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ANALYSIS OF FORMULAS FOR NUMERICAL DIFFERENTIATION OF FUNCTIONS WITH LARGE GRADIENTS

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Abstract: The issue of numerical differentiation of a function of one variable in the presence of a boundary layer is considered. The relevance of the study is related to the fact that in the presence of large gradients of the function, the error of classical formulas of numerical differentiation on a uniform grid can be significant. In order to ensure that the formula error does not increase due to large gradients of the function, two approaches are considered: the use of classical formulas of numerical differentiation on grids that thicken in the boundary layer region and the construction of formulas on a uniform grid that are exact on the boundary layer component responsible for large gradients of the function. The formulas on Shishkin and Bakhvalov meshes, widely used in constructing difference schemes in the presence of a boundary layer, are studied. A comparison of the approaches is carried out.

Keywords: function of one variable, large gradients, numerical differentiation formula, Shishkin mesh, Bakhvalov mesh, special numerical formula for derivative, error estimation.

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1 Introduction

Application classical polynomial numerical differentiation formulas [1] on a uniform grid in the presence of a boundary layer can lead to significant errors [2]. Therefore, it is necessary to construct numerical differentiation formulas whose errors do not increase due to large gradients of the function in the boundary layer region.

To construct formulas that take the presence of a boundary layer into account, two approaches were used: using numerical differentiation formulas that are exact on the boundary layer component of the function [2]– [5], and using classical polynomial numerical differentiation formulas on Shishkin [6] and Bakhvalov [7] meshes, which become denser in the boundary layer region.

Numerical differentiation formulas on the Shishkin mesh were studied, for example, in [8], [9]. In [8] a difference scheme was used to find the solution of a boundary value problem for a second-order an ordinary differential equation with a small parameter ε at the highest derivative. Based on the grid solution, the first derivative was calculated. An estimate of the relative error in calculating the derivative was obtained, uniform in the parameter ε.

In [9], the issue of calculating the derivative of a function with large gradients in an exponential boundary layer is considered. On each interval $[x_m, x_{m+k-1}]$ of the Shishkin mesh, the classical formula with k nodes in the grid sample for the derivative is applied. The relative error in calculating the n-th derivative in [9] is given by multiplying the absolute error by ε^n. This corresponds to the fact that on the interval under consideration, $|u^{(n)}(x)| \leq C/\varepsilon^n$. However, on the intervals $[x_m, x_{m+k-1}]$, on which the derivatives of the function $u(x)$ are bounded, multiplying by ε^n to calculate the relative error is incorrect. In this case, we estimate the absolute error.

In [10], estimates of the relative error of the classical numerical differentiation formula were obtained on the Bakhvalov mesh with a modification from [11] for each interval $[x_m, x_{m+k-1}]$. As in the case of the Shishkin mesh, on intervals outside the boundary layer region it is more correct to obtain the estimate of the absolute error.

Now we will discuss existing results on the development of numerical differentiation formulas that are exact on the boundary layer component responsible for large function gradients.

In [2], a decomposition of the function is used, in which the component responsible for large function gradients is known up to a factor. An interpolation formula with an arbitrarily number of interpolation nodes k, is constructed on a uniform grid; this formula is exact on the boundary layer component. A uniform error estimate for this interpolation formula over the boundary layer component was obtained in [4]. Based on differentiation of the constructed interpolant, a numerical differentiation formula with k nodes in a grid template for the derivative is constructed in [2]; this formula is exact on the boundary layer component of the function.

Previously, the extraction of the boundary layer component was used in [12] and [13] to construct a difference scheme with the property of uniform convergence in the parameter ε when solving a singularly perturbed boundary value problem.

In this paper, we continue the analysis of numerical differentiation formulas for functions with large gradients. We will conduct a comparative analysis of the approaches under consideration.

By C and C_j, we will mean positive constants independent of the boundary layer component $\Phi(x)$, its derivatives, and the number of grid intervals N. In the case of an exponential boundary layer, these constants are independent of ε. We will constrain various quantities to a single constant C_j, if clear from the text. We will assume that $f = O(g)$ if for some constant $C \quad |f| \le C|g|$; $f = O^*(g)$ if $f = O(g)$ and $g = O(f)$. Let us denote $K = 2(1-\varepsilon)$.

2 Application of the classical formula for numerical differentiation

Let the function $u(x)$ satisfy the decomposition:

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

where the components $q(x)$ and $\Phi(x)$ are not explicitly specified and the derivative estimates for them hold:

$$|q^{(n)}(x)| \le C_1, \quad |\Phi^{(n)}(x)| \le \frac{C_1}{\varepsilon^n} e^{-\alpha x/\varepsilon}, \quad 0 \le n \le k,\ \alpha > 0, \varepsilon \in (0,1]. \tag{2}$$

According to (2), the regular component $q(x)$ has derivatives bounded up to a given order k, while the derivatives of the boundary-layer component $\Phi(x)$ are not uniformly bounded in the parameter ε.

The decomposition (1) for an arbitrarily given k was developed in [6] for the solution $u(x)$ of a singularly perturbed problem:

$$\varepsilon u''(x) + a_1(x)u'(x) - a_2(x)u(x) = f(x), \quad u(0) = A,\ u(1) = B, \tag{3}$$

where $a_1(x) \ge \alpha > 0, a_2(x) \ge 0,\ \varepsilon \in (0,1]$, the functions a_1, a_2, f are sufficiently smooth. This decomposition was used in [6] and other works to estimate the error of difference schemes.

We apply the decomposition (1) to estimate the error of polynomial numerical differentiation formulas in the presence of a boundary layer.

We define a grid on the interval $[0,1]$:

$$\Omega^h = \{x_0 = 0,\ x_j = x_{j-1} + h_j, j = 1, \dots, N,\ x_N = 1\}.$$

We assume that the function $u(x)$, which has the decomposition (1), is defined at the nodes of the grid Ω^h, $u_j = u(x_j)$.

Let the original interval $[0,1]$ be divided into disjoint intervals $[x_m, x_{m+k-1}]$, on which we will construct numerical differentiation formulas with k nodes in the template for the derivative. In (2), we define k as the number of nodes in the template formula for calculating the derivative.

Let $L_{m,k}(u,x)$ be the Lagrange polynomial for $u(x)$, $\{x_m,\dots,x_{m+k-1}\}$ be the interpolation nodes on the interval $[x_m,x_{m+k-1}]$. Classical difference formulas for calculating derivatives are constructed based on differentiating the Lagrange polynomial [1]:

$$u^{(n)}(x)\approx L^{(n)}_{m,k}(u,x), n<k,\ x\in[x_m,x_{m+k-1}]. \tag{4}$$

In accordance with [14, p. 117] the error estimate is valid:

$$|u^{(n)}(x)-L^{(n)}_{m,k}(u,x)|\le C_0\max_s|u^{(k)}(s)|\max_j h_j^{k-n},\ x,s\in[x_m,x_{m+k-1}] \tag{5}$$

for some constant C_0, where $k>n\ge 0,\ j=m+1,\dots,m+k-1$.

Now let's focus on the case of a uniform grid with step h. From (5) it follows that the absolute error in calculating derivatives based on the application of formula (4) is of order $O(h^{k-n})$, if the derivative $u^{(k)}(x)$ is uniformly bounded.

In the exponential boundary layer region from (2), (5), for some constant C_2, we have the error estimate:

$$\varepsilon^n\Big|u^{(n)}(x)-L^{(n)}_{m,k}(u,x)\Big|\le C_2\Big(\frac{h}{\varepsilon}\Big)^{k-n},\ x\in[x_m,x_{m+k-1}],n\ge 0. \tag{6}$$

According to (6), for $\varepsilon\le h$, the relative error can be significant. We show that the estimate (6) is achievable. Let $u(x)=e^{-x/\varepsilon}, x\in[0,1]$. We write out the formula for the derivative:

$$u'(x)\approx\frac{u_j-u_{j-1}}{h},\ x\in[x_{j-1},x_j]. \tag{7}$$

In the case of formula (7) with $\varepsilon=h$, despite the smallness of h, we have:

$$\varepsilon\big|\frac{u_1-u_0}{h}-u'(0)\big|=e^{-1}.$$

Thus, in the case of a uniform grid, the relative error of classical polynomial formulas for numerical differentiation can be significant if the function has large gradients.

2.1. Error estimation on the Shishkin mesh. Given the decomposition (1) − (2), we define the Shishkin mesh [6]. Let's set the parameter σ :

$$\sigma=\min\Big\{\frac{1}{2},\frac{k\varepsilon}{\alpha}\ln N\Big\} \tag{8}$$

and grid steps of Ω^h:

$$h_j=h=\frac{2\sigma}{N},\ 1\le j\le\frac{N}{2};\ h_j=H=\frac{2(1-\sigma)}{N},\ \frac{N}{2}<j\le N. \tag{9}$$

In (8) k corresponds to the number of nodes in the sample for the derivative, α corresponds to the condition $a_1(x)\ge\alpha>0$ in (3). According to (9), in the case $\sigma=1/2$, the grid is uniform. We assume that the interval $[0,1]$ is covered by disjoint intervals $[x_m,x_{m+k-1}]$, and that each interval lies entirely within or outside the interval $[0,\sigma]$. This is true if N is a multiple of $2(k-1)$.

We estimate the error in calculating the derivative by applying formula (4) on each interval $[x_m, x_{m+k-1}]$ of the Shishkin mesh.

Theorem 1. *Let the function $u(x)$ satisfy the decomposition (1)–(2), and let the grid Ω^h correspond to (8), (9). Then, for all $x \in [x_m, x_{m+k-1}]$, depending on the values of m and σ, one of the error estimates holds for some constant C:*

$$\varepsilon^n \Big| u^{(n)}(x) - L^{(n)}_{m,k}(u,x) \Big| \leq C \Big(\frac{\ln N}{N} \Big)^{k-n}, \ x_{m+k-1} \leq \sigma, \ \sigma < \frac{1}{2}, \tag{10}$$

$$\varepsilon^n \Big| L^{(n)}_{m,k}(u,x) - u^{(n)}(x) \Big| \leq \frac{C}{N^k} e^{-\alpha(x_m-\sigma)/\varepsilon} + \frac{C\varepsilon^n}{N^{k-n}}, \ x_m \geq \sigma, \quad \sigma < \frac{1}{2}, \tag{11}$$

$$\Big| L^{(n)}_{m,k}(u,x) - u^{(n)}(x) \Big| \leq C \frac{(\ln N)^k}{N^{k-n}}, \ \sigma = \frac{1}{2}. \tag{12}$$

Proof. Taking into account (8), (9), we obtain that in the boundary layer region $[0, \sigma]$, the estimate (6) turns into the relative error estimate (10).

Let us dwell on the estimate (11), applied outside the boundary layer region $[0, \sigma]$. We use the estimate:

$$\varepsilon^n \Big| L^{(n)}_{m,k}(\Phi,x) - \Phi^{(n)}(x) \Big| \leq \varepsilon^n |L^{(n)}_{m,k}(\Phi,x)| + \varepsilon^n |\Phi^{(n)}(x)|. \tag{13}$$

In accordance with (2), (8) for $x_m \geq \sigma$ we have

$$\varepsilon^n |\Phi^{(n)}(x)| \leq \frac{C_1}{N^k} e^{-\alpha(x_m-\sigma)/\varepsilon}, \ x \in [x_m, x_{m+k-1}]. \tag{14}$$

The Lagrange polynomial on the interval $[x_m, x_{m+k-1}]$ has the form [1]:

$$L_{m,k}(\Phi,x) = \sum_{j=m}^{m+k-1} \Phi_j P_{j,m}(x), \ \Phi_j = \Phi(x_j), \ P_{j,m}(x) = \prod_{\substack{i=m \\ i \neq j}}^{m+k-1} \frac{x - x_i}{x_j - x_i}.$$

For the derivative of the Lagrange polynomial for some constant C_2 we have

$$\Big| L^{(n)}_{m,k}(\Phi,x) \Big| = \Big| \sum_{j=m}^{m+k-1} \Phi_j P^{(n)}_{j,m}(x) \Big| \leq \frac{C_2}{H^n} \max_{m \leq j \leq m+k-1} |\Phi_j|, \tag{15}$$

where H corresponds to (9). Taking into account (2), (9), for $x_m \geq \sigma$ we obtain from (15)

$$|L^{(n)}_{m,k}(\Phi,x)| \leq \frac{C_3}{N^{k-n}} e^{-\alpha(x_m-\sigma)/\varepsilon} \tag{16}$$

for some constant C_3.

Taking into account (2), (13), (14), (16), for $x_m \geq \sigma$ we obtain the estimate:

$$\varepsilon^n \Big| L^{(n)}_{m,k}(\Phi,x) - \Phi^{(n)}(x) \Big| \leq \frac{C_1}{N^k} e^{-\alpha(x_m-\sigma)/\varepsilon} + \varepsilon^n \frac{C_3}{N^{k-n}} e^{-\alpha(x_m-\sigma)/\varepsilon},$$
$$x \in [x_m, x_{m+k-1}]. \tag{17}$$

Given (17) and the estimate (5) in the case of the regular component $q(x)$, for some constant C we obtain the estimate (11).

It remains to consider the case where in (8) $\sigma = 1/2$, in which case the grid Ω^h becomes uniform. Then from (8) it follows that $\varepsilon \geq \alpha/(2k \ln N)$. Taking this inequality into account in the estimate (6), we obtain the estimate (12). The theorem is proved. □

According to (11), as $(x_m - \sigma)$ increases, that is, as we move away from the boundary layer region, the relative error estimate on the interval $[x_m, x_{m+k-1}]$ transforms into an absolute error estimate of order $O(1/N^{k-n})$.

2.2. Error estimation on the Bakhvalov mesh. We assume that the decomposition (1) − (2) holds for the function $u(x)$. We define the Bakhvalov mesh [7] taking into account the modification [11].

We define the parameter σ :

$$\sigma = \min\Big\{\frac{1}{2}, -\frac{k\varepsilon}{\alpha}\ln\varepsilon\Big\}, \varepsilon \leq e^{-1}. \tag{18}$$

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

Let $\sigma < 1/2$. We define nodes on the interval $[0, \sigma]$, where, according to (1) − (2), the function $u(x)$ has large gradients:

$$x_j = -\frac{k\varepsilon}{\alpha}\ln\Big[1 - 2(1-\varepsilon)\frac{j}{N}\Big],\ j = 0, 1, \ldots, \frac{N}{2}. \tag{19}$$

From (19) it follows that $x_{N/2} = \sigma$. On the interval $[\sigma, 1]$, we define the grid as uniform, $h_j = 2(1-\sigma)/N$, where $j = N/2+1, ..., N$. Taking into account (19), we obtain

$$h_j = \frac{k\varepsilon}{\alpha}\ln\Big[1 + \frac{2(1-\varepsilon)}{N - 2(1-\varepsilon)j}\Big],\ j = 1, 2, \ldots, \frac{N}{2}. \tag{20}$$

The sequence of steps $\{h_j\}$ in (20) is strictly increasing. It is easy to show that for some constant C the following estimate holds:

$$h_j \leq \frac{C}{N},\ j = 1, 2, \ldots, N. \tag{21}$$

In accordance with the following theorem we obtain estimates of the error on the Bakhvalov mesh.

Theorem 2. *Let the decomposition (1) − (2) hold for the function $u(x)$, and let the grid Ω^h correspond to the Bakhvalov mesh defined above. Then, for all $x \in [x_m, x_{m+k-1}]$, depending on the values of m and σ, one of the error estimates holds for some constant C:*

$$\varepsilon^n \Big|u^{(n)}(x) - L^{(n)}_{m,k}(u,x)\Big| \leq C\Big[\Big(\varepsilon + \frac{K(k-1)}{N}\Big)^k \ln^{k-n}\Big(1 + \frac{K}{N\varepsilon}\Big) + \frac{\varepsilon^n}{N^{k-n}}\Big],$$
$$K = 2(1-\varepsilon), \quad x_{m+k-1} = \sigma, \tag{22}$$

$$\varepsilon^n \Big|u^{(n)}(x) - L^{(n)}_{m,k}(u,x)\Big| \leq \frac{C}{N^{k-n}}, \quad x_{m+k-1} < \sigma, \tag{23}$$

$$\Big|u^{(n)}(x) - L^{(n)}_{m,k}(u,x)\Big| \leq \frac{C}{N^{k-n}}, \quad x_m \geq \sigma,\ \sigma < \frac{1}{2}, \tag{24}$$

$$\left|u^{(n)}(x) - L^{(n)}_{m,k}(u,x)\right| \le \frac{C}{N^{k-n}},\ \ \sigma = \frac{1}{2}. \tag{25}$$

Proof. Taking into account (2), (21), from inequality (5) we obtain that for some constant C_0 for all m

$$\left|q^{(n)}(x) - L^{(n)}_{m,k}(q,x)\right| \le \frac{C_0}{N^{k-n}},\ \ x \in [x_m, x_{m+k-1}]. \tag{26}$$

Let's consider various cases for the interval $[x_m, x_{m+k-1}]$.

We will dwell on the estimate (22), when $x_{m+k-1} = \sigma$. In this case $m = N/2 - k + 1$. Taking into account (19), for a given m we have

$$x_m = -\frac{k\varepsilon}{\alpha} \ln\Big(\varepsilon + \frac{K(k-1)}{N}\Big). \tag{27}$$

Then

$$e^{-\alpha x_m/\varepsilon} = \Big(\varepsilon + \frac{K(k-1)}{N}\Big)^k. \tag{28}$$

From (20) it follows

$$h_{N/2} = \frac{k\varepsilon}{\alpha} \ln\Big(1 + \frac{K}{N\varepsilon}\Big). \tag{29}$$

Taking into account estimates (2), (26), (28), (29) in (5), we obtain estimate (22).

Let us consider the case $x_{m+k-1} < \sigma$. Then $m + k - 1 = N/2 - l$, where $l > 0$. Then, in accordance with (20)

$$h_{m+k-1} = \frac{k\varepsilon}{\alpha} \ln\Big[1 + \frac{K}{N\varepsilon + Kl}\Big]. \tag{30}$$

Considering (28), (30) from (5) we obtain

$$\varepsilon^n \left|\Phi^{(n)}(x) - L^{(n)}_{m,k}(\Phi,x)\right| \le C\Big(\varepsilon + \frac{K(k-1)}{N}\Big)^k \ln^{k-n}\Big(1 + \frac{K}{N\varepsilon + Kl}\Big). \tag{31}$$

Taking into account (26), (31), we obtain estimate (23).

Let's dwell on the estimate (24). For $x_m \ge \sigma$, in accordance with (2), (18), (21), for some constant C_1, the estimate $|u^{n)}(x)| \le C_1$ holds for all $n < k$ and $x \in [x_m, x_{m+k-1}]$. Then from (5), we obtain the estimate (24).

Let's dwell on the assessment (25). In the case $\sigma = 1/2$ the grid Ω^h is uniform. Let us prove that in this case $\varepsilon \ge C_0 > 0$ for some constant C_0.

According to (18), for $\sigma = 1/2$ the inequality $-\varepsilon \ln \varepsilon \ge \alpha/(2k)$ holds. Let us set $A = \min\{\alpha/(2k), e^{-1}\}$. The function $f(x) = -x \ln x$ increases on the interval $[0, e^{-1}]$, therefore $A = -C_0 \ln C_0$ for some positive constant C_0, where $C_0 \le e^{-1}$. Given the increasing $f(x)$ and the inequality $-\varepsilon \ln \varepsilon \ge -C_0 \ln C_0$, we obtain $\varepsilon \ge C_0 > 0$.

Thus, in the case $\sigma = 1/2$, the estimate $\varepsilon \ge C_0 > 0$ holds. Then, in accordance with the decomposition (1), the derivatives of the function $u(x)$ are bounded uniformly in ε. Hence, on an arbitrary interval $[x_m, x_{m+k-1}]$, in accordance with (5), (21), for some constant C, the error estimate (25) holds. The theorem is proved. □

The estimate (22) is simplified depending on the relationship between N and ε. For $\varepsilon \le C/N$ from (22) for some constant C_0 it follows

$$\varepsilon^n \Big| u^{(n)}(x) - L^{(n)}_{m,k}(u,x) \Big| \le C_0 \Big[\frac{1}{N^k} \ln^{k-n} \Big(1 + \frac{K}{N\varepsilon}\Big) + \frac{\varepsilon^n}{N^{k-n}} \Big],$$

$$x \in [x_m, x_{m+k-1}],\ x_{m+k-1} = \sigma. \tag{32}$$

The estimate (32) corresponds to the step $h_{N/2}$ of the Bakhvalov mesh defined in (29).

3 Numerical Differentiation Formulas Exact on the Boundary Layer Component

On a uniform grid, we investigate numerical differentiation formulas that are exact on the boundary layer component responsible for large gradients of the function. The construction of such formulas is based on differentiating an interpolant that is exact on the boundary layer component [2], [4].

We assume that for a sufficiently smooth function $u(x)$ the following decomposition holds:

$$u(x) = p(x) + \gamma \Phi(x),\ x \in [0,1], \tag{33}$$

where $p(x)$ is a regular component with bounded derivatives up to order k, $\Phi(x)$ is a boundary layer component, which is a general function and is responsible for large gradients of the function $u(x)$. The function $\Phi(x)$ is assumed to be known, $p(x)$ and γ are not specified, for some constant C $|\gamma| \le C$.

According to [13], for an arbitrarily given k, the decomposition (33) can be constructed for the solution of the problem (3). In this case

$$\Phi(x) = e^{-\beta x/\varepsilon},\ \varepsilon \in (0,1], \tag{34}$$

where $\beta > 0, \beta = a_1(0)$ where $a_1(x)$ corresponds to (3). For the derivatives of the regular component $p(x)$, the following estimates hold [13]:

$$|p^{(n)}(x)| \le C_0 \Big[1 + \frac{1}{\varepsilon^{n-1}} e^{-\alpha x/\varepsilon}\Big], n \le k, \tag{35}$$

where α corresponds to the condition $a_1(x) \ge \alpha > 0$. According to (34), (35), the derivative $p'(x)$ is bounded uniformly in ε, the derivatives of the function $\Phi(x)$ increase with decreasing ε, $\varepsilon \in (0,1]$.

A.M. Il'in in [12] proposed fitting a difference scheme to the boundary layer component (34), achieving the uniform convergence of the scheme in the parameter ε.

We use a similar approach when constructing formulas for the numerical differentiation of functions with decomposition (33). The function $\Phi(x)$ can correspond to the presence of an exponential, power-law boundary layer, or another singularity [3].

In [2], the interpolation formula for a function with decomposition (33), which is exact on the component $\Phi(x)$, is constructed:

$$L_{\Phi,k}(u,x) = L_{m,k-1}(u,x) + \frac{[x_m,\dots,x_{m+k-1}]u}{[x_m,\dots,x_{m+k-1}]\Phi}\Big[\Phi(x) - L_{m,k-1}(\Phi,x)\Big], \quad x \in [x_m, x_{m+k-1}], \tag{36}$$

where $L_{m,k}(u,x)$ is the Lagrange polynomial defined before formula (4), $[x_m,\dots,x_{m+k-1}]u$ is the divided difference [1] for function $u(x)$, k is the number of interpolation nodes, $k \geq 2$.

The formula (36), according to [4], can be written as:

$$L_{\Phi,k}(u,x) = L_{m,k}(u,x) + \frac{[x_m,\dots,x_{m+k-1}]u}{[x_m,\dots,x_{m+k-1}]\Phi}\Big[\Phi(x) - L_{m,k}(\Phi,x)\Big], \quad x \in [x_m, x_{m+k-1}], \tag{37}$$

To prevent the denominator in (37) from vanishing, we impose the constraint:

$$\Phi^{(k-1)}(x) \neq 0, \;\; x \in (x_m, x_{m+k-1}).$$

Formula (37) is an interpolation formula with nodes $x_m, x_{m+1}, \dots, x_{m+k-1}$ and exact on polynomials of degree $(k-2)$ and on the function $\Phi(x)$.

By differentiating (37) in [4], a numerical differentiation formula is constructed that is exact on the boundary layer component $\Phi(x)$:

$$u^{(n)}(x) \approx L^{(n)}_{\Phi,k}(u,x) = L^{(n)}_{m,k}(u,x) + \frac{\Delta^{k-1}u_m}{\Delta^{k-1}\Phi_m}\Big[\Phi^{(n)}(x) - L^{(n)}_{m,k}(\Phi,x)\Big], \tag{38}$$

where $x \in [x_m, x_{m+k-1}]$, $n < k$, $\Delta^{k-1}u_m$ is the finite difference for the function $u(x)$ [1, p. 65], defined by the relations:

$$\Delta u_m = u_{m+1} - u_m, \Delta^j u_m = \Delta(\Delta^{j-1}u_m).$$

We propose to estimate the error of formula (38) based on the following theorem.

Theorem 3. *Let the function $u(x)$ satisfy the decomposition* (33)*, the constant D_k is defined such that $0 < 1/D_k \leq C_1$ for some constant C_1 and the following estimate holds:*

$$G = \frac{h^{k-2}}{D_k} \int\limits_{x_m}^{x_{m+k-1}} |\Phi^{(k)}(t)|\,dt \Big/ |\Delta^{k-1}\Phi_m| \leq C_2 \tag{39}$$

for some constant C_2. Then, for some constant C, for all $x \in [x_m, x_{m+k-1}]$, the following error estimate holds:

$$\frac{1}{D_k}\Big|L^{(n)}_{\Phi,k}(u,x) - u^{(n)}(x)\Big| \leq Ch^{k-n-1}\Big[\frac{1}{D_k}\int\limits_{x_m}^{x_{m+k-1}} |p^{(k)}(t)|\,dt + \int\limits_{x_m}^{x_{m+k-2}} |p^{(k-1)}(t)|\,dt\Big]. \tag{40}$$

Proof. In [5], a theorem was proved according to which, if condition (39) is satisfied for some constant C_2, then for all $x \in [x_m, x_{m+k-1}]$, the following estimate holds:

$$\frac{1}{D_k}\Big|L^{(n)}_{\Phi,k}(u,x) - u^{(n)}(x)\Big| \le \frac{1}{D_k}\Big|L^{(n)}_{m,k}(p,x) - p^{(n)}(x)\Big| +$$
$$+\frac{C_2}{h^{n-1}}\Big|L_{m,k-1}(p, x_{m+k-1}) - p(x_{m+k-1})\Big|. \tag{41}$$

According to [5, formula (3.8)], there exists a constant C_3 such that for an arbitrary sufficiently smooth function $v(x)$ the following estimate holds:

$$|L^{(n)}_{m,k}(v,x) - v^{(n)}(x)| \le C_3 h^{k-n-1} \int\limits_{x_m}^{x_{m+k-1}} |v^{(k)}(t)|\,dt \tag{42}$$

for all $x \in [x_m, x_{m+k-1}]$. Applying the estimate (42) for $v(x) = p(x)$, from (41) we obtain the estimate (40), which proves the theorem. □

Let us consider an example of applying Theorem 3. Consider the case $k = 2, n = 1$. We assume that for a sufficiently smooth function $u(x)$, the decomposition (33) holds, and

$$\Phi'(x) \ne 0, x \in (x_m, x_{m+1}) \tag{43}$$

and for some constant D_2, the following estimate holds:

$$|\Phi''(x)| \le D_2|\Phi'(x)|,\ x \in [x_m, x_{m+1}]. \tag{44}$$

Let us write down the formula (38) in the case of $k = 2,\ n = 1:$

$$u'(x) \approx L'_{\Phi,2}(u,x) = \frac{u_{m+1} - u_m}{\Phi_{m+1} - \Phi_m}\Phi'(x), x \in [x_m, x_{m+1}]. \tag{45}$$

According to (39), in the case under consideration

$$G = \frac{1}{D_2}\int\limits_{x_m}^{x_{m+1}} |\Phi''(s)|\,ds \Big/ |\Phi_{m+1} - \Phi_m|. \tag{46}$$

Taking into account (43), (44), from (46) we obtain that $G \le 1$.

So, the condition (39) is satisfied when $C_2 = 1$. In accordance with Theorem 3, the estimate (40) holds, which in the case under consideration has the form:

$$\Big|\frac{u_{m+1} - u_m}{\Phi_{m+1} - \Phi_m}\Phi'(x) - u'(x)\Big| \le C \int\limits_{x_m}^{x_{m+1}} |p''(t)|\,dt. \tag{47}$$

Thus, we have obtained an estimate of the error (47) of formula (45) under constraints (43), (44).

In the case of an exponential boundary layer, when relations (34), (35) are valid, from (47) we obtain an estimate of the relative error:

$$\varepsilon\Big|\frac{u_{m+1} - u_m}{\Phi_{m+1} - \Phi_m}\Phi'(x) - u'(x)\Big| \le C_1 h,\ x \in [x_m, x_{m+1}] \tag{48}$$

for some constant C_1.

Thus, applying Theorem 3, we obtained error estimates (47), (48).

In [5], in the case of an exponential boundary layer and $k = n + 1$, the following error estimate was obtained for formula (38):

$$\varepsilon^n \left| L^{(n)}_{\Phi,k}(u, x) - u^{(n)}(x) \right| \leq Ch, \; x \in [x_m, x_{m+k-1}]. \quad (49)$$

By differentiating (36), we can verify that for $k = n + 1$, formula (38) is significantly simplified:

$$u^{(n)}(x) \approx L^{(n)}_{\Phi,k}(u, x) = \frac{\Delta^n u_m}{\Delta^n \Phi_m} \Phi^{(n)}(x), \quad x \in [x_m, x_{m+k-1}].$$

4 Results of numerical experiments

We define the function:

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

The function $u(x)$ corresponds to the decompositions (1), (33), $\Phi(x) = e^{-x/\varepsilon}$.

We present the results of numerical experiments calculating the second derivative of the function $u(x)$ on the intervals $[x_m, x_{m+2}]$, covering the interval $[0, 1]$.

We will dwell on the application of the classical formula:

$$u''(x) \approx L''_{m,3}(u, x) = \frac{2u_m}{h_{m+1}(h_{m+1} + h_{m+2})} - \frac{2u_{m+1}}{h_{m+1}h_{m+2}} +$$

$$+ \frac{2u_{m+2}}{h_{m+2}(h_{m+1} + h_{m+2})}, \; m = 0, 2, \ldots, N - 2, \; x \in [x_m, x_{m+2}] \quad (50)$$

and the formula on a uniform grid, exact on the boundary layer component:

$$u''(x) \approx L''_{\Phi,3}(u, x) = \frac{u_m - 2u_{m+1} + u_{m+2}}{\Phi_m - 2\Phi_{m+1} + \Phi_{m+2}} \Phi''(x), \quad x \in [x_m, x_{m+2}]. \quad (51)$$

In the tables, $ae - j$ denotes $a \times 10^{-j}$.

Table 1 shows the error

$$\Delta_{\varepsilon,N} = \varepsilon^2 \max_m \max_j |L''_{m,3}(u, \tilde{x}_{j,m}) - u''(\tilde{x}_{j,m})|$$

when calculated using formula (50) for the uniform grid, where $\tilde{x}_{j,m}$ are the nodes of the interval $[x_m, x_{m+2}]$ of a grid condensed by a factor of four.

According to the calculation results, the error does not decrease with increasing number of grid intervals N, if $\varepsilon = 1/N$. This confirms that applying classical numerical differentiation formulas on a uniform grid to functions with large gradients can lead to significant errors.

Let's consider the calculation results using formula (50) on the Shishkin and Bakhvalov meshes.

Tables 2-3 show the error $\Delta_{\varepsilon,N}$ and the calculated order of accuracy

$$M_{\varepsilon,N} = \log_2 \frac{\Delta_{\varepsilon,N}}{\Delta_{\varepsilon,2N}}$$

for the Shishkin and Bakhvalov meshes.

The calculation results on the Shishkin mesh, presented in Table 2, are consistent with the error estimate (10) for $k = 3, n = 2$.

The results of calculations on the Bakhvalov mesh, presented in Table 3, correspond to an error of the order of $O(1/N)$, which is consistent with the estimate (23) for $k = 3, n = 2$.

Table 4 shows the error in calculating $\tilde{\Delta}_{\varepsilon,N}$ using formula (51), where

$$\tilde{\Delta}_{\varepsilon,N} = \varepsilon^2 \max_m \max_j |L''_{\Phi,3}(u, \tilde{x}_{j,m}) - u''(\tilde{x}_{j,m})|.$$

According to the errors presented in Table 4, the order of accuracy of formula (51) is close to the first order, which corresponds to the estimate (49) in the case $k = 3, n = 2$.

TABLE 1. Error of the classical formula (50) on a uniform grid

ε	N					
	16	32	64	128	256	512
1	$1.74e-1$	$8.74e-2$	$4.38e-2$	$2.19e-2$	$1.10e-2$	$5.48e-3$
16^{-1}	$2.26e-1$	$1.19e-1$	$6.10e-2$	$3.09e-2$	$1.55e-2$	$7.79e-3$
32^{-1}	$4.00e-1$	$2.23e-1$	$1.18e-1$	$6.07e-2$	$3.08e-2$	$1.55e-2$
64^{-1}	$6.35e-1$	$3.95e-1$	$2.22e-1$	$1.18e-1$	$6.06e-2$	$3.08e-2$
128^{-1}	$8.61e-1$	$6.30e-1$	$3.93e-1$	$2.21e-1$	$1.17e-1$	$6.06e-2$
256^{-1}	$9.77e-1$	$8.57e-1$	$6.27e-1$	$3.91e-1$	$2.21e-1$	$1.17e-1$
512^{-1}	$1.00e+0$	$9.77e-1$	$8.55e-1$	$6.26e-1$	$3.91e-1$	$2.20e-1$

TABLE 2. Error and order of accuracy of the formula (50) on the Shishkin mesh

ε	N					
	16	32	64	128	256	512
1	$1.74e-1$	$8.74e-2$	$4.38e-2$	$2.19e-2$	$1.10e-2$	$5.48e-3$
	1.00	1.00	1.00	1.00	1.00	1.00
16^{-1}	$3.50e-1$	$2.58e-1$	$1.68e-1$	$9.17e-2$	$4.79e-2$	$2.45e-2$
	0.44	0.62	0.88	0.94	0.97	0.98
32^{-1}	$3.50e-1$	$2.58e-1$	$1.74e-1$	$1.09e-1$	$6.52e-2$	$3.77e-2$
	0.44	0.57	0.67	0.74	0.79	0.83
64^{-1}	$3.50e-1$	$2.58e-1$	$1.74e-1$	$1.09e-1$	$6.52e-2$	$3.77e-2$
	0.44	0.57	0.67	0.74	0.79	0.83

TABLE 3. Error and order of accuracy of the formula (50) on the Bakhvalov mesh

ε	N					
	16	32	64	128	256	512
1	$1.74e-1$	$8.74e-2$	$4.38e-2$	$2.19e-2$	$1.10e-2$	$5.48e-3$
	1.00	1.00	1.00	1.00	1.00	1.00
16^{-1}	$2.38e-1$	$1.30e-1$	$6.76e-2$	$3.45e-2$	$1.74e-2$	$8.75e-3$
	0.87	0.94	0.97	0.99	0.99	1.00
32^{-1}	$2.44e-1$	$1.34e-1$	$6.98e-2$	$3.56e-2$	$1.80e-2$	$9.04e-3$
	0.87	0.94	0.97	0.99	0.99	1.00
64^{-1}	$2.48e-1$	$1.36e-1$	$7.08e-2$	$3.62e-2$	$1.83e-2$	$9.18e-3$
	0.87	0.94	0.97	0.99	0.99	1.00
128^{-1}	$2.49e-1$	$1.37e-1$	$7.14e-2$	$3.64e-2$	$1.84e-2$	$9.25e-3$
	0.87	0.94	0.97	0.99	0.99	1.00

TABLE 4. Error of formula (51) on a uniform grid

ε	N					
	16	32	64	128	256	512
1	$5.29e-1$	$2.59e-1$	$1.28e-1$	$6.39e-2$	$3.19e-2$	$1.59e-2$
16^{-1}	$1.15e-2$	$5.30e-3$	$2.55e-3$	$1.25e-3$	$6.20e-4$	$3.08e-4$
32^{-1}	$6.45e-3$	$2.78e-3$	$1.30e-3$	$6.26e-4$	$3.08e-4$	$1.53e-4$
64^{-1}	$4.21e-3$	$1.58e-3$	$6.87e-4$	$3.22e-4$	$1.56e-4$	$7.66e-5$
128^{-1}	$3.74e-3$	$1.03e-3$	$3.90e-4$	$1.71e-4$	$8.02e-5$	$3.88e-5$
256^{-1}	$6.48e-3$	$9.04e-4$	$2.54e-4$	$9.69e-5$	$4.26e-5$	$2.00e-5$
512^{-1}	$4.11e-2$	$1.53e-3$	$2.22e-4$	$6.30e-5$	$2.42e-5$	$1.06e-5$

5 Conclusion

Approaches to constructing numerical differentiation formulas in the presence of a boundary layer are investigated. The problem is that using classical polynomial numerical differentiation formulas on a uniform grid can lead to significant errors when the function has large gradients. To prevent errors from increasing due to large gradients of the function, two approaches are considered: using classical polynomial numerical differentiation formulas on Shishkin and Bakhvalov meshes, which become denser in the region of large gradients of the function, and constructing special numerical differentiation formulas on a uniform grid that are exact on the boundary layer component of the function. Such approaches are widely used in constructing difference schemes for singularly perturbed problems whose convergence is uniform with respect to a small parameter. New error estimates are obtained for classical numerical differentiation formulas on Shishkin and Bakhvalov meshes. The obtained estimates are uniform with respect to the small parameter. An approach to estimating the error of numerical differentiation formulas that are exact on the boundary layer component of a function is proposed. Error estimates for numerical differentiation formulas constructed using the approaches under consideration are compared. The results of computational experiments corresponding to the obtained error estimates are presented.

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