

NONCLASSICAL BOUNDARY CONDITIONS FOR QUINTIC SPLINES

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UDC 519.65

We study the influence of nonclassical boundary conditions on the accuracy of approximation of a smooth function by a quintic spline of class C^4 on a uniform mesh of a segment. We give an asymptotic analysis and compare different boundary conditions. Bibliography: 15 titles.

Introduction

Definition of splines. Assume that we are given the values of a function $f_i = f(x_i)$, $i = \overline{0, N}$, at nodes of the uniform mesh

$$\Delta : x_i = x_0 + ih, \quad i = \overline{0, N}; \quad x_0 = a, \quad h = (b - a)/N,$$

on a segment $[a, b]$. By a *quintic interpolation spline* we mean a function $S(x)$ such that

- 1) $S(x) \in C^4[a, b]$,
- 2) $S(x)$ is a polynomial of the fifth degree on each interval $[x_i, x_{i+1}]$, $i = \overline{0, N-1}$,
- 3) $S(x_i) = f_i$, $i = \overline{0, N}$.

Quintic splines are useful if we need to approximate a function or its derivatives (of the first, second, and third order) with higher accuracy in comparison with cubic splines. Furthermore, using quintic splines, it is possible to approximate the fourth and fifth order derivatives which vanish in the case of cubic splines.

Necessity of boundary conditions. To define an interpolation spline $S(x)$ in a unique way, we need to impose additional conditions [1]. Usually, such conditions are given as some conditions on the derivatives of spline at the endpoints of $[a, b]$ and are referred to as *boundary conditions*. There are two conditions at each endpoint.

If a periodic function $f(x)$ is interpolated, then for such an extra conditions we can take the periodicity condition for the corresponding interpolation spline, namely, $S^{(\alpha)}(x_0) = S^{(\alpha)}(x_N)$, $\alpha = 1, 2, 3, 4$. We note that the periodic case has been studied well. In particular, as shown in

[2], for a periodic quintic spline interpolating a periodic function $f(x) \in C^{12}[a, b]$ the following asymptotic relations hold:

$$S(x) = f(x) + \frac{h^6}{6!} \gamma(t) f^{(6)}(x) + \frac{h^7}{7!} \delta(t) f^{(7)}(x) + O(h^8), \quad x \in [x_i, x_{i+1}], \quad (1)$$

where

$$\gamma(t) = \frac{1}{2} t^2 (1-t)^2 (1+2t-2t^2), \quad \delta(t) = t(1-t)(1-2t)(3t^4 - 6t^3 + 3t + 1), \quad t = \frac{x - x_i}{h}.$$

Furthermore, in the periodic case, for splines of an arbitrary degree with uniform mesh unimproved pointwise estimates for the approximation error were obtained in [3], where also the difficulty of the problem with nonperiodic boundary conditions was emphasized.

An asymptotic analysis of different boundary conditions, where the exact values of some derivatives of $f(x) \in C^7[a, b]$ are given at the endpoints of $[a, b]$, was performed in [4], where the following counterparts of (1) in the nonperiodic case were also obtained:

$$S(x) = f(x) + \frac{h^6}{6!} \gamma_{i,N}(t) f^{(6)}(x) + O(h^7), \quad x \in [x_i, x_{i+1}], \quad i = \overline{0, N-1}, \quad (2)$$

where $\gamma_{i,N}(t)$ depend on the number of interval, the number of nodes, and the type of boundary conditions. It is clear that the approximation error for the spline $\|S - f\|_C$ as $h \rightarrow 0$ is determined by the quantity $\|\gamma_{i,N}\|_C$. Therefore, the natural question arises: What boundary conditions are optimal in the sense $\|\gamma_{i,N}\|_C$ should be minimal. In [4], we give a comparative analysis of the behavior of $\|\gamma_{i,N}\|_C$ depending on the boundary conditions and present optimal boundary conditions in the sense of accuracy

$$S^{(\alpha)}(x_i) = f^{(\alpha)}(x_i), \quad \alpha = 1, 3, \quad i = 0, 1, N-1, N. \quad (3)$$

It is shown that for the optimal boundary conditions

$$\gamma_{i,N}(t) = \gamma(t) = \frac{1}{2} t^2 (1-t)^2 (1+2t-2t^2). \quad (4)$$

For constructing quintic splines one can use a family of boundary conditions [5] which requires no additional information except for the initial data. These conditions have the form

$$\begin{aligned} m_i + \alpha m_{i+1} + \beta m_{i+2} + \gamma m_{i+3} &= p'_i(x_i) + \alpha p'_i(x_{i+1}) + \beta p'_i(x_{i+2}) + \gamma p'_i(x_{i+3}), \quad i = 0, 1, \\ m_i + \alpha m_{i-1} + \beta m_{i-2} + \gamma m_{i-3} &= p'_{i-5}(x_i) + \alpha p'_{i-5}(x_{i-1}) + \\ &+ \beta p'_{i-5}(x_{i-2}) + \gamma p'_{i-5}(x_{i-3}), \quad i = N, N-1. \end{aligned}$$

Here, $m_i = S'(x_i)$, $i = \overline{0, N}$; $p_i(x)$ is an interpolation polynomial of the fifth degree such that $p_i(x_k) = f_k$, $k = \overline{i, i+5}$. The parameters α, β, γ are chosen in such a way that under the interpolation of $f(x) \in C^7[a, b]$ the following estimate holds:

$$\|S^{(r)} - f^{(r)}\|_C = O(h^{6-r}), \quad r = \overline{0, 5}. \quad (5)$$

The study of boundary conditions without requirement of the exact values of the derivatives of an interpolated function at the endpoints of $[a, b]$ was further studied in [6], where it was shown

that the estimate (5) remains valid for splines of degree 4 interpolating a function $f(x) \in C^7[a, b]$ with the boundary conditions

$$\int_{x_i}^{x_{i+1}} S(x) dx = \int_{x_i}^{x_{i+1}} p_i(x) dx, \quad i = 0, 1, N-2, N-1.$$

For quintic splines $s(x) \in C^4[0, 1]$ interpolating $f(x) \in C^6[0, 1]$ on a uniform mesh $x_i = x_0 + ih$, $i = \overline{0, N}$; $x_0 = 0$, $h = 1/N$, satisfying the initial data

$$\begin{aligned} s(\alpha_i) &= f(\alpha_i), & s(\beta_i) &= f(\beta_i), & i &= \overline{0, N-1}, \\ s''(x_i) &= f''(x_i), & i &= \overline{0, N}, \end{aligned}$$

where $\alpha_i = x_i + h/3$, $\beta_i = x_i + 2h/3$, and the boundary conditions

$$s'(x_0) = f'(x_0), \quad s'(x_N) = f'(x_N),$$

the following estimate was obtained in [7]:

$$|s(x) - f(x)| \leq K \frac{h^6}{6!} \|f^{(6)}\|_{C[0, 1]}, \quad x \in [0, 1].$$

For quintic splines and boundary conditions required the continuity of the fifth order derivative of the spline at points near the endpoints of the interpolation segment

$$S^{(5)}(x_i - 0) = S^{(5)}(x_i + 0), \quad i = 1, 2, N-2, N-1$$

under the assumption that $f \in C^6(\mathbb{R}_+)$ is bounded and the step is sufficiently small $h \rightarrow 0$, the following error estimate was obtained in [8]:

$$\sup_{x \in \mathbb{R}_+} |f^{(r)}(x) - S^{(r)}(x)| \leq c_f h^{6-r}.$$

In this paper, we analyze boundary conditions for an interpolation quintic spline, where only one derivative or no derivatives are given at each of the endpoints of $[a, b]$.

1 Construction of Quintic Splines

At points $x \in [x_i, x_{i+1}]$, $i = \overline{0, N-1}$, the spline $S(x)$ can be represented as [9]:

$$\begin{aligned} S(x) &= f_i(1-t)^3(1+3t+6t^2) + f_{i+1}t^3(10-15t+6t^2) + hm_i(1-t)^3t(1+3t) \\ &+ hm_{i+1}t^3(1-t)(3t-4) + \frac{h^2}{2}M_i(1-t)^3t^2 + \frac{h^2}{2}M_{i+1}t^3(1-t)^2, \end{aligned} \quad (6)$$

where $m_i = S'(x_i)$, $M_i = S''(x_i)$. We assume that the number of interpolation points is at least 4, i.e., $N \geq 3$. By the continuity of the third and fourth order derivatives of $S(x)$, we see that

M_i are connected with m_i, f_i by the relations [10]

$$M_{i-1} = \frac{1}{16h} [-111m_{i-1} - 227m_i - 79m_{i+1} - 3m_{i+2}] + \frac{1}{16h^2} [-235f_{i-1} + 65f_i + 155f_{i+1} + 15f_{i+2}], \quad (7)$$

$$M_i = \frac{1}{16h} [3m_{i-1} - 33m_i - 29m_{i+1} - m_{i+2}] + \frac{1}{16h^2} [15f_{i-1} - 85f_i + 65f_{i+1} + 5f_{i+2}], \quad (8)$$

$$M_{i+1} = \frac{1}{16h} [m_{i-1} + 29m_i + 33m_{i+1} - 3m_{i+2}] + \frac{1}{16h^2} [5f_{i-1} + 65f_i - 85f_{i+1} + 15f_{i+2}], \quad (9)$$

$$M_{i+2} = \frac{1}{16h} [3m_{i-1} + 79m_i + 227m_{i+1} + 111m_{i+2}] + \frac{1}{16h^2} [15f_{i-1} + 155f_i + 65f_{i+1} - 235f_{i+2}]. \quad (10)$$

Substituting (8), (9) into (6) for $x \in [x_i, x_{i+1}]$, $i = \overline{1, N-2}$, we find

$$S(x) = f_{i-1}\varphi_1(t) + f_i\varphi_2(t) + f_{i+1}\varphi_2(1-t) + f_{i+2}\varphi_1(1-t) + hm_{i-1}\psi_1(t) + hm_i\psi_2(t) - hm_{i+1}\psi_2(1-t) - hm_{i+2}\psi_1(1-t), \quad (11)$$

where

$$\varphi_1 = t^2(1-t)^2(15-10t)/32, \quad \varphi_2 = (1-t)^2(32+64t+11t^2-42t^3)/32, \\ \psi_1 = t^2(1-t)^2(3-2t)/32, \quad \psi_2 = t(1-t)^2(32+31t-34t^2)/32.$$

Similar expressions for splines at the boundary intervals $[x_0, x_1]$ and $[x_{N-1}, x_N]$ are obtained from (6) by substituting M_i and M_{i+1} from (7), (8) and (9), (10). Namely, for $x \in [x_0, x_1]$

$$S(x) = f_0\varphi_3(t) + f_1\varphi_4(t) + f_2\varphi_5(t) + f_3\varphi_6(t) + hm_0\psi_3(t) + hm_1\psi_4(t) + hm_2\psi_5(t) + hm_3\psi_6(t), \quad (12)$$

where

$$\varphi_3 = (1-t)^2(32+64t-139t^2+58t^3)/32, \quad \psi_3 = t(1-t)^2(18t^2-47t+32)/32, \\ \varphi_4 = t^2(65+40t-115t^2+42t^3)/32, \quad \psi_4 = t^2(1-t)(-98t^2+293t-227)/32, \\ \varphi_5 = t^2(1-t)^2(155-90t)/32, \quad \psi_5 = t^2(1-t)^2(50t-79)/32, \\ \varphi_6 = t^2(1-t)^2(15-10t)/32, \quad \psi_6 = t^2(1-t)^2(2t-3)/32.$$

For $x \in [x_{N-1}, x_N]$ we have

$$S(x) = f_N\varphi_3(1-t) + f_{N-1}\varphi_4(1-t) + f_{N-2}\varphi_5(1-t) + f_{N-3}\varphi_6(1-t) - hm_N\psi_3(1-t) - hm_{N-1}\psi_4(1-t) - hm_{N-2}\psi_5(1-t) - hm_{N-3}\psi_6(1-t). \quad (13)$$

To define the spline $S(x)$ completely, it is necessary to find the coefficients m_i , $i = \overline{0, N}$, satisfying the relations [11]

$$m_{i-2} + 26m_{i-1} + 66m_i + 26m_{i+1} + m_{i+2} = g_i, \quad i = \overline{2, N-2}, \quad (14)$$

where

$$g_i = \frac{1}{h} [-5f_{i-2} - 50f_{i-1} + 50f_{i+1} + 5f_{i+2}]. \quad (15)$$

The relations (14) and (15) are valid since (8) and (9) with the same indices coincide.

The system (14) is indefinite ($N-3$ equations and $N+1$ unknowns) and should be completed with four equations following from the boundary conditions on $S(x)$.

2 Boundary Conditions

The boundary conditions considered in [4] can be formally divided into two groups.

1. The classical conditions, where two different derivatives of the interpolated function are given at the points x_0 and x_N

$$\begin{cases} S^{(\alpha)}(x_0) = f_0^{(\alpha)}, & S^{(\beta)}(x_0) = f_0^{(\beta)}, \\ S^{(\alpha)}(x_N) = f_N^{(\alpha)}, & S^{(\beta)}(x_N) = f_N^{(\beta)}, \end{cases} \quad \alpha \in \{1, 2, 3\}, \quad \alpha < \beta \leq 4, \quad (16)$$

where $f_i^{(\alpha)} = f^{(\alpha)}(x_i)$.

2. The two-point conditions, where any derivatives of the interpolated function are given at the points x_0, x_1, x_{N-1}, x_N

$$\begin{cases} S^{(\alpha)}(x_0) = f_0^{(\alpha)}, & S^{(\beta)}(x_1) = f_1^{(\beta)}, \\ S^{(\alpha)}(x_N) = f_N^{(\alpha)}, & S^{(\beta)}(x_{N-1}) = f_{N-1}^{(\beta)}, \end{cases} \quad \alpha, \beta \in \{1, 2, 3, 4\}. \quad (17)$$

As was already mentioned, the main lack of these boundary conditions is that we have to be given with the exact values of derivatives of the interpolated function. In this paper, we weaken this requirement in the sense that either no values of derivatives are given at the endpoints or at most one derivative can be given at each endpoint. Namely, we consider boundary conditions of the following types.

1. Approximation of the derivatives of $f(x)$ in the classical conditions (16):

$$\begin{cases} S^{(\alpha)}(x_0) = \tilde{f}_0^{(\alpha)}, & S^{(\beta)}(x_0) = \tilde{f}_0^{(\beta)}, \\ S^{(\alpha)}(x_N) = \tilde{f}_N^{(\alpha)}, & S^{(\beta)}(x_N) = \tilde{f}_N^{(\beta)}, \end{cases} \quad \alpha \in \{1, 2, 3\}, \quad \alpha < \beta \leq 4, \quad (18)$$

and in the two-point conditions (17):

$$\begin{cases} S^{(\alpha)}(x_0) = \tilde{f}_0^{(\alpha)}, & S^{(\beta)}(x_1) = \tilde{f}_1^{(\beta)}, \\ S^{(\alpha)}(x_N) = \tilde{f}_N^{(\alpha)}, & S^{(\beta)}(x_{N-1}) = \tilde{f}_{N-1}^{(\beta)}, \end{cases} \quad \alpha, \beta \in \{1, 2, 3, 4\}, \quad (19)$$

where $\tilde{f}_i^{(\alpha)}$ are approximations of derivatives and they should be chosen in such a way that

$$f_i^{(\alpha)} - \tilde{f}_i^{(\alpha)} = O(h^{6-\alpha}), \quad \alpha = \overline{1, 4}. \quad (20)$$

2. The continuity condition for of the fifth order derivative of the (not-a-knot) spline at the points $x_1, x_2, x_{N-2}, x_{N-1}$:

$$\begin{cases} S^{(5)}(x_1 - 0) = S^{(5)}(x_1 + 0), & S^{(5)}(x_2 - 0) = S^{(5)}(x_2 + 0), \\ S^{(5)}(x_{N-1} - 0) = S^{(5)}(x_{N-1} + 0), & S^{(5)}(x_{N-2} - 0) = S^{(5)}(x_{N-2} + 0) \end{cases},$$

or at the points $x_1, x_3, x_{N-3}, x_{N-1}$:

$$\begin{cases} S^{(5)}(x_1 - 0) = S^{(5)}(x_1 + 0), & S^{(5)}(x_3 - 0) = S^{(5)}(x_3 + 0), \\ S^{(5)}(x_{N-1} - 0) = S^{(5)}(x_{N-1} + 0), & S^{(5)}(x_{N-3} - 0) = S^{(5)}(x_{N-3} + 0). \end{cases}.$$

3. The combined conditions, where the exact values of derivatives of $f(x)$ are given at the points x_0, x_N and the continuity condition for the fifth order derivative of the spline is imposed at the points x_1, x_{N-1} :

$$\begin{cases} S^{(\alpha)}(x_0) = f_0^{(\alpha)}, & S^{(5)}(x_1 - 0) = S^{(5)}(x_1 + 0), \\ S^{(\alpha)}(x_N) = f_N^{(\alpha)}, & S^{(5)}(x_{N-1} - 0) = S^{(5)}(x_{N-1} + 0), \end{cases} \quad \alpha \in \{1, 2, 3, 4\}.$$

All the boundary conditions are given at both endpoints in a symmetric way. This means that the type of boundary conditions is the same at both endpoints, i.e., if the conditions $S'(x_0) = f'_0$ and $S^{(5)}(x_1 - 0) = S^{(5)}(x_1 + 0)$ are given at the left endpoint, then the conditions $S'(x_N) = f'_N$ and $S^{(5)}(x_{N-1} - 0) = S^{(5)}(x_{N-1} + 0)$ are imposed at the right endpoint.

Following [4], we code types of boundary conditions by $abcd$, where a, c means the number of points at which the derivatives are given or are assumed to be continuous and b, d means the order of derivatives at points a, c respectively.

To emphasize that the approximate value of derivatives is given, we use the notation ap . For example, $0213ap$ means that boundary conditions have the form $S''(x_0) = \tilde{f}''_0, S'''(x_1) = \tilde{f}'''_1$.

2.1. Approximation of derivatives. The relations (18) and (19) include difference approximations of derivatives. First, we note that the indicated accuracy of these approximations is necessary for preventing the decrease of maximal possible order of approximation $O(h^6)$ of a function by quintic splines. Second, we are naturally interested only in approximations on the minimal pattern (6 points).

We consider a Lagrange polynomial of the fifth degree constructed from the nodes $x_i, x_{i+1}, \dots, x_{i+5}$ and represented in the Newton form

$$\begin{aligned} L_i(x) = & f_i + f[x_{i+1}, x_i](x - x_i) + f[x_{i+2}, x_{i+1}, x_i](x - x_{i+1})(x - x_i) \\ & + f[x_{i+3}, x_{i+2}, x_{i+1}, x_i](x - x_{i+2})(x - x_{i+1})(x - x_i) \\ & + f[x_{i+4}, x_{i+3}, x_{i+2}, x_{i+1}, x_i](x - x_{i+3})(x - x_{i+2})(x - x_{i+1})(x - x_i) \\ & + f[x_{i+5}, x_{i+4}, x_{i+3}, x_{i+2}, x_{i+1}, x_i](x - x_{i+4})(x - x_{i+3})(x - x_{i+2})(x - x_{i+1})(x - x_i), \end{aligned}$$

where $f[x_{i+k}, x_{i+k-1}, \dots, x_i]$ are separated differences of order $k = 1, 2, \dots, 5$. It is known [13] that

$$L_i^{(\alpha)}(x) - f^{(\alpha)}(x) = O(h^{6-\alpha}).$$

Therefore, all the required difference approximations satisfying (20) are obtained by

$$\tilde{f}_k^{(\alpha)} = L_i^{(\alpha)}(x_k),$$

where $i = 0$ for $k = 0, 1$ and $i = N - 5$ for $k = N - 1, N$.

The differential approximations of the derivatives at the left endpoint have the form

$$\begin{aligned}\tilde{f}'_0 &= [-137f_0 + 300f_1 - 300f_2 + 200f_3 - 75f_4 + 12f_5]/60h, \\ \tilde{f}''_0 &= [45f_0 - 154f_1 + 214f_2 - 156f_3 + 61f_4 - 10f_5]/12h^2, \\ \tilde{f}'''_0 &= [-17f_0 + 71f_1 - 118f_2 + 98f_3 - 41f_4 + 7f_5]/4h^3, \\ \tilde{f}^{(4)}_0 &= [3f_0 - 14f_1 + 26f_2 - 24f_3 + 11f_4 - 2f_5]/h^4, \\ \tilde{f}'_1 &= [-12f_0 - 65f_1 + 120f_2 - 60f_3 + 20f_4 - 3f_5]/60h, \\ \tilde{f}''_1 &= [10f_0 - 15f_1 - 4f_2 + 14f_3 - 6f_4 + f_5]/12h^2, \\ \tilde{f}'''_1 &= [-7f_0 + 25f_1 - 34f_2 + 22f_3 - 7f_4 + f_5]/4h^3, \\ \tilde{f}^{(4)}_1 &= [2f_0 - 9f_1 + 16f_2 - 14f_3 + 6f_4 - f_5]/h^4.\end{aligned}$$

Similar approximations of derivatives at the right endpoint have the form

$$\begin{aligned}\tilde{f}'_{N-1} &= [12f_N + 65f_{N-1} - 120f_{N-2} + 60f_{N-3} - 20f_{N-4} + 3f_{N-5}]/60h, \\ \tilde{f}''_{N-1} &= [10f_N - 15f_{N-1} - 4f_{N-2} + 14f_{N-3} - 6f_{N-4} + f_{N-5}]/12h^2, \\ \tilde{f}'''_{N-1} &= [7f_N - 25f_{N-1} + 34f_{N-2} - 22f_{N-3} + 7f_{N-4} - f_{N-5}]/4h^3, \\ \tilde{f}^{(4)}_{N-1} &= [2f_N - 9f_{N-1} + 16f_{N-2} - 14f_{N-3} + 6f_{N-4} - f_{N-5}]/h^4, \\ \tilde{f}'_N &= [137f_N - 300f_{N-1} + 300f_{N-2} - 200f_{N-3} + 75f_{N-4} - 12f_{N-5}]/60h, \\ \tilde{f}''_N &= [45f_N - 154f_{N-1} + 214f_{N-2} - 156f_{N-3} + 61f_{N-4} - 10f_{N-5}]/12h^2, \\ \tilde{f}'''_N &= [17f_N - 71f_{N-1} + 118f_{N-2} - 98f_{N-3} + 41f_{N-4} - 7f_{N-5}]/4h^3, \\ \tilde{f}^{(4)}_N &= [3f_N - 14f_{N-1} + 26f_{N-2} - 24f_{N-3} + 11f_{N-4} - 2f_{N-5}]/h^4.\end{aligned}$$

2.2. Equations obtained from the boundary conditions. Using the expressions for the derivatives of a spline following from (6) and the expressions (7)–(10), we find the following relations in terms of m_i which are equivalent to the boundary conditions (16) (these equations were earlier obtained in [4]):

$$m_0 = g_{1,0}, \quad m_N = g_{1,N}, \tag{21}$$

where $g_{1,0} = f'_0$, $g_{1,N} = f'_N$;

$$\begin{cases} 111m_0 + 227m_1 + 79m_2 + 3m_3 = g_{2,0}, \\ 3m_{N-3} + 79m_{N-2} + 227m_{N-1} + 111m_N = g_{2,N}, \end{cases} \tag{22}$$

where

$$\begin{aligned}g_{2,0} &= 235f[x_0, x_1] + 170f[x_1, x_2] + 15f[x_2, x_3] - 16hf''_0, \\ g_{2,N} &= 15f[x_{N-3}, x_{N-2}] + 170f[x_{N-2}, x_{N-1}] + 235f[x_{N-1}, x_N] + 16hf''_N;\end{aligned}$$

$$\begin{cases} 18m_0 + 65m_1 + 26m_2 + m_3 = g_{3,0}, \\ m_{N-3} + 26m_{N-2} + 65m_{N-1} + 18m_N = g_{3,N}, \end{cases} \quad (23)$$

where

$$\begin{aligned} g_{3,0} &= 50f[x_0, x_1] + 55f[x_1, x_2] + 5f[x_2, x_3] + \frac{2}{3}h^2 f_0''', \\ g_{3,N} &= 5f[x_{N-3}, x_{N-2}] + 55f[x_{N-2}, x_{N-1}] + 50f[x_{N-1}, x_N] + \frac{2}{3}h^2 f_N'''; \end{aligned}$$

$$\begin{cases} 83m_0 + 391m_1 + 179m_2 + 7m_3 = g_{4,0}, \\ 7m_{N-3} + 179m_{N-2} + 391m_{N-1} + 83m_N = g_{4,N}, \end{cases} \quad (24)$$

where

$$\begin{aligned} g_{4,0} &= 255f[x_0, x_1] + 370f[x_1, x_2] + 35f[x_2, x_3] - \frac{4}{3}h^3 f_0^{(4)}, \\ g_{4,N} &= 35f[x_{N-3}, x_{N-2}] + 370f[x_{N-2}, x_{N-1}] + 255f[x_{N-1}, x_N] + \frac{4}{3}h^3 f_N^{(4)}. \end{aligned}$$

The equations for m_i corresponding to the two-point boundary conditions (17) were partially derived above: (21)–(24). The equations at the points x_1 and x_{N-1} are obtained in the same way as the equation at the points x_0, x_N and have the form

$$m_1 = g_{1,1}, \quad m_{N-1} = g_{1,N-1}, \quad (25)$$

where $g_{1,1} = f_1'$, $g_{1,N-1} = f_{N-1}'$;

$$\begin{cases} 3m_0 - 33m_1 - 29m_2 - m_3 = g_{2,1}, \\ m_{N-3} + 29m_{N-2} + 33m_{N-1} - 3m_N = g_{2,N-1}, \end{cases} \quad (26)$$

where

$$\begin{aligned} g_{2,1} &= 15f[x_0, x_1] - 70f[x_1, x_2] - 5f[x_2, x_3] + 16hf_1'', \\ g_{2,N-1} &= 5f[x_{N-3}, x_{N-2}] + 70f[x_{N-2}, x_{N-1}] - 15f[x_{N-1}, x_N] + 16hf_{N-1}''; \end{aligned}$$

$$\begin{cases} m_0 + 8m_1 + m_2 = g_{3,1}, \\ m_{N-2} + 8m_{N-1} + m_N = g_{3,N-1}, \end{cases} \quad (27)$$

where

$$\begin{aligned} g_{3,1} &= 5f[x_0, x_1] + 5f[x_1, x_2] - \frac{2}{3}h^2 f_1''', \\ g_{3,N-1} &= 5f[x_{N-2}, x_{N-1}] + 5f[x_{N-1}, x_N] - \frac{2}{3}h^2 f_{N-1}'''; \end{aligned}$$

$$\begin{cases} 7m_0 + 99m_1 + 71m_2 + 3m_3 = g_{4,1}, \\ 3m_{N-3} + 71m_{N-2} + 99m_{N-1} + 7m_N = g_{4,N-1}, \end{cases} \quad (28)$$

where

$$g_{4,1} = 35f[x_0, x_1] + 130f[x_1, x_2] + 15f[x_2, x_3] + \frac{4}{3}h^3 f_1^{(4)},$$

$$g_{4,N-1} = 15f[x_{N-3}, x_{N-2}] + 130f[x_{N-2}, x_{N-1}] + 35f[x_{N-1}, x_N] - \frac{4}{3}h^3 f_{N-1}^{(4)}.$$

Equations (21)–(28) contain the exact values of derivatives of $f_k^{(m)}$. To obtain an equation for the boundary conditions (18), (19), we need to replace $f_k^{(m)}$ with the approximate values of the derivatives $\tilde{f}_k^{(m)}$ obtained from the difference approximation by the above formulas.

2.3. The not-a-knot conditions. At $x \in [x_i, x_{i+1}]$, $i = \overline{0, N-1}$, the fifth order derivative of the spline $S(x)$ has the form

$$S^{(5)}(x) = \frac{720}{h^5}(f_{i+1} - f_i) - \frac{360}{h^4}(m_{i+1} + m_i) + \frac{60}{h^3}(M_{i+1} - M_i), \quad (29)$$

i.e., it is constant on each segment $[x_i, x_{i+1}]$. Substituting (29) into the continuity condition for the fifth order derivative $S^{(5)}(x_i - 0) = S^{(5)}(x_i + 0)$, we find

$$6(m_{i+1} - m_{i-1}) - h(M_{i+1} - 2M_i + M_{i-1}) = \frac{12}{h}(f_{i+1} - 2f_i + f_{i-1}). \quad (30)$$

Expressing $M = (M_0, M_1, \dots, M_N)^T$ in terms of $m = (m_0, m_1, \dots, m_N)^T$ in accordance with (7)–(10), we obtain two different representations of (30):

$$5m_{i-1} + 33m_i + 21m_{i+1} + m_{i+2} = 5f[x_{i+2}, x_{i+1}] + 38f[x_{i+1}, x_i] + 17f[x_i, x_{i-1}], \quad (31)$$

$$m_{i-2} + 21m_{i-1} + 33m_i + 5m_{i+1} = 17f[x_{i+1}, x_i] + 38f[x_i, x_{i-1}] + 5f[x_{i-1}, x_{i-2}]. \quad (32)$$

Equation (31) is applied for $i = 1, N-3, N-2$, whereas (32) is used for $i = 2, 3, N-1$. The right-hand sides of both equations are denoted by $g_{5,i}$.

The difference between the boundary conditions 1525 and 1535 consists in the following. Using the conditions 1525, we find a large continuous, up to the fifth order derivative, part of the spline on $[x_0, x_3], [x_{N-3}, x_N]$, whereas, if we use the condition 1535, we find two large parts on $[x_0, x_2], [x_2, x_4]$ and $[x_{N-4}, x_{N-2}], [x_{N-2}, x_N]$. We note that equation for the combined boundary conditions was, in fact, obtained in the previous sections.

3 Systems of Equations for m_i

Adding the equations obtained from the boundary conditions of each type to Equations (14), we obtain a closed system of equations with respect to the unknowns m_i :

$$Am = g, \quad (33)$$

where $m = (m_0, \dots, m_N)^T$ and $g = (g_0, g_1, g_2, \dots, g_{N-2}, g_{N-1}, g_N)^T$. Moreover, the components g_2, \dots, g_{N-2} of g are the same for all boundary conditions and are computed by formula (15), whereas g_0, g_1, g_{N-1}, g_N depend on the type of boundary conditions.

For boundary conditions 0315 we have the system of equations

$$\begin{pmatrix} 269 & 248 & 13 & & & & & & \\ 97 & 309 & 129 & 5 & & & & & \\ 1 & 26 & 66 & 26 & 1 & & & & \\ & & & \ddots & & & & & \\ & & & & 1 & 26 & 66 & 26 & 1 \\ & & & & & 5 & 129 & 309 & 97 \\ & & & & & & 13 & 248 & 269 \end{pmatrix} \begin{pmatrix} m_1 \\ m_2 \\ m_3 \\ \vdots \\ m_{N-3} \\ m_{N-2} \\ m_{N-1} \end{pmatrix} = \begin{pmatrix} 18g_{5,1} - 5g_{3,0} \\ 5g_2 - g_{5,1} \\ g_3 \\ \vdots \\ g_{N-3} \\ 5g_{N-2} - g_{5,N-1} \\ 18g_{5,N-1} - 5g_{3,N} \end{pmatrix}. \quad (38)$$

The unknowns m_0, m_N are found by solving the system of equations (38) in accordance with the formulas

$$m_0 = \frac{1}{18} [g_{3,0} - 65m_1 - 26m_2 - m_3],$$

$$m_N = \frac{1}{18} [g_{3,N} - 65m_{N-1} - 26m_{N-2} - m_{N-3}].$$

For boundary conditions 0415 we have the system of equations

$$\begin{pmatrix} 2000 & 1206 & 49 & & & & & & \\ 1221 & 3231 & 1274 & 49 & & & & & \\ 1 & 26 & 66 & 26 & 1 & & & & \\ & & & \ddots & & & & & \\ & & & & 1 & 26 & 66 & 26 & 1 \\ & & & & & 49 & 1274 & 3231 & 1221 \\ & & & & & & 49 & 1206 & 2000 \end{pmatrix} \begin{pmatrix} m_2 \\ m_3 \\ m_4 \\ \vdots \\ m_{N-4} \\ m_{N-3} \\ m_{N-2} \end{pmatrix} = \begin{pmatrix} g_2^{0415} \\ g_3^{0415} \\ g_4 \\ \vdots \\ g_{N-4} \\ m_{N-3}^{0415} \\ g_{N-2}^{0415} \end{pmatrix}, \quad (39)$$

where

$$g_2^{0415} = \frac{49}{5}(5g_2 - g_{5,1}) - \frac{97}{80}(83g_{5,1} - 5g_{4,0}), \quad g_3^{0415} = 49g_3 - \frac{1}{16}(83g_{5,1} - 5g_{4,0}),$$

$$g_{N-2}^{0415} = \frac{49}{5}(5g_{N-2} - g_{5,N-1}) - \frac{97}{80}(83g_{5,N-1} - 5g_{4,N}), \quad g_{N-3}^{0415} = 49g_{N-3} - \frac{1}{16}(83g_{5,N-1} - 5g_{4,N}).$$

The unknowns m_0, m_1, m_{N-1}, m_N are found by solving the system of equations (39) in accordance with the formula

$$m_1 = \frac{1}{49} [(83g_{5,1} - 5g_{4,0})/16 - 53m_2 - 3m_3],$$

$$m_{N-1} = \frac{1}{49} [(83g_{5,N-1} - 5g_{4,N})/16 - 53m_{N-2} - 3m_{N-3}],$$

$$m_0 = \frac{1}{83} [g_{4,0} - 391m_1 - 179m_2 - 7m_3],$$

$$m_N = \frac{1}{83} [g_{4,N} - 391m_{N-1} - 179m_{N-2} - 7m_{N-3}].$$

The matrices of all the above systems have diagonal dominance. Thus, for all the types of boundary conditions under consideration we can guarantee the existence, uniqueness, and possibility of computing solutions by the stable 5-point sweeping method. [9].

4 Asymptotics of Approximation Error

The asymptotic representations (2) for the error of approximation by a spline $S(x)$ in the case of the classical boundary conditions were obtained in [4], where the proof was based on the diagonal dominance in the systems for m_i . Since the same fact occurs in the case of the boundary conditions under consideration, we can repeat the reasoning of [4] to obtain (2).

However, since we cannot explicitly indicate the functions $\gamma_{i,N}(t)$ for each type of boundary conditions, for further consideration we use numerical experiments. The functions $\gamma_{i,N}(t)$ are independent of $f(x)$. Therefore, setting $f(x) = x^6$ and taking into account that $f^{(6)}(x) = 6!$, $f^{(k)}(x) \equiv 0$, $k \geq 7$, from (2) we find

$$S(x) = f(x) + h^6 \gamma_{i,N}(t),$$

from which we find the sought function $\gamma_{i,N}(t)$:

$$\gamma_{i,N}(t) = \frac{1}{h^6} (S(x) - x^6). \quad (40)$$

We note that $x^6 - S(x)$ is called a monospline [9].

We show that $\gamma_{i,N}(t)$ are bounded. We consider the system (33) for constructing a spline with boundary conditions 0102ap. We introduce a spline $H(x)$, $x \in [x_0, x_N]$, interpolating f_i , f'_i , $i = \overline{0, N}$, at the nodes and taking the following form on each segment $[x_i, x_{i+1}]$, $i = \overline{1, N-2}$:

$$\begin{aligned} H(x) = & f_{i-1} \varphi_1(t) + f_i \varphi_2(t) + f_{i+1} \varphi_2(1-t) + f_{i+2} \varphi_1(1-t) \\ & + h f'_{i-1} \psi_1(t) + h f'_i \psi_2(t) - h f'_{i+1} \psi_2(1-t) - h f'_{i+2} \psi_1(1-t). \end{aligned}$$

On $[x_0, x_1]$ and $[x_{N-1}, x_N]$, the spline $H(x)$ is expressed by

$$\begin{aligned} H(x) = & f_0 \varphi_3(t) + f_1 \varphi_4(t) + f_2 \varphi_5(t) + f_3 \varphi_6(t) \\ & + h f'_0 \psi_3(t) + h f'_1 \psi_4(t) + h f'_2 \psi_5(t) + h f'_3 \psi_6(t), \\ H(x) = & f_N \varphi_3(1-t) + f_{N-1} \varphi_4(1-t) + f_{N-2} \varphi_5(1-t) + f_{N-3} \varphi_6(1-t) \\ & - h f'_N \psi_3(1-t) - h f'_{N-1} \psi_4(1-t) - h f'_{N-2} \psi_5(1-t) - h f'_{N-3} \psi_6(1-t). \end{aligned}$$

Taking the polynomial x^6 for $f(x)$ and repeating the argument of [4], we find

$$H(x) - x^6 = h^6 \gamma(t), \quad x \in [x_i, x_{i+1}], \quad i = \overline{0, N-1}.$$

Taking into account that $\|\gamma\|_C = 3/64$, we obtain the estimate

$$\|H - x^6\|_C \leq \frac{3}{64} h^6. \quad (41)$$

We consider the difference $S(x) - H(x)$. For $x \in [x_i, x_{i+1}]$, $i = \overline{1, N-2}$, we have

$$\begin{aligned} S(x) - H(x) = & h[(m_{i-1} - f'_{i-1}) \psi_1(t) + (m_i - f'_i) \psi_2(t) \\ & - (m_{i+1} - f'_{i+1}) \psi_2(1-t) - (m_{i+2} - f'_{i+2}) \psi_1(1-t)]. \end{aligned} \quad (42)$$

The vector on the right-hand side of the system is equal to $g = (g_{1,0}, g_{2,0}, g_2, \dots, g_{2,N}, g_{1,N})^T$. Subtracting Af' , $f' = (f'_0, \dots, f'_N)^T$, from both sides of (33), we find

$$A(m - f') = g - Af'. \quad (43)$$

Let us estimate the components of $g - Af'$. By the Taylor formula,

$$\begin{aligned} g_{1,0} - (Af')_0 &= 120h^5, \\ g_{2,0} - (Af')_1 &= 9144h^5, \\ g_i - (Af')_i &= 0, \quad i = \overline{2, N-2}, \\ g_{2,N} - (Af')_{N-1} &= 9144h^5, \\ g_{1,N} - (Af')_N &= 120h^5. \end{aligned}$$

We denote by $\|z\|_\infty = \max_i |z_i|$ and $\|A\| = \max_i \sum_j |a_{ij}|$ the norms of a vector $z = (z_0, \dots, z_N)^T$ and a matrix $A = (a_{ij})$. Since the matrix A of the system (33) for constructing a spline with boundary conditions 0102ap has diagonal dominance, equal to 1, we have [9] $\|A^{-1}\| \leq 1$. Therefore,

$$\|m - f'\|_\infty \leq \|g - Af'\|_\infty,$$

and, consequently,

$$\|m - f'\|_\infty \leq 9144h^5.$$

The functions $\psi_1(t)$, $\psi_2(t)$, $t \in [0, 1]$, can be estimated from above as follows:

$$\|\psi_1\|_C \leq 0,005, \quad \|\psi_2\|_C \leq 0,18.$$

As a result, from (42) we obtain the estimate

$$\|S - H\|_C \leq h\|m - f'\|_\infty(2\|\psi_1\|_C + 2\|\psi_2\|_C) \leq 3383,28h^6. \quad (44)$$

Since $\|S - x^6\|_C \leq \|S - H\|_C + \|H - x^6\|_C$, from (41), (44) for (40) we get

$$\|\gamma_{i,N}\|_C \leq 3383,33, \quad i = \overline{1, N-2}.$$

For $i = 0, (N-1)$ similar arguments lead to the estimate $\|\gamma_{i,N}\|_C \leq 5806,49$. Thus, the functions $\gamma_{i,N}(t)$ are bounded in the case of boundary conditions 0102ap. In the remaining cases, the boundedness of $\gamma_{i,N}(t)$ is proved in a similar way.

We present the results of numerical experiment of calculating values of the functions $\gamma_{i,N}(t)$ and their maxima for different boundary conditions. Computations are performed on $[-1, 1]$. It should be noted that the functions $\gamma_{i,N}(t)$ fastly converge to the limit values $\gamma_{i,\infty}(t)$ as N increases for any boundary conditions and that all functions fastly converge to $\gamma(t) = \frac{1}{2}t^2(1-t)^2(1+2t-2t^2)$ far from the endpoints of $[a, b]$. Thereby the well known fact of local influence of boundary conditions on the behavior of the spline is confirmed, at least, in asymptotics.

Tables 1 and 2 consist of the values of $\max_i \|\gamma_{i,80}\|_C$ for different boundary conditions. These values are, in fact, the same as $\max_i \|\gamma_{i,\infty}\|_C$. In Table 1, for the sake of brevity the code of boundary condition is divided into two parts: the first part (the first column of the table) means the order of derivative at the point x_0 , whereas the second part (the first row of the table) means the order of derivative at the points x_0 and x_1 for the classical and two-point boundary conditions respectively. For example, for boundary conditions 0213ap we have $\max_i \|\gamma_{i,\infty}\|_C \approx 17,2278$. The empty cells of the table mean the absence of boundary conditions of the corresponding type (for example, 0202ap) or repetition of some other condition (for example, 0203ap and 0302ap).

We note that for all boundary conditions with 6-point difference approximations of derivatives (cf. Table 1) the asymptotic behavior of $\gamma_{i,N}(t)$ is considerably worse than in the case of the not-a-knot conditions 1525 (cf. Table 2). For boundary conditions of type $0X15ap$, $X = 1, 2, 3, 4$, the situation is similar since $\max_i \|\gamma_{i,\infty}\|_C \in [14, 7545, 16, 5224]$. Thus, it is not reasonable to use conditions with difference approximations of derivatives; it suffices to consider only boundary conditions 1525.

TABLE 1. Values of $\max_i \|\gamma_{i,80}\|_C$ for boundary conditions with difference approximations of derivatives.

	02	03	04	11	12	13	14
01	16,8471	16,7938	16,7310	17,1490	16,0806	17,0406	16,3908
02		16,6531	16,5207	17,3063	15,9410	17,2278	16,0169
03			16,2318	17,4722	15,8901	17,5733	15,7305
04				17,6377	15,8785	18,0879	15,6004

TABLE 2. Values of $\max_i \|\gamma_{i,80}\|_C$ for boundary conditions with continuous fifth order derivative at one or two points.

1525	1535	0115	0215	0315	0415
9,8340	15,8112	0,7006	1,3749	2,7981	6,0206

The results in Tables 1 and 2 show that the combined boundary conditions are optimal. Among two variants of the not-a-knot conditions 1525 and 1535, the better is the condition 1525. We also considered the so-called not-a-knot conditions 2535. However, such conditions are not of great importance since $\max_i \|\gamma_{i,\infty}\|_C \approx 128,4$, which is considerably worse than the case of conditions 1525.

We note that all the boundary conditions considered in this paper are worse in the sense of accuracy than the optimal conditions in [4] because $\max_i \|\gamma_{i,\infty}\|_C > \|\gamma\|_C = 3/64$. However, the considered conditions are more useful in practice since they require less information about derivatives of the interpolated function.

5 Interpolation of the Runge Function. Numerical Experiment

As an example, we consider interpolation of the Runge function [14]

$$f(x) = \frac{1}{1 + 25x^2} \quad (45)$$

on a uniform mesh on $[-1, 1]$. Lagrange polynomials taken for interpolation in this example turn out to be divergent [14, 15]. Let us consider quintic splines for interpolation. Tables 3–6 represent the error of approximation of the Runge function by splines with different boundary conditions.

Assume that the Runge function is interpolated by quintic splines on a uniform mesh with different N . Then $e_1 = \|S - f\|_{C[-1,1]}$ is the same for all boundary conditions and attains the

maximum at the middle of $[-1, 1]$, where the boundary conditions do not practically affect the approximation error. The corresponding data are given in Table 3. However, near the endpoints, the influence becomes considerable, and the behavior of errors $S(x) - f(x)$ near the endpoints looks like the behavior of $\gamma_{i,N}(t)$.

TABLE 3. Values of e_1 for all boundary conditions with different N .

N	20	40	80	160
e_1	$1,60 \times 10^{-4}$	$3,14 \times 10^{-5}$	$2,48 \times 10^{-7}$	$3,05 \times 10^{-9}$

Now, we consider interpolation of the Runge function (45) by quintic splines on a uniform mesh on $[0, 1]$ and study the behavior of the approximation error. If we use the boundary conditions with six-point approximations of derivatives for $N = 20$, then the norms of approximation error are practically the same: $e_2 = \|S - f\|_{C[0,1]} \in [1, 21 \times 10^{-3}, 1, 31 \times 10^{-3}]$. In this case, the error graphs are practically undistinguishable.

Table 4 presents errors in the case of boundary conditions including the continuity of the fifth order derivative of the spline at one or two points. The error attains the maximum near the point 0.

TABLE 4. Values of e_2 for boundary conditions with the fifth order derivative for $N = 20$.

1525	1535	0115	0215	0315	0415
$9,73 \times 10^{-4}$	$1,21 \times 10^{-4}$	$3,98 \times 10^{-5}$	$5,81 \times 10^{-5}$	$7,04 \times 10^{-5}$	$5,19 \times 10^{-5}$

In the case $N = 20$, it turns out that the error in the case of conditions 1535 is considerably less than that for conditions 1525. It can look like a contradiction with the above conclusion about the advantage of conditions 1525 in comparison with condition 1535. However, the error asymptotic can be observable only for large N , whereas we have $N = 20$ in the example with the Runge function. The results for large N are presented in Tables 5 and 6.

TABLE 5. Values of e_2 for boundary conditions with approximation of derivatives with different N .

N	e_2
40	$[8,80 \times 10^{-6}, 9,71 \times 10^{-6}]$
80	$[5,07 \times 10^{-7}, 5,33 \times 10^{-7}]$
160	$[1,26 \times 10^{-8}, 1,35 \times 10^{-8}]$
320	$[2,19 \times 10^{-10}, 2,36 \times 10^{-10}]$

TABLE 6. Values of e_2 for boundary conditions with continuity of the 5th order derivative for different N .

N	1525	1535	0115	0215	0315	0415
40	$7,94 \times 10^{-7}$	$3,67 \times 10^{-5}$	$1,49 \times 10^{-6}$	$3,01 \times 10^{-6}$	$6,41 \times 10^{-6}$	$1,49 \times 10^{-5}$
80	$3,87 \times 10^{-7}$	$1,73 \times 10^{-7}$	$3,68 \times 10^{-8}$	$7,25 \times 10^{-8}$	$1,49 \times 10^{-7}$	$3,25 \times 10^{-7}$
160	$8,31 \times 10^{-9}$	$1,11 \times 10^{-8}$	$6,33 \times 10^{-10}$	$1,24 \times 10^{-9}$	$2,53 \times 10^{-9}$	$5,47 \times 10^{-9}$
320	$1,4 \times 10^{-10}$	$2,15 \times 10^{-10}$	$1,01 \times 10^{-11}$	$1,99 \times 10^{-11}$	$4,04 \times 10^{-11}$	$8,71 \times 10^{-11}$

The above results show that the use of quintic splines on a uniform mesh allows us to approximate the Runge function with high accuracy.

In this paper, we used only 6-point approximations for derivatives in the optimal conditions (3). From the theoretical point of view, 7-point approximations of derivatives, could yield the same error asymptotics as $h \rightarrow 0$ as in the case of the optimal boundary conditions. However, the results below show that this fact holds, generally speaking, for very small h .

We consider the quantity

$$AR = \frac{e_2}{\max_i \|\gamma_{i,N}(t)f^{(6)}(x)h^6/6!\|_C}.$$

It is obvious that $\lim_{h \rightarrow 0} AR = 1$. This fact is also confirmed by the results (cf. Table 7) of numerical experiment with the optimal boundary conditions 0111 and conditions $0111\widetilde{ap}$ (with 7-point approximations of the first order derivatives). However, for conditions $0111\widetilde{ap}$, the convergence rate AR satisfies the relation $AR \approx 1$ only for very small h .

Similar results are obtained by for the remaining types of optimal boundary conditions (3).

TABLE 7. Values of AR for boundary conditions $0111\widetilde{ap}$ and 0111 with different N .

N	$0111\widetilde{ap}$	0111
25	42,5300	1,1635
50	123,6195	0,9584
100	80,1194	1,0070
200	25,9438	1,0026
400	7,4697	1,0007
800	2,5577	1,0002
1600	1,3709	1,0009

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Submitted on July 10, 2015