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FORMULAS OF NUMERICAL DIFFERENTIATION ON A UNIFORM MESH FOR FUNCTIONS WITH THE EXPONENTIAL BOUNDARY LAYER

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Abstract. It is known that the solution of a singularly perturbed problem corresponds to the function with large gradients in a boundary layer. The application of Lagrange polynomial on a uniform mesh to interpolate such functions leads to large errors. To achieve the error estimates uniform with respect to a small parameter, we can use either a polynomial interpolation on a mesh which condenses in a boundary layer or we can use special interpolation formulas which are exact on a boundary layer component of the interpolating function. In this paper, we construct and study the formulas of numerical differentiation based on the interpolation formulas which are exact on a boundary layer component. We obtained the error estimates which are uniform with respect to a small parameter. Some numerical results validating the theoretical estimates are discussed.

Key words. Function of one variable, exponential boundary layer, formulas of numerical differentiation, an error estimate.

1. Introduction

Singularly perturbed problems are used for modeling convection-diffusion processes with dominant convection therefore the question of numerical solution of such problems is relevant. Solutions of singularly perturbed problems have large gradients in a boundary layer, thus application of classical difference schemes leads to large errors. To construct the difference schemes which converge uniformly with respect to a small parameter ε, there are two basic approaches based on papers A. M. Ilyin [1] and N. S. Bakhvalov [2].

In [1], it is proposed to construct difference schemes based on a fitting to the boundary layer component. These schemes are known as the exponential fitting schemes and were constructed in many works, for example in monographs [3,4] and the references therein. The schemes of arbitrarily high ε-uniform order of accuracy on a uniform mesh were constructed in [5,6]. According to [7] the exponential fitted scheme on a uniform mesh is ε-uniformly accurate in the case of an elliptic problem with regular boundary layers.

In [2], it is proposed to apply classical difference scheme on a special mesh that condenses in a boundary layer. This approach was developed in [8–15] and in a number of other works.

The question of construction of numerical differentiation formulas for functions with large gradients in a boundary layer is relevant too, because the use of classical formulas based on a differentiation of the Lagrange polynomial [16] leads to large errors. We can use the approaches used to construct difference schemes which converge ε-uniformly to create the acceptable numerical differentiation formulas.

The approach based on application of classical numerical differentiation formulas on meshes that condense in a boundary layer was investigated in [17–21] and some other works. In [17], an ordinary convection-diffusion equation is considered. The

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upwind scheme on the Shishkin and the Bakhvalov meshes with the property of ε-uniform convergence was used. To calculate the first derivative of the solution of differential problem, the authors used the solution of difference scheme and one-sided difference formula. The estimate of the relative error in a boundary layer and the estimate of the absolute error outside a boundary layer were obtained. These estimates are ε-uniform. In [20], this approach was applied to solve numerically a weakly coupled system of two singularly perturbed convection-diffusion second order ordinary differential equations on the Shishkin mesh. In [18, 19], the error of difference formulas on the Shishkin mesh for the derivatives of the solution of a singularly perturbed elliptic problem was investigated. In [21], the difference scheme on the Shishkin mesh for a linear singularly perturbed parabolic convection-diffusion problem was investigated. Similarly to [17] the error of the numerical differentiation formulas at mesh nodes was estimated.

In this paper, we study a problem of numerical differentiation on a uniform mesh by the use of a fitting of the difference formulas to the component responsible for the large gradients of the function in a boundary layer. The study of this approach is of interest for the following reasons. Difference schemes on uniform meshes are applicable to the numerical solution of a number of singularly perturbed problems as was mentioned above. Difference formulas for derivatives with the exponential fitting can be successfully applied to construct difference schemes and splines which converge ε-uniformly. It can be necessary in the case of initial or boundary conditions in a boundary layer region to approximate the first or the second derivatives. We applied such approach in [22, 23]. In [24], special difference formulas for approximation of derivatives were used to construct exact difference schemes but this method was not applied to singularly perturbed problems.

We assume that a function $u(x)$ has the decomposition:

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

where the functions $u(x)$, $p(x)$, $\Phi(x)$ are sufficiently smooth, the boundary layer component $\Phi(x)$ is known and responsible for the large gradients of the function $u(x)$, the function $p'(x)$ is uniformly bounded. We also assume that the constant γ and the function $p(x)$ are unknown but the estimates of certain derivatives of the function $p(x)$ are known.

In [25], the decomposition (1) of the solution of a singularly perturbed boundary value problem was investigated. The authors applied the decomposition to prove a uniform convergence of the difference scheme.

To construct the example of decomposition (1), we consider a singularly perturbed problem

$$\varepsilon u''(x) + a(x)u'(x) - b(x)u(x) = f(x), \qquad u(0) = A, \quad u(1) = B, \tag{2}$$

where $a(x) \geqslant \alpha_0 > 0$, $b(x) \geqslant 0$, $\varepsilon \in (0, 1]$, functions a, b, f are sufficiently smooth, the constant α_0 is separated from zero. It is known [25] that for small values of parameter ε a solution of the problem (2) has exponential boundary layer near $x = 0$ and the function $u(x)$ has the form (1). If we specify

$$\Phi(x) = e^{-a_0\,x/\varepsilon}, \quad a_0 = a(0), \quad \gamma = -\varepsilon u'(0)/a_0,$$

then there are the estimates $|p'(x)| \leqslant C_0$, $|\gamma| \leqslant C_0$, where the constant C_0 is independent of ε. In this case the derivatives $p^{(j)}(x)$, $j \geqslant 2$ can be unbounded for small value ε but the function $\gamma\Phi(x)$ is responsible for the main growth of $u(x)$ in a boundary layer. For this reason, we construct formulas of numerical differentiation that are exact on the function $\Phi(x)$. We also study an accuracy of such formulas in the case of the exponential boundary layer under conditions that $\Phi(x) = e^{-\alpha x/\varepsilon}$, $\alpha > 0$, $\varepsilon \in (0, 1]$, the constant α is separated from zero.

Let us give a review of the papers in which this approach was applied. In [26], it is shown in the case $u(x) = e^{-x/\varepsilon}$, $x \in [0, 1]$ that the relative error of classical formula for the first derivative $u'(x) \approx (u_n - u_{n-1})/h$ in the case $\varepsilon = h$ on the first interval of mesh has an order $O(1)$ independently of h. In [26], the numerical differentiation formula on two nodes which is exact on a boundary layer component is constructed in the case of the exponential boundary layer and it is proved that the relative error of that formula has an order $O(h)$ uniformly with respect to ε. In [27], for a function of the form (1) the numerical differentiation formula on two nodes was constructed.

In [28], non-polynomial interpolation formula with arbitrarily given number of the interpolation nodes for a function of the form (1) is constructed. The proposed interpolant is exact on the boundary layer component $\Phi(x)$. Numerical differentiation formulas based on a differentiation of the proposed interpolant are obtained to calculate derivatives of the function $u(x)$. The constructed formulas of numerical differentiation with arbitrarily given number of nodes are exact on the boundary layer component $\Phi(x)$. However in [28], the ε-uniform error estimates of the constructed formulas are absent. In [29], to calculate the first and the second derivatives at nodes of mesh in the case of the exponential layer component, ε-uniform estimates of the relative error of the numerical differentiation formulas are obtained.

Notation. Let $\|f\|_{[a,\,b]} = \max\limits_{x \in [a,\,b]} |f(x)|$. Here C, sometimes subscripted, denotes a generic positive constant which is independent of the perturbation parameter ε and the step size of the mesh.

2. Problem

We assume that the function $u(x)$ has the form (1) and Ω^h is a uniform mesh of the considered interval

$$\Omega^h = \{x_n : \; x_n = n\,h, \; n = 0, 1, \dots, N, \; x_0 = 0, \; x_N = 1\}.$$

We also assume that the function $u(x)$ is given at the nodes $x_n \in \Omega^h$. Let us denote $u_n = u(x_n)$.

The formula of numerical differentiation which is exact on the boundary layer component $\Phi(x)$, for a function of the form (1) is constructed in [28]. The formula for computation of the j^{th}-derivative of the function $u(x)$ on the interval $[x_m, \, x_{m+k-1}]$ has the form

$$\text{(3)} \quad L^{(j)}_{\Phi,\,k}(u, x) = L^{(j)}_{k-1}(u, x) + \frac{[x_m, \, x_{m+1}, \dots, x_{m+k-1}]u}{[x_m, \, x_{m+1}, \dots, x_{m+k-1}]\Phi} \left(\Phi^{(j)}(x) - L^{(j)}_{k-1}(\Phi, x) \right),$$

where $j \geqslant 0$, $L_{k-1}(u, x)$ is the Lagrange polynomial interpolating the function $u(x)$ on $(k-1)$ nodes $x_m, \; x_{m+1}, \; \dots, \; x_{m+k-2}$, $L^{(j)}_{k-1}(u, x)$ is the j^{th}-derivative of Lagrange polynomial $L_{k-1}(u, x)$ and $[x_m, x_{m+1}, \dots, x_{m+k-1}]u$ is the divided difference of the function $u(x)$ [30, p. 340].

Further we investigate the formula (3) for function of the form (1), in the case $\Phi(x) = e^{-\alpha\, x/\varepsilon}$, $\alpha > 0$, $\varepsilon \in (0, 1]$ for the first derivative ($j = 1$) on $k = 2, \; 3$ and for the second derivative ($j = 2$) on $k = 3, \; 4$.

3. Formulas of numerical differentiation for the first derivative

3.1. Formula of numerical differentiation for the first derivative on two nodes. We consider the formula (3) in the case $j=1$, $k=2$

$$L'_{\Phi,\,2}(u,x)=\frac{u_n-u_{n-1}}{\Phi_n-\Phi_{n-1}}\Phi'(x),\qquad x\in[x_{n-1},\,x_n]. \tag{4}$$

Assume that the condition $\Phi'(x)\neq 0,\ x\in(x_{n-1},\,x_n)$ is fulfilled. Then the formula (4) is correctly defined.

In [26], the formula (4) in the case $\Phi(x)=e^{-\alpha\,x/\varepsilon}$ is investigated and the following error estimate is proved

$$\varepsilon|L'_{\Phi,2}(u,x)-u'(x)|\leqslant Ch,\qquad x\in[x_{n-1},\,x_n],\quad n=1,2,\dots,N. \tag{5}$$

Further we obtain the estimate (5) in the integral form and specify the constant C.

Theorem 3.1. *Let $\Phi(x)=e^{-\alpha\,x/\varepsilon}$. Then for $n=1,2,\dots,N$ one has*

$$\begin{aligned}\varepsilon|L'_{\Phi,2}(u,x)-u'(x)|&\leqslant \alpha\int\limits_{x_{n-1}}^{x_n}|p'(t)|\,dt+\varepsilon\int\limits_{x_{n-1}}^{x_n}|p''(t)|\,dt\leqslant\\ &\leqslant h\left(\alpha\,\|p'\|_{[x_{n-1},\,x_n]}+\varepsilon\,\|p''\|_{[x_{n-1},\,x_n]}\right),\qquad x\in[x_{n-1},\,x_n].\end{aligned} \tag{6}$$

Proof. Taking into account that the formula (4) is exact on $\Phi(x)$, we obtain

$$\varepsilon|L'_{\Phi,2}(u,x)-u'(x)|\leqslant\varepsilon|L'_{\Phi,2}(p,x)-L'_2(p,x)|+\varepsilon|L'_2(p,x)-p'(x)|. \tag{7}$$

At first, we estimate the second term in (7). Then one has

$$\begin{aligned}\varepsilon|L'_2(p,x)-p'(x)|&=\varepsilon\left|\frac{p_n-p_{n-1}}{h}-p'(x)\right|=\varepsilon|p'(s)-p'(x)|\leqslant\\ &\leqslant\varepsilon\int\limits_{x_{n-1}}^{x_n}|p''(t)|\,dt\leqslant\varepsilon\,h\,\|p''\|_{[x_{n-1},x_n]},\qquad s\in[x_{n-1},\,x_n].\end{aligned} \tag{8}$$

For the first term in (7) it is satisfied

$$\begin{aligned}\varepsilon\left|L'_{\Phi,\,2}(p,x)-L'_2(p,x)\right|&=|p_n-p_{n-1}|\left|\frac{\varepsilon\,\Phi'(x)}{\Phi_n-\Phi_{n-1}}-\frac{\varepsilon}{h}\right|=\\ &=\left|\int\limits_{x_{n-1}}^{x_n}p'(t)\,dt\right|\,|F_{1,\,2}(x)|\,,\qquad F_{1,\,2}(x)=\frac{\varepsilon\,\Phi'(x)}{\Phi_n-\Phi_{n-1}}-\frac{\varepsilon}{h}.\end{aligned} \tag{9}$$

Then substituting $\Phi(x)=e^{-\alpha\,x/\varepsilon}$ into the function $F_{1,\,2}(x)$, one obtains

$$F_{1,\,2}(x)=\frac{\varepsilon}{h}\left(-\frac{\frac{\alpha\,h}{\varepsilon}\,e^{-\frac{\alpha\,x}{\varepsilon}}}{e^{-\frac{\alpha\,x_n}{\varepsilon}}-e^{-\frac{\alpha\,x_{n-1}}{\varepsilon}}}-1\right).$$

We show that $|F_{1,\,2}(x_n)|\leqslant\alpha$. Let $t=\alpha\,h/\varepsilon$ then

$$F_{1,\,2}(x_n)=\frac{\alpha}{t}\left(\frac{t}{e^t-1}-1\right),\qquad |F_{1,\,2}(x_n)|=\alpha\left|\frac{t-e^t+1}{t(e^t-1)}\right|=\alpha\,\frac{e^t-t-1}{t(e^t-1)}\leqslant\alpha.$$

It is analogically verified that $|F_{1,\,2}(x_{n-1})|\leqslant\alpha$. Taking into account that the function $F_{1,\,2}(x)$ is decreasing, we obtain

$$|F_{1,\,2}(x)|\leqslant\alpha,\qquad x\in[x_{n-1},\,x_n].$$

Then from (9) one has

$$\varepsilon|L'_{\Phi,2}(p,x) - L'_2(p,x)| \leqslant \alpha \int\limits_{x_{n-1}}^{x_n} |p'(t)|\,dt \leqslant \alpha\, h\, \|p'\|_{[x_{n-1},x_n]}. \tag{10}$$

Thus the estimate (6) follows from (7), (8) and (10). □

3.2. Formula of numerical differentiation for the first derivative on three nodes. We consider classical formula of numerical differentiation for the first derivative

$$u'(x) \approx L'_3(u,x) = \frac{u_{n+1} - u_{n-1}}{2h} + \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2}(x - x_n), \tag{11}$$

where $x \in [x_{n-1},\, x_{n+1}]$.

Let $u(x) = e^{-x/\varepsilon}$. Then in the case $\varepsilon = h$ one has

$$\varepsilon\,|(-3u_0 + 4u_1 - u_2)/(2h) - u'(0)| = \big|(-1.5 + 2e^{-1} - 0.5e^{-2}) - (-1)\big| \approx 0.168.$$

We obtained that in the case $\varepsilon = h$ the relative error of the formula (11) can be large for small values of h.

Now we consider the formula (3) in the case $k = 3$, $j = 1$

$$L'_{\Phi,3}(u,x) = \frac{u_n - u_{n-1}}{h} + \frac{u_{n-1} - 2u_n + u_{n+1}}{\Phi_{n-1} - 2\Phi_n + \Phi_{n+1}} \left(\Phi'(x) - \frac{\Phi_n - \Phi_{n-1}}{h} \right), \tag{12}$$

where $x \in [x_{n-1},\, x_{n+1}]$. Assume that the condition $\Phi''(x) \neq 0$, $x \in (x_{n-1},\, x_{n+1})$ is fulfilled. Then the formula (12) is correctly defined.

Theorem 3.2. *Let $\Phi(x) = e^{-\alpha\, x/\varepsilon}$. Then for $n = 1, 2, \ldots, N-1$ one has*

$$\begin{gathered} \varepsilon|L'_{\Phi,3}(u,x) - u'(x)| \leqslant \min\{\alpha\, h, \varepsilon\} \left(2 \int\limits_{x_{n-1}}^{x_{n+1}} |p''(t)|\; dt + \right. \\ \left. + \frac{5}{4\,\alpha} \max\{\alpha\, h, \varepsilon\} \int\limits_{x_{n-1}}^{x_{n+1}} |p'''(t)|\; dt \right) \leqslant 2\, h \min\{\alpha\, h, \varepsilon\} \Big(2\, \|p''\|_{[x_{n-1},\, x_{n+1}]} + \\ + \frac{5}{4\,\alpha} \max\{\alpha\, h, \varepsilon\}\, \|p'''\|_{[x_{n-1},\, x_{n+1}]} \Big), \qquad x \in [x_{n-1},\, x_{n+1}]. \end{gathered} \tag{13}$$

Proof. Since the formula (12) is exact on $\Phi(x)$ we obtain

$$\begin{gathered} \varepsilon(L'_{\Phi,3}(u,x) - u'(x)) = \varepsilon(L'_{\Phi,3}(p,x) - p'(x)) = \\ = \varepsilon(L'_{\Phi,3}(p,x) - L'_3(p,x)) + \varepsilon(L'_3(p,x) - p'(x)). \end{gathered} \tag{14}$$

In order to estimate the second term in (14) we use the Taylor formula with the integral form of the remainder

$$|L_3'(p,x)-p'(x)| = \left|\frac{p_{n+1}-p_{n-1}}{2h} - p'(x_n) + \frac{p_{n+1}-2p_n+p_{n-1}}{h^2}(x-x_n)-\right.$$

$$\left.-p'(x)+p'(x_n)\right| \leqslant \frac{1}{4\,h}\left|\int\limits_{x_{n-1}}^{x_n} p'''(t)(x_{n-1}-t)^2\,dt + \int\limits_{x_n}^{x_{n+1}} p'''(t)(x_{n+1}-t)^2\,dt\right| +$$

$$+\left|\int\limits_{x_n}^{x}\left(\frac{p_{n+1}-2p_n+p_{n-1}}{h^2} - p''(s)\right)ds\right| \leqslant \frac{h}{4}\int\limits_{x_{n-1}}^{x_{n+1}} |p'''(t)|\;dt+$$

$$+\left|\int\limits_{x_n}^{x}(p''(r)-p''(s))\;ds\right| \leqslant \frac{h}{4}\int\limits_{x_{n-1}}^{x_{n+1}} |p'''(t)|\;dt + \left|\int\limits_{x_n}^{x}\int\limits_{s}^{r} p'''(t)\,dt\,ds\right| \leqslant$$

$$\leqslant \frac{5}{4}\,h\int\limits_{x_{n-1}}^{x_{n+1}} |p'''(t)|\;dt, \qquad r\in[x_{n-1},\,x_{n+1}].$$

Therefore, one has

$$\varepsilon|L_3'(p,x)-p'(x)| \leqslant \frac{5}{4}\,\varepsilon\,h\int\limits_{x_{n-1}}^{x_{n+1}} |p'''(t)|\;dt \leqslant \frac{5}{2}\,\varepsilon\,h^2\,\|p'''\|_{[x_{n-1},\,x_{n+1}]}\,. \tag{15}$$

In order to estimate the first term in (14) we use the Taylor formula with the integral form of the remainder

$$\varepsilon\left|L_{\Phi,3}'(p,x)-L_3'(p,x)\right| = \varepsilon\left|\frac{p_{n-1}-2p_n+p_{n+1}}{\Phi_{n-1}-2\Phi_n+\Phi_{n+1}}\left(\Phi'(x)-\frac{\Phi_n-\Phi_{n-1}}{h}\right)-\right.$$

$$\left.-\frac{(p_{n-1}-2p_n+p_{n+1})(2x-x_n-x_{n-1})}{2h^2}\right| =$$

$$= |p_{n-1}-2p_n+p_{n+1}|\left|\frac{\varepsilon(\Phi'(x)-(\Phi_n-\Phi_{n-1})/h)}{\Phi_{n-1}-2\Phi_n+\Phi_{n+1}} - \frac{\varepsilon(2x-x_n-x_{n-1})}{2h^2}\right| =$$

$$= \left|\int\limits_{x_n}^{x_{n+1}} p''(t)(x_{n+1}-t)\,dt + \int\limits_{x_n}^{x_{n-1}} p''(t)(x_{n-1}-t)\,dt\right| |F_{1,3}(x)|\,,$$

where the function $F_{1,3}(x)$ corresponds to the expression in the last module. Therefore, one has

$$\begin{aligned}\varepsilon|L_{\Phi,3}'(p,x)-L_3'(p,x)| &\leqslant h\,|F_{1,3}(x)|\int\limits_{x_{n-1}}^{x_{n+1}} |p''(t)|\;dt \leqslant \\ &\leqslant 2\,h^2\,\|p''\|_{[x_{n-1},\,x_{n+1}]}\;|F_{1,3}(x)|\,.\end{aligned} \tag{16}$$

Substituting $\Phi(x)=e^{-\alpha\,x/\varepsilon}$ into the function $F_{1,\,3}(x)$, we obtain

$$F_{1,\,3}(x)=\frac{\varepsilon\left(-\alpha\,\varepsilon^{-1}e^{-\frac{\alpha\,(x-x_n)}{\varepsilon}}-\left(1-e^{\frac{\alpha\,h}{\varepsilon}}\right)/h\right)}{e^{-\frac{\alpha\,h}{\varepsilon}}-2+e^{\frac{\alpha\,h}{\varepsilon}}}-\frac{\varepsilon(2x-x_n-x_{n-1})}{2h^2}. \tag{17}$$

We show that on any interval $[x_{n-1},\,x_{n+1}]\subset[0,\,1]$ the function $F_{1,\,3}(x)$ is bounded uniformly with respect to ε. Let $t=\alpha\,h/\varepsilon$. Then from (17) at the node x_{n-1} we yield

$$F_{1,\,3}(x_{n-1})=\alpha\,\frac{\varepsilon}{\alpha\,h}\left(\frac{e^{\frac{\alpha\,h}{\varepsilon}}-1-\frac{\alpha\,h}{\varepsilon}\,e^{\frac{\alpha\,h}{\varepsilon}}}{e^{-\frac{\alpha\,h}{\varepsilon}}-2+e^{\frac{\alpha\,h}{\varepsilon}}}+\frac{1}{2}\right)=\alpha\,\frac{3e^t-2te^t+e^{-t}-4}{2t(e^{-t}-2+e^t)}.$$

Since for $t\geqslant 0$ the estimate $\varphi_1(t)=3e^t-2te^t+e^{-t}-4\leqslant 0$ is satisfied then we obtain

$$|F_{1,\,3}(x_{n-1})|=\alpha\,\frac{2te^t-3e^t-e^{-t}+4}{2t(e^{-t}-2+e^t)}. \tag{18}$$

One can show that the function $\varphi_2(t)=2t(e^{-t}-2+e^t)-(2te^t-3e^t-e^{-t}+4)$ and the function $\varphi_3(t)=2(e^{-t}-2+e^t)-(2te^t-3e^t-e^{-t}+4)$ are nonnegative in the case $t\geqslant 0$, therefore, from (18) one has

$$|F_{1,\,3}(x_{n-1})|\leqslant\alpha,\qquad |F_{1,\,3}(x_{n-1})|\leqslant\frac{\alpha}{t}=\frac{\varepsilon}{h},$$

consequently, it is satisfied

$$h|F_{1,\,3}(x_{n-1})|\leqslant\min\{\alpha\,h,\varepsilon\}. \tag{19}$$

It is analogically verified that

$$h|F_{1,\,3}(x_{n+1})|\leqslant\min\{\alpha\,h,\varepsilon\}. \tag{20}$$

Now we investigate the function $F_{1,\,3}(x)$ at the stationary point x_d. It follows from (17) that

$${F_{1,\,3}}'(x)=\frac{\alpha^2\,e^{-\frac{\alpha\,(x-x_n)}{\varepsilon}}}{\varepsilon(e^{-\frac{\alpha\,h}{\varepsilon}}-2+e^{\frac{\alpha\,h}{\varepsilon}})}-\frac{\varepsilon}{h^2}.$$

Therefore, one has

$$e^{-\frac{\alpha\,x_d}{\varepsilon}}=\frac{e^{-\frac{\alpha\,h}{\varepsilon}}-2+e^{\frac{\alpha\,h}{\varepsilon}}}{(\alpha\,h/\varepsilon)^2}\,e^{-\frac{\alpha\,x_n}{\varepsilon}}=\frac{e^{-\frac{2\alpha\,h}{\varepsilon}}-2\,e^{-\frac{\alpha\,h}{\varepsilon}}+1}{(\alpha\,h/\varepsilon)^2}\,e^{-\frac{\alpha\,x_{n-1}}{\varepsilon}}. \tag{21}$$

Since $e^{-\frac{\alpha\,h}{\varepsilon}}-2+e^{\frac{\alpha\,h}{\varepsilon}}\geqslant(\alpha\,h/\varepsilon)^2$ is satisfied then $x_d\leqslant x_n$. Taking into account that $e^{-\frac{2\alpha\,h}{\varepsilon}}-2\,e^{-\frac{\alpha\,h}{\varepsilon}}+1\leqslant(\alpha\,h/\varepsilon)^2$ holds, we obtain $x_d\geqslant x_{n-1}$. It follows that $x_d\in[x_{n-1},\,x_n]$. From (17) and (21) we obtain

$$F_{1,\,3}(x_d)=\alpha\,\frac{\varepsilon}{\alpha\,h}\left(\frac{e^{\frac{\alpha\,h}{\varepsilon}}-1-\varepsilon\,(e^{-\frac{\alpha\,h}{\varepsilon}}-2+e^{\frac{\alpha\,h}{\varepsilon}})/(\alpha\,h)}{e^{-\frac{\alpha\,h}{\varepsilon}}-2+e^{\frac{\alpha\,h}{\varepsilon}}}-\frac{1}{2}\left(1+\frac{2(x_d-x_n)}{h}\right)\right)$$

$$=\alpha\,\frac{t(e^t-e^{-t})+(\delta t-2)(e^{-t}-2+e^t)}{2t^2(e^{-t}-2+e^t)},$$

where $\delta=2(x_n-x_d)/h$.

Since $\delta\geqslant 0$, we have $\varphi_7(t)=t(e^t-e^{-t})+(\delta t-2)(e^{-t}-2+e^t)\geqslant 0$ in the case $t\geqslant 0$. Thus, it follows that

$$|F_{1,\,3}(x_d)|=\alpha\,\frac{t(e^t-e^{-t})+(\delta t-2)(e^{-t}-2+e^t)}{2\,t^2(e^{-t}-2+e^t)}. \tag{22}$$

We prove $t \geqslant \delta/2$. In order to do this we consider the function $\theta_1(t) = t^2\, e^{t^2} - (e^{-t} - 2 + e^t)$ and prove $\theta_1(t) \geqslant 0$. For $t \geqslant 0$ one has

$$\theta_1(0) = 0, \qquad {\theta_1}'(t) = 2t\, e^{t^2} + 2t^3\, e^{t^2} + e^{-t} - e^t, \qquad {\theta_1}'(0) = 0,$$
$${\theta_1}''(t) = (2e^{t^2} - e^{-t} - e^t) + (10t^2 + 4t^4)\, e^{t^2} = \theta_{11}(t) + \theta_{12}(t),$$

where $\theta_{12}(t) = (10t^2 + 4t^4)\, e^{t^2} \geqslant 0$ and $\theta_{11}(t) = 2e^{t^2} - e^t - e^{-t}$. For $t \geqslant 0$ we obtain

$$\theta_{11}(0) = 0, \qquad {\theta_{11}}'(t) = 4t\, e^{t^2} - e^t + e^{-t}, \qquad {\theta_{11}}'(0) = 0,$$

$${\theta_{11}}''(t) = 8t^2e^{t^2} + 4e^{t^2} - e^t - e^{-t} = 8t^2e^{t^2} + (e^t - e^{-t}) + 2e^t(2e^{t^2-t} - 1) =$$

$$= 8t^2e^{t^2} + (e^t - e^{-t}) + 2e^t(e^{t^2-t+\ln 2} - 1) >$$

$$> 2e^t(e^{t^2-t+1/4} - 1) = 2e^t(e^{(t-1/2)^2} - 1) \geqslant 0.$$

It follows that for $t \geqslant 0$ we have $\theta_{11}(t) \geqslant 0$. Therefore, one has $\theta_1(t) \geqslant 0$. Then we obtain

$$e^{-\frac{\alpha\, x_d}{\varepsilon}} = \frac{e^{-\frac{\alpha\, h}{\varepsilon}} - 2 + e^{\frac{\alpha\, h}{\varepsilon}}}{(\alpha\, h/\varepsilon)^2}\, e^{-\frac{\alpha\, x_n}{\varepsilon}} \leqslant e^{(\alpha\, h/\varepsilon)^2}\, e^{-\frac{\alpha\, x_n}{\varepsilon}},$$

hence, the estimate $x_d \geqslant -\alpha\, h^2/\varepsilon + x_n$ holds, therefore, $t \geqslant \delta/2$ is satisfied.

One can show in the case $t \geqslant 0$ that the function $\varphi_8(t) = 2\, t^2(e^{-t} - 2 + e^t) - (t(e^t - e^{-t}) + (\delta t - 2)(e^{-t} - 2 + e^t))$ is nonnegative by taking into account that the estimate $t \geqslant \delta/2$ holds true.

One can also show in the case $t \geqslant 0$ that the function $\varphi_9(t) = 4\, t(e^{-t} - 2 + e^t) - (t(e^t - e^{-t}) + (\delta t - 2)(e^{-t} - 2 + e^t))$ is nonnegative by taking into account that the estimate $\delta \leqslant 2$ holds true.

Since $\varphi_8(t) \geqslant 0$ and $\varphi_9(t) \geqslant 0$, from (22) we get

$$|F_{1,\,3}(x_d)| \leqslant \alpha, \qquad |F_{1,\,3}(x_d)| \leqslant \frac{2\,\alpha}{t} = \frac{2\,\varepsilon}{h},$$

therefore, one has

$$h|F_{1,\,3}(x_d)| \leqslant \min\{\alpha\, h, 2\,\varepsilon\} \leqslant 2\, \min\{\alpha\, h, \varepsilon\}. \tag{23}$$

Thus, from (16), (19), (20), (23) we obtain

$$\varepsilon|L'_{\Phi,3}(p,x) - L'_3(p,x)| \leqslant 2\, \min\{\alpha\, h, \varepsilon\} \int\limits_{x_{n-1}}^{x_{n+1}} |p''(t)|\, dt \leqslant \tag{24}$$

$$\leqslant 4\, h \min\{\alpha\, h, \varepsilon\}\, \|p''\|_{[x_{n-1},\, x_{n+1}]}\,.$$

Then the estimate (13) follows from (14), (15) and (24). □

4. Formulas of numerical differentiation for the second derivative

4.1. Formula of numerical differentiation for the second derivative on three nodes. We consider classical formula of numerical differentiation for the second derivative

$$u''(x) \approx L''_3(u,x) = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2}, \qquad x \in [x_{n-1},\, x_{n+1}]. \tag{25}$$

Let $u(x) = e^{-x/\varepsilon}$. Then in the case $\varepsilon = h$ we have

$$\varepsilon^2 \left|(u_0 - 2u_1 + u_2)/h^2 - u''(0)\right| \approx 0.6.$$

We notice that in this case $\varepsilon \leqslant h$ the relative error of the formula (25) can be large.

Now we consider the formula (3) in the case $k = 3,\ j = 2$

$$L''_{\Phi,3}(u,x) = \frac{u_{n-1} - 2u_n + u_{n+1}}{\Phi_{n-1} - 2\Phi_n + \Phi_{n+1}} \Phi''(x), \qquad x \in [x_{n-1},\, x_{n+1}]. \tag{26}$$

Assume that the condition $\Phi''(x) \neq 0,\ x \in (x_{n-1},\, x_{n+1})$ is fulfilled. Then the formula (26) is correctly defined.

Theorem 4.1. *Let $\Phi(x) = e^{-\alpha\, x/\varepsilon}$. Then for $n = 1, 2, \ldots, N-1$ one has*

$$\begin{gathered}\varepsilon^2 |L''_{\Phi,3}(u,x) - u''(x)| \leqslant \left(3\,\alpha \, \max\{\alpha\, h, \varepsilon\} \int\limits_{x_{n-1}}^{x_{n+1}} |p''(t)|\; dt + \right. \\ \left. + 2\,\varepsilon^2 \int\limits_{x_{n-1}}^{x_{n+1}} |p'''(t)|\; dt \right) \leqslant 2\,h \left(3\,\alpha\, \max\{\alpha\, h, \varepsilon\}\, \|p''\|_{[x_{n-1},\, x_{n+1}]} + \right. \\ \left. + 2\,\varepsilon^2\, \|p'''\|_{[x_{n-1},\, x_{n+1}]} \right), \quad x \in [x_{n-1},\, x_{n+1}].\end{gathered} \tag{27}$$

Proof. Since the formula (26) is exact on $\Phi(x)$ we have

$$\begin{gathered}\varepsilon^2 (L''_{\Phi,3}(u,x) - u''(x)) = \varepsilon^2 (L''_{\Phi,3}(p,x) - p''(x)) = \\ = \varepsilon^2 (L''_{\Phi,3}(p,x) - L''_3(p,x)) + \varepsilon^2 (L''_3(p,x) - p''(x)).\end{gathered} \tag{28}$$

In order to estimate the second term in (28) we use the Taylor formula with the integral form of the remainder

$$\begin{gathered}|L''_3(p,x) - p''(x)| = \left| \frac{p_{n+1} - 2p_n + p_{n-1}}{h^2} - p''(x_n) + p''(x_n) - p''(x) \right| \leqslant \\ \leqslant \frac{1}{2h^2} \left| \int\limits_{x_n}^{x_{n+1}} p'''(t)(x_{n+1} - t)^2\, dt - \int\limits_{x_{n-1}}^{x_n} p'''(t)(t - x_{n-1})^2\, dt \right| + \\ + \left| \int\limits_{x}^{x_n} p'''(t)\, dt \right| \leqslant 2 \int\limits_{x_{n-1}}^{x_{n+1}} |p'''(t)|\; dt.\end{gathered}$$

Therefore, one has

$$\varepsilon^2 |L''_3(p,x) - p''(x)| \leqslant 2\,\varepsilon^2 \int\limits_{x_{n-1}}^{x_{n+1}} |p'''(t)|\; dt \leqslant 4\,\varepsilon^2\, h\, \|p'''\|_{[x_{n-1},\, x_{n+1}]}\,. \tag{29}$$

In order to estimate the first term in (28) we use the Taylor formula with the integral form of the remainder

$$\varepsilon^2 \left|L''_{\Phi,3}(p,x) - L''_3(p,x)\right| = \varepsilon^2 \left|\frac{p_{n-1}-2p_n+p_{n+1}}{\Phi_{n-1}-2\Phi_n+\Phi_{n+1}}\Phi''(x) - \right.$$

$$\left. -\frac{p_{n-1}-2p_n+p_{n+1}}{h^2}\right| = |p_{n-1}-2p_n+p_{n+1}| \left|\frac{\varepsilon^2\Phi''(x)}{\Phi_{n-1}-2\Phi_n+\Phi_{n+1}} - \frac{\varepsilon^2}{h^2}\right| =$$

$$= \left|\int\limits_{x_n}^{x_{n+1}} p''(t)(x_{n+1}-t)\,dt + \int\limits_{x_n}^{x_{n-1}} p''(t)(x_{n-1}-t)\,dt\right| |F_{2,\,3}(x)|\,,$$

where the function $F_{2,\,3}(x)$ corresponds to the expression in the last module. Therefore, one has

$$\varepsilon^2|L''_{\Phi,3}(p,x) - L''_3(p,x)| \leqslant h\,|F_{2,\,3}(x)| \int\limits_{x_{n-1}}^{x_{n+1}} |p''(t)|\,dt \leqslant \tag{30}$$

$$\leqslant 2\,h^2\,\|p''\|_{[x_{n-1},\,x_{n+1}]}\,|F_{2,\,3}(x)|\,.$$

Substituting $\Phi(x) = e^{-\alpha\,x/\varepsilon}$ into the function $F_{2,\,3}(x)$ we obtain

$$F_{2,\,3}(x) = \frac{\alpha^2\,e^{-\frac{\alpha\,(x-x_n)}{\varepsilon}}}{e^{-\frac{\alpha\,h}{\varepsilon}} - 2 + e^{\frac{\alpha\,h}{\varepsilon}}} - \frac{\varepsilon^2}{h^2}. \tag{31}$$

We show that on any interval $[x_{n-1},\,x_{n+1}] \subset [0,\,1]$ the function $F_{2,\,3}(x)$ is bounded uniformly with respect to ε. Let $t = \alpha\,h/\varepsilon$ then from (31) at the node x_{n-1} we yield

$$F_{2,\,3}(x_{n-1}) = \alpha^2\left(\frac{e^{\frac{\alpha\,h}{\varepsilon}}}{e^{-\frac{\alpha\,h}{\varepsilon}} - 2 + e^{\frac{\alpha\,h}{\varepsilon}}} - \frac{\varepsilon^2}{\alpha^2\,h^2}\right) = \alpha^2\,\frac{e^t(t^2-1)+2-e^{-t}}{t^2(e^{-t}-2+e^t)}.$$

Since for $t \geqslant 0$ the estimate $\psi_1(t) = e^t(t^2-1)+2-e^{-t} \geqslant 0$ is satisfied then we obtain

$$|F_{2,\,3}(x_{n-1})| = \alpha^2\,\frac{e^t(t^2-1)+2-e^{-t}}{t^2(e^{-t}-2+e^t)}. \tag{32}$$

On can show that the function $\psi_2(t) = 3t^2(e^{-t}-2+e^t) - (e^t(t^2-1)+2-e^{-t})$ is nonnegative in the case $t \geqslant 1$, and in the case $0 \leqslant t < 1$ the function $\psi_3(t) = 3t(e^{-t}-2+e^t) - (e^t(t^2-1)+2-e^{-t})$ is nonnegative. Then from (32) we yield

$$|F_{2,\,3}(x_{n-1})| \leqslant 3\alpha^2, \quad \alpha\,h \geqslant \varepsilon; \qquad |F_{2,\,3}(x_{n-1})| \leqslant \frac{3\,\alpha^2}{t} = 3\,\alpha\,\frac{\varepsilon}{h}, \quad \alpha\,h < \varepsilon,$$

therefore, it is satisfied

$$h|F_{2,\,3}(x_{n-1})| \leqslant 3\,\alpha\,\max\{\alpha\,h, \varepsilon\}. \tag{33}$$

Now we estimate $F_{2,\,3}(x_{n+1})$. It follows from (31) that

$$F_{2,\,3}(x_{n+1}) = \alpha^2\,\frac{t^2e^{-t}+2-e^t-e^{-t}}{t^2(e^{-t}-2+e^t)}.$$

Since the following function $\psi_4(t)$ can be presented in the form

$$\psi_4(t) = e^t + e^{-t} - 2 - t^2e^{-t} = (e^{t/2} - e^{-t/2} + te^{-t/2})(e^{t/2} - e^{-t/2} - te^{-t/2}),$$

and the function $\psi_{42}(t) = e^{t/2} - e^{-t/2} - te^{-t/2}$ is nonnegative for $t \geqslant 0$ then one has $\psi_4(t) \geqslant 0$ for $t \geqslant 0$. Therefore, we obtain

$$|F_{2,3}(x_{n+1})| = \alpha^2 \frac{e^t + e^{-t} - 2 - t^2 e^{-t}}{t^2(e^{-t} - 2 + e^t)}. \tag{34}$$

Since the following function $\psi_5(t)$ can be presented in the form

$$\psi_5(t) = t(e^{-t} - 2 + e^t) - (e^t + e^{-t} - 2 - t^2 e^{-t}) = (t-1)(e^{-t} - 2 + e^t) + t^2 e^{-t},$$

then $\psi_5(t) \geqslant 0$ for $t \geqslant 1$. Next, it is easy to verify that $\psi_5(t) \geqslant 0$ for $0 \leqslant t \leqslant 1$. Therefore, one has $\psi_5(t) \geqslant 0$ for $t \geqslant 0$.

Taking into account that in the case $t \geqslant 0$ the function $\psi_5(t)$ and the function $\psi_6(t) = (e^{-t} - 2 + e^t) - (e^t + e^{-t} - 2 - t^2 e^{-t})$ are nonnegative then it follows from (34) that

$$|F_{2,3}(x_{n+1})| \leqslant \frac{\alpha^2}{t} = \alpha\,\frac{\varepsilon}{h}, \qquad |F_{2,3}(x_{n+1})| \leqslant \frac{\alpha^2}{t^2} = \frac{\varepsilon^2}{h^2},$$

therefore, one has

$$h^2 |F_{2,3}(x_{n+1})| \leqslant \varepsilon \min\{\alpha\, h, \varepsilon\}. \tag{35}$$

It follows from (31) that

$$F_{2,3}{}'(x) = -\frac{\alpha^3\, e^{-\frac{\alpha\,(x - x_n)}{\varepsilon}}}{\varepsilon(e^{-\frac{\alpha\, h}{\varepsilon}} - 2 + e^{\frac{\alpha\, h}{\varepsilon}})} < 0, \qquad x \in [x_{n-1},\, x_{n+1}],$$

then taking into account (33) and (35), from (30) we obtain

$$\begin{aligned} \varepsilon^2 |L''_{\Phi,3}(p,x) - L''_3(p,x)| &\leqslant 3\,\alpha\, \max\{\alpha\, h, \varepsilon\} \int\limits_{x_{n-1}}^{x_{n+1}} |p''(t)|\, dt \leqslant \\ &\leqslant 6\,\alpha\, h \max\{\alpha\, h, \varepsilon\}\, \|p''\|_{[x_{n-1},\, x_{n+1}]}\,. \end{aligned} \tag{36}$$

Then the estimate (27) follows from (28), (29) and (36). □

4.2. Formula of numerical differentiation for the second derivative on four nodes. We consider classical formula of numerical differentiation for the second derivative

$$L''_4(u,x) = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} + \frac{u_{n+2} - 3u_{n+1} + 3u_n - u_{n-1}}{h^3}(x - x_n), \tag{37}$$

where $x \in [x_{n-1},\, x_{n+2}]$.

Similarly to analysis of the error of the formula (25), it can be shown that the error of the formula (37) is of order $O(1)$ in the case $\varepsilon = h$.

Now we consider the formula (3) in the case $k = 4$, $j = 2$

$$\begin{aligned} L''_{\Phi,4}(u,x) = {}& \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} + \\ &+ \frac{u_{n+2} - 3u_{n+1} + 3u_n - u_{n-1}}{\Phi_{n+2} - 3\Phi_{n+1} + 3\Phi_n - \Phi_{n-1}} \left(\Phi''(x) - \frac{\Phi_{n-1} - 2\Phi_n + \Phi_{n+1}}{h^2} \right), \end{aligned} \tag{38}$$

where $x \in [x_{n-1},\, x_{n+2}]$. Assume that the condition $\Phi'''(x) \neq 0$, $x \in (x_{n-1},\, x_{n+2})$ is fulfilled. Then the formula (38) is correctly defined.

Theorem 4.2. *Let* $\Phi(x) = e^{-\alpha\, x/\varepsilon}$*. Then for* $n = 1, 2, \dots, N-2$ *one has*

$$\varepsilon^2 |L''_{\Phi,\,4}(u,x) - u''(x)| \leqslant h \left(C_1\, \varepsilon^2 \int\limits_{x_{n-1}}^{x_{n+2}} |p^{(4)}(s)|\, ds + \right.$$

$$\left. + C_2 \max\{\alpha\, h, \varepsilon\} \int\limits_{x_{n-1}}^{x_{n+2}} |p^{(3)}(s)|\, ds \right) \leqslant 3\, h^2 \left(C_1\, \varepsilon^2 \|p^{(4)}\|_{[x_{n-1},\, x_{n+2}]} + \right. \tag{39}$$

$$\left. + C_2 \max\{\alpha\, h, \varepsilon\} \|p^{(3)}\|_{[x_{n-1},\, x_{n+2}]} \right), \quad x \in [x_{n-1},\, x_{n+2}],$$

where $C_1 = 19/6$*,* $C_2 = 12\, e^3\, \alpha$*.*

Proof. The formula (38) is exact on the function $\Phi(x)$, therefore we have

$$\begin{aligned} &\varepsilon^2 (L''_{\Phi,4}(u,x) - u''(x)) = \varepsilon^2 (L''_{\Phi,4}(p,x) - p''(x)) = \\ &= \varepsilon^2 (L''_{\Phi,4}(p,x) - L''_4(p,x)) + \varepsilon^2 (L''_4(p,x) - p''(x)). \end{aligned} \tag{40}$$

Let us consider the relative error corresponding to the first term in (40) in the form

$$\varepsilon^2 (L''_{\Phi,4}(p,x) - L''_4(p,x)) = \frac{1}{h} (p_{n+2} - 3p_{n+1} + 3p_n - p_{n-1})\, F_{2,\,4}(x), \tag{41}$$

where

$$F_{2,\,4}(x) = \varepsilon^2 h \left(\frac{\Phi''(x) - (\Phi_{n-1} - 2\Phi_n + \Phi_{n+1})/h^2}{\Phi_{n+2} - 3\Phi_{n+1} + 3\Phi_n - \Phi_{n-1}} - \frac{x - x_n}{h^3} \right).$$

Applying the Taylor formula with the integral form of the remainder at the node x_n for $p(x_{n\pm1})$ and $p(x_{n+2})$, we yield

$$|p_{n+2} - 3p_{n+1} + 3p_n - p_{n-1}| \leqslant \frac{3}{2}\, h^2 \int\limits_{x_{n-1}}^{x_{n+2}} |p^{(3)}(s)|\, ds. \tag{42}$$

Substituting $\Phi(x) = e^{-\alpha\, x/\varepsilon}$ into the function $F_{2,\,4}(x)$ we obtain

$$F_{2,\,4}(x) = \frac{\varepsilon^2 \left(1 - e^{-\frac{\alpha\, h}{\varepsilon}}\right)^2 - \alpha^2 h^2 e^{-\frac{\alpha (x - x_{n-1})}{\varepsilon}}}{h \left(1 - e^{-\frac{\alpha\, h}{\varepsilon}}\right)^3} - \frac{\varepsilon^2}{h^2}(x - x_n). \tag{43}$$

Let us consider the case $\alpha\, h/\varepsilon \geqslant 1$. Then $1 - e^{-\alpha\, h/\varepsilon} \geqslant 1 - e^{-1}$. It follows from (43) that

$$|F_{2,\,4}(x)| \leqslant \alpha^2 \left(\left(\frac{\varepsilon}{\alpha\, h}\right)^2 \frac{h}{1 - e^{-1}} + \frac{h}{(1 - e^{-1})^3} + \left(\frac{\varepsilon}{\alpha\, h}\right)^2 |x - x_n| \right) \leqslant 8\, \alpha^2 h. \tag{44}$$

Let us consider the case $\alpha\, h/\varepsilon < 1$. It follows from (43) that

$$F_{2,\,4}(x) = \frac{\varepsilon^2 h \left(1 - e^{-\frac{\alpha\, h}{\varepsilon}}\right)^2 - \varepsilon^2 (x - x_n) \left(1 - e^{-\frac{\alpha\, h}{\varepsilon}}\right)^3 - \alpha^2 h^3\, e^{-\frac{\alpha (x - x_{n-1})}{\varepsilon}}}{h^2 \left(1 - e^{-\frac{\alpha\, h}{\varepsilon}}\right)^3}. \tag{45}$$

Next, we raise $(1 - e^{-\alpha h/\varepsilon})$ to the second and the third powers in the numerator of the formula (45) and apply the Maclaurin series expansion with the Lagrange form of the remainder for exponential functions.

Then we combine the like terms and obtain

$$F_{2,4}(x)=\frac{\alpha^4h^3}{\varepsilon^2(1-e^{-\alpha h/\varepsilon})^3}\left(\left(\frac{1}{12}+\frac{\Delta}{2}-\frac{\Delta^2}{2}\right)+\right.$$
$$\left.+\frac{\alpha\,h}{\varepsilon}\left(\left(\frac{1}{60}-\frac{\Delta}{40}\right)e^{-s_1}+\left(\frac{4\,\Delta}{5}-\frac{4}{15}\right)e^{-s_2}-\frac{81\,\Delta}{40}\,e^{-s_3}+\frac{\Delta^3}{6}\,e^{-s_4}\right)\right), \tag{46}$$

where $s_1\in(0,\,\alpha\,h/\varepsilon)$, $s_2\in(0,\,2\,\alpha\,h/\varepsilon)$, $s_3,\,s_4\in(0,\,3\,\alpha\,h/\varepsilon)$, $\Delta=(x-x_n)/h$.

The following inequality for $t\in[0,1]$ is valid

$$1-e^{-t}\geqslant e^{-1}\,t,$$

therefore, it follows from (46) that

$$|F_{2,4}(x)|\leqslant\alpha\,e^3\,\varepsilon\left(\frac{11}{12}+\frac{\alpha\,h}{\varepsilon}\,\frac{811}{120}\right)\leqslant 8\,e^3\,\alpha\,\varepsilon. \tag{47}$$

Taking into account the estimates (44), (47), we obtain

$$|F_{2,4}(x)|\leqslant 8\,e^3\,\alpha\,\max\{\alpha\,h,\,\varepsilon\},\qquad x\in[x_{n-1},\,x_{n+2}]. \tag{48}$$

It follows from (41), (42), (48) that

$$\varepsilon^2|L''_{\Phi,4}(p,x)-L''_4(p,x)|\leqslant 12\,e^3\,\alpha\,h\,\max\{\alpha\,h,\varepsilon\}\int\limits_{x_{n-1}}^{x_{n+2}}|p^{(3)}(s)|\,ds\leqslant$$
$$\leqslant 36\,e^3\,\alpha\,h^2\,\max\{\alpha\,h,\varepsilon\}\,\|p'''\|_{[x_{n-1},\,x_{n+2}]}. \tag{49}$$

In order to estimate the second term of the right-hand (40) we transform the formula (37) and yield

$$L''_4(p,x)-p''(x)=\left(\frac{p_{n+1}-2p_n+p_{n-1}}{h^2}-p''_n\right)+$$
$$+\int\limits_{x}^{x_n}\left(p^{(3)}(s)-\frac{p_{n+2}-3p_{n+1}+3p_n-p_{n-1}}{h^3}\right)ds. \tag{50}$$

Applying the Taylor formula with the integral form of the remainder at the node x_n for $p(x_n\pm h)$, we obtain

$$\left|\frac{p_{n+1}-2p_n+p_{n-1}}{h^2}-p''_n\right|\leqslant\frac{h}{6}\int\limits_{x_{n-1}}^{x_{n+1}}|p^{(4)}(s)|\,ds\leqslant\frac{h^2}{3}\,\|p^{(4)}\|_{[x_{n-1},\,x_{n+1}]}. \tag{51}$$

It is known that for some $s_0\in[x_{n-1},\,x_{n+2}]$ it is satisfied

$$p_{n+2}-3p_{n+1}+3p_n-p_{n-1}=h^3p^{(3)}(s_0),$$

therefore, for the second term in (50) one has

$$\left|\int\limits_{x}^{x_n}\left(p^{(3)}(s)-\frac{p_{n+2}-3p_{n+1}+3p_n-p_{n-1}}{h^3}\right)ds\right|\leqslant 3\,h\int\limits_{x_{n-1}}^{x_{n+2}}|p^{(4)}(s)|\,ds\leqslant$$
$$\leqslant 9\,h^2\,\|p^{(4)}\|_{[x_{n-1},\,x_{n+2}]}. \tag{52}$$

Substituting (51), (52) into (50), we obtain

$$|L_4''(p,x) - p''(x)| \leqslant \frac{h}{6} \int\limits_{x_{n-1}}^{x_{n+1}} |p^{(4)}(s)|\,ds + 3\,h \int\limits_{x_{n-1}}^{x_{n+2}} |p^{(4)}(s)|\,ds \leqslant \tag{53}$$

$$\leqslant \frac{28}{3}\,h^2\,\|p^{(4)}\|_{[x_{n-1},\,x_{n+2}]}.$$

Then the estimate (39) follows from (40), (49) and (53). □

Notice 1. In this paper, the numerical differentiation formulas which are exact on a boundary layer component of the differentiable function $u(x)$ are investigated. Outside the boundary layer where the derivatives of $u(x)$ become uniformly bounded, we can use the classical numerical differentiation formulas $L_k^{(j)}(u,x)$ to calculate the derivatives $u^{(j)}(x)$.

For example, let us consider the formula to calculate the first derivative

$$u'(x) \approx L_2'(u,x) = \frac{u_n - u_{n-1}}{h}, \qquad x \in [x_{n-1},\, x_n].$$

Then the following estimate is fulfilled

$$\left|\frac{u_n - u_{n-1}}{h} - u'(x)\right| \leqslant h\,\|u''\|_{[x_{n-1},\,x_n]}.$$

If it begins with some n the following estimate is valid

$$\Phi''(x) = \frac{\alpha^2}{\varepsilon^2}\,e^{-\frac{\alpha\,x}{\varepsilon}} \leqslant 1 \qquad x \geqslant x_{n-1},$$

then there is a constant C_0 such that the estimate $\|u''\|_{[x_{n-1},\,x_n]} \leqslant C_0$ holds true. Therefore, the following estimate is satisfied for $x \in [x_{n-1}, x_n]$

$$\left|\frac{u_n - u_{n-1}}{h} - u'(x)\right| \leqslant C_0\,h \qquad x_{n-1} \geqslant -\frac{2\,\varepsilon}{\alpha}\ln\frac{\varepsilon}{\alpha}\,.$$

Notice 2. The approach proposed here can be extended to two-dimensional case. In [31], a generalization of one-dimensional formula (3) in the case $j = 0$ is studied. We can use analogously the two-dimensional interpolation formula from [31] to construct a two-dimensional formula of numerical differentiation. Such formula can be applied to approximate derivatives in the case of elliptic problem with regular boundary layers.

5. Numerical results

Example 1. We consider the following function

$$u(x) = e^{-\frac{5\,x}{\varepsilon}} + 4\,cos\left(\frac{\pi\,x}{2}\right) + \frac{1}{x+1}, \quad x \in [0,\,1].$$

Let us define the error norms

$$\Delta_{L,\,N,\,k}^{(j)} = \max_{\substack{i=0,\,1,\,\dots,\,4(k-1)\\ l=0,\,k-1,\,\dots,\,N-k+1}} \varepsilon^j\,|L_k^{(j)}(u, x_{l+i/4}) - u^{(j)}(x_{l+i/4})|,$$

$$\Delta_{\Phi,\,N,\,k}^{(j)} = \max_{\substack{i=0,\,1,\,\dots,\,4(k-1)\\ l=0,\,k-1,\,\dots,\,N-k+1}} \varepsilon^j\,|L_{\Phi,\,k}^{(j)}(u, x_{l+i/4}) - u^{(j)}(x_{l+i/4})|,$$

where $x_{l+1/2} = (x_l + x_{l+1})/2$, $x_{l+1/4} = (x_l + x_{l+1/2})/2$, $x_{l+3/4} = (x_{l+1/2} + x_{l+1})/2$ and other fractional nodes are similarly defined. Thus, the error norm is calculated as maximum of the error at all nodes of the fined mesh which can be obtained from the given mesh by dividing each mesh interval into four equal parts.

Table 1 contains the error norm $\Delta^{(1)}_{L,N,3}$ of classical numerical differentiation formula for the first derivative (left table) and the error norm $\Delta^{(1)}_{\Phi,N,3}$ of the proposal formula (right table) for various values of N and ε.

TABLE 1. The error norm $\Delta^{(1)}_{L,N,3}$ of classical numerical differentiation formula for the first derivative (in the left) and $\Delta^{(1)}_{\Phi,N,3}$ of the proposal formula (in the right).

3ε	N				3ε	N			
	48	192	768	3072		48	192	768	3072
3	1.75e−2	1.16e−3	7.37e−5	4.62e−6	3	6.69e−3	4.12e−4	2.57e−5	1.60e−6
2^{-2}	1.13e+0	1.30e−1	9.60e−3	6.27e−4	2^{-2}	7.96e−3	4.05e−4	2.39e−5	1.47e−6
2^{-4}	3.51e+0	1.13e+0	1.30e−1	9.60e−3	2^{-4}	1.28e−2	4.98e−4	2.53e−5	1.49e−6
2^{-5}	4.25e+0	2.32e+0	4.18e−1	3.63e−2	2^{-5}	1.53e−2	6.19e−4	2.72e−5	1.52e−6
2^{-8}	4.91e+0	4.63e+0	3.51e+0	1.13e+0	2^{-8}	1.76e−2	1.04e−3	5.00e−5	2.00e−6
2^{-10}	4.98e+0	4.91e+0	4.63e+0	3.51e+0	2^{-10}	1.79e−2	1.10e−3	6.49e−5	3.13e−6
2^{-13}	5.00e+0	4.99e+0	4.95e+0	4.81e+0	2^{-13}	1.80e−2	1.12e−3	6.96e−5	4.22e−6
2^{-14}	5.00e+0	4.99e+0	4.98e+0	4.91e+0	2^{-14}	1.80e−2	1.12e−3	6.99e−5	4.31e−6

From Table 1 follows that the error of classical numerical differentiation formula (11) is $O(h^2)$ only in the case $h < \varepsilon$ but the error of the proposal formula (12) is uniform with respect to ε. These results correspond to the estimates obtained in Theorem 3.2.

Table 2 contains the error norm $\Delta^{(2)}_{L,N,3}$ of classical numerical differentiation formula for the second derivative (left table) and the error norm $\Delta^{(2)}_{\Phi,N,3}$ of the proposal formula (right table) for various values of N and ε.

TABLE 2. The error norm $\Delta^{(2)}_{L,N,3}$ of classical numerical differentiation formula for the second derivative (in the left) and $\Delta^{(2)}_{\Phi,N,3}$ of the proposal formula (in the right).

3ε	N				3ε	N			
	48	192	768	3072		48	192	768	3072
3	2.57e+0	6.72e−1	1.70e−1	4.26e−2	3	9.81e−1	2.38e−1	5.92e−2	1.48e−2
2^{-2}	1.69e+1	6.56e+0	1.87e+0	4.83e−1	2^{-2}	1.19e−1	2.05e−2	4.64e−3	1.13e−3
2^{-4}	2.40e+1	1.69e+1	6.56e+0	1.87e+0	2^{-4}	8.75e−2	7.44e−3	1.28e−3	2.90e−4
2^{-5}	2.48e+1	2.16e+1	1.12e+1	3.57e+0	2^{-5}	8.90e−2	5.77e−3	7.27e−4	1.50e−4
2^{-8}	2.50e+1	2.49e+1	2.40e+1	1.69e+1	2^{-8}	8.98e−2	5.60e−3	3.42e−4	2.97e−5
2^{-10}	2.50e+1	2.50e+1	2.49e+1	2.40e+1	2^{-10}	8.99e−2	5.62e−3	3.50e−4	2.14e−5
2^{-13}	2.50e+1	2.50e+1	2.50e+1	2.50e+1	2^{-13}	8.99e−2	5.62e−3	3.51e−4	2.19e−5
2^{-14}	2.50e+1	2.50e+1	2.50e+1	2.50e+1	2^{-14}	8.99e−2	5.62e−3	3.51e−4	2.19e−5

From Table 2 follows that the error of classical numerical differentiation formula (25) is $O(h)$ only in the case $h < \varepsilon$ but the error of the proposal formula (26) is uniform with respect to ε. These results correspond to the estimates obtained in Theorem 4.1.

Table 3 contains the error norm $\Delta^{(2)}_{L,N,4}$ of classical numerical differentiation formula for the second derivative (left table) and the error norm $\Delta^{(2)}_{\Phi,N,4}$ of the proposal formula (right table) for various values of N and ε.

TABLE 3. The error norm $\Delta^{(2)}_{L,N,4}$ of classical numerical differentiation formula for the second derivative (in the left) and $\Delta^{(2)}_{\Phi,N,4}$ of the proposal formula (in the right).

3ε	N			
	48	192	768	3072
3	$2.40e{-1}$	$1.63e{-2}$	$1.04e{-3}$	$6.53e{-5}$
2^{-2}	$1.10e{+1}$	$1.61e{+0}$	$1.29e{-1}$	$8.56e{-3}$
2^{-4}	$2.30e{+1}$	$1.10e{+1}$	$1.61e{+0}$	$1.29e{-1}$
2^{-5}	$2.45e{+1}$	$1.85e{+1}$	$4.75e{+0}$	$4.73e{-1}$
2^{-8}	$2.50e{+1}$	$2.49e{+1}$	$2.30e{+1}$	$1.10e{+1}$
2^{-10}	$2.50e{+1}$	$2.50e{+1}$	$2.49e{+1}$	$2.30e{+1}$
2^{-13}	$2.50e{+1}$	$2.50e{+1}$	$2.50e{+1}$	$2.50e{+1}$
2^{-14}	$2.50e{+1}$	$2.50e{+1}$	$2.50e{+1}$	$2.50e{+1}$

3ε	N			
	48	192	768	3072
3	$3.31e{-2}$	$2.00e{-3}$	$1.24e{-4}$	$7.78e{-6}$
2^{-2}	$4.15e{-3}$	$1.78e{-4}$	$1.01e{-5}$	$6.18e{-7}$
2^{-4}	$3.21e{-3}$	$6.50e{-5}$	$2.78e{-6}$	$1.58e{-7}$
2^{-5}	$3.34e{-3}$	$5.12e{-5}$	$1.58e{-6}$	$8.16e{-8}$
2^{-8}	$3.41e{-3}$	$5.31e{-5}$	$7.85e{-7}$	$1.59e{-8}$
2^{-10}	$3.41e{-3}$	$5.34e{-5}$	$8.31e{-7}$	$1.23e{-8}$
2^{-13}	$3.41e{-3}$	$5.34e{-5}$	$8.35e{-7}$	$1.30e{-8}$
2^{-14}	$3.41e{-3}$	$5.34e{-5}$	$8.35e{-7}$	$1.30e{-8}$

From Table 3 follows that the error of classical numerical differentiation formula (37) is $O(h^2)$ only in the case $h < \varepsilon$ but the error of the proposal formula (38) is uniform with respect to ε. These results correspond to the estimates obtained in Theorem 4.2.

Example 2. We consider the following function

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

We note that this function is the exact solution of the problem

$$\begin{aligned} &\varepsilon\, u'(x) + (1+x)\, u(x) = -\frac{\varepsilon\,\pi}{2}\, sin\left(\frac{\pi\, x}{2}\right) + (1+x)\; cos\left(\frac{\pi\, x}{2}\right), \\ &u(0) = 2, \qquad x \in [0,\, 1], \end{aligned}$$

and in this case $\Phi(x) = e^{-\frac{x}{\varepsilon}}$ and $\gamma = 1$ in the representation (1).

Table 4 contains the error norm $\Delta^{(1)}_{L,N,3}$ of classical numerical differentiation formula for the first derivative (left table) and the error norm $\Delta^{(1)}_{\Phi,N,3}$ of the proposal formula (right table) for various values of N and ε.

From Table 4 follows that the error of classical numerical differentiation formula (11) is $O(h^2)$ only in the case $h < \varepsilon$ but the error of the proposal formula (12) is uniform with respect to ε. These results correspond to the estimates obtained in Theorem 3.2.

Table 5 contains the error norm $\Delta^{(2)}_{L,N,3}$ of classical numerical differentiation formula for the second derivative (left table) and the error norm $\Delta^{(2)}_{\Phi,N,3}$ of the proposal formula (right table) for various values of N and ε.

From Table 5 follows that the error of classical numerical differentiation formula (25) is $O(h)$ only in the case $h < \varepsilon$ but the error of the proposal formula (26) is uniform with respect to ε. These results correspond to the estimates obtained in Theorem 4.1.

Conclusion

The numerical differentiation formulas which are exact on a boundary layer component of the function with large gradients in an exponential boundary layer

TABLE 4. The error norm $\Delta^{(1)}_{L,N,3}$ of classical numerical differentiation formula for the first derivative (in the left) and $\Delta^{(1)}_{\Phi,N,3}$ of the proposal formula (in the right).

3ε	N = 48	192	768	3072
3	5.13e−4	3.21e−5	2.00e−6	1.25e−7
2^{-2}	1.37e−2	9.45e−4	6.05e−5	3.81e−6
2^{-4}	1.63e−1	1.64e−2	1.17e−3	7.55e−5
2^{-5}	3.78e−1	5.70e−2	4.61e−3	3.08e−4
2^{-8}	9.06e−1	6.34e−1	1.68e−1	1.73e−2
2^{-10}	9.77e−1	9.06e−1	6.34e−1	1.68e−1
2^{-13}	9.97e−1	9.88e−1	9.53e−1	8.13e−1
2^{-14}	9.99e−1	9.94e−1	9.77e−1	9.06e−1

3ε	N = 48	192	768	3072
3	5.87e−4	3.70e−5	2.32e−6	1.45e−7
2^{-2}	2.46e−3	1.84e−4	1.20e−5	7.58e−7
2^{-4}	5.30e−3	6.76e−4	5.00e−5	3.26e−6
2^{-5}	3.98e−3	1.10e−3	9.59e−5	6.51e−6
2^{-8}	9.70e−4	2.90e−4	3.54e−4	4.35e−5
2^{-10}	1.05e−3	6.06e−5	8.10e−5	8.89e−5
2^{-13}	1.07e−3	6.61e−5	3.99e−6	2.97e−6
2^{-14}	1.07e−3	6.65e−5	4.09e−6	1.51e−6

TABLE 5. The error norm $\Delta^{(2)}_{L,N,3}$ of classical numerical differentiation formula for the second derivative (in the left) and $\Delta^{(2)}_{\Phi,N,3}$ of the proposal formula (in the right).

3ε	N = 48	192	768	3072
3	7.39e−2	1.85e−2	4.62e−3	1.15e−3
2^{-2}	1.70e−1	4.57e−2	1.16e−2	2.93e−3
2^{-4}	5.77e−1	2.05e−1	5.66e−2	1.45e−2
2^{-5}	8.02e−1	3.72e−1	1.13e−1	2.97e−2
2^{-8}	9.95e−1	9.38e−1	5.99e−1	2.16e−1
2^{-10}	9.99e−1	9.96e−1	9.39e−1	6.00e−1
2^{-13}	1.00e+0	1.00e+0	9.99e−1	9.84e−1
2^{-14}	1.00e+0	1.00e+0	1.00e+0	9.96e−1

3ε	N = 48	192	768	3072
3	8.46e−2	2.13e−2	5.33e−3	1.33e−3
2^{-2}	3.29e−2	9.07e−3	2.32e−3	5.83e−4
2^{-4}	2.45e−2	9.02e−3	2.46e−3	6.30e−4
2^{-5}	1.48e−2	8.10e−3	2.43e−3	6.33e−4
2^{-8}	1.06e−3	1.62e−3	1.61e−3	5.79e−4
2^{-10}	1.07e−3	2.59e−4	4.17e−4	4.04e−4
2^{-13}	1.07e−3	6.69e−5	3.65e−5	4.13e−5
2^{-14}	1.07e−3	6.69e−5	1.62e−5	2.01e−5

are investigated. The numerical differentiation formulas are considered to calculate the first derivative on two and three nodes and the second derivative on three and four nodes. The ε-uniform estimates of the relative error for these formulas are obtained. Numerical results are given to confirm the theoretical results.

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