Approaches to the calculation of derivatives of functions with large gradients in the boundary layer under the values at the grid nodes

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Abstract. A problem of approximation the derivatives of functions with large gradients in the exponential boundary layer is investigated. The application of classical formulas of numerical differentiation to such functions leads to significant errors. The approaches based on the application of special formulas of numerical differentiation on a uniform grid and polynomial formulas of numerical differentiation on the Shishkin mesh, condensed in the boundary layer, are discussed. An approach based on the differentiation of splines approximating the original function with large gradients is studied similarly. With this approach, the derivatives are found as smooth functions of their argument.

1. Introduction

The problem of calculating the derivatives of functions with large gradients in the boundary layer region is investigated. Such functions correspond to the solution of a singularly perturbed boundary value problem with a small parameter $\varepsilon$ at the highest derivative [1]. Various convection-diffusion processes with predominant convection are modeled on the basis of singularly perturbed problems. Therefore, the problem of constructing numerical differentiation formulas, the error of which does not depend on the large gradients of the function in the boundary layer, is relevant.

Our problem is the calculation the derivatives of such function by its values at the grid nodes. These values can be obtained on the basis of the application of a difference scheme for solving singularly perturbed boundary value problem. The influence of computing inaccuracies in the work is not investigated. It is known that the use of classical formulas of numerical differentiation on the uniform grid to functions with large gradients can lead to significant errors.

The approaches developed in this paper based on the application of the classical formulas of numerical differentiation on Shishkin mesh, condensed in the boundary layer, and using non-polynomial formulas of numerical differentiation, exact for the boundary layer component. The possibility of using splines to calculate derivatives is investigated also.

Now we introduce the notations. Let $\varepsilon \in (0, 1]$ be a positive parameter. Denote by $S(\Omega, k, 1)$ the space of polynomial splines of degree $k$ and defect 1 on the mesh $\Omega$. By $C$ and $C_j$ we mean positive constants that do not depend on the parameter $\varepsilon$ and the number of mesh intervals.
In this case, the same symbol $C_j$ can denote different constants. We define the norm of the function $||u|| = \max_x |u(x)|$, $x \in [0, 1]$.

2. The fitting the formulas to the boundary layer component

Let the function $u(x)$ be decomposed

$$u(x) = p(x) + \gamma \Phi(x), \quad x \in [0, 1],$$

where the function $u(x)$ is sufficiently smooth, the component $\Phi(x)$ of the boundary layer is known, sufficiently smooth and has large gradients in the boundary layer, the regular component $p(x)$ has bounded derivatives up to some order, the constant $\gamma$ and the function $p(x)$ are unknown.

We note that the representation (1) is valid for the solution of a singularly perturbed problem

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

where $a(x) \geq a_0 > 0$, $b(x) \geq 0$, $\varepsilon \in (0, 1]$, functions $a, b, f$ are smooth enough, the constant $a_0$ is separated from zero. If we set

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

then for some $C_0$ there are the estimates $|\gamma|^2 \leq C_0$, $|\gamma| \leq C_0$. We note that the derivatives of function $\Phi(x)$ increase unlimited with decreasing $\varepsilon$.

Let the function (1) be given at the nodes of the uniform grid $\Omega^h = \{x_n = nh, n = 0, 1, \ldots, N, Nh = 1\}$. The problem is to compute the derivatives of the function $u(x)$ by its values at the nodes of the grid $\Omega^h$. Let $u_n = u(x_n)$, $n = 0, 1, \ldots, N$.

Now we show that the application of classical formulas on a uniform grid is unacceptable to calculate the derivatives of functions with large gradients. Consider the formula

$$u'(x) \approx \frac{u_n - u_{n-1}}{h}, \quad x_{n-1} \leq x \leq x_n.$$

Let us $u(x) = e^{-x/\varepsilon}$. Then $\varepsilon|(u_1 - u_0)/h - u'(0)| = e^{-1}$ if $\varepsilon = h$. So, the relative error of the formula does not decrease as $h \to 0$, $\varepsilon = h$.

In [2] the interpolation formula, which is exact for the component $\Phi(x)$, is proposed. The component $\Phi(x)$ gives the basic growth of the function $u(x)$ in the boundary layer. Differentiation of the constructed interpolant leads to formulas of numerical differentiation using values of the function on $k$ grid nodes:

$$L_{\Phi,k}^{(j)}(u, x) = L_{k-1}^{(j)}(u, x) + \frac{[x_m, x_{m+1}, \ldots, x_{m+k-1}]u}{[x_m, x_{m+1}, \ldots, x_{m+k-1}]\Phi_{k-1}^{(j)}(\Phi(x))},$$

where $x_m \leq x \leq x_{m+k-1}$, $j \geq 0$, $L_{k-1}(u, x)$ is the Lagrange polynomial for the function $u(x)$ with $(k-1)$ nodes $x_m, x_{m+1}, \ldots, x_{m+k-2}$, and $[x_m, x_{m+1}, \ldots, x_{m+k-1}]u$ is the divided difference for the function $u(x)$. The formula (3) is exact on the component $\Phi(x)$. In [3] are investigated special cases of this formula for $j = 1, 2, k = 2, 3, 4$.

For an example, let’s look at the case $j = 2, k = 4$. Then

$$L_{\Phi,4}^{(j)}(u, x) = \frac{u_{n-1} - 2u_n + u_{n+1}}{h^2} + \frac{u_{n-2} - 3u_n + 3u_{n+1} - u_{n+2}}{h^2}(\Phi(x) - \Phi_{n-1} - 2\Phi_n + \Phi_{n+1}),$$

where $x \in [x_{n-1}, x_{n+2}], \Phi^{(3)}(x) \neq 0$.

**Theorem 1.** Let us $\Phi(x) = e^{-\alpha x/\varepsilon}$, $\alpha > 0$. Then for some constant $C$

$$\varepsilon^2|L_{\Phi,4}^{(j)}(u, x) - u''(x)| \leq C h^2(\varepsilon^2||p^{(4)}|| + (h + \varepsilon)||p^{(3)}||), \quad x \in [x_{n-1}, x_{n+2}].$$

The proof of this theorem is based on the fact that the proposed difference formula for the derivative $u''(x)$ is exact on the boundary layer component $\Phi(x)$ and it remains to estimate the error on the regular component $p(x)$. 

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3. Polynomial formulas for the derivatives on Shishkin mesh

In this section we assume that the function \( u(x) \) is representable in the form:

\[
u(x) = q(x) + \Phi(x), \quad x \in [0, 1],
\]

where for the components \( q(x) \), \( \Phi(x) \) the following estimates hold

\[
|q^{(j)}(x)| \leq C_1, \quad |\Phi^{(j)}(x)| \leq \frac{C_1}{x^j} e^{-\alpha x/\varepsilon}, \quad 0 \leq j \leq m_0.
\]

As is known \([1]\), the decomposition (4) is valid for the solution of the problem (2).

In accordance with \([1]\) we define on the interval \([0, 1]\) a piecewise-uniform mesh

\[
\Delta = \{x_n : x_n = x_{n-1} + h_n, \quad n = 1, 2, \ldots, N, \quad x_0 = 0, \quad x_N = 1\}
\]

with the step \( h_n \) in the boundary layer \([0, \sigma]\) and with the step \( H \) outside the boundary layer

\[h_n = h = \frac{2\sigma}{N}, \quad 1 \leq n \leq \frac{N}{2}; \quad h_n = H = \frac{2(1 - \sigma)}{N}, \quad \frac{N}{2} < n \leq N, \quad \sigma \in (0, 1/2].\]

We will construct difference formulas for calculating the derivatives on sub-intervals with \( k \) nodes covering the interval \([0, 1]\). Assume that \( N \) is a multiple of \( 2(k - 1) \), so that each sub-interval is entirely inside or outside the boundary layer region \([0, \sigma]\), \( \sigma = x_N/2\).

Thus, we split the interval \([0, 1]\) into \( N/(k - 1) \) sub-intervals:

\[
[0, 1] = \bigcup_{m=0, k-1}^{N-k+1} [x_m, x_{m+k-1}].
\]

To construct the difference formula for the derivative on the interval \([x_m, x_{m+k-1}]\), we perform the interpolation of the function \( u(x) \) on this interval by the Lagrange polynomial \( L_k(u, x) \).

We define

\[
\sigma = \min \left\{ \frac{1}{2}, \frac{k \varepsilon}{\alpha \ln N} \right\}.
\]

**Theorem 2.** Let the function \( u(x) \) has the representation (4), \( m_0 = k + j \), where \( k \) is the number of nodes in the difference formula for the derivative and \( j \) is the number of the calculated derivative. Let \( \Delta \) corresponds to (6). Then for some constant \( C \) on each interval \([x_m, x_{m+k-1}]\) for \( m = 0, k-1, \ldots, N - k + 1 \) one of the error estimates is valid

\[
\varepsilon^j |u^{(j)}(x) - L_k^{(j)}(u, x)| \leq C \left( \frac{\ln N}{N} \right)^{k-j}, \quad j \geq 0, \quad \sigma < 1/2, \quad x_{m+k-1} \leq \sigma,
\]

\[
\varepsilon^j |u^{(j)}(x) - L_k^{(j)}(u, x)| \leq C \left[ \frac{1}{Nk} e^{-\alpha(x_m-\sigma)/\varepsilon} + \frac{\varepsilon^j}{N^{k-j}} \right], \quad j \geq 0, \quad \sigma < 1/2, \quad x_m \geq \sigma,
\]

\[
\varepsilon^j |u^{(j)}(x) - L_k^{(j)}(u, x)| \leq C \left( \min \left( \frac{\ln N}{N}, \frac{1}{N\varepsilon} \right) \right)^{k-j}, \quad j \geq 0, \quad \sigma = 1/2.
\]

The proof of this theorem is based on the use of decomposition (4), properties of the mesh (6) and on known relationship:

\[
u^{(j)}(x) - L_k^{(j)}(u, x) = \sum_{i=0}^{j} \frac{j!}{(j-i)!} w_k^{(j-i)}(x) \underbrace{x, \ldots, x, x_m, \ldots, x_{m+k-1}}_{(i+1) \text{ times}}, \quad j \geq 0,
\]

where \( w_k(x) = (x - x_m)(x - x_{m+1}) \cdots (x - x_{m+k-1}) \). The estimates (8)–(10) are \( \varepsilon \)-uniform.
4. An application of a cubic spline on the Shishkin mesh
We assume that for the interpolated function $u(x)$ is valid the decomposition (4) and in (5)
$0 \leq j \leq 4$. We define the mesh $\Delta$ in accordance with (6) and

$$\sigma = \min \left\{ \frac{1}{2}, \frac{4\varepsilon}{\alpha} \ln N \right\}. $$

Let $S(x, u) \in S(\Delta, 3, 1)$ be the interpolation cubic spline on $\Delta$ constructed from the conditions

$$S(x_n, u) = u(x_n), \ 0 \leq n \leq N,\ S'(0, u) = u'(0),\ S'(1, u) = u'(1).$$

In [4] the estimation of the interpolation error by the spline $S(x, u)$ is obtained. It is proved that the error grows with decreasing $\varepsilon$ and this estimation is not improved.

However, a cubic spline on the Shishkin mesh can be used for the calculation of the derivatives of the function (4) in accordance with the following theorem.

**Theorem 3.** Suppose that the function $u(x)$ has the representation (4) and the mesh corresponds to (6). Then for some constant $C$ one of the error estimates is valid:

$$\varepsilon |u'(x) - S'(x, u)| \leq C \frac{\ln^3 N}{N^3}, \ x \leq \sigma,$$

$$|u'(x) - S'(x, u)| \leq C \left[ \frac{1}{N^3} + \frac{1}{\varepsilon N^3} e^{-\alpha(x-\sigma)/\varepsilon} + \frac{1}{\varepsilon N^3} e^{-\beta(n-N/2)} \right], \ x > \sigma,$$

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

$$|u''(x) - S''(x, u)| \leq C \left[ \frac{1}{N^3} + \frac{1}{\varepsilon^2 N^3} e^{-\alpha(x-\sigma)/\varepsilon} + \frac{1}{\varepsilon N^3} e^{-\beta(n-N/2)} \right], \ x > \sigma.$$

Consequently, in the region of the boundary layer the relative error is $\varepsilon$-uniform and outside the region of large gradients the absolute error is $\varepsilon$-uniform.

5. An application of an exponential spline on a uniform grid
Suppose that the decomposition (1) holds for the function $u(x)$,

$$|p^{(j)}(x)| \leq C_1, \ 0 \leq j \leq 4, \Phi(x) = e^{-\alpha x/\varepsilon}, \ \alpha > 0, \ x \in [0, 1].$$

(11)

We define the space of generalized splines

$$SL(\Omega^h, 3, 1) = \{ S(x) \in C^2[0, 1] : S(x) = a_n + b_n x + c_n x^2 + d_n e^{-\alpha x/\varepsilon}, \ x \in [x_n, x_{n+1}], \ 0 \leq n < N \}. $$

We construct an exponential interpolation spline $S_\Phi(x; u) \in SL(\Omega^h, 3, 1)$ for the function $u(x)$ from interpolation conditions

$$S_\Phi(x_n; u) = u(x_n), \ 0 \leq n \leq N,\ S'_\Phi(0; u) = u'(0),\ S''_\Phi(1; u) = u''(1).$$

(12)

**Theorem 4.** For a function $u(x)$, having the decomposition (1) with conditions (11), there exists a unique interpolation spline $S_\Phi(x; u) \in SL(\Omega^h, 3, 1)$ satisfying conditions (12), and for some constant $C$ and $j = 0, 1, 2$ the following estimates hold

$$\| S_\Phi^{(j)}(x; u) - u^{(j)}(x) \|_{C[0,1]} \leq C \min \left\{ h^{3-j}, \frac{h^{1-j}}{\varepsilon} \right\}, \ \varepsilon \in (0, 1].$$

(13)
Consider the case \( \varepsilon \). The values of the basis functions \( N_j \) is true for 10 equal parts. We define the relative error in computing the cubic spline on a uniform grid \( \Omega^h \). The estimate (13) is true for \( j = 0 \), therefore \( |g(x)| \leq C \min \{h^3, h^2/\varepsilon \} \). Taking into account that the non-negative basis functions \( N_{n,3}(x) \) in the sum are equal to unity, we have \( |\beta_n| \leq C \min \{h^3, h^4/\varepsilon \} \). Taking into account the property of basis splines \( N_{n,k}(x) = (N_{n,k-1}(x) - N_{n+1,k-1}(x))/h \), we obtain from (14) the estimate (13) for \( j = 1 \). The case \( j = 2 \) is treated similarly. It proves Theorem 4.

### 6. Results of numerical experiments

We define a function

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

Let \( \tilde{x}_i \) be the nodes of the grid obtained from the original grid dividing each grid interval into 10 equal parts. We define the relative error in computing the \( j \)-th derivative for given \( \varepsilon \) and \( N \) on the basis of the spline \( S(x, u) \):

\[
\Delta_j(\varepsilon, N) = \varepsilon^j \max_i |S^{(j)}(\tilde{x}_i, u) - u^{(j)}(\tilde{x}_i)|
\]

and the accuracy orders: calculated \( CR_j(\varepsilon, N) \) and theoretical \( M_{N,k} \):

\[
CR_j(\varepsilon, N) = \log_2 \frac{\Delta_j(\varepsilon, N/2)}{\Delta_j(\varepsilon, N)} \quad \text{and} \quad M_{N,j} = \log_2 \left( \frac{\ln^{4-j}(N/2)}{(N/2)^{4-j}} \right).
\]

Table 1 shows \( \Delta_1(\varepsilon, N) \) and \( CR_1(\varepsilon, N) \) when calculating the first derivative in depending on the values of \( \varepsilon \) and \( N \) on the basis of the cubic spline \( S(x, u) \) on the uniform grid \( \Omega^h \).

Table 2 shows \( \Delta_1(\varepsilon, N) \) and \( CR_1(\varepsilon, N) \) when calculating the first derivative based on cubic spline \( S(x, u) \) on Shishkin mesh. In the last line the table gives theoretical orders of accuracy \( M_{N,1} \).

Table 3 shows absolute errors and computed orders of accuracy in the calculation of the first derivative on the basis of exponential spline \( S_\Phi(x; u) \) on a uniform grid.

The results of the calculations are in agreement with the estimates of errors.
Table 2. Relative errors and accuracy orders, the cubic spline on Shishkin mesh

| ε  | 2^4  | 2^5  | 2^6  | 2^7  | 2^8  |
|----|------|------|------|------|------|
| 1  | 1.11 \times 10^{-4} | 1.38 \times 10^{-5} | 1.72 \times 10^{-6} | 2.16 \times 10^{-7} | 2.70 \times 10^{-8} |
| 10^{-3} | 3.61 \times 10^{-2} | 1.39 \times 10^{-3} | 4.07 \times 10^{-4} | 9.81 \times 10^{-5} | 2.07 \times 10^{-5} |
| 10^{-4} | 3.61 \times 10^{-2} | 1.39 \times 10^{-3} | 4.07 \times 10^{-4} | 9.81 \times 10^{-5} | 2.07 \times 10^{-5} |

Table 3. Absolute errors and accuracy orders, the exponential spline on a uniform grid

| ε  | 2^4  | 2^5  | 2^6  | 2^7  | 2^8  |
|----|------|------|------|------|------|
| 1  | 2.36 \times 10^{-4} | 2.91 \times 10^{-5} | 3.61 \times 10^{-6} | 4.49 \times 10^{-7} | 5.60 \times 10^{-8} |
| 10^{-3} | 7.76 \times 10^{-2} | 1.92 \times 10^{-3} | 4.58 \times 10^{-4} | 1.04 \times 10^{-4} | 2.14 \times 10^{-4} |
| 10^{-4} | 7.32 \times 10^{-2} | 2.00 \times 10^{-3} | 5.00 \times 10^{-4} | 1.24 \times 10^{-4} | 3.04 \times 10^{-4} |

7. Conclusion
The problem of calculating the derivatives of a function of one variable having large gradients in the boundary layer region and given at the grid nodes is investigated. In the construction of numerical differentiation formulas for such functions, two approaches are considered: the application of polynomial formulas on the Shishkin mesh and the construction of special formulas that are exact on the boundary layer component responsible for the basic growth of the function in the boundary layer. Also, an approach based on the differentiation of a spline interpolating a given function is proposed. With this approach, a cubic spline is considered on a Shishkin mesh and an exponential spline on a uniform grid. Estimates of the error of the considered approaches are given. These estimates are uniform in a small parameter. The results of numerical experiments are consistent with the obtained error estimates.

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