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Adaptive formulas of numerical differentiation of functions with large gradients

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Abstract. There are constructed formulas for the numerical differentiation of functions of one variable with large gradients. Formulas are based on the fitting to the singular component responsible for the large gradients of the function. The singular component is considered as a function of the general form. The error estimates of the difference formulas for calculating first and second derivatives are obtained. The results of the calculations are given.

1. Introduction

It is known that the solutions of singularly perturbed problems that simulate convective-diffusion processes with predominant convection, have large gradients in the boundary layer region. Formulas of numerical differentiation based on Lagrange polynomials unacceptable in the case of functions with large gradients in the boundary layer [1]. In this connection the problem of constructing numerical differentiation formulas that take into account the asymptotic behavior of a differentiable function in the boundary layer [2] is urgent. For example, solutions of singularly perturbed problems have large gradients in the region of the boundary layer.

In [3] the question of constructing approximation schemes using the finite volume method is considered, taking into account the well-known asymptotic behavior of the solution of two-dimensional singularly perturbed elliptic problem. To approximate the fluxes, it is proposed to apply a formula that is exact on the singular component of the solution. In [4] built an interpolation formula with an arbitrarily specified number of interpolation nodes, exact on the singular component. Differentiation of the constructed interpolant produces numerical differentiation formulas that are exact on the singular component. differentiable function.

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In this paper, we study the numerical differentiation formulas based on fitting to the component responsible for the large gradients of the function.

We assume that for the function $u(x)$ the following decomposition is valid

$$u(x) = p(x) + \gamma\Phi(x), \; x \in [a, b], \tag{1}$$

where $p(x)$ is a regular component with bounded derivatives up to a certain order, $\Phi(x)$ is a singular component with large gradients in a some region. The component $\Phi(x)$ is assumed to be known, $p(x)$ and γ are not specified.

For example, the solution of the singularly perturbed boundary value problem has the decomposition (1) [2, 5] with $\Phi(x) = e^{-mx/\varepsilon}$, where $m > 0$, $\varepsilon \in (0, 1]$, $x \in [0, 1]$.

The solution of the problem

$$u'' + \frac{1}{x}u' - b(x)u = f(x), \; \varepsilon < x < 1, \; u(\varepsilon) = A, u(1) = B$$

has the decomposition (1) with $\Phi(x) = \ln x$, $x \in (\varepsilon, 1]$, $\gamma = \varepsilon u'(\varepsilon)$. Here $b(x) \geq 0, \varepsilon \in (0, 1]$.

By C and C_j we mean positive constants independent of the singular component $\Phi(x)$, of its derivatives and of the grid step. In cases of exponential boundary layer and logarithmic singularities, these constants do not depend on small parameter ε and grid step. Different quantities we can limit by one constant C.

2. Fitting a formula to a singular component

Let the function $u(x)$ be representable as (1) and given at nodes of a uniform grid. Application to a function with large gradients of classical interpolation formulas, formulas of numerical differentiation and integration can lead to significant errors [1, 6]. Denote by $I(u, x)$ the interpolation, numerical differentiation or integration operator. Let $I^h(u, x)$ be the classical formula for the approximation of $I(u, x)$, based on the use of Lagrange polynomials. Then

$$|I(u, x) - I^h(u.x)| \leq |I(p, x) - I^h(p, x)| + |\gamma||I(\Phi, x) - I^h(\Phi, x)|. \tag{2}$$

We define an adaptive formula that is exact on the component $\Phi(x)$:

$$I_\Phi(u, x) = \frac{I^h(u, x)}{I^h(\Phi, x)} I(\Phi, x). \tag{3}$$

We assume that $I^h(\Phi, x) \neq 0$. This restriction can be achieved by choosing the regular component $p(x)$. The formula (3) was applied in [3] for solving the problem of numerical integration. Easy to get an estimate

$$\Big|I_\Phi(u, x) - I(u, x)\Big| \leq \Big|I^h(p, x) - I(p, x)\Big| + |I^h(p, x)|\Big|\frac{I(\Phi, x) - I^h(\Phi, x)}{I^h(\Phi, x)}\Big|. \tag{4}$$

From the comparison (2) and (4) it follows that the formula $I_\Phi(u, x)$ is more accurate if $|I^h(p, x)| \ll |I^h(\Phi, x)|$.

3. Adaptive formulas for numerical differentiation

3.1. Formula with two nodes for calculating the first derivative

Let Ω^h be a uniform grid of interval $[a, b]$:

$$\Omega^h = \{x_n : \; x_n = a + nh, n = 0, 1, \ldots, N, \; x_N = b\}, \; \Delta_n = [x_{n-1}, x_n].$$

We assume that a function $u(x)$ of the form (1) is given at the nodes of mesh Ω^h, $u_n = u(x_n)$.

We now show the ineffectiveness of applying the classical formula for the derivative in the case of a function of the form (1). Let's set $\Phi(x) = \ln x, x \in [\varepsilon, 1]$. Let be $\varepsilon = h$. Then $\varepsilon|(u_1 - u_0)/h - u'(\varepsilon)| = 1 - \ln 2$. So, for $h \to 0$, the relative error of the classical formula for the first derivative does not decrease if $\varepsilon = h$. The problem of constructing special formulas for numerical differentiation of functions of the form (1) is urgent.

Now we'll obtain an adaptive formula for numerical differentiation based on formulas (3). Let us $I^h(u, x) = (u_n - u_{n-1})/h,\ x \in [x_{n-1}, x_n]$. Suggesting $\Phi'(x) \neq 0$, and using (3), we get the formula that is exact on the singular component $\gamma\Phi(x)$:

$$u'(x) \approx L'_{\Phi,2}(u, x) = \frac{u_n - u_{n-1}}{\Phi_n - \Phi_{n-1}} \Phi'(x),\ x \in [x_{n-1}, x_n]. \tag{5}$$

Suppose that

$$|\Phi'(x)| \leq B_n,\ x \in [x_{n-1}, x_n].$$

Lemma 1 *Suppose that for some constant* G_n

$$\frac{\int\limits_{x_{n-1}}^{x_n} |\Phi''(s)|\, ds}{B_n|\Phi_n - \Phi_{n-1}|} \leq G_n. \tag{6}$$

Then

$$\Big|\frac{L'_{\Phi,2}(u, x) - u'(x)}{B_n}\Big| \leq G_n \int\limits_{x_{n-1}}^{x_n} |p'(s)|\, ds + \frac{1}{B_n} \int\limits_{x_{n-1}}^{x_n} |p''(s)|\, ds,\ x \in [x_{n-1}, x_n]. \tag{7}$$

Proof. Taking into account that the formula (5) is exact on $\Phi(x)$, we obtain

$$L'_{\Phi,2}(u, x) - u'(x) = \frac{p_n - p_{n-1}}{\Phi_n - \Phi_{n-1}} \Big[\Phi'(x) - \frac{\Phi_n - \Phi_{n-1}}{h}\Big] + \Big(\frac{p_n - p_{n-1}}{h} - p'(x)\Big). \tag{8}$$

Using the estimate

$$\Big|\Phi'(x) - \frac{\Phi_n - \Phi_{n-1}}{h}\Big| \leq \int\limits_{x_{n-1}}^{x_n} |\Phi''(s)|\, ds,$$

we have (7) from (8). The lemma is proved.

Remark 1. Let us consider the case of exponential boundary layer when $\Phi(x) = e^{-mx/\varepsilon}$, $\varepsilon, m > 0,\ x \in [0, 1]$. Let's set $B_n = m/\varepsilon$. Then the estimate (6) will be fulfilled if $G_n = 1$. From (7) for some constant C we obtain

$$\varepsilon\Big|L'_{\Phi,2}(u, x) - u'(x)\Big| \leq Ch,\ x \in [x_{n-1}, x_n]. \tag{9}$$

Remark 2. Let us $\Phi(x) = \ln x,\ x \in [\varepsilon, 1]$. We define $B_n = 1/x_{n-1}$ and obtain

$$\frac{\int\limits_{x_{n-1}}^{x_n} |\Phi''(s)|\, ds}{B_n|\Phi_n - \Phi_{n-1}|} = \frac{1 - x_{n-1}/x_n}{\ln \frac{x_n}{x_{n-1}}} \leq 1.$$

We obtain that the condition (6) is fulfilled when $G_n = 1$. In this case we obtain an estimate of the error (9).

3.2. Difference formula for the second derivative

Write the classical difference formula to calculate the second derivative, using the values of the function at the three grid nodes:

$$u''(x) \approx \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2}, \ x \in [x_{n-1}, x_{n+1}]. \tag{10}$$

It can be shown that in the case of a function of the form (1) the relative error of the formula (10) can be of the order of $O(1)$. Based on the formula (3), we obtain the difference formula that is exact on the singular component $\gamma\Phi(x)$:

$$u''(x) \approx L''_{\Phi,3}(u, x) = \frac{u_{n+1} - 2u_n + u_{n-1}}{\Phi_{n+1} - 2\Phi_n + \Phi_{n-1}}\Phi''(x), \ x \in [x_{n-1}, x_{n+1}]. \tag{11}$$

Below we assume that

$$\Phi''(x) \neq 0, x \in (x_{n-1}, x_{n+1}), \ |\Phi''(x)| \leq D_n, \ x \in [x_{n-1}, x_{n+1}]. \tag{12}$$

Lemma 2 *Suppose that for some constant G_n:*

$$\frac{h}{D_n}\frac{\int\limits_{x_{n-1}}^{x_{n+1}} |\Phi'''(s)|\, ds}{|\Phi_{n+1} - 2\Phi_n + \Phi_{n-1}|} \leq G_n. \tag{13}$$

Then

$$\Big|\frac{L''_{\Phi,3}(u, x) - u''(x)}{D_n}\Big| \leq \frac{3G_n}{2}\int\limits_{x_{n-1}}^{x_{n+1}} |p''(s)|\, ds + \frac{3}{2D_n}\int\limits_{x_{n-1}}^{x_{n+1}} |p'''(s)|\, ds, \ x \in [x_{n-1}, x_{n+1}]. \tag{14}$$

Proof. Taking into account that the formula (11) is exact on $\Phi(x)$, we obtain

$$L''_{\Phi,3}(u, x) - u''(x) = L''_{\Phi,3}(p, x) - p''(x) =$$

$$= (p_{n+1} - 2p_n + p_{n-1})\Big[\frac{1}{\Phi_{n+1} - 2\Phi_n + \Phi_{n-1}}\Phi''(x) - \frac{1}{h^2}\Big] + \Big(\frac{p_{n+1} - 2p_n + p_{n-1}}{h^2} - p''(x)\Big). \tag{15}$$

We write the first term of the formula (15) as

$$Q_1 = (p_{n+1} - 2p_n + p_{n-1})\frac{\Phi''(x) - (\Phi_{n+1} - 2\Phi_n + \Phi_{n-1})/h^2}{\Phi_{n+1} - 2\Phi_n + \Phi_{n-1}}. \tag{16}$$

Using (13), from (16) we get

$$\Big|\frac{Q_1}{D_n}\Big| \leq \frac{3G_n}{2}\int\limits_{x_{n-1}}^{x_{n+1}} |p''(s)|\, ds. \tag{17}$$

For the second term in (15) we have

$$\Big|\frac{p_{n+1} - 2p_n + p_{n-1}}{h^2} - p''(x)\Big| \leq \frac{3}{2}\int\limits_{x_{n-1}}^{x_{n+1}} |p'''(s)|\, ds. \tag{18}$$

From (15), (17), (18) we obtain (14). The lemma is proved.

Remark 3. By analogy with the remarks 1, 2 based on estimates (14) it can be shown that in cases $\Phi(x) = e^{-mx/\varepsilon}$ and $\Phi(x) = \ln x$ for some constant C the following error estimate holds

$$\varepsilon^2\Big|L''_{\Phi,3}(u, x) - u''(x)\Big| \leq Ch.$$

3.3. Three-node formula for the first derivative

On the interval $[x_{n-1}, x_{n+1}]$, we write out a three-node formula for the first derivative:

$$L'_{\Phi,3}(u,x) = \frac{u_{n+1}-u_{n-1}}{2h} + \frac{u_{n+1}-2u_n+u_{n-1}}{\Phi_{n+1}-2\Phi_n+\Phi_{n-1}}\Big[\Phi'(x) - \frac{\Phi_{n+1}-\Phi_{n-1}}{2h}\Big]. \tag{19}$$

The formula (19) is exact on singular component $\Phi(x)$.

Lemma 3 *Let the following conditions be true*

$$\Phi''(x) \neq 0,\ |\Phi'''(x)| \le q|\Phi''(x)|,\ x \in (x_{n-1}, x_{n+1}). \tag{20}$$

Then

$$\Big|L'_{\Phi,3}(u,x) - u'(x)\Big| \le \frac{7}{4}h \int\limits_{x_{n-1}}^{x_{n+1}} \Big[q|p''(s)| + |p'''(s)|\Big]\, ds. \tag{21}$$

Proof. We write the error in the form

$$L'_{\Phi,3}(u,x) - u'(x) = L'_{\Phi,3}(p,x) - p'(x) = \Big(L'_{\Phi,3}(p,x) - L'_3(p,x)\Big) + \Big(L'_3(p,x) - p'(x)\Big) \tag{22}$$

and estimate each term, where $L'_3(p,x)$ is three-node polynomial formula for the first derivative. We use the condition (20) to estimate the first term:

$$\Big|L'_{\Phi,3}(p,x) - L'_3(p,x)\Big| \le \frac{7}{4}|p_{n+1}-2p_n+p_{n-1}|\times$$

$$\times \frac{\int\limits_{x_n}^{x_{n+1}} (x_{n+1}-s)|\Phi'''(s)|\, ds + \int\limits_{x_{n-1}}^{x_n} (s-x_{n-1})|\Phi'''(s)|\, ds}{\Big|\int\limits_{x_n}^{x_{n+1}} (x_{n+1}-s)\Phi''(s)\, ds + \int\limits_{x_{n-1}}^{x_n} (s-x_{n-1})\Phi''(s)\, ds\Big|} \le \frac{7}{4}qh \int\limits_{x_{n-1}}^{x_{n+1}} |p''(s)|\, ds.$$

The estimate of the second term in (22) is known. It proves the lemma.

It follows from lemma 3 that in cases $\Phi(x) = e^{-mx/\varepsilon}$ and $\Phi(x) = \ln x,\ x \ge \varepsilon > 0$ the following error estimate is valid

$$\varepsilon\Big|L'_{\Phi,3}(u,x) - u'(x)\Big| \le Ch \int\limits_{x_{n-1}}^{x_{n+1}} \Big[|p''(s)| + \varepsilon|p'''(s)|\Big]\, ds.$$

4. The formula for the derivative in two-dimensional case

Let for a sufficiently smooth function $u(x,y)$ in the region $\Omega = [0,1]\times[0,1]$ the following representation is true:

$$u(x,y) = p(x,y) + \gamma(y)\Phi(x), \tag{23}$$

where $p(x,y)$ is a regular component with bounded derivatives up to some order, $\Phi(x)$ is a known function with large gradients. The functions $p(x,y), \gamma(y)$ in the decomposition (23) are not specified. Such a decomposition is valid for the solution of the elliptic problem with a boundary layer with respect to the variable x [7].

Let Ω^h be the rectangular grid of the domain Ω :

$$\Omega^h = \{(x_i, y_j),\ x_i = ih_1,\ i = 0,1,\dots,N_1,\ x_j = jh_2,\ j = 0,1,\dots,N_2\}.$$

Set the cell $K_{i,j}$: $K_{i,j} = [x_i, x_{i+1}] \times [y_j, y_{j+1}]$.

We assume that the function $u(x, y)$ of the form (23) is given at nodes of the uniform grid Ω^h and construct a formula of numerical differentiation in the cell $K_{i,j}$.

Based on the differentiation of a two-dimensional interpolant that is exact on $\Phi(x)$, we construct a new formula for calculating the derivative

$$\frac{\partial u}{\partial x}(x,y) \approx L'_{\Phi.x}(u,x,y) = \Big(u_{i+1,j+1} - u_{i,j+1} - u_{i+1,j} + u_{i,j}\Big)\frac{\Phi'(x)}{\Phi_{i+1}-\Phi_i} \times \frac{y-y_j}{h_2} +$$

$$+\Big(u_{i+1,j} - u_{i,j}\Big)\frac{\Phi'(x)}{\Phi_{i+1}-\Phi_i}, \ (x,y) \in K_{i,j}. \tag{24}$$

Lemma 4 *Let* $|\Phi'(x)| \le B_i, x \in [x_i, x_{i+1}]$ *and for some constant* G_i

$$\frac{\int\limits_{x_i}^{x_{i+1}} |\Phi''(s)|\, ds}{B_i|\Phi_{i+1}-\Phi_i|} \le G_i.$$

Then

$$\frac{1}{B_i}|L'_{\Phi,x}(u,x,y) - u'_x(x,y)| \le 3h_1 \max_{(s,t)} |p'_x(s,t)|G_i + \frac{2}{B_i}\Big(\max_{s,t}|p''_{xx}(s,t)|h_1 + \max_{s,t}|p''_{xy}(s,t)|h_2\Big).$$

Remark 4. Let $\Phi(x) = e^{-mx/\varepsilon}$ or $\Phi(x) = \ln x$. Then $B_i = C/\varepsilon$.

Consider the problem

$$\frac{\partial^2 u}{\partial r^2} + \frac{1}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial \phi^2} = f(r,\phi), \tag{25}$$

$$u(\varepsilon,\phi) = \Psi_1(\phi), \ u(1,\phi) = \Psi_2(\phi), \tag{26}$$

where $\varepsilon \le r \le 1, \ 0 \le \phi \le 2\pi$, functions $f(r,\phi), \Psi_1(\phi), \Psi_2(\phi)$ are smooth enough.

The problem (25)-(26) models the steady-state filtration of the fluid to the well, while ε is a parameter proportional to the relative diameter of the well. The solution of the problem (25)-(26) has large gradients near the boundary $r = \varepsilon$ and can be represented as

$$u(r,\phi) = p(r,\phi) + \gamma(\phi)\ln r,$$

where functions $p(r,\phi), \gamma(\phi)$ have bounded first derivatives with respect to their arguments. Therefore, the formula (24) can be used to calculate the derivative of $u(r,\phi)$ with respect to r. At the same time, the error estimate holds

$$\varepsilon|L'_{\Phi,r}(u,r,\phi) - u'_r(r,\phi)| \le C(h_1+h_2), \ (r,\phi) \in K_{i,j}, \ i,j = 0,1,\ldots,N-1.$$

5. Numerical results

Consider the function

$$u(x) = cos(\pi x) + e^{-x/\varepsilon}, \ \ 0 \le x \le 1, \ \varepsilon > 0.$$

Table 1 shows the norm of error

$$\Delta = \varepsilon \max_n |u'(x_n) - L'_3(u,x_n)|, \ 0 \le n \le N$$

of polynomial three-node formula for the first derivative. The error is not ε-uniform.

Table 2 shows the norm of error for the constructed formula (19). The second order of accuracy is confirmed, which corresponds to the estimate (21).

Table 1. The error of the classic three-node formula

ε	N					
	10	10^2	10^3	10^4	10^5	10^6
1	$5.04e-2$	$5.07e-4$	$5.07e-6$	$5.07e-8$	$5.39e-10$	$3.27e-10$
10^{-1}	$2.06e-2$	$1.36e-3$	$1.63e-5$	$1.66e-7$	$1.67e-9$	$3.65e-11$
10^{-2}	$5.14e-4$	$2.37e-2$	$1.37e-3$	$1.63e-5$	$1.66e-7$	$1.67e-9$
10^{-3}	$5.14e-5$	$2.24e-6$	$2.37e-2$	$1.36e-3$	$1.63e-5$	$1.66e-7$
10^{-4}	$5.14e-6$	$5.17e-8$	$2.27e-6$	$2.37e-2$	$1.37e-3$	$1.63e-5$
10^{-5}	$5.14e-7$	$5.17e-9$	$5.17e-11$	$2.27e-6$	$2.37e-2$	$1.37e-3$

Table 2. The error of the three-node formula (19)

ε	N					
	10	10^2	10^3	10^4	10^5	10^6
1	$5.39e-2$	$5.42e-4$	$5.42e-6$	$5.42e-8$	$5.75e-10$	$7.35e-11$
10^{-1}	$1.66e-2$	$1.72e-4$	$1.72e-6$	$1.72e-8$	$1.74e-10$	$3.13e-11$
10^{-2}	$4.80e-3$	$1.59e-4$	$1.64e-6$	$1.65e-8$	$1.65e-10$	$3.80e-12$
10^{-3}	$4.81e-4$	$4.93e-5$	$1.60e-6$	$1.64e-8$	$1.65e-10$	$1.85e-12$
10^{-4}	$4.81e-5$	$4.93e-6$	$4.93e-7$	$1.59e-8$	$1.64e-10$	$1.66e-12$
10^{-5}	$4.81e-6$	$4.93e-7$	$4.93e-8$	$4.93e-9$	$1.59e-10$	$1.65e-12$

6. Conlusion

Developed adaptive formulas for the numerical differentiation of a function of one variable with large gradients. By construction, the formulas are exact on the singular component, which is responsible for the large gradients of the function. The constructed formula of the first order of accuracy was generalized to the two-dimensional case. Estimates of errors of the constructed formulas are obtained. It is confirmed by results of numerical experiments.

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References

[1] Zadorin A I 2007 Interpolation method for the boundary layer problem *Sib. Zh. Vychisl. Mat.* **10** 267-275

[2] 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)

[3] Gurieva Y L and Il'in V P 2001 Modified finite volume method for singularly perturbed boundary value problems *Vychisl. Tekhnol., Special Issue: Proceedings of International Conference RDAMM-2001* **6** 245-252

[4] Zadorin A I and Zadorin N A 2012 Interpolation formula for functions with a boundary layer component and its application to derivatives calculation *Siberian Electronic Math. Reports* **9** 445-455

[5] Kellog R B and Tsan A 1978 Analysis of some difference approximations for a singular perturbation problem without turning points *Mathematics of Computation* **32** 1025-1039

[6] Zadorin A I 2016 Interpolation formulas for functions with large gradients in the boundary layer and their application *Modeling and Analysis of Information Systems* **23** 377-384

[7] Roos H G, Stynes M and Tobiska L 2008 *Numerical Methods for Singularly Perturbed Differential Equations, Convection-Diffusion and Flow problems* (Berlin: Springer)