): 65L10

ABSTRACT

The numerical solution of singularly perturbed second order linear two-point boundary value problems is studied. A method is proposed that uses a weighted combination of the backward and forward divided difference, such that the boundary layer behavior is represented accurately. In a turning point region -with diameter $O(\varepsilon^{\frac{1}{2}})$- an accurate approximation can be obtained when a local mesh with $h = O(\varepsilon^{\frac{1}{2}})$ is applied. A maximum principle applies to the approximate solution if it does for the exact solution. In addition,the method is easy to implement.

1. INTRODUCTION

A large number of physical problems give rise to singular perturbation problems, i.e. differential equations in which the highest derivative is multiplied by a small parameter. This occurs for initial value problems as well as for boundary value problems. In both cases the use of standard methods for solving the differential equations is impossible or highly inefficient. For initial value problems this situation led to the development of methods for the so-called *stiff differential equations*. For boundary value problems much work has been done in the field of pure analysis and often solutions can be computed in the form of an asymptotic expansion in terms of the small parameter. A large number of interesting phenomena has been discovered and analysed. In this place we mention the work of Visik and Lyusternik [1957], Eckhaus and De Jager [1966] and Eckhaus [1972] on boundary layer problems in more dimensions and the work of O'Malley [1970] and Ackerberg and O'Malley [1970] on boundary value problems with a turning point in a one-dimensional domain.

In contrast with the large number of publications which appeared on the numerical solution of stiff differential equations for initial value problems, only a few papers on the numerical solution of singularly perturbed boundary value problems are known to the author -although it is expected that this is a rapidly developing field.

The purpose of this paper is to describe a finite difference method for solving the two-point boundary value problem of the form

$$\varepsilon y''(x) + f(x)\, y'(x) - g(x)\, y(x) = k(x) \tag{1.a}$$

$$y(a) = \alpha, \quad y(b) = \beta, \tag{1.b}$$

where ε is a small positive parameter.

The same problem was considered by Pearson [1968], Il'in [1969] and Miranker and Morreeuw [1973], and a related problem was treated by Dorr [1970,1971]. Pearson [1968] introduced a variable net, using two-sided differences. Il'in [1969] multiplied the small parameter ε by a factor γ,

depending on ε, $f(x)$ and the uniform mesh spacing h. This factor γ is chosen such that the solution of the homogeneous problem is represented exactly. Dorr [1970] exploits the use of one-sided differences and Miranker [1973] makes use of the known analytic properties of the solution, in particular in the neighborhood of a turning point of the differential equation.

In this paper we introduce a new method that couples most benefits of the known methods with an utmost simplicity. The method uses the common three-point difference approximation to $y''(x_i)$ and introduces a new three-point difference approximation to $y'(x_i)$, which is a weighted combination of the backward and forward divided difference. The only disadvantage seems to be the low order of accuracy; although some may have the opinion that low order methods are inherent to the efficient solution of this kind of problems.

2. THE METHOD

The main difficulty in the numerical solution of singular perturbation problems is to obtain a difference approximation that is asymptotically correct for $\varepsilon \to 0$. It is well-known that replacing the first derivative $y'(x)$ by central differences is not suitable for small ε/h when the second derivative is approximated in the usual way by

$$y_{x\bar{x}} = (y_{i+1}-2y_i+y_{i-1})/h^2. \tag{2}$$

Moreover, for fixed h and $f(x) \neq 0$, and $\varepsilon \to 0$, no resemblance at all exists between the solution of the differential equation and the solution of the difference equation.

This difficulty can be dealt with by the use of a directional divided difference operator [cf. Dorr, 1970]

$$y_{\hat{x}} = \begin{cases} (y_{i+1}-y_i)/h & \text{if } f(x_i) > 0, \\ (y_i-y_{i-1})/h & \text{if } f(x_i) \leq 0. \end{cases} \tag{3}$$

Instead of this discrete choice between the forward and backward divided difference we introduce the Weighted One-Side Differences (WOSD) method

$$(4) \qquad y_{\tilde{x}} = ((1+\alpha_i)\, y_{i+1} - 2\alpha_i y_i - (1-\alpha_i)\, y_{i-1})/(2h),$$

with $\alpha_i \in [-1,+1]$.

We notice that this contains the forward, the backward and the central differences, depending on the value of the parameter α_i.

The parameter α_i is chosen, depending on ε, f and h, such that

1) the local maximum principle holds for the solution of the difference equation whenever it holds for the differential equation [cf. Dorr, Parter and Shampine, 1973];
2) the boundary layer behavior of the solution of the differential equation is accurately represented by the solution of the difference equation.

3. THE MAXIMUM PRINCIPLE

In order to obtain a difference approximation that satisfies the local maximum principle [cf. Brandt, 1973] we take α_i such that the (tridiagonal) matrix (a_{ij}), which results from the discretization

$$(5) \qquad -\varepsilon y_{x\bar{x}} - f y_{\tilde{x}} + gy = -k, \qquad g \geq 0,$$

is of positive type [cf. Ciarlet, 1970]. This requires (definition of positive type) $-a_{i,i+1} \leq 0$, $-a_{i,i-1} \leq 0$ and $-a_{i,i+1} - a_{i,i} - a_{i,i-1} \geq 0$, for all i with $a < x_i < b$, where

$$(6) \qquad \begin{aligned} a_{i,i+1} &= \frac{\varepsilon}{h^2} + \frac{(1+\alpha_i)\, f(x_i)}{2h}, \\ a_{i,i} &= \frac{-2\varepsilon}{h^2} - \frac{2\alpha_i f(x_i)}{2h} - g(x_i), \\ a_{i,i-1} &= \frac{\varepsilon}{h^2} - \frac{(1-\alpha_i)\, f(x_i)}{2h}. \end{aligned}$$

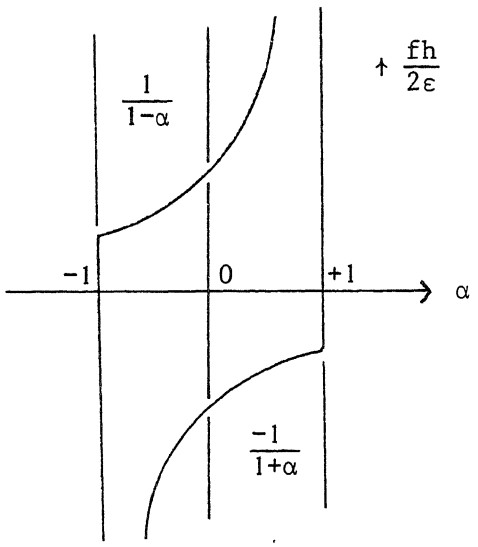
In the sequel we will omit the index i of α_i and we will write f for $f(x_i)$.

Since $g \geq 0$, the requirements read

$$\left.\begin{aligned} 2\varepsilon + (1+\alpha)\ fh &\geq 0 \\ 2\varepsilon - (1-\alpha)\ fh &\geq 0 \end{aligned}\right\}$$

or

$$\frac{-1}{1+\alpha} \leq \frac{fh}{2\varepsilon} \leq \frac{1}{1-\alpha} \quad . \tag{7}$$



In this way we get bounds for the parameter α depending on the value of fh/ε.

We notice that the method of directional divided differences is one particular choice of a (discontinuous) function $\alpha(fh/\varepsilon)$ which satisfies the maximum principle. Other choices for the function $\alpha(fh/\varepsilon)$, such that the maximum principle holds for the numerical solution, are e.g.

$$\alpha = \tanh\left(\frac{hf}{2\varepsilon}\right)$$

or

$$\alpha = \frac{2}{\pi} \arctan\left(\frac{hf}{2\varepsilon}\right) \quad .$$

Respectively, this is verified by

$$-\frac{1}{1+\alpha} < \operatorname{arctanh}(\alpha) < \frac{1}{1-\alpha}$$

and

$$\frac{-1}{1+\alpha} < \tan\left(\frac{\pi\alpha}{2}\right) < \frac{1}{1-\alpha} .$$

An advantage of this kind of choice of α, as compared with the directional divided difference of Dorr, is that for $fh \ll \varepsilon$ the WOSD-method approaches the 2nd order accuracy of the central difference approximation.

4. EXPONENTIAL FITTING

The freedom left in the choice of the function $\alpha(fh/\varepsilon)$ will be exploited to obtain a good representation of boundary layer behavior. To this end we recall that the WKB-analysis of the homogeneous equation (1) gives an asymptotic approximation to the solution for small ε. Away from a zero of $f(x)$ this yields -to first order- two approximate solutions

$$y_1 = \exp\{-\int^x g(t)/f(t)\ dt\} \tag{8}$$

$$y_2 = (f(x))^{-1} \exp\{-\frac{1}{\varepsilon}\int^x f(t)\ dt + \int^x g(t)/f(t)\ dt\}. \tag{9}$$

The function $y_1(x)$ represents the solution of the reduced equation $f(x)\ y'(x) - g(x)\ y(x) = 0$, and $y_2(x)$ describes the boundary layer behavior (at the left-hand end for $f(x) > 0$ and at the right-hand end for $f(x) < 0$). For $\varepsilon g \ll f^2$ the first term in the exponent of y_2 dominates and the boundary layer behavior is approximated by

$$C \exp\{-\frac{1}{\varepsilon}\int^x f(t)\ dt\}.$$

This suggests to choose $\alpha(fh/\varepsilon)$ such that the solution of

(10) $\varepsilon y'' + f y' = 0$

is represented exactly.

(Note that the same principle of exponential fitting is well-known in the numerical solution of stiff initial value problems.)

Hence we take

$$\frac{2\varepsilon - (1-\alpha)\, fh}{2\varepsilon + (1+\alpha)\, fh} = \exp(-\frac{fh}{\varepsilon}),$$

i.e.

(11) $$\alpha(\frac{fh}{2\varepsilon}) = -\frac{2\varepsilon}{fh} + \coth(\frac{fh}{2\varepsilon}).$$

This function $\alpha(z)$ is easily computed since it allows a Taylor series expansion around the origin

(12) $$\alpha(z) = \frac{z}{3} - \frac{z^3}{45} + \frac{2z^5}{945} - \frac{z^7}{4725} + \ldots \quad .$$

It is readily seen that $\alpha(z)$ satisfies

(13) $$\frac{-1}{1+\alpha(z)} \le z \le \frac{1}{1-\alpha(z)}$$

and hence this choice of α satisfies the condition for preserving the maximum principle properties.

5. THE ALGORITHM

The algorithm we propose now follows immediately. A set of nodal points $\{x_i\}_{i=0}^{N}$, $x_0 = a$, $x_N = b$ is chosen in advance and the differential equation is replaced by the linear system

$$a_{i,i+1}\, y_{i+1} + a_{i,i}\, y_i + a_{i,i-1}\, y_{i-1} = k(x_i), \quad i=1,2,\ldots,N-1$$

with

$$a_{i,i+1} = \frac{2}{(h+k)h} + \frac{f(x_i)\ (1+\alpha_i)}{2h} ,$$

$$a_{i,i-1} = \frac{2\varepsilon}{(h+k)k} - \frac{f(x_i)\ (1-\alpha_i)}{2k} ,$$

(14)
$$a_{i,i} = g(x_i) - a_{i,i+1} - a_{i,i-1} ,$$

$$\alpha_i = \coth\left(\frac{(h+k)\ f(x_i)}{4\varepsilon}\right) - \frac{4\varepsilon}{(h+k)\ f(x_i)} ,$$

$$h = x_{i+1} - x_i \quad \text{and} \quad k = x_i - x_{i-1}.$$

The discrete maximum principle is also satisfied for the non-uniform net. However, for a correct representation of the boundary layer, a uniform mesh is required *locally*; i.e. where the boundary layer is significant, the small region has to be covered by a (coarse or fine) uniform net.

6. ACCURACY IN THE TURNING POINT REGIONS

It is clear that, for $\alpha \neq 0$, the method is only a first order method, i.e. the discretization error is $O(h)$. From O'Malley [1970] we know that in the common case of a turning point x_0 ($f(x_0) = 0$, $f'(x_0) \neq 0$, $-g(x_0)/f'(x_0)$ is not a positive integer) the turning point region is $O(\sqrt{\varepsilon})$. In this region a rapid change of the solution may be expected. It is therefore reasonable that, for approximation of the solution in this region, we take locally $h = O(\sqrt{\varepsilon})$ but h small compared with $\sqrt{\varepsilon}$.
Since $f(x_0) = 0$ and $f'(x_0) \neq 0$ we also have $f(x) = O(\sqrt{\varepsilon})$. Hence $\frac{fh}{2\varepsilon} = O(1)$ and small as compared with 1. This implies $\alpha \approx \frac{fh}{6\varepsilon}$ and the WOSD-method approaches to the method with central differences which is second order. Thus a reasonable good approximation of the solution in the turning point region can be obtained by using a local mesh $O(\sqrt{\varepsilon})$.

7. NUMERICAL RESULTS

In this last section we characterize the errors, which arise when our method is applied to a number of model problems. All computations discussed in this section were performed on a CDC CYBER 73/28 computer.

7.1. Global accuracy

First we give two examples to show that the global accurary of the method is first order for large hf/ε and second order for small hf/ε. To this end we plot the logarithm of the error, $e = \max_i |y(x_i) - y_i|$, versus the logarithm of the mesh width h.

We take two examples also given by Miranker and Morreeuw [1973].

Example 1. (see fig. 1)

Differential equation

$$\varepsilon y'' + |x|\, y' - y = -(1+\pi^2\varepsilon)\cos(\pi x) - \pi|x|\sin(\pi x); \quad x \in [-1,+1]. \tag{15}$$

Exact solution

$$y = \cos(\pi x).$$

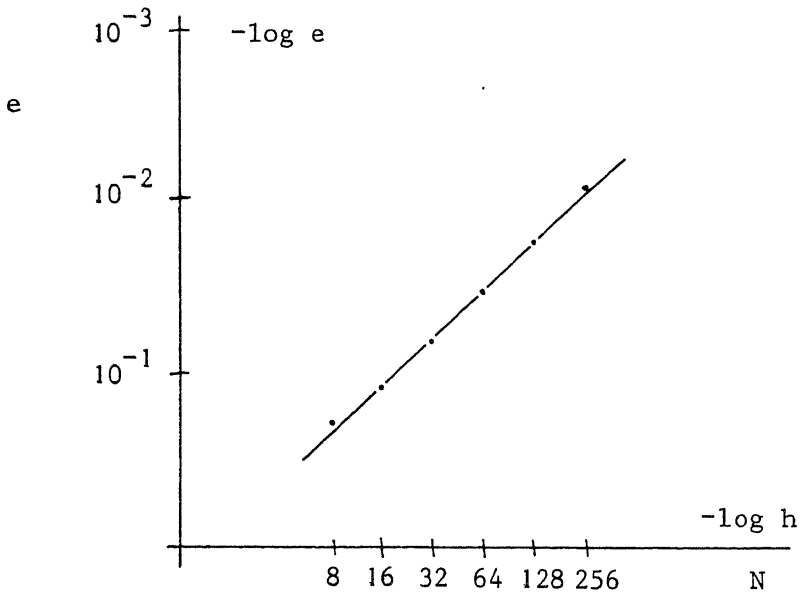


Figure 1: Example 1: $\varepsilon = 10^{-8}$. -log (e) versus -log(h).

Example 2. (see fig. 2)

Differential equation

$$y'' + |x|\, y' - y = 12\varepsilon x^2 + 4|x|\, x^3 - x^4, \qquad x \in [-1,+1]. \tag{16}$$

Exact solution

$$y = x^4.$$

From fig. 2 it can be seen that the method approaches second order accuracy for small values of fh/ε.

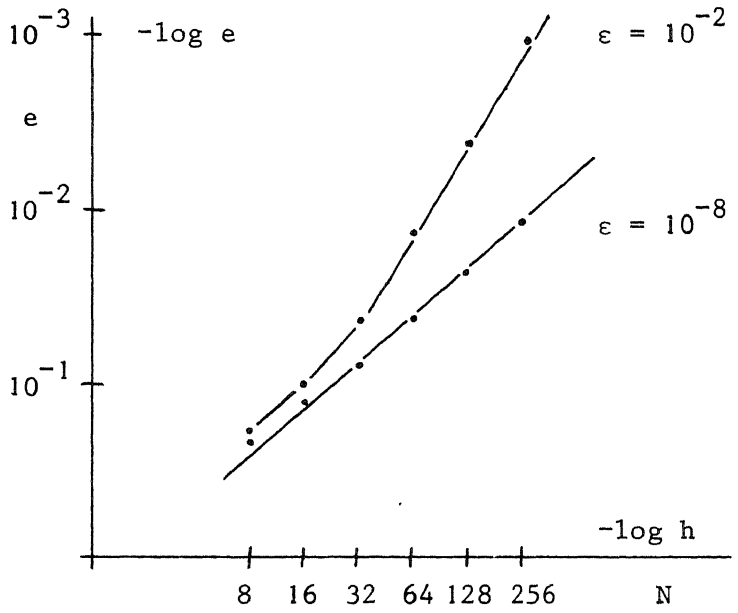


Figure 2: Example 2: $\varepsilon = 10^{-8}$, $\varepsilon = 10^{-2}$. $-\log(e)$ versus $-\log(h)$.

7.2. Accuracy in the turning point region

Here we take the following differential equation as an example

$$\varepsilon y'' + xy' = 0, \qquad x \in [-1,+1]. \tag{17}$$

Exact solution

$$y(x) = 1.5 + 0.5\ \mathrm{erf}(x/\sqrt{2\varepsilon}).$$

For small values of ε, a coarse mesh ignores the internal boundary layer at $x = 0$. This may flatter the results when $\max_i |y(x_i) - y_i|$ is taken as a measure for the quality of the approximation to $y(x)$. For an accurate description of $y(x)$ we need a local refinement of the mesh in the turning point region. Here, for computational purposes, we take this region $(-4\sqrt{\varepsilon}, 4\sqrt{\varepsilon})$.

In the experiments we take an (equidistant) mesh for $[-1, -4\sqrt{\varepsilon}]$ and $[4\sqrt{\varepsilon}, +1]$ and we take a finer (equidistant) mesh on $(-4\sqrt{\varepsilon}, 4\sqrt{\varepsilon})$.

In the tables 1, 2 and 3 we give for resp. $\varepsilon = 10^{-2}, 10^{-4}, 10^{-8}$ the values of $e = \max_i |y(x_i) - y_i|$ for 2×m1 mesh intervals outside and m2 mesh intervals inside the turning point region. In the tables we denote $2.56_{10}-3$ by 2.56(-3).

In figure 3 the logarithm of the mesh width in the turning point region is plotted versus -ln(e) for the case $\varepsilon = 10^{-8}$. The direction of the straight line clearly shows the second order accuracy.

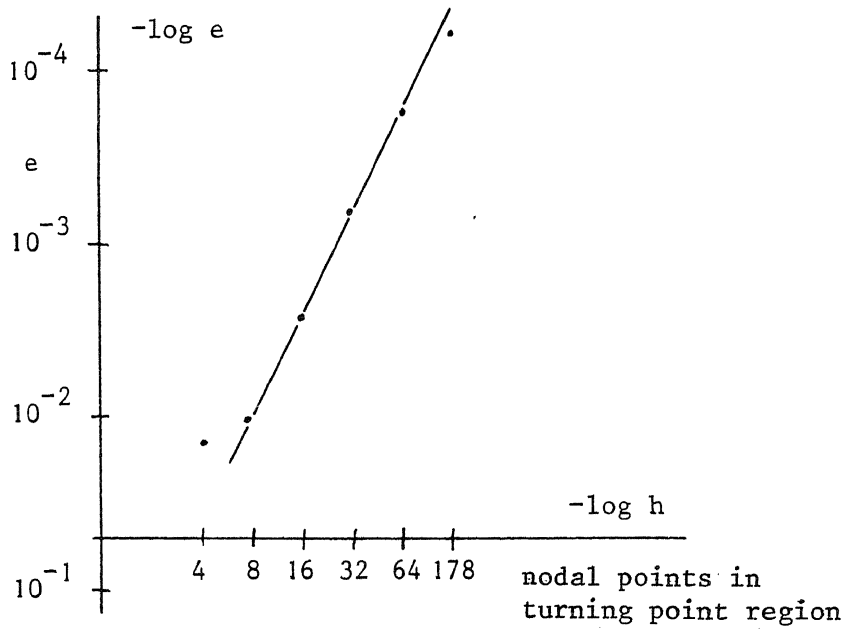


Figure 3: $10^{-8}\ y'' + xy' = 0$, $x \in [-1,+1]$, $y(-1) = 1$, $y(1) = 2$.
log(e) versus log(h).

m1 \ m2	4	8	16	32	64	128
3	1.38(-2)	1.07(-2)	2.57(-3)	6.50(-4)	1.76(-4)	5.85(-5)
6	1.37(-2)		2.56(-3)	6.41(-4)	1.67(-4)	4.88(-5)
12				6.35(-4)	1.60(-4)	4.22(-5)
24			2.56(-3)	6.32(-4)	1.58(-4)	4.01(-5)
48	1.37(-2)	1.07(-2)	2.55(-3)	6.32(-4)	1.58(-4)	3.94(-5)

Table 1: $\max_i |y(x_i) - y_i|$ for $\varepsilon = 10^{-2}$.

m1 \ m2	4	8	16	32	64	128
3	1.38(-2)	1.07(-2)	2.58(-3)	6.53(-4)	1.79(-4)	6.23(-5)
6						
12						6.23(-5)
24						6.21(-5)
48	1.38(-2)	1.07(-2)	2.57(-3)	6.50(-4)	1.76(-4)	5.85(-5)

Table 2: $\max_i |y(x_i) - y_i|$ for $\varepsilon = 10^{-4}$.

m1 \ m2	4	8	16	32	64	128
3	1.38(-2)	1.07(-2)	2.58(-3)	6.53(-4)	1.79(-4)	6.23(-5)
6						
12						
24						
48	1.38(-2)	1.07(-2)	2.58(-3)	6.53(-4)	1.79(-4)	6.23(-5)

Table 3: $\max_i |y(x_i) - y_i|$ for $\varepsilon = 10^{-8}$.

m1 \ m2	4	8	16	32	64	128
3	11	15	23	39	71	135
6	17	21	29	45	77	141
12	29	33	41	57	89	153
24	53	57	65	81	113	177
48	101	105	113	129	161	225

Table 4: The total number of meshpoints (2*m1+m2+1).

7.3. Some other turning point problems

Here we consider the differential equation

$$\varepsilon y'' + axy' - by = 0 \quad , \quad x \in [-1,+1],\ y(-1) = 1,\ y(+1) = 2, \tag{18}$$

with constant coefficients, $a = \pm 1$, $b > 0$ and $0 < \varepsilon << 1$. It is clear from theoretical considerations (as it is, in fact, from the numerical experiment), that the algorithm gives excellent approximation for $a = -1$. More interesting are examples with $a = +1$.

We denote by $y^*(x)$ the asymptotic solution for $\varepsilon \to 0$ of equation (18) with $a = +1$. Outside the turning point region this solution reads

$$y^*(x) = \begin{cases} |x|^b & \text{for } x < 0 \\ 2|x|^b & \text{for } x > 0, \end{cases} \tag{19}$$

in addition

$$y^*(0) = O(\varepsilon^{b/2}). \tag{20}$$

In table 4 we give (for $b = 0.5$, 1, 1.0001 and 2) the values of $e = \max_{|x_i| > 4\sqrt{\varepsilon}} |y^*(x_i) - y_i|$ for different values of ε; m2 mesh intervals were taken inside the turning point region $(-4\sqrt{\varepsilon}, +4\sqrt{\varepsilon})$ and m1 mesh intervals at each side, outside the turning point region.

b	ε	m1 = 64, m2 = 32		m1 = 32, m2 = 16	
		e	y(0)	e	y(0)
.5	1.(-1)	1.04(-2)	7.00(-1)	3.17(-3)	6.91(-1)
	1.(-2)	9.18(-3)	3.89(-1)	9.65(-3)	3.85 -1)
	1.(-3)	9.86(-3)	2.17(-1)	1.70(-2)	2.13(-1)
	1.(-4)	1.76(-2)	1.18(-1)	3.37(-2)	1.12(-1)
	1.(-6)	4.01(-2)	2.68(-2)	5.74(-2)	2.12(-2)
	1.(-8)	2.90(-2)	3.40(-3)	3.87(-2)	2.43(-3)
1.	1.(-1)	2.48(-4)	3.77(-1)	2.46(-4)	3.74(-1)
	1.(-2)	2.12(-6)	1.19(-1)	2.06(-6)	1.18(-1)
	1.(-3)	5.90(-7)	3.77(-2)	4.00(-7)	3.75(-2)
	1.(-4)	5.44(-8)	1.19(-2)	4.22(-9)	1.18(-2)
	1.(-6)	4.97(-14)	1.19(-3)	2.84(-14)	1.18(-3)
	1.(-8)	4.26(-14)	1.19(-4)	1.42(-14)	1.18(-4)
1.0001	1.(-1)	2.52(-4)	3.77(-1)	2.46(-4)	3.74(-1)
	1.(-2)	4.35(-6)	1.19(-1)	4.41(-6)	1.18(-1)
	1.(-3)	1.96(-6)	3.77(-2)	2.75(-6)	3.74(-2)
	1.(-4)	1.41(-6)	1.19(-2)	2.58(-6)	1.18(-2)
	1.(-6)	1.40(-6)	1.19(-3)	2.26(-6)	1.18(-3)
	1.(-8)	1.40(-6)	1.19(-4)	2.67(-6)	1.18(-4)
2.	1.(-1)	5.72(-2)	1.40(-1)	8.89(-2)	1.48(-1)
	1.(-2)	1.69(-2)	1.50(-2)	1.79(-2)	1.53(-2)
	1.(-3)	6.74(-3)	1.57(-3)	1.33(-2)	1.72(-3)
	1.(-4)	7.39(-3)	1.93(-4)	1.46(-2)	2.46(-4)
	1.(-6)	7.66(-3)	6.84(-6)	1.51(-2)	1.23(-5)
	1.(-8)	7.69(-3)	5.60(-7)	1.51(-2)	1.11(-6)

Table 4

In figure 4 we show the computed value of $-\log(y(0))$ plotted against $-\log(\varepsilon)$. This shows that the asymptotic relation (20) is realized numerically for values $\varepsilon > {}_{10}{}^{-4}$. For b = 1 (i.e. the case where the asymptotic solution outside the turning point region is linear) relation (20) is satisfied exactly even for $\varepsilon << 10^{-4}$. (Data used from table 4.)

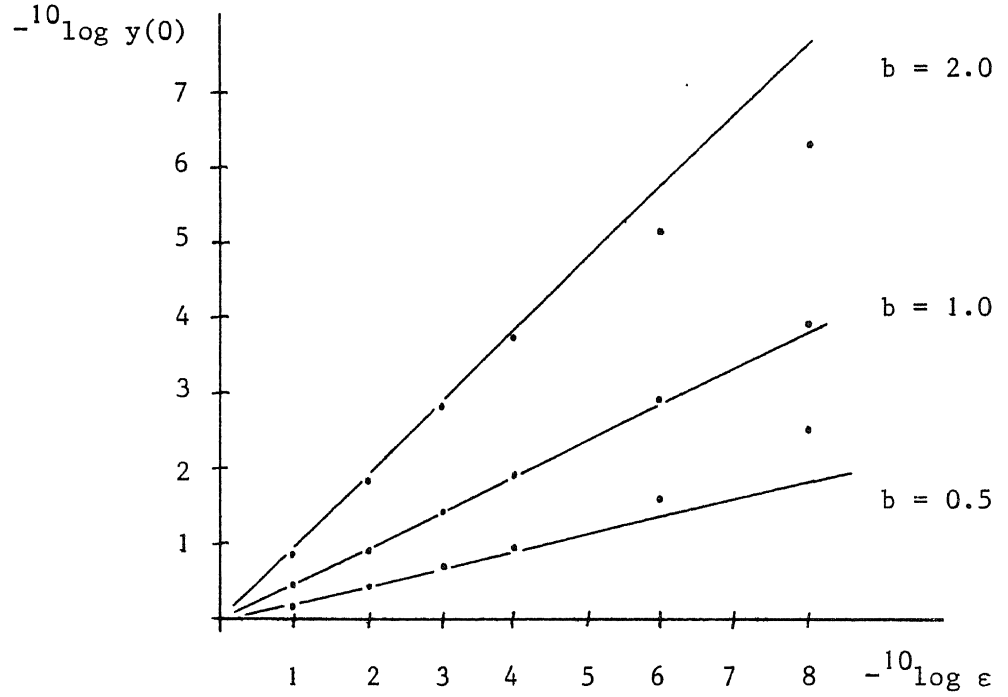


Figure 4: The computed value of y(0) as a function of ε.

REFERENCES

Ackerberg, R.C. & O'Malley, R.E. [1970]. *Boundary layer problems exhibiting resonance*. Studies in Appl. Math. 49 (1970) 277.

Brandt, A. [1973]. *Generalized local maximum principles for finite difference operators*. Math. Comp. 27 (1973) 685.

Ciarlet, P.G. [1970]. *Discrete maximum principle for finite difference operators*. Aequationes Math. 4 (1970) 338.

Dorr, F.W. [1970]. *The numerical solution of singular perturbations of boundary value problems*. SIAM J. Numer. Anal. 7 (1970) 281.

Dorr, F.W. [1971]. *An example of ill-conditioning in the numerical solution of singular perturbation problem*. Math. Comp. 25 (1970) 271.

Dorr, F.W., Parter, S.V. and Shampine, L.F. [1973]. *Applications of the maximum principle to singular perturbation problems*. SIAM Rev. 15 (1973) 43.

Eckhaus, W. & de Jager, E.M. [1966]. *Asymptotic solutions of singular perturbation problems for linear differential equations of elliptic type*. Arch. Rational Mech. Anal. 23 (1966) 26.

Eckhaus, W. [1972]. *Boundary layers in linear elliptic singular perturbation problems*. SIAM Rev. 14 (1972) 225.

Il'in, A.M. [1969]. *Differencing scheme for a differential equation with a small parameter affecting the highest derivative*. Mat. Zametki 6 (1969) 237; transl.: Math. Notes Acad. Sc. USSR 6 (1969) 596.

Miranker, W.L. & Morreeuw, J.P. [1973]. *Semi-analytic numerical studies of turning points arising in stiff boundary value problems*. IBM Research report, RC 4458 (1973).

O'Malley, R.E. [1970]. *On boundary value problems for a singular perturbed differential equation with a turning point*. SIAM J. Math. Anal. 4 (1970) 479.

Pearson, C.E. [1968a]. *On a differential equation of boundary layer type*. J. of Math. and Physics 47 (1968) 134.

Pearson, C.E. [1968b]. *On nonlinear ordinary differential equations of boundary layer type*. J. of Math. and Physics 47 (1968) 351.

Visik, M.I. & Lyusternik, L.A. [1957]. *Regular degeneration and boundary layer for linear differential equations with small parameter*. Uspehi. Mat. Nauk. (1957); Amer. Math. Soc. Transl. 2.20 (1962).