The spline approach to the calculation of derivatives on the Bakhvalov mesh in the presence of a boundary layer

Alexander Zadorin
Sobolev Institute of Mathematics
Novosibirsk, 630090, Russia
zadorin@ofim.oscsbras.ru

Nikita Zadorin
Sobolev Institute of Mathematics
Novosibirsk, 630090, Russia
nik-zadorin@yandex.ru

Abstract

The problem of calculating the derivatives of a function with large gradients in the region of an exponential boundary layer is considered. To do this, it is proposed to construct a cubic spline on the Bakhvalov grid, which thickens in the boundary layer. We study the convergence of the derivatives of the constructed spline to the derivatives of the function given at the grid nodes. Error estimates are obtained taking into account uniformity in a small parameter. The obtained error estimates are confirmed by the results of computational experiments.

1 Introduction

Various convective-diffusion processes with prevailing convection are modeled on the basis of boundary value problems for equations with a small parameter ε before the highest derivative. Solutions to such problems have large gradients, which leads to the loss of accuracy of classical difference schemes, interpolation formulas, and numerical differentiation formulas.

Difference schemes that have the property of convergence uniform in the parameter ε are constructed in some papers. Difference schemes on Shishkin mesh [1] and on Bakhvalov mesh [2] are widely used. Of interest is the development of formulas for numerical differentiation in the presence of a boundary layer. The problem is that the application of classical polynomial formulas to functions with large gradients leads to significant errors [3].

In [4], [5], a cubic spline was studied on the Shishkin mesh. Error estimates are obtained that are uniform with respect to the parameter ε. In [6], the cubic spline on the Shishkin mesh is used to calculate derivatives with respect to the function values at the mesh nodes. Relative error estimates are obtained uniformly in ε. In [7] an analog of a cubic spline is constructed on a uniform grid. This spline is exact on the singular component of the interpolated function. An interpolation error estimate is obtained that is uniform with respect to the small parameter ε.

In this paper, we study the possibility of using a cubic spline on a Bakhvalov mesh for the approximate calculation of derivatives of functions with large gradients in the boundary layer.

Let the function $u(x)$ be representable in the form:

$$u(x) = p(x) + \Phi(x),\ x \in [0, 1], \tag{1}$$

where

$$|p^{(j)}(x)| \le C_1, \quad |\Phi^{(j)}(x)| \le \frac{C_1}{\varepsilon^j} e^{-\alpha x/\varepsilon},\ 0 \le j \le 4, \tag{2}$$

In: Sergei S. Goncharov, Yuri G. Evtushenko (eds.): Proceedings of the Workshop on Applied Mathematics and Fundamental Computer Science 2020 , Omsk, Russia, 30-04-2020, published at http://ceur-ws.org

where the functions $p(x)$ and $\Phi(x)$ are not explicitly defined, $\alpha > 0, \varepsilon \in (0, 1]$, constant C_1 is independent of ε. According to (2), the regular component $p(x)$ has bounded derivatives to the fourth order, and the boundary-layer component $\Phi(x)$ has derivatives that are not uniformly bounded with the respect to the parameter ε. According to [1], the representation (1) with constraints (2) is valid for the solution of the boundary value problem for a second-order differential equation with a small parameter ε with the highest derivative.

Let us show the relevance of developing difference formulas for calculating derivatives with respect to function values at mesh nodes if the function has the representation (1). The classical difference formula with two nodes for the derivative has the form:

$$u'(x) \approx L_2'(u, x) = \frac{u_n - u_{n-1}}{h}, \quad x_{n-1} \le x \le x_n. \tag{3}$$

Let $u(x) = e^{-x/\varepsilon}$. Then with $\varepsilon = h$ it will be $\varepsilon|(u_1 - u_0)/h - u'(0)| = e^{-1}$. The relative error of the formula (3) does not decrease with mesh step decreasing. We need to develop formulas for numerical differentiation with accuracy that is uniform with respect to the parameter ε.

By C and C_j we mean positive constants independent of the parameter ε and the number of mesh nodes N.

2 Setting of the non-uniform mesh

Let Ω^h be a mesh on the interval $[0, 1]$:

$$\Omega^h = \{x_n : x_n = x_{n-1} + h_n, \ n = 1, \dots, N, \ x_0 = 0, \ x_N = 1\}.$$

We assume that the function $u(x)$ of the form (1) is defined at the nodes of the mesh, $u_n = u(x_n), \ n = 0, 1, 2, \dots, N$.

Set Ω^h as a Bakhvalov mesh [2] with the nodes $x_n = g(n/N), \ n = 0, 1, \dots, N$, where the function $g(t)$ is defined as follows:

$$g(t) = -\frac{4\varepsilon}{\alpha} \ln \Big[1 - 2(1 - \varepsilon)t\Big], 0 \le t \le \frac{1}{2}, \ \varepsilon \le e^{-1}, \tag{4}$$

$$g(t) = \sigma + (2t - 1)(1 - \sigma), \quad 1/2 \le t \le 1. \tag{5}$$

For $\varepsilon \le e^{-1}$ we set the parameter σ

$$\sigma = \min\Big\{\frac{1}{2}, -\frac{4\varepsilon}{\alpha} \ln \varepsilon\Big\}. \tag{6}$$

With this setting of σ derivative $\Phi^{(4)}(x)$ is ε-uniformly bounded for $x \ge \sigma$.

For $\varepsilon > e^{-1}$ we set $\sigma = 1/2$. For $\sigma = 1/2$ we set the mesh Ω^h uniform.

So let the conditions be met: $\varepsilon \le e^{-1}$ and $\sigma < 1/2$. In accordance with the relations (4)– (6) define a mesh Ω^h with nodes $x_n = g(n/N)$. Given (4), (5), we obtain

$$x_n = -\frac{4\varepsilon}{\alpha} \ln \Big[1 - 2(1 - \varepsilon)n/N\Big], n = 0, 1, \dots, \frac{N}{2}, \tag{7}$$

$$x_n = \sigma + (2n/N - 1)(1 - \sigma), \ n = N/2, \dots, N.$$

Given (7), we obtain that in the boundary layer region

$$h_n = \frac{4\varepsilon}{\alpha} \ln \Big[1 + \frac{2(1 - \varepsilon)/N}{1 - 2(1 - \varepsilon)n/N}\Big], \ n = 1, 2, \dots, N/2. \tag{8}$$

It is easy to verify that the sequence of steps $h_n, \ n = 1, 2, \dots, N/2$ – is strictly increasing. From (8) it follows that

$$h_{N/2} = \frac{4\varepsilon}{\alpha} \ln \Big[1 + \frac{2(1 - \varepsilon)}{N\varepsilon}\Big].$$

Therefore, for some constant C_2 there is an estimate:

$$h_n \le \frac{C_2}{N}, \ n = 1, 2, \dots, N. \tag{9}$$

3 Cubic spline on the Bakhvalov mesh

On the constructed mesh Ω^h we define a cubic spline $S(u,x) \in C^2[0,1]$ [8]

$$S(u,x) = \frac{(x_n - x)^3}{6h_n} M_{n-1} + \frac{(x - x_{n-1})^3}{6h_n} M_n +$$

$$+ \Big(\frac{u_n}{h_n} - \frac{M_n h_n}{6}\Big)(x - x_{n-1}) + \Big(\frac{u_{n-1}}{h_n} - \frac{M_{n-1} h_n}{6}\Big)(x_n - x),$$

where $M_n = S''(u, x_n)$ and these coefficients are found from the system of equations:

$$\frac{h_n}{6} M_{n-1} + \frac{h_n + h_{n+1}}{3} M_n + \frac{h_{n+1}}{6} M_{n+1} = \frac{u_{n+1} - u_n}{h_{n+1}} - \frac{u_n - u_{n-1}}{h_n},$$

$$n = 1, 2, \ldots, N-1, \quad M_0 = u''(0), \ M_N = u''(1). \tag{10}$$

Theorem 1. *For some constant C for all $x \in [0,1]$ following error estimates are valid:*

$$\varepsilon^2 |S''(u,x) - u''(x)| \le \ \min\Big\{\frac{C}{N^2}(N\varepsilon + 2)\ln\Big[1 + \frac{2}{N\varepsilon}\Big], \frac{C}{N}\Big\}, \tag{11}$$

$$\varepsilon |S'(u,x) - u'(x)| \le \ \frac{C}{N^2}(N\varepsilon + 2)\ln^2\Big[1 + \frac{2}{N\varepsilon}\Big]. \tag{12}$$

Proof. First, we estimate the error $z_n = M_n - u''(x_n)$. Given (10), we get that $\{z_n\}$ is a solution of the system:

$$\frac{h_n}{6} z_{n-1} + \frac{h_n + h_{n+1}}{3} z_n + \frac{h_{n+1}}{6} z_{n+1} = F_n, \ n = 1, 2, \ldots, N-1, \quad z_0 = 0, \ z_N = 0, \tag{13}$$

where

$$F_n = \frac{u_{n+1} - u_n}{h_{n+1}} - \frac{u_n - u_{n-1}}{h_n} - \frac{h_n}{6} u''_{n-1} - \frac{h_n + h_{n+1}}{3} u''_n - \frac{h_{n+1}}{6} u''_{n+1}.$$

Given the Taylor series expansion with a remainder term in integral form, we obtain

$$F_n = \int\limits_{x_n}^{x_{n+1}} \Big[\frac{1}{2h_{n+1}}(x_{n+1} - s)^2 - \frac{h_{n+1}}{6}\Big] u'''(s)\,ds - \int\limits_{x_{n-1}}^{x_n} \Big[\frac{1}{2h_n}(s - x_{n-1})^2 - \frac{h_n}{6}\Big] u'''(s)\,ds. \tag{14}$$

Represent F_n in the form

$$F_n = F_n^1 - F_n^2, \quad F_n^2 = \int\limits_{x_{n-1}}^{x_n} \Big[\frac{1}{2h_n}(s - x_{n-1})^2 - \frac{h_n}{6}\Big] u'''(s)\,ds.$$

Given that with $u'''(s) = const$ $\ F_n^1 = F_n^2 = 0$, we get

$$F_n^2 = \int\limits_{x_{n-1}}^{x_n} \Big[\frac{1}{2h_n}(s - x_{n-1})^2 - \frac{h_n}{6}\Big] \int\limits_{x_{n-1}}^{s} u^{(4)}(t)\,dt\,ds. \tag{15}$$

From (15) we obtain

$$|F_n^2| < \frac{2}{3} h_n^2 \int\limits_{x_{n-1}}^{x_n} |u^{(4)}(t)|\,dt. \tag{16}$$

From (16) we get

$$\frac{|F_n^2|}{h_{n+1}} < \frac{2}{3} h_n \int\limits_{x_{n-1}}^{x_n} |u^{(4)}(s)|\,ds. \tag{17}$$

Case $n \le N/2$. Given the representation (1) with constraints (2), for some constant C we get

$$\frac{|F_n^2|}{h_{n+1}} \le C\frac{h_n}{\varepsilon^3}\Big(e^{-\alpha x_{n-1}/\varepsilon} - e^{-\alpha x_n/\varepsilon}\Big) + Ch_n^2. \tag{18}$$

Let's set $K = 2(1-\varepsilon)$. From (18), (7), (9) we obtain

$$\varepsilon^2\frac{|F_n^2|}{h_{n+1}} \le \frac{C_2}{N}\Big(1 - \frac{K(n-1)}{N}\Big)\ln\Big[1 + \frac{K}{N-Kn}\Big] + \frac{C}{N^2}. \tag{19}$$

Given (19) and the boundedness of the derivatives of the function $u(x)$ outside the boundary layer region, for some constant C_0 we get:

$$\varepsilon^2\frac{|F_n^2|}{h_{n+1}} \le \frac{C_0}{N^2},\ n < \frac{N}{2}. \tag{20}$$

$$\varepsilon^2\frac{|F_n^2|}{h_{n+1}} \le \frac{C_0}{N^2}(N\varepsilon+2)\ln\Big[1+\frac{2}{N\varepsilon}\Big],\ n = \frac{N}{2}. \tag{21}$$

$$\frac{|F_n^2|}{h_{n+1}} \le \frac{C_0}{N^2},\ n > \frac{N}{2}. \tag{22}$$

Given the estimates (20)–(22) and the fact that $\varepsilon^2|F_n^1|/h_{n+1}$ satisfies the same estimates, we obtain

$$\varepsilon^2\max_n\frac{|F_n|}{h_{n+1}} \le \frac{C}{N^2}(N\varepsilon+2)\ln\Big[1+\frac{2}{N\varepsilon}\Big].$$

From (14) implies

$$\varepsilon^2\max_n|F_n| \le \frac{C}{N^2}.$$

Therefore,

$$\varepsilon^2\max_n\frac{|F_n|}{h_{n+1}} \le \gamma = \min\Big\{\frac{C}{N^2}(N\varepsilon+2)\ln\Big[1+\frac{2}{N\varepsilon}\Big], \frac{C}{N}\Big\}. \tag{23}$$

We proceed to estimation of z_n from (13). Divide the ratio (13) by h_{n+1} and get

$$\frac{h_n}{6h_{n+1}}z_{n-1} + \Big[\frac{1}{3} + \frac{h_n}{3h_{n+1}}\Big]z_n + \frac{1}{6}z_{n+1} = \frac{F_n}{h_{n+1}},\ n = 1,\dots,N-1, z_0 = 0,\ z_N = 0. \tag{24}$$

The matrix of the system (24) has a strict diagonal predominance in rows with the prevalence index $1/6$, therefore, by the estimate (23) we get

$$\varepsilon^2\max_n|M_n - u''(x_n)| \le 6\gamma. \tag{25}$$

Let's estimate the error in calculating of the second derivative at an arbitrary point $x \in [x_{n-1}, x_n]$. It is easy to get

$$S''(u,x) - u''(x) = z_{n-1} + (z_n - z_{n-1})\frac{x - x_{n-1}}{h_n} + u''_{n-1} + (u''_n - u''_{n-1})\frac{x - x_{n-1}}{h_n} - u''(x). \tag{26}$$

Given an estimate (25) in (26) for $\varepsilon^2 z_n$ and an estimate of the error of the linear interpolation formula for the function $u''(x)$

$$\Big|u''_{n-1} + (u''_n - u''_{n-1})\frac{x - x_{n-1}}{h_n} - u''(x)\Big| \le h_n\int\limits_{x_{n-1}}^{x_n}|u^{(4)}(s)|\,ds$$

of the form (17), for some constant C we obtain

$$\varepsilon^2|S''(u,x) - u''(x)| \le C\gamma,\ x \in [x_{n-1}, x_n],\ n \le N/2.$$

It proves the estimate (11) for $x \in [x_{n-1}, x_n],\ n \le N/2$.

When $x \in [x_{n-1}, x_n],\ n > N/2$ an estimate (11) is correct, because the derivatives of the function $u(x)$ to the fourth order are ε-uniformly bounded.

Now let's get the estimate of error in the calculation of the first derivative.

Let $z(x) = S(u,x) - u(x),\ x \in [x_{n-1}, x_n]$. Due to the interpolation condition, there is $s \in (x_{n-1}, x_n)$: $z'(s) = 0$. Then, by the mean value theorem, there is $s_0 :\ z'(x) - z'(s) = z''(s_0)(x-s)$. Given (8), (11) we obtain the estimate (12). The theorem is proved.

Remark. For $\varepsilon \geq C/N$ from (11), (12) follows

$$\varepsilon |S'(u,x) - u'(x)| \leq \frac{C}{N^2},\ \varepsilon^2 |S''(u,x) - u''(x)| \leq \frac{C}{N^2},$$

for $\varepsilon = 1$ error estimates coincide with known estimates in the regular case.

4 Results of numerical experiments

Let us compare the accuracy in the calculation of derivatives based on spline interpolation when constructing a cubic spline on a uniform grid, Shishkin and Bakhvalov meshes.

Set the Shishkin mesh [1]:

$$\sigma = \min\left\{\frac{1}{2}, \frac{4\varepsilon}{\alpha}\ln N\right\},\ h_n = \frac{2\sigma}{N},\ n \leq \frac{N}{2};\ h_n = \frac{2(1-\sigma)}{N},\ n > \frac{N}{2}.$$

According to [6], in the case of a function of the form (1) and the Shishkin mesh for some constant C the following error estimates hold

$$\varepsilon^j |u^{(j)}(x) - S^{(j)}(x,u)| \leq C\frac{\ln^{4-j} N}{N^{4-j}},\quad x \in [0,1],\ j = 1,2. \tag{27}$$

Table 1: The error in calculating the first derivative on a uniform grid

ε	N					
	16	32	64	128	256	512
1	$3.84e-5$	$4.81e-6$	$6.01e-7$	$7.52e-8$	$9.40e-9$	$1.17e-9$
10^{-1}	$4.61e-3$	$6.29e-4$	$8.18e-5$	$1.04e-5$	$1.32e-6$	$1.65e-7$
10^{-2}	$8.85e-1$	$2.59e-1$	$5.36e-2$	$8.59e-3$	$1.20e-3$	$1.58e-4$
10^{-3}	$1.22e+1$	6.09	2.92	1.23	$4.00e-1$	$9.21e-2$
10^{-4}	$1.22e+2$	$6.09e+1$	$3.05e+1$	$1.53e+1$	7.63	3.73

Table 2: The error in calculating the first derivative on the Shishkin mesh

ε	N					
	16	32	64	128	256	512
1	$3.84e-5$	$4.81e-6$	$6.01e-7$	$7.52e-8$	$9.40e-9$	$1.17e-9$
10^{-1}	$4.61e-3$	$6.29e-4$	$8.18e-5$	$1.04e-5$	$1.32e-6$	$1.65e-7$
10^{-2}	$1.35e-1$	$2.45e-2$	$3.65e-3$	$4.94e-4$	$6.41e-5$	$8.15e-6$
10^{-3}	$3.16e-1$	$6.86e-2$	$1.13e-2$	$1.60e-3$	$2.12e-4$	$2.73e-5$
10^{-4}	$5.37e-1$	$1.35e-1$	$2.45e-2$	$3.65e-3$	$4.94e-4$	$6.41e-5$
10^{-5}	$7.78e-1$	$2.19e-1$	$4.36e-2$	$6.83e-3$	$9.46e-4$	$1.24e-4$

We define a function of the form (1)

$$u(x) = \cos\frac{\pi x}{2} + e^{-x/\varepsilon},\ x \in [0,1],\ \varepsilon \in (0,1].$$

Tables 1–3 show the relative error

$$\Delta_{N,\varepsilon} = \varepsilon \max_{n,j}\left|S'(u, \tilde{x}_{n,j}) - u'(\tilde{x}_{n,j})\right|$$

when calculating the first derivative of the function $u(x)$ in cases of a uniform mesh, Shishkin mesh and Bakhvalov mesh. Here $\tilde{x}_{n,j}$ are nodes of the condensed mesh, obtained from the division of each mesh interval $[x_{n-1}, x_n]$

into 10 equal parts. In tables $e - m$ means 10^{-m}. The results of calculations on the Bakhvalov mesh for all values ε and N give a third order of accuracy, which is not lower than the order of accuracy by estimate (12). The results of calculations on the Shishkin mesh are consistent with the estimate (27).

Table 4 shows the relative error

$$\Delta_{N,\varepsilon} = \varepsilon^2 \max_{n,j} \left| S''(u, \tilde{x}_{n,j}) - u''(\tilde{x}_{n,j}) \right|$$

for computing the second derivative of the function $u(x)$ in the case of the Bakhvalov mesh. Numerical results on the Bakhvalov mesh for all values of ε and N give a second order of accuracy,

Table 5 similarly shows the relative error for computing the second derivative of the function $u(x)$ in the case of the Shishkin mesh.

The calculation results show the unacceptability of using a cubic spline on a uniform mesh to calculate derivatives. The calculation error on the Bakhvalov mesh is lower than on the Shishkin mesh.

Table 3: The error in calculating the first derivative on the Bakhvalov mesh

ε	N					
	16	32	64	128	256	512
1	$3.84e-5$	$4.81e-6$	$6.01e-7$	$7.52e-8$	$9.40e-9$	$1.17e-9$
10^{-1}	$4.61e-3$	$6.29e-4$	$8.18e-5$	$1.04e-5$	$1.32e-6$	$1.65e-7$
10^{-2}	$2.78e-3$	$3.42e-4$	$4.25e-5$	$5.29e-6$	$6.60e-7$	$8.24e-8$
10^{-3}	$2.86e-3$	$3.52e-4$	$4.36e-5$	$5.43e-6$	$6.78e-7$	$8.47e-8$
10^{-4}	$2.87e-3$	$3.53e-4$	$4.37e-5$	$5.45e-6$	$6.80e-7$	$8.49e-8$

Table 4: The error in calculating the second derivative on the Bakhvalov mesh

ε	N					
	16	32	64	128	256	512
1	$2.15e-3$	$5.37e-4$	$1.34e-4$	$3.36e-5$	$8.41e-6$	$2.10e-6$
10^{-1}	$2.50e-2$	$6.91e-3$	$1.81e-3$	$4.64e-4$	$1.17e-4$	$2.95e-5$
10^{-2}	$1.81e-2$	$4.64e-3$	$1.17e-3$	$2.96e-4$	$7.42e-5$	$1.86e-5$
10^{-3}	$1.84e-2$	$4.72e-3$	$1.20e-3$	$3.01e-4$	$7.55e-5$	$1.89e-5$
10^{-4}	$1.84e-2$	$4.73e-3$	$1.20e-3$	$3.02e-4$	$7.56e-5$	$1.89e-5$

Table 5: The error in calculating the second derivative on the Shishkin mesh

ε	N					
	16	32	64	128	256	512
1	$2.15e-3$	$5.37e-4$	$1.34e-4$	$3.36e-5$	$8.41e-6$	$2.10e-6$
10^{-1}	$2.50e-2$	$6.91e-3$	$1.81e-3$	$4.64e-4$	$1.17e-4$	$2.95e-5$
10^{-2}	$1.90e-1$	$7.10e-2$	$2.15e-2$	$5.90e-3$	$1.54e-3$	$3.94e-4$
10^{-3}	$3.02e-1$	$1.31e-1$	$4.40e-2$	$1.27e-2$	$3.40e-3$	$8.77e-4$
10^{-4}	$3.91e-1$	$1.90e-1$	$7.10e-2$	$2.15e-2$	$5.90e-3$	$1.54e-3$
10^{-5}	$4.56e-1$	$2.49e-1$	$1.00e-1$	$3.21e-2$	$9.02e-3$	$2.38e-3$

5 Conclusion

The problem of calculating the derivatives of a function having large gradients in the region of an exponential boundary layer is considered. To do this, it is proposed to construct a cubic spline under the values of the function in the grid nodes. Error estimates are obtained in calculating the derivatives in the case of the Bakhvalov mesh. A numerical comparison is made of the accuracy of calculating derivatives on a uniform grid, Shishkin and

Bakhvalov meshes. It is shown that the use of the Bakhvalov mesh gives more accurate results. The use of a uniform grid is not acceptable.

6 Acknowledgements

The reported work of Zadorin N.A. was funded by RFBR, project number 19-31-60009. The work of Zadorin A.I. was funded by program of fundamental scientific researches of the SB RAS 1.1.3., project 0314-2019-0009.

References

[1] G.I. Shishkin *Mesh Approximations of Singularly Perturbed Elliptic and Parabolic Equations.* Yekaterinburg-Ural. Otd. Ross. Akad. Nauk, 1992 (in Russian).

[2] N.S. Bakhvalov The optimization of methods of solving boundary value problems with a boundary layer. *USSR Comput. Math. Math. Phys.* 9(4):139-166, 1969.

[3] A.I. Zadorin, N.A. Zadorin Spline interpolation on a uniform mesh for functions with a boundary-layer component. *Comput. Math. Math. Phys.* 50(2):211-223, 2010.

[4] I.A. Blatov, A.I. Zadorin, E.V. Kitaeva On interpolation by cubic splines of the functions with a boundary layers. *CEUR Workshop Proceedings.* 1638:515-520, 2016.

[5] I.A. Blatov, A.I. Zadorin, E.V. Kitaeva Cubic spline interpolation of functions with high gradients in boundary layers. *Comput. Math. Math. Phys.* 57(1):7-25, 2017.

[6] I.A. Blatov, A.I. Zadorin, E.V. Kitaeva Approximation of a function and its derivatives on the basis of cubic spline interpolation in the presence of a boundary layer. *Comput. Math. Math. Phys.* 59(3):343-354, 2019.

[7] I.A. Blatov, A.I. Zadorin, E.V. Kitaeva On the parameter-uniform convergence of exponential spline interpolation in the presence of a boundary layer. *Comput. Math. Math. Phys.* 58(3):348-363, 2018.

[8] Yu.S. Zavyalov, B.N. Kvasov, V. L. Miroshnichenko *Methods of Spline Functions.* Moscow-Nauka, 1981 (in Russian).