New approaches to constructing quadrature formulas for functions with large gradients

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Abstract. The problem of numerical integration of functions with large gradients in the boundary layer is studied. The use of the Newton-Cotes formulas on a uniform grid to integrate such functions can lead to significant errors. The article investigates approaches to the construction of quadrature formulas, the error of which does not increase due to large gradients of the function in the boundary layer. The following approaches are considered: the construction of quadrature formulas that are exact on the singular component responsible for the growth of the function in the boundary layer, the application of the Newton-Cotes formulas on the Shishkin and Bakhvalov meshes, minimization the error of the quadrature formula due to the construction of nodes. The investigated approaches are new, partially reflected in the publications. The results of computational experiments are presented.

1. Introduction

The problem of the numerical integration of functions with large gradients is of interest, because the accuracy of the Newton-Cotes formulas in the case of such functions can significantly decrease [1]. In [1] it is shown that the application of the composed Newton-Cotes quadrature formula in the presence of an exponential boundary layer can lead to errors of the order of \( O(h) \), despite the increase the number of nodes of the basic quadrature formula. For example, the composed Simpson formula in the regular case has an error of the order of \( O(h^4) \), and in the presence of a boundary layer, the error becomes of the order of \( O(h) \), where \( h \) is the grid step.

Thus, in the case of a uniform grid, it is unacceptable to use the Newton-Cotes formulas for the numerical integration of functions with large gradients. In this work, we investigate approaches to construct a quadrature formula so that its error does not depend on large gradients of the function in the boundary layer. We consider new approaches based on fitting the quadrature formula to the singular component of the integrable function and on the use of classical formulas on grids that are condensed in the boundary layer. Meshes of Bakhvalov N.S. [2] and Shishkin G.I. [3] are widely used to construct uniformly converging difference schemes for singularly perturbed problems. Let’s consider the use of these meshes for constructing quadrature formulas.

By \( C \) and \( C_j \) we mean positive constants that do not depend on the singular component of the function being integrated, in particular, on the small parameter \( \epsilon \), and on the number of grid nodes. We can use the same constant \( C \) to estimate different quantities.
2. Fitting the Newton-Cotes formula to the singular component

Consider the question of constructing a quadrature formula for calculating the integral

\[ I(u) = \int_{a}^{b} u(x) \, dx \]  

in the case of the function \( u(x) \) having the representation:

\[ u(x) = p(x) + \gamma \Phi(x), \quad x \in [a, b]. \]  

We assume that the function \( u(x) \) is sufficiently smooth, the singular component \( \Phi(x) \) is known, is sufficiently smooth, its derivatives are not uniformly bounded, the regular component \( p(x) \) is bounded together with the derivatives to some of order, the constant \( \gamma \) and \( p(x) \) are not specified. The decomposition (2) holds for the solution of a singularly perturbed boundary value problem:

\[ \varepsilon u''(x) + a_1(x)u'(x) - a_2(x)u(x) = f(x), \quad u(0) = A, \quad u(1) = B, \]  

where \( a_1(x) \geq \alpha > 0, \) \( a_2(x) \geq 0, \) \( \varepsilon > 0, \) functions \( a_1, a_2, f \) are smooth enough. According to \([3] – [5]\), for small values of the parameter \( \varepsilon \) the solution of the problem (3) has an exponential boundary layer at the boundary \( x = 0 \) and the function \( u(x) \) satisfies the representation (2) when specifying \( \Phi(x) = e^{-a_1(0)\varepsilon^{-1}x}. \)

Let’s set equally spaced nodes \( \{x_1, x_2, \ldots, x_k\} \) of quadrature formula for calculating integral (1), where \( x_j = a + (j-1)h, \) \( 1 \leq j \leq k, \) \( x_k = b. \) We denote \( u_j = u(x_j). \)

Let us define the Lagrange interpolation polynomial:

\[ L_j(u, x) = \sum_{n=1}^{j} u_n \prod_{i=1, i \neq n}^{j} \frac{x - x_i}{x_n - x_i}. \]

In \([6]\) on the interval \([a, b]\) the following formula for interpolation of function of the form (2) was constructed:

\[ L_{\Phi,k}(u, x) = L_{k-1}(u, x) + \frac{[x_1, x_2, \ldots, x_k]u}{[x_1, x_2, \ldots, x_k] \Phi} \left[ \Phi(x) - L_{k-1}(\Phi, x) \right], \]

where \( x_1, x_2, \ldots, x_k \) are interpolation nodes, \([x_1, x_2, \ldots, x_k]u \) is divided difference for the function \( u(x) \) \([7]\). The formula (4) is exact on the singular component \( \Phi(x). \)

According to \([7]\), for some \( s \in (a, b) \)

\[ [x_1, x_2, \ldots, x_k] \Phi = \Phi^{(k-1)}(s)/(k-1)!. \]

Therefore, the formula (4) is correct, if \( \Phi^{(k-1)}(x) \neq 0, \) for \( x \in (a, b). \)

In \([8]\) the following lemma is proved.

**Lemma 1** Let

\[ \Phi^{(k-1)}(x) \neq 0, \quad \Phi^{(k)}(x) \neq 0, \quad k \geq 2, \quad x \in (a, b). \]

Then

\[ |L_{\Phi,k}(u, x) - u(x)| \leq 2 \max_s |p^{(k-1)}(s)| h^{k-1}, \quad x, s \in [a, b]. \]
The interpolation formula (4) can be written as

\[ L_{\Phi,k}(u,x) = L_k(u,x) + \frac{[x_1, x_2, \ldots, x_k]u}{[x_1, x_2, \ldots, x_k] \Phi} \left[ \Phi(x) - L_k(\Phi, x) \right]. \]  

(5)

Applying the formula (5), we construct a quadrature formula that is exact on the singular component \( \Phi(x) \):

\[ S_{\Phi,k}(u) = S_k(u) + \frac{[x_1, x_2, \ldots, x_k]u}{[x_1, x_2, \ldots, x_k] \Phi} \left[ \int_a^b \Phi(x) \, dx - S_k(\Phi) \right], \]  

(6)

where

\[ S_k(u) = \int_a^b L_k(u, x) \, dx \]  

(7)

is closed Newton-Cotes formula with \( k \) nodes.

Based on Lemma 1, we can prove the following theorem.

**Theorem 1** Let

\[ \Phi^{(k-1)}(x) \neq 0, \, \Phi^{(k)}(x) \neq 0, \, k \geq 2, \, x \in (a,b). \]

Then

\[ \left| S_{\Phi,k}(u) - \int_a^b u(x) \, dx \right| \leq 2(b-a) \max_s |p^{(k-1)}(s)| \varepsilon^k, \, x, s \in [a,b]. \]  

(8)

The estimate (8) does not depend on the singular component \( \Phi(x) \) and its derivatives. Note that the conditions of theorem 1 are satisfied, for example, in the case of an exponential boundary layer, when on the interval \([0, 1]\) \( \Phi(x) = e^{-\alpha x/\varepsilon} \).

3. **Newton-Cotes formula on the Shishkin mesh**

We assume that the integrable function \( u(x) \) can be represented as

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

(9)

where

\[ |p^{(j)}(x)| \leq C_1, \, |\Phi^{(j)}(x)| \leq \frac{C_1}{\varepsilon^j} e^{-\alpha x/\varepsilon}, \, 0 \leq j \leq m, \]  

(10)

where the functions \( p(x) \) and \( \Phi(x) \) are not explicitly given, \( \alpha > 0, \varepsilon > 0 \), some constant \( C_1 \) does not depend on \( \varepsilon \). According to (10), the regular component \( p(x) \) has derivatives bounded up to the order \( m \), and the singular component \( \Phi(x) \) has derivatives that are not uniformly bounded in the parameter \( \varepsilon \). In this section, \( m = k \) is the number of nodes of the applied quadrature formula. According to [3], [9], submission (9) with constraints (10) is valid for the solution of problem (3).

Quadrature Newton-Cotes formula on the Shishkin mesh for numerical integration of functions with large gradients researched in [10].

Let’s set the Shishkin mesh [3]

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

(11)

with steps

\[ h_n = \frac{2\sigma}{N}, \, 1 \leq n \leq \frac{N}{2}; \, h_n = \frac{2(1-\sigma)}{N}, \, \frac{N}{2} < n \leq N. \]
Let’s set
\[
\sigma = \min \left\{ \frac{1}{2}, \frac{k \varepsilon}{\alpha} \ln N \right\}. \tag{12}
\]

We assume that \(N\) is a multiple of \(2(k-1)\) and divide the original interval \([0, 1]\) into \(N/(k-1)\) intervals
\[
[0, 1] = \bigcup_{m=0}^{N/(k-1) N/k} [x_m, x_{m+k-1}].
\]

On each interval \([x_m, x_{m+k-1}]\) we construct the Newton-Cotes formula \(S_{m,k}(u)\) with nodes \(x_m, \ldots, x_{m+k-1}\) by analogies with (7). Note that by the constraint on \(N\), each the interval \([x_m, x_{m+k-1}]\) is completely in the region \([0, \sigma]\) or outside it.

Let us define a composed quadrature formula on the interval \([0, 1]\):
\[
S_k(u) = \sum_{m=0}^{N/(k-1) N/k} S_{m,k}(u). \tag{13}
\]

**Theorem 2** Let the function \(u(x)\) have a representation (9) with constraints (10) for \(m = k\). Then for the formula (13) on the mesh (11) for some constant \(C\), the following error estimates are valid
\[
|I(u) - S_k(u)| \leq \frac{C}{N^k} \left[ 1 + \varepsilon \ln^{k+1} N \right] \text{ if } \varepsilon < \frac{\alpha}{2k \ln N}, \tag{14}
\]
\[
|I(u) - S_k(u)| \leq \frac{C}{N^k} \min \left\{ \frac{1}{\varepsilon^k}, \ln k, N \right\} \text{ if } \varepsilon \geq \frac{\alpha}{2k \ln N}. \tag{15}
\]

The proof of the theorem 2 is based on an estimate of the error of the Lagrange polynomial on the Shishkin mesh. In the general case, the estimate of the interpolation error by the Lagrange polynomial is known. In order for the error estimate to be uniform in a small parameter \(\varepsilon\), the interpolation error on functions \(p(x)\) and \(\Phi(x)\) is estimated separately, taking into account the estimates (10).

In the regular case, when the function \(u(x)\) has bounded derivatives, the composed Newton-Cotes formula has error of order \(O(1/N^k)\). The obtained error estimates (14), (15) are close to the error estimate in the regular case, when the parameter \(\varepsilon\) is close to one or to zero.

4. **Formula of trapeziums on the Bakhvalov mesh**

We assume that the function \(u(x)\) satisfies the representation (9)-(10) with \(m = 2\). Let’s set the nodes of the Bakhvalov mesh \([2], [11]::
\[
x_n = -\frac{r \varepsilon}{\alpha} \ln \left[ 1 - 2(1 - \varepsilon)n/N \right], \quad n = 0, 1, \ldots, N/2, \quad \varepsilon \leq e^{-1}, \tag{16}
\]
\[
x_n = \sigma + (2n/N - 1)(1 - \sigma), \quad n = N/2, \ldots, N, \tag{17}
\]
\[
\sigma = \min \{1/2, -\frac{r \varepsilon}{\alpha} \ln \varepsilon\}, \quad r \geq 2. \tag{18}
\]

For \(\varepsilon \geq e^{-1}\) the grid on the interval \([0, 1]\) is set uniform.

Let us define a formula for piecewise linear interpolation, on the grid interval \([x_{n-1}, x_n]\), having the form
\[
L_2(u, x) = u_{n-1} + \frac{x - x_{n-1}}{h_n} (u_n - u_{n-1}).
\]

In [12] the following lemma is proved.
Lemma 2 Let the function \( u(x) \) have the representation (9)-(10) with \( m = 2, r \geq 2 \). Then on the mesh with nodes (16)-(18) for some constant \( C \) the error estimate is valid

\[
|u(x) - L_2(u, x)| \leq \frac{C}{N^2}, \quad x \in [0, 1].
\]

Taking into account lemma 2, for an arbitrary grid interval we obtain the error estimate

\[
\left| \int_{x_{n-1}}^{x_n} u(x) \, dx - \frac{u_{n-1} + u_n}{2} \right| \leq \frac{C}{N^3}.
\]

Therefore, for the composed formula of trapeziums, the following estimate is valid

\[
\left| \int_0^1 u(x) \, dx - \sum_{n=1}^{N} \frac{u_{n-1} + u_n}{2} \right| \leq \frac{C}{N^2}.
\]

The Newton-Cotes formulas on the Bakhvalov mesh have not been previously studied. The error of other Newton-Cotes formulas can be estimated in a similar way.

5. Gaussian formula in the presence of a boundary layer

Gaussian formulas have a higher order of accuracy; therefore, it is of interest to apply them to functions with large gradients in the boundary layer. We assume that the integrable function \( u(x) \) has a representation (9) with constraints (10) for \( m = 2k \).

Let us estimate the error of the composite formula when the Gauss formula is applied on each base interval, the nodes of which are the roots of the Legendre polynomial. For the intervals on which the basic Gauss formulas are constructed, it is proposed to take the intervals of the Shishkin mesh. Then these intervals will be quite small in the boundary layer. We studied the Gauss formula for such function \( u(x) \) in [13].

Let us show that the intervals for the basic Gauss quadrature formula cannot be taken without taking into account their dense in the boundary layer. To do this, consider the Gauss formula \( S(u) \) with one node on the interval \([0, h]\) and estimate the error on the singular component \( \Phi(x) = e^{-x/\varepsilon} \). We have

\[
I(\Phi) = \int_0^h \Phi(x) \, dx \approx S(\Phi) = h \Phi(h/2).
\]

For the error \( \Delta \), the following relation is valid:

\[
\Delta = |I(\Phi) - h \Phi(h/2)| = |\varepsilon(1 - e^{-h/\varepsilon}) - he^{-h/(2\varepsilon)}|.
\]

Therefore, \( \Delta = O(h^3) \) for \( \varepsilon = 1 \) and \( \Delta \approx \varepsilon \) for \( \varepsilon \ll h \). It can be shown that for \( \varepsilon \leq h \) Gauss formulas with a different number of nodes have similar properties.

Let’s define a quadrature formula. We set the Shishkin mesh of the form (11) with

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

where \( k \) is the number of nodes of the basic Gauss quadrature formula.

Let \([x_{n-1}, x_n]\) be an arbitrary interval of the Shishkin mesh. Let’s set

\[
I_n(u) = \int_{x_{n-1}}^{x_n} u(x) \, dx.
\]
Then
\[ I(u) = \sum_{n=1}^{N} I_n(u). \]

Let \( S_{n,k}(u) \) be a Gauss formula with \( k \) nodes for the integral \( I_n(u) \):
\[
S_{n,k}(u) = \frac{x_n - x_{n-1}}{2} \sum_{j=1}^{k} D_j u(x_{n,j}), \quad S_k(u) = \sum_{n=1}^{N} S_{n,k}(u),
\]
where the nodes \( x_{n,j} \) on the interval \([x_{n-1}, x_n]\) are defined through the roots of the Legendre polynomial of degree \( k \).

**Theorem 3** Let the function \( u(x) \) satisfy representation (9)–(10) for \( m = 2k \). Then for the composite Gauss formula \( S_k(u) \) on the Shishkin mesh with \( \sigma \) from (19), the following error estimates hold
\[
|I(u) - S_k(u)| \leq \frac{C}{N^{2k}} \left[ 1 + \varepsilon \ln^{2k+1} N \right], \quad \text{if} \quad \varepsilon < \alpha/(4k \ln N),
\]
\[
|I(u) - S_k(u)| \leq \frac{C}{N^{2k}} \left( \min\{\varepsilon^{-1}, \ln N\} \right)^{2k}, \quad \text{if} \quad \varepsilon \geq \alpha/(4k \ln N),
\]
where \( C \) is some constant.

The proof is based on the well-known error estimate for the Gauss formula [7]
\[
|I_n(u) - S_{n,k}(u)| \leq \frac{(x_n - x_{n-1})^{2k+1}(k!)^4}{(2k)!^3(2k + 1)} M_{2k}, \quad M_{2k} = \max_{x \in [x_{n-1}, x_n]} |u^{(2k)}(x)|,
\]
by using decomposition (9)–(10) and the Shishkin mesh.

Note that the resulting error estimate is close to the known error estimate for the Gauss formula in the regular case, when the error is of the order of \( O(1/N^{2k}) \).

### 6. Optimizing the nodes of the quadrature formula

Let the function \( u(x) \) have large gradients in the exponential boundary layer and on the interval \([0, 1]\) it has the representation (9). On each grid interval \([x_{n-1}, x_n]\) we apply the Newton-Cotes formula with \( k \) uniformly spaced nodes. We assume that \( x_0 = 0, x_N = 1 \), and the nodes \( x_n, \ n = 1, 2, \ldots, N - 1 \) will be found on the basis of minimizing the error of the composite quadrature formula. This approach is described in [7] in the regular case using the trapezoid formula as an example. We propose its application in the presence of an exponential boundary layer. Previously, we investigated this approach in [14].

Let \( S_{k,n}(u) \) be the Newton-Cotes quadrature formula with \( k \) nodes, applied on the interval \([x_{n-1}, x_n]\). Then for the error of this formula the following estimate holds
\[
|S_{k,n}(u) - I_n(u)| \leq C(x_n - x_{n-1})^{k+1} \max_{s \in [x_{n-1}, x_n]} |u^{(k)}(s)|.
\]

Let us define a composite quadrature formula
\[
S_k(u) = \sum_{n=1}^{N} S_{k,n}(u).
\]
Let $|u^{(k)}(x)| \leq F(x)$. Then according to (20)

$$|I(u) - S_k(u)| \leq C \sum_{n=1}^{N} \max_{x \in [x_{n-1}, x_n]} F(x) (x_n - x_{n-1})^{k+1}. \quad (22)$$

We will find the nodes $x_n$ in the form $x_n = g(n/N)$ based on minimizing the error in (22). To do this, we replace the sum on the right-hand side (22) by an integral and proceed to minimize the integral

$$\int_{0}^{1} (g'(t))^{k+1} F(g(t)) \, dt = \int_{0}^{1} (t'(g))^{-k} F(g) \, dg = \int_{0}^{1} G(g, t, t') \, dg. \quad (23)$$

The integral (23) is minimized by solving the Euler equation [7]

$$\frac{d}{dg} \left( \frac{\partial G}{\partial t'} \right) - \frac{\partial G}{\partial t} = 0. \quad (24)$$

Considering (23), we get

$$F(g)(g'(t))^{k+1} = M_1. \quad (24)$$

It remains to solve the equation (24) and find the unknown constants from the boundary conditions.

Considering the conditions (10), we define

$$F(x) = 1 + \frac{1}{\varepsilon} e^{-\alpha x/\varepsilon}. \quad (25)$$

We find the function $g(t)$ separately in the domain $[0, \sigma]$, where we take $F(x) = \frac{1}{\varepsilon} e^{-\alpha x/\varepsilon}$ and beyond, where $F(x) = 1$.

As a result, we find the grid nodes:

$$x_n = -\frac{(k+1)\varepsilon}{\alpha} \ln \left[ 1 - 2(1 - \varepsilon) \frac{n}{N} \right], \quad n = 0, \ldots, \frac{N}{2}, \quad (25)$$

$$\sigma = -\frac{(k+1)\varepsilon}{\alpha} \ln \varepsilon, \quad (26)$$

$$x_n = 2\sigma - 1 + 2(1 - \sigma) n/N, \quad n > \frac{N}{2}. \quad (27)$$

**Theorem 4** Let the function $u(x)$ have the representation (9), grid nodes correspond to (25) – (27). Then for some constant $C$

$$|I(u) - S_k(u)| \leq C \frac{n^{k}}{N}. \quad (28)$$

The proof of this theorem is based on the estimate (20). The error of the quadrature formula is estimated separately for the components $p(x)$ and $\Phi(x)$. Estimates of the derivatives of these functions (10) are used. The step $h_n = x_n - x_{n-1}$ is estimated based on formulas for grid nodes (25 – (27). As a result, we obtain the estimate (28).

**Remark 1** We got that the minimum error of the composite Newton-Cotes formula is attained on the Bakhvalov’s mesh, as (16), (17). According to Theorem 4, the error estimate is uniform in a parameter $\varepsilon$. The order of accuracy is the same as in the regular case when the function $u(x)$ does not have large gradients.
In a similar way, the case is considered when the Gaussian quadrature formula with \( k \) nodes is applied on each interval \([x_{n-1}, x_n]\). For the Gauss formula \( G_{k,n}(u) \), applied on the interval \([x_{n-1}, x_n]\), we use the error estimate \cite{7}

\[
|G_{k,n}(u) - I_n(u)| \leq C(x_n - x_{n-1})^{2k+1} \max_{s \in [x_{n-1}, x_n]} |u^{(2k)}(s)|.
\]

Carrying out the optimal choice of nodes by analogy with the case of the Newton-Cotes formula, we obtain

\[
\sigma_1 = -\frac{(2k + 1)\varepsilon}{\alpha} \ln \varepsilon,
\]

\[
x_n = -\frac{(2k + 1)\varepsilon}{\alpha} \ln \left[ 1 - 2(1 - \varepsilon)n/N \right], \quad n = 0, 1, 2, \ldots, N/2,
\]

\[
x_n = 2\sigma_1 - 1 + 2(1 - \sigma_1)n/N, \quad n = N/2, N/2 + 1, \ldots, N.
\]

**Theorem 5** Let the function \( u(x) \) have the representation (9), grid nodes correspond to (30) – (31). Then for some constant \( C \)

\[
|I(u) - G_k(u)| \leq \frac{C}{N^{2k}}, \quad G_k(u) = \sum_{n=1}^{N} G_{k,n}(u).
\]

### 7. Results of numerical experiments

Consider a function

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

In tables \( \varepsilon - m \) means \( 10^{-m} \).

**Table 1.** The error of the composite three-nodes Newton-Cotes formula on the uniform grid

| \( \varepsilon \) | \( N \) |
|---|---|
|   | 16 | 32 | 64 | 128 | 256 | 512 |
| 1  | 0.38e-6 | 0.24e-7 | 0.15e-8 | 0.93e-10 | 0.58e-11 | 0.36e-12 |
| 10^{-1} | 0.81e-4 | 0.52e-5 | 0.33e-6 | 0.21e-7 | 0.12e-8 | 0.81e-10 |
| 10^{-2} | 0.12e-1 | 0.23e-2 | 0.25e-3 | 0.19e-4 | 0.13e-5 | 0.80e-7 |
| 10^{-3} | 0.20e-1 | 0.94e-2 | 0.42e-2 | 0.16e-2 | 0.41e-3 | 0.55e-4 |
| 10^{-4} | 0.21e-1 | 0.10e-1 | 0.51e-2 | 0.25e-2 | 0.12e-2 | 0.55e-3 |
| 10^{-5} | 0.21e-1 | 0.10e-1 | 0.52e-2 | 0.26e-2 | 0.13e-2 | 0.64e-3 |

Table 1 shows the error of the composite Newton-Cotes formula with three nodes on a uniform grid. The order of accuracy decreases from the fourth to the first with decreasing \( \varepsilon \). Numerical results show that it is unacceptable to apply the Newton-Cotes formulas on a uniform grid in the case of small values of the parameter \( \varepsilon \).

Table 2 shows the error of the composite formula with three nodes, exact on the singular component (6). Outside the boundary layer region, the Simpson formula is applied. The order of accuracy is reduced from fourth to third with decreasing \( \varepsilon \). This corresponds to Theorem 1, given that Simpson’s formula can be viewed as a four-nodes formula when the middle node is double.

Numerical results on the application of the Newton-Cotes formula on the Shishkin mesh are given in \cite{10}. These results confirm the estimates (14), (15).
Table 2. The error of the composite modified three-nodes formula (6)

| $\varepsilon$ | $N$   |
|---------------|-------|
|               | 16    | 32    | 64    | 128   | 256   | 512   |
| $10^{-1}$     | 0.12e - 3 | 0.85e - 6 | 0.53e - 7 | 0.33e - 8 | 0.21e - 9 | 0.13e - 10 |
| $10^{-2}$     | 0.30e - 3 | 0.24e - 4 | 0.16e - 5 | 0.10e - 6 | 0.61e - 8 | 0.38e - 9  |
| $10^{-3}$     | 0.37e - 3 | 0.45e - 4 | 0.50e - 5 | 0.72e - 6 | 0.80e - 7 | 0.62e - 8  |
| $10^{-4}$     | 0.39e - 3 | 0.49e - 4 | 0.61e - 5 | 0.75e - 6 | 0.90e - 7 | 0.10e - 7  |
| $10^{-5}$     | 0.39e - 3 | 0.50e - 4 | 0.62e - 5 | 0.78e - 6 | 0.97e - 7 | 0.12e - 7  |

Table 3. The error of the composite three-nodes Newton-Cotes formula on the optimal mesh

| $\varepsilon$ | $N$   |
|---------------|-------|
|               | 16    | 32    | 64    | 128   | 256   | 512   |
| $10^{-3}$     | 6.0e - 7 | 3.5e - 8 | 2.2e - 9 | 1.3e - 10 | 8.8e - 12 | 3.7e - 13 |
| $10^{-4}$     | 3.6e - 7 | 2.2e - 8 | 1.4e - 9 | 8.5e - 11 | 5.3e - 12 | 3.3e - 13 |
| $10^{-5}$     | 3.3e - 7 | 2.1e - 8 | 1.3e - 9 | 8.1e - 11 | 5.0e - 12 | 3.2e - 13 |
| $10^{-6}$     | 3.3e - 7 | 2.1e - 8 | 1.3e - 9 | 8.0e - 11 | 5.0e - 12 | 3.1e - 13 |

Table 4. The error of the composite Gauss formula with three nodes

| $\varepsilon$ | $N$   |
|---------------|-------|
|               | 4     | 8     | 16    | 32    | 64    | 128   |
| $1$           | 1.09e - 9 | 1.69e - 11 | 2.64e - 13 | 4.21e - 15 | 2.22e - 16 | -     |
| $10^{-1}$     | 9.91e - 6 | 1.80e - 7 | 2.92e - 9 | 4.60e - 11 | 7.21e - 13 | 1.10e - 14 |
| $10^{-2}$     | 1.77e - 5 | 3.39e - 6 | 3.48e - 7 | 2.26e - 8 | 1.09e - 9  | 4.36e - 11 |
| $10^{-3}$     | 1.72e - 6 | 3.40e - 7 | 3.49e - 8 | 2.28e - 9 | 1.09e - 10 | 4.36e - 12 |
| $10^{-4}$     | 1.04e - 7 | 3.30e - 8 | 3.47e - 9 | 2.26e - 10| 1.09e - 11 | 4.36e - 13 |
| $10^{-5}$     | 5.78e - 8 | 2.25e - 9 | 3.31e - 10| 2.23e - 11| 1.09e - 12 | 4.36e - 14 |
| $10^{-6}$     | 7.39e - 8 | 8.22e - 10| 1.68e - 11| 1.98e - 12| 1.05e - 13 | 4.77e - 15 |
| $10^{-7}$     | 7.55e - 8 | 1.13e - 9 | 1.46e - 11| 5.68e - 13| 8.32e - 15 | 2.22e - 16 |

Table 3 shows the error of the composite Simpson formula (21) using the optimal grid. The order of accuracy is fourth uniformly in $\varepsilon$, which corresponds to (28) with $k = 4$.

Table 4 shows the error of the Gauss composite formula with three nodes using the Shishkin mesh. The calculation results show that the order of accuracy close to six, which corresponds to Theorem 3.

The results show that of the formulas under consideration, the application of the Gauss formula gives the most accurate results.

8. Conclusion

The analysis of the available approaches to the construction of quadrature formulas for the numerical integration of functions with large gradients in the boundary layer is carried out. We studied the construction of quadrature formulas, the error of which does not increase in the presence of a boundary layer region of large gradients. Approaches based on the construction of formulas that are exact on the rapidly growing singular component of the integrable function and on the use of classical quadrature formulas on the Shishkin and Bakhvalov meshes thickening in the boundary layer. We considered the issue of minimizing the error of quadrature formulas by specifying nodes. The estimates of the error, confirmed by the results of computational experiments, are given.
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References
[1] Zadorin A I and Zadorin N A 2011 Quadrature formulas for functions with a boundary-layer component Comput. Math. Math. Phys. 51 pp 1837-1846
[2] Bakhvalov N S 1969 The optimization of methods of solving boundary value problems with a boundary layer USSR Comput. Math. Math. Phys. 9(4) pp 139-166
[3] Shishkin G I 1992 Grid Approximations of Singularly Perturbed Elliptic and Parabolic Equations (Yekaterinburg: Ural. Otd. Ross. Akad. Nauk) (in Russian)
[4] Miller J J H, O’Riordan E and Shishkin G I 2012 Fitted Numerical Methods for Singular Perturbation Problems: Error Estimates in the Maximum Norm for Linear Problems in One and Two Dimensions (Singapore: World Scientific)
[5] Kellogg R B and Tsan A 1978 Analysis of some difference approximations for a singular perturbation problems without turning points Math. Comput. 32 pp 1025-1039
[6] Zadorin A I and Zadorin N A 2012 Interpolation formula for functions with a boundary layer component and its application to derivatives calculation Sib. Electron. Math. Rep. 9 pp 445-455
[7] Bakhvalov N S, Zhidkov N P and Kobelkov G M 1987 Numerical Methods ( Moscow: Nauka ) (in Russian)
[8] Zadorin N A 2020 Non-polynomial interpolation of functions in the presence of a boundary layer Journal of Physics: Conf. Series 1441 012179
[9] Linss T 2001 The necessity of Shishkin decompositions Applied Mathematics Letters 14 pp 891-896
[10] Zadorin A I 2015 Lagrange interpolation and Newton-Cotes formulas for functions with boundary layer components on piecewise-uniform grids Numer. Anal. Appl. 8(3) pp 235-247
[11] Linss T 2010 Layer-Adapted Meshes for Reaction-Convection-Diffusion Problems ( Berlin: Springer-Verlag )
[12] Blatov I A and Zadorin N A 2019 Interpolation on the Bakhvalov mesh in the presence of an exponential boundary layer Uchenye Zapiski Kazanskogo Universiteta. Seriya Fiziko-Matematicheskie Nauki 161 (4) pp 497-508 (In Russian)
[13] Zadorin A I 2016 Gauss quadrature on a piecewise uniform mesh for functions with large gradients in a boundary layer Sib. Electron. Math. Rep. 13 pp 101-110 (In Russian)
[14] Zadorin A I 2020 Optimization of nodes of Newton-Cotes formulas in the presence of an exponential boundary layer Journal of Physics: Conf. Series 1546 012107