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Journal of Computational and Applied Mathematics 478 (2026) 117240

Contents lists available at ScienceDirect

Journal of Computational and Applied Mathematics

journal homepage: www.elsevier.com/locate/cam

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ARTICLE INFO

Keywords:
Cubic spline
Natural spline
Error estimate
Condition number

ABSTRACT

In this paper a fourth order asymptotically optimal error bound for a new cubic interpolating spline function, denoted by Q-spline, is derived for the case that only function values at given points are used but not any derivative information. The bound seems to be stronger than earlier error bounds for cubic spline interpolation in such setting such as the not-a-knot spline. A brief analysis of the conditioning of the end conditions of cubic spline interpolation leads to a modification of the not-a-knot spline, and some numerical examples suggest that the interpolation error of this revised not-a-knot spline generally is comparable to the near optimal Q-spline and lower than for the not-a-knot spline when the mesh size is small.

1. Introduction

Given knots $x_0 < x_1 < \ldots < x_n$ and a function $f : [x_0, x_n] \to \mathbb{R}$, an interpolating function s is searched for with $s(x_i) = f_i := f(x_i)$ for $0 \le i \le n$. Throughout, it is assumed that f is four times continuously differentiable on $[x_0, x_n]$ and that $n \ge 5$.

Possibly the most famous result concerning cubic spline functions is the following Lemma:

Lemma 1. *The cubic spline function with either the first derivative or the second derivative specified at both end points is the unique function that minimizes the integral of the square of the second derivative among all interpolating C^2-functions with the same end conditions.*

When there are no end conditions then the natural spline s with $s''(x_0) = s''(x_n) = 0$ minimizes the integral of the square of the second derivative among all interpolating C^2-functions, an observation that dates back to [3].

Lemma 1 is also true for the periodic spline when f is periodic with period $x_n - x_0$; see, for example, [5], Chapter 2.4. In the following only the case is considered where f is not necessarily periodic.

- The case $s''(x_i) = 0$ for $i = 0$ and $i = n$ often is denoted by **natural spline** in the literature and when $s'(x_i) = f'(x_i)$ for $i = 0$ and $i = n$ are given, this is often denoted by **clamped spline**. Following this common notation, the cubic spline interpolant with end conditions $s''(x_i) = f''(x_i)$ for $i = 0$ and for $i = n$ will be denoted by **clamped natural spline** in the following.

Apart from the smoothness of the cubic spline function established in Lemma 1 also an appealing error estimate is known. Setting $\|f^{(4)}\|_\infty := \max_{\xi \in [x_0, x_n]} |f^{(4)}(\xi)|$ the following error estimate is given in [2]:

Lemma 2. *For $x \in [x_0, x_n]$ the clamped spline and also the clamped natural spline s satisfy*

$$|s(x) - f(x)| \le \frac{5}{384} \|f^{(4)}\|_\infty h^4$$

with $h := \max_{1 \le i \le n}(x_i - x_{i-1})$. This result is best possible.

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https://doi.org/10.1016/j.cam.2025.117240
Received 7 July 2025; Received in revised form 13 November 2025
Available online 4 December 2025

To put the above lemma into perspective, in Lemma 3 below it is compared to a third order polynomial approximation that uses only function values and that also allows for an error estimate in terms of the fourth derivative $f^{(4)}$.

Lemma 3. *Let f be four times continuously differentiable on $[x_0, x_n]$. Based on the data $f(x_i)$ for $0 \le i \le n$, an approximation of $f(x)$ for $x \in [x_1, x_{n-1}]$ is possible by an interpolating cubic polynomial p such that*

$$|p(x) - f(x)| \le \tfrac{3}{128} \|f^{(4)}\|_\infty h^4$$

with $h := \max_{1\le i\le n}(x_i - x_{i-1})$.

For $x \in [x_0, x_1]$ or $x \in [x_{n-1}, x_n]$

$$|p(x) - f(x)| \le \tfrac{1}{24} \|f^{(4)}\|_\infty h^4$$

Both estimates are best possible.

Proof. When x coincides with x_i for some i there is nothing to show. Let $x \in (x_1, x_{n-1})$. Choose i such that $x \in (x_i, x_{i+1})$ and let p be the cubic polynomial interpolating f at $x_{i-1}, x_i, x_{i+1}, x_{i+2}$. The standard error bound for polynomial interpolation states that

$$f(x) - p(x) = \frac{f^{(4)}(\xi)}{24}\omega(x) \quad \text{with} \quad \omega(x) = \prod_{j=i-1}^{i+2}(x - x_j) \tag{1}$$

and with $\xi \in (x_{i-1}, x_{i+2})$. Observe that $\|\omega\|_\infty$ increases when, for example, x_{i-1} is reduced while x_i, x_{i+1}, and x_{i+2} remain unchanged. Thus, when maximizing $\|\omega\|_\infty$ one can assume without loss of generality that all mesh points have maximum distance $x_{k+1} - x_k = h$ for all k. Straightforward calculations then show that $|\omega(x)| \le \frac{9}{16}h^4$ for $x \in [x_i, x_{i+1}]$. The first statement of the lemma follows when inserting this into (1).

Similarly, for $x \in [x_0, x_1]$, the term $\omega(x)$ is given by $\omega(x) = \prod_{j=0}^{4}(x - x_j)$ and straightforward calculations show that $|\omega(x)| \le h^4$. Likewise also for $x \in [x_{n-1}, x_n]$.

When interpolating the function f with $f(x) \equiv x^4$, the fourth derivative is constant so that (1) implies that the bounds given in Lemma 1 are best possible. ☐

For points x near the end points it is not surprising that the spline approximation using derivative information at the end points has a lower error estimate than cubic interpolation, but also for points near the middle of $[x_0, x_n]$ the constant term for the spline approximation $\frac{5}{384} \approx 0.0130 < 0.0234 \approx \frac{3}{128}$ is better than for the cubic interpolation. (The constant term at the end points is $\frac{1}{24} \approx 0.0417$.)

Apart from that, in general, the piecewise cubic interpolation referred to in Lemma 3 also is not differentiable at the knots x_i for $1 \le i \le n-1$.

Both, Lemma 1 and Lemma 2 refer to the case that either f' or f'' is known at the end points. When neither the derivative information for f is available nor f is known to be periodic, the spline s of choice often is either the not-a-knot spline or the natural spline. The natural spline always has second derivative zero at the end points, $s''(x_0) = s''(x_n) = 0$ independent of the second derivative of f at these points. As detailed in Corollary 1 below, when $f''(x_0)$ or $f''(x_n)$ are nonzero this results in a lower approximation accuracy of f by s near x_0 or near x_n. Also for the not-a-knot spline there seem to be no error estimates comparable to Lemma 2 when an irregular mesh is used.

Not-a-knot splines on a regular grid with constant distances $x_i - x_{i-1}$ are considered for example in [6]. By an optimal placement of two additional not-a-knot-nodes, an explicit error bound as in Lemma 2 could be derived with constant 10.85/384 compared to 5/384 in Lemma 2. Earlier, in [1] it was shown that cubic spline interpolation with the not-a-knot end condition converges to any C^2-interpolant on arbitrary irregular meshes when the mesh size goes to zero, but no explicit error rates are given. Here, an attempt is made to define an interpolating cubic spline function along with an explicit error estimate without using any additional points or any derivative information at the end points.

Before addressing possible replacements of the conditions for the natural spline or the not-a-knot spline, the condition number of possible alternative end conditions is addressed next.

2. Ill-conditioning of end conditions

For illustration in this section $n = 50$ equidistant mesh points with distance 1 are considered first. Since there are two degrees of freedom, the various interpolating cubic spline functions always differ by multiples of two splines s_1 and s_2 satisfying $s_1(x_i) = s_2(x_i) = 0$ for $0 \le i \le n$ and

$$s_1'(x_0) = 1, \;\; s_1''(x_0) = 2\sqrt{3}, \qquad \text{and} \qquad s_2'(x_0) = 1, \;\; s_2''(x_0) = -2\sqrt{3}.$$

(The initial values $\pm 2\sqrt{3}$ are chosen at will, what matters is that s_1 and s_2 are linearly independent of each other.)

The existence of such functions s_1 and s_2 implies the following observation concerning possible generalizations of Lemma 2:

Note 1. Without the specification of some form of end condition there does not exist any finite number $T = T(f, h)$ such that an interpolating cubic spline function s for some given function f and some given mesh size h always satisfies $\|f - s\|_\infty \le T$.

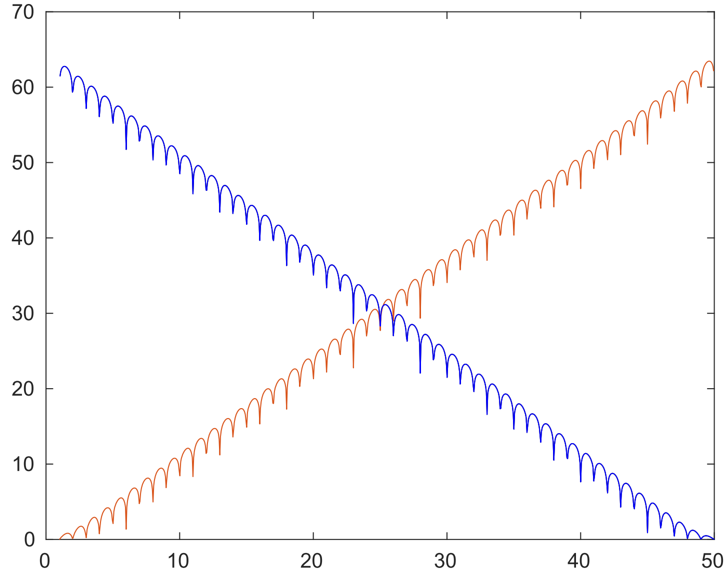

Fig. 1. Exact values of $\ln(|s_1|+1)$ in red and of $\ln(4 \cdot 10^{28}|s_2|+1)$ in blue. The logarithmic scale translates the exponential growth/decay of the oscillations of $|s_1|$ or $|s_2|$ to a linear growth/decay rate.

(This is so because arbitrary multiples of s_1 and s_2 can be added to an interpolating cubic spline without changing the interpolation property.)

On the interval $[x_0, x_1] = [0, 1]$ the function s_1 takes the form

$$s_1(x) = (x - x_0) + \sqrt{3}(x - x_0)^2 - (1 + \sqrt{3})(x - x_0)^3$$

where the coefficient of $(x - x_0)^3$ is the negative of the sum of the other two coefficients, so that $s_1(x_0) = s_1(x_1) = 0$. From this it follows that

$$s_1'(x_1) = 1 + 2\sqrt{3} - 3(1 + \sqrt{3}) = -(2 + \sqrt{3})$$

and

$$s_1''(x_1) = 2\sqrt{3} - 6(1 + \sqrt{3}) = -6 - 4\sqrt{3} = -(2 + \sqrt{3}) \cdot 2\sqrt{3}.$$

Thus, the first and second derivative of s_1 at x_1 are $-(2 + \sqrt{3})$ times the values at x_0, and again, the coefficient of $(x - x_1)^3$ for s_1 on the interval $[x_1, x_2]$ is the negative of the sum of the coefficients for $(x - x_1)$ and $(x - x_1)^2$. Inductively, the values of s_1 multiply by $-(2 + \sqrt{3})$ each time the variable x passes from $[x_{i-1}, x_i]$ to $[x_i, x_{i+1}]$. The graph of s_1 oscillates and the absolute values "explode" for large values of x.

Likewise,

$$s_2(x) = (x - x_0) - \sqrt{3}(x - x_0)^2 + (\sqrt{3} - 1)(x - x_0)^3,$$

with $s_2'(x_1) = \sqrt{3} - 2$ and $s_2''(x_1) = (\sqrt{3} - 2)s_2''(x_0)$. Both derivatives are multiplied by $\sqrt{3} - 2 \approx -0.268$, and the graph of s_2 rapidly converges to zero for large values of x.

Fig. 1 illustrates the exponential growth of s_1 and the exponential decay of s_2 for large values of x. The function s_2 is scaled by a factor $4 \cdot 10^{28}$ to match the range of s_1, and since $s_1(x_i) = s_2(x_i) = 0$, not $\ln(\text{abs}(s_1))$ but $\ln(\text{abs}(s_1)+1)$ is plotted; likewise for s_2. (At the knots x_i the values $\ln(\text{abs}(s_1)+1)$ go down to zero. In Fig. 1 the mesh points used for the plot are chosen disjoint from the knots x_i so that the lines in the figure do not go down to zero at all x_i.)

The numerical computation of the coefficients of s_2 starting from $[x_0, x_1]$ and extending to $[x_i, x_{i+1}]$ for $i = 1, 2, \ldots, 50$ is highly unstable. The exact values (derived above) coincide with the data shown in Fig. 1. The numerical values for s_2 computed by the above procedure are depicted in Fig. 2, and first behave as predicted but rounding errors accumulate and the numerical values for $|s_2|$ grow exponentially for $i \geq 17$. (The errors also grow exponentially for $i \leq 17$ but are still too small to be seen in Figure 2.) Here, the values of $\ln(\text{abs}(s_2)+\text{eps})$ are plotted where eps is the machine precision so that small values of s_2 can be identified on the plot.

To explain this behavior let the representation of s_2 on the interval $[x_i, x_{i+1}]$ be denoted by

$$s_2(x) = b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3 \qquad \text{for } x \in [x_i, x_{i+1}].$$

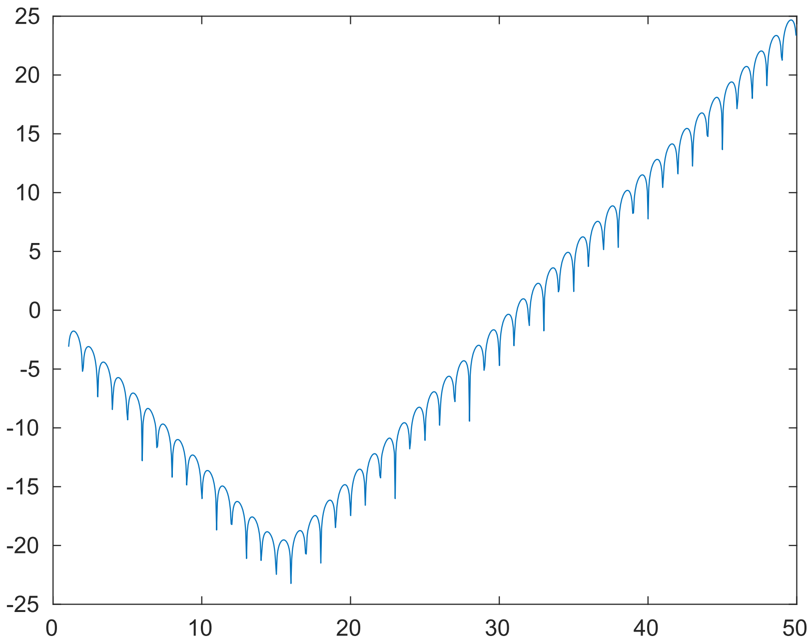

Fig. 2. Computed values of $\ln(|s_2| + \mathrm{eps})$ starting computations from the left; near $x = 15$ the exponential accumulation of the rounding errors becomes visible.

Then $d_i = -(a_i + b_i)$ can be treated as an auxiliary variable, while b_i, c_i satisfy the discrete linear dynamical system

$$\begin{bmatrix} b_{i+1} \\ c_{i+1} \end{bmatrix} = \begin{bmatrix} -2 & -1 \\ -3 & -2 \end{bmatrix} \begin{bmatrix} b_i \\ c_i \end{bmatrix} =: \; A \begin{bmatrix} b_i \\ c_i \end{bmatrix}.$$

The eigenvalues of A are just the two numbers $-(2+\sqrt{3})$ and $\sqrt{3}-2$, and the coefficients of s_1 and of s_2 yield the associated eigenvectors. Due to rounding errors, the numerical coefficients converge to multiples of the eigenvector for the eigenvalue with the larger absolute value; this is what can be seen in Fig. 2. (The graph of s_2 in Fig. 1 was computed starting at the right end point, and the numerical values roughly correspond to the exact values known from the analysis of the dynamical system.) We note that replacing $s(x)$ by $\check{s}(x) := s(h^{-1}x)$ for some mesh size $h > 0$, then the k-th derivative of $\check{s}$ is $\check{s}^{(k)}(x) = h^{-k}s^{(k)}(x)$. The growth factor $-(2+\sqrt{3})$ when moving from $[x_i, x_{i+1}]$ to $[x_{i+1}, x_{i+2}]$ remains the same.

The situation is quite similar when the mesh is not uniform. In Fig. 3, the same number of mesh points was chosen from a uniform distribution on the same interval. Again, two spline functions s_1 and s_2 are defined with end values 1 and $2\sqrt{3}$ for the first and second derivative either on left (s_1) or on the right (s_2). Again there is some form of exponential growth either when x increases, or when x decreases.

Using slightly different definitions of s_1 and s_2, it was observed in [2] that linear combinations of s_1 and s_2 generally have large oscillating function values near x_0 and near x_n, and comparatively very small absolute function values in the middle. Summarizing we obtain the following observations:

Note 2. Finding a spline function s where the values of s' and s'' are given, either both at x_0 or both at x_n, is an extremely ill-conditioned problem.

Such "asymmetric" end conditions as in Note 2 will not be used in the sequel; instead "symmetric" end conditions will be considered that treat both ends of the interval $[x_0, x_n]$ the same way.

A second observation can also be made:

Note 3. If two interpolating spline functions $\hat{s}$ and $\bar{s}$ for a function f on the points $x_0 < \ldots < x_n$ are given with moderate values $\|\hat{s} - f\|_\infty$ and $\|\bar{s} - f\|_\infty$ then for $x \in [x_0, x_n]$ sufficiently far from both end points the difference $|\hat{s}(x) - \bar{s}(x)|$ is tiny.

Indeed, $\hat{s}$ and $\bar{s}$ differ by a linear combination of s_1 and s_2, and by assumption, the difference has moderate function values near the end points since else at least one of the values $\|s - f\|_\infty$ would be large. As observed above, this linear combination of s_1 and s_2 has tiny function values for points $x \in [x_0, x_n]$ sufficiently far from both end points. Thus, for such x both spline functions $\hat{s}$ and $\bar{s}$ have similarly strong approximation properties as stated in Lemma 2 for the clamped natural spline – not only for the function values, but as detailed in [2] also for the first two derivatives. Without quantifying[1] this observation exactly, it will be referred to as **consistent spline property** in the motivation of the revised not-a-knot spline in Section 4.

[1] An exact quantification can be derived for regular meshes based on the eigenfunctions s_1, s_2 examined in this section.

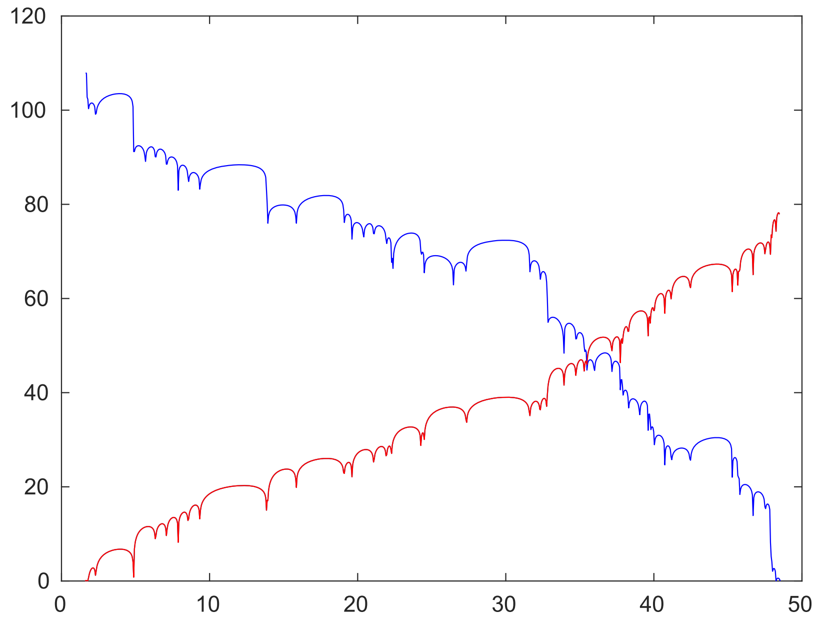

Fig. 3. Graph of $\ln(|s_1|+1)$ in red (starting left) and of $\ln(|s_2|+1)$ in blue (starting right) on an irregular mesh.

3. Approximating the clamped natural spline

Lemma 2 provides an excellent approximation guarantee for the clamped natural spline when the exact values of $f''(x_0)$ and $f''(x_n)$ are known. This leads to the question, in how far approximate values κ_0 and κ_n used in place of $f''(x_0)$ and $f''(x_n)$ lead to splines with tight approximation guarantees as well. This question is considered next.

Definition 1. Let $x_0 < x_1 < \ldots < x_n$ and $f \in C^4([x_0, x_n])$ be given, and set $h := \max_{1\le i\le n}(x_i - x_{i-1})$. Further let κ_0, κ_n be given such that $|\kappa_0 - f''(x_0)| \le R\|f^{(4)}\|_\infty h^2$ and $|\kappa_n - f''(x_n)| \le R\|f^{(4)}\|_\infty h^2$ for some fixed constant R. Then the cubic spline s for f on $x_0, \ldots, x_n$ with $s''(x_0) = \kappa_0$ and $s''(x_n) = \kappa_n$ is called an **R-approximate clamped natural spline**.

Theorem 1. *For $x \in [x_0, x_n]$ any R-approximate clamped natural spline s satisfies*

$$|s(x) - f(x)| \le \left(\frac{5}{384} + \frac{R}{8}\right)\|f^{(4)}\|_\infty h^4.$$

Proof. Let s_{cn} be the clamped natural spline and let s be the R-approximate clamped natural spline. Setting $s_\Delta := s_{cn} - s$ it follows from Lemma 1 for $x \in [x_0, x_n]$ that

$$|f(x) - s(x)| \le |f(x) - s_{cn}(x)| + |s_\Delta(x)| \le \frac{5}{384}\|f^{(4)}\|_\infty h^4 + |s_\Delta(x)|$$

To bound $|s_\Delta(x)|$ let $\mu_i := (x_i - x_{i-1})/(x_{i+1} - x_{i-1})$ and $\lambda_i := (x_{i+1} - x_i)/(x_{i+1} - x_{i-1})$ for $1 \le i \le n-1$ and denote the second derivatives of s_Δ at x_i by $M_i := s''_\Delta(x_i)$ for $0 \le i \le n$. In the literature, the quantities M_i are called moments. By construction, $s_\Delta(x_i) = 0$ for $0 \le i \le n$, and by Definition 1, $|M_0| \le R\|f^{(4)}\|_\infty h^2$, same as for $|M_n|$. Adapting standard arguments as in Theorem I.3.5 in [7], the (rectangular) linear system for the moments M_i for s_Δ can be stated as

$$\begin{pmatrix} \mu_1 & 2 & \lambda_1 & & & \\ & \mu_2 & 2 & \lambda_2 & & \\ & & \ddots & \ddots & \ddots & \\ & & & \mu_{n-1} & 2 & \lambda_{n-1} \end{pmatrix}\begin{pmatrix} M_0 \\ \vdots \\ \vdots \\ M_n \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix}$$

where the right hand side follows from $s_\Delta(x_i) = 0$ for all i. Since M_0 and M_n are fixed, this is equivalent to

$$\begin{pmatrix} 2 & \lambda_1 & & & \\ \mu_2 & 2 & \lambda_2 & & \\ & \ddots & \ddots & \ddots & \\ & & \mu_{n-2} & 2 & \lambda_{n-2} \\ & & & \mu_{n-1} & 2 \end{pmatrix}\begin{pmatrix} M_1 \\ \vdots \\ \vdots \\ \vdots \\ M_{n-1} \end{pmatrix} = \begin{pmatrix} -\mu_1 M_0 \\ 0 \\ \vdots \\ 0 \\ -\lambda_{n-1} M_n \end{pmatrix}.$$

Let the (square) matrix on the left be denoted by A. Then, since $\mu_i, \lambda_i > 0, \quad \mu_i + \lambda_i = 1$, the matrix A is strictly diagonally dominant and $\|Az\|_\infty \ge \|z\|_\infty$ for all $z \in \mathbb{R}^n$. Hence, it follows that $|M_i| \le R\|f^{(4)}\|_\infty h^2$ for all i.

Since s_Δ has zeros at x_i and at x_{i+1} and since its second derivative is bounded by $R\|f^{(4)}\|_\infty h^2$, its absolute value on any interval $[x_i, x_{i+1}]$ for $0 \le i \le n-1$ cannot exceed $\frac{1}{8}(x_{i+1} - x_i)^2\, R\|f^{(4)}\|_\infty h^2 \le \frac{R}{8}\|f^{(4)}\|_\infty h^4$.
□

3.1. Estimating $f''(x_0)$ and $f''(x_n)$

We begin with a simple estimate of $f''(x_0)$ assuming only the continuity of $f^{(4)}$ but not the existence of higher derivatives: To this end the second derivative at x_0 of the cubic interpolant through x_0, x_1, x_2, x_4 is computed. (Of course, an analogous estimate applies to $f''(x_n)$ as well.)

Lemma 4. *Let p be the polynomial of degree at most 3 that interpolates f at $x_0 < x_1 < x_2 < x_3$. If f is four times continuously differentiable on $[x_0, x_3]$ and $h := \max_{0\le i\le 2}(x_{i+1} - x_i)$, then*

$$|p''(x_0) - f''(x_0)| = \left|\frac{f^{(4)}(\xi)}{24}\,\omega''(x)\big|_{x=x_0}\right| \le \left|\frac{11}{12} f^{(4)}(\xi)h^2\right|$$

where $\xi \in (x_0, x_3)$ and $\omega(x) := \prod_{j=0}^{3}(x - x_j)$.

Proof. For completeness a short proof using standard arguments is given:

Straightforward calculations lead to $0 < |\omega''(x_0)| \le 22h^2$. Let $K := \frac{f''(x_0)-p''(x_0)}{\omega''(x_0)}$ and consider the function

$$\tilde f(x) := f(x) - p(x) - K\omega(x).$$

By construction, $\tilde f$ has the four zeros x_0, x_1, x_2, x_3. By Rolle's theorem, $\tilde f'$ has three zeros in (x_0, x_3), and $\tilde f''$ has two zeros in (x_0, x_3). By definition of K, also $\tilde f''(x_0) = 0$. Hence $\tilde f'''$ also has two zeros in (x_0, x_3) and $\tilde f^{(4)}$ also has (at least) one zero ξ in (x_0, x_3). Since $\omega^{(4)}(x) \equiv 24$ it follows that

$$0 = \tilde f^{(4)}(\xi) = f^{(4)}(\xi) - 0 - 24K,$$

i.e., $K = f^{(4)}(\xi)/24$ or, by definition of K,

$$f''(x_0) - p''(x_0) = \frac{f^{(4)}(\xi)}{24}\omega''(x_0)$$

from which the claim follows by the bound on $|\omega''(x_0)|$. □

Using the estimates of the above lemma yields an R-approximate clamped natural spline with $R = \frac{22}{24} = \frac{11}{12}$.

3.2. Improving the estimate of $f''(x_0)$ and $f''(x_n)$

In view of the proof of Theorem 1, a sharper approximation of $f''(x_0)$ and $f''(x_n)$ would immediately result in a sharper error estimate for $\|s - f\|_\infty$.

To start with, only the available interpolation data and the unknown bound of $\|f^{(4)}\|_\infty$ is used without assuming the existence of $\|f^{(5)}\|_\infty$.

For determining the cubic polynomial of Lemma 4 one can compute the Newton interpolation table of divided differences for f with support points $x_0, \dots, x_3$. Then, a fifth point x_4 is added. The fourth divided difference $f[x_0, x_1, x_2, x_3, x_4] =: \rho$ is the exact value $\frac{f^{(4)}(\xi)}{24}$ for some point $\xi \in (x_0, x_4)$. When forming $\tilde f$ with $\tilde f(x) \equiv f(x) - \rho(x - x_0)^4$ it follows that $\tilde f(\xi)^{(4)} = 0$ and that the first three derivatives of f and of $\tilde f$ at $x = x_0$ coincide.

By construction there is a worst case bound, $\|\tilde f^{(4)}\|_\infty \le 2\|f^{(4)}\|_\infty$, and since $\tilde f(\xi)^{(4)} = 0$ we may hope that on the interval $[x_0, x_3]$ we have in fact $\|\tilde f^{(4)}\|_\infty < \|f^{(4)}\|_\infty$, possibly much smaller.

We can then form the cubic interpolation $\tilde c$ of $\tilde f$ on $[x_0, x_1, x_2, x_3]$ and use $\tilde c''(x_0)$ as estimate for $f''(x_0)$. Likewise for the estimate of $f''(x_n)$. The approximate clamped natural spline using these estimates for $f''(x_0)$ and $f''(x_n)$ is called **Q-spline** in the sequel – being based on a quartic correction term $-\rho(x - x_0)^4$. It will at most double the approximation error R compared to the spline based on Lemma 4, but will hopefully reduce it instead.

To quantify this hope one can revisit the divided differences observing that the first divided difference also satisfies the relation

$$f[x_0, x_1] := \frac{f[x_1]-f[x_0]}{x_1-x_0} = \int_0^1 f'(x_0 + t(x_1 - x_0))dt.$$

It coincides with the value $f'(\xi^{(1)})$ for some $\xi^{(1)} \in [x_0, x_1]$ but it can also be seen as the average value of f' on $[x_0, x_1]$. Likewise the k-th divided differences form certain average values of the k-th derivatives of f divided by "$k!$". Estimating the changes of such average value of $f^{(4)}$ can be done "in principle" without using the fifth derivative, but this seems to be very tedious. Since in practical applications the situation is rare that the fourth derivative exists but the fifth does not, the following simpler analysis assuming the existence of the fifth derivative is detailed:

Define $\|f^{(5)}\|_\infty := \infty$ if the fifth derivative of f is not continuous and else set $\|f^{(5)}\|_\infty$ as maximum absolute value of $f^{(5)}$ on $[x_0, x_4]$. Observe that the cubic interpolation $\tilde c$ coincides with the degree-at-most-4-polynomial $\tilde p$ that interpolates $\tilde f$ at $x_0, \dots, x_4$. (The divided differences for a function f linearly depend on f so that the fourth divided difference for $\tilde f$ is zero.) When $\|f^{(5)}\|_\infty$ is finite, a proof analogous to the one of Lemma 4 yields that

$$|\tilde p''(x_0) - f''(x_0)| \le R\left|f^{(5)}(\xi)h^2\right|$$

where $\xi \in (x_0, x_4)$ and $R = R(h) = \frac{5h}{12}$. (The bound on $|\omega''(x_0)|$ is given by $50h^5$ which is divided by factorial of 5 leading to $\frac{5h}{12}h^4$.)

Summarizing, we obtain the following theorem:

Theorem 2. *Let $x_0 < x_1 < \ldots < x_n$ with $n \geq 4$ be given and a four times continuously differentiable function $f : [x_0, x_n] \to \mathbb{R}$. Define*

$$\|f^{(5)}\|_\infty := \begin{cases} \infty & \text{if the fifth derivative of } f \text{ is not continuous} \\ \max_{x\in[x_0,x_4]\cup[x_{n-4},x_n]} |f^{(5)}(x)| & \text{else} \end{cases}$$

(If $f^{(5)}$ does not exist it is interpreted as not continuous.) Approximate $f''(x_0)$ by $p''(x_0)$ where p is the fourth order polynomial interpolating f on $x_0, \ldots, x_4$. Likewise for $f''(x_n)$. Let s be the Q-spline using these approximate values in place of $f''(x_0)$ and $f''(x_n)$. For $x \in [x_0, x_n]$ the spline s then satisfies

$$|s(x) - f(x)| \leq \left(\frac{5}{384} + \frac{R}{8}\right)\|f^{(4)}\|_\infty h^4.$$

where $R = \min\{\frac{11}{6}, \frac{5h\|f^{(5)}\|_\infty}{12\|f^{(4)}\|_\infty}\}$.

(In the trivial case that $\|f^{(4)}\|_\infty = 0$ it follows that also $\|f^{(5)}\|_\infty = 0$ and the ratio $\frac{5h\|f^{(5)}\|_\infty}{12\|f^{(4)}\|_\infty}$ in Theorem 2 can be replaced with 0.)

The bound in Theorem 2 is not best possible but it is always a fourth order approximation, and when $f^{(5)}$ exists and is continuous at both end points, then for $h \to 0$ it is arbitrarily close to the best possible bound derived in [2] – but (!) without using any derivative information. To our knowledge this is the only explicit fourth order bound on the error of a cubic spline approximation on an arbitrary set of knots in the absence of any derivative information.

The natural spline in turn only is a second order approximation as noted in the next corollary.

Corollary 1. *Under the assumptions of Theorem 2, the error of the natural spline s (with $s''(x_0) = s''(x_n) = 0$) is of the exact order h^2 when $|f''(x_0)| + |f''(x_n)| > 0$.*

Proof. Assume without loss of generality that $f''(x_0) = \delta > 0$. The $O(h^2)$ upper bound for the error can be established as in the proof of Theorem 2 using that $|s''(x_0) - f''(x_0)| = |f''(x_0)| = O(1)$ rather than $O(h^2)$. For the lower bound observe that for small h the inequality $0.8\delta \leq f''(x) \leq 1.2\delta$ for $x \in [x_0, x_1]$ is true. Since s'' is linear on $[x_0, x_1]$ with $s''(x_0) = 0$, either $s''(x) - f''(x) < -0.2\delta$ for $x \in [x_0, x_0 + \frac{h}{4}]$ or $s''(x) - f''(x) > 0.2\delta$ for $x \in [x_1 - \frac{h}{4}, x_1]$. Both lead to an order h^2 maximum value of $|s''(x) - f''(x)|$ for $x \in [x_0, x_1]$. □

3.2.1. A heuristic error bound

When $n \geq 5$, lower bounds for $\|f^{(4)}\|_\infty/24$ and for $\|f^{(5)}\|_\infty/120$ can be computed by the fourth and fifth divided differences for f near x_0. Using these values as estimates for the true values leads to an error bound where the term R in Theorem 2 can be estimated as $R \lessapprox \min\left\{\frac{11}{6}, \frac{25h|f[x_0,x_1,x_2,x_3,x_4,x_5]|}{12|f[x_0,x_1,x_2,x_3,x_4]|}\right\}$ with $h := \max_{0\leq i\leq 4}(x_{i+1} - x_i)$. (Likewise for the other end point x_n.)

4. A revised not-a-knot spline

By Theorem 2, for small h, the Q-spline is optimal or near optimal. To be of practical relevance however, a spline must be found that improves over the not-a-knot spline (**NAK-spline**) in more general situations, also for large h and irregular data points. We observe at first that it is impossible to improve over the NAK-spline in *all* situations, because f might just happen to be equal to the NAK-spline or might be a very close C^4-approximation to the NAK-spline. The numerical results in the next section show an approximation quality of the NAK-spline that is comparable to the (nearly optimal) Q-spline. A possible explanation for this observation might be the consistent spline property that was observed in Section 2 In the interval $[x_0, x_2]$ the NAK-spline is a cubic interpolating function with somewhat good approximation properties to the first two derivatives of f at x_2 due to the consistent spline property. To further improve this approximation, the observation can be used that the fourth divided difference $f[x_0, x_1, x_2, x_3, x_4] =: \rho$ of f generates some average value of $f^{(4)}/24$ on (x_0, x_4). If $f^{(4)}$ was constant on (x_0, x_4), the best piecewise constant approximation s''' of f''' would not require s''' to be continuous at x_1 (as in the case of the NAK-spline) but that the jump of s''' at x_1 is roughly given by $\delta_1 := 12\rho(x_2 - x_0) = \frac{1}{2}f^{(4)} \cdot (x_2 - x_0)$. (This is the best staircase approximation of a linear function with slope $f^{(4)}$ for any choice of $x_1 \in (x_0, x_2)$.) The revised not-a-knot-spline (**RNAK-spline**) therefore requires a jump δ_1 of s''' at x_1. And again, similarly for the jump δ_2 of s''' at x_{n-1}.

4.1. A practical safeguard

For the RNAK-spline, the jumps δ_1 and δ_2 of s''' at the points x_1 and x_{n-1} are based on a finite difference estimate of $f^{(4)}$.

When the mesh sizes $x_{i+1} - x_i$ near the end points are sufficiently small, this indeed seems to be an improvement over the NAK-spline, as illustrated in Section 5 But when the changes in the fourth derivative $f^{(4)}$ of f on the interval (x_0, x_4) or on (x_{n-4}, x_n) are large, it may happen that the finite difference estimate of $f^{(4)}$ is poor and that the NAK-spline leads to a better approximation than the RNAK-spline. In order to reduce the chances that this happens, a finite difference estimate of the fifth derivative can be used to damp the jump of s''' at the point x_1 or x_{n-1} when the estimate of $|f^{(5)}|$ is large. The following heuristic safety-criterion is independent of scalings $f(.) \mapsto \lambda f(.)$ or $f(.) \mapsto f(\lambda\,.)$. As in Section 3.2.1 it is based on the quotient of $f_{(5)}$ and $f_{(4)}$ where $f_{(k)} := f[x_0, \ldots, x_k]$ is the k-th divided difference for $k \geq 1$.

The value of ρ in the definition of the RNAK-spline is $\rho = f_{(4)} = f^{(4)}(\xi)/24$ for some point $\xi \in (x_0, x_4)$. This is used as an approximation of the average value of $f^{(4)}/24$ on the interval (x_0, x_2). If $f_{(4)} \cdot f_{(5)} > 0$ indicating a growth of $|f^{(4)}|$ on (x_0, x_4) with smaller

Table 1
Errors $\|s - f\|_\infty$ for $f(x) \equiv \sin(x)$ on $[0, \pi]$, equidistant knots.

# knots	6	12	24	48	96
NAT-spline	4.5e-4	1.8e-5	9.1e-7	5.2e-8	3.1e-09
NAK-spline	2.7e-3	5.5e-5	1.4e-6	5.2e-8	3.1e-09
Q-spline	2.2e-3	4.0e-5	9.6e-7	5.2e-8	3.1e-09
RNAK-spline	1.6e-3	1.8e-5	9.1e-7	5.2e-8	3.1e-09

Table 2
Errors $\|s - f\|_\infty$ for $f(x) \equiv \sin(x)$ on $[\pi/4, 5\pi/4]$, equidistant knots.

# knots	6	12	24	48	96
NAT-spline	1.4e-2	2.9e-3	6.5e-4	1.6e-4	3.8e-5
NAK-spline	4.3e-3	1.7e-4	7.9e-6	4.3e-7	2.5e-8
Q-spline	1.6e-3	5.5e-5	2.2e-6	1.1e-7	6.0e-9
RNAK-spline	6.6e-4	4.6e-5	9.1e-7	5.2e-8	3.1e-9

Table 3
Errors $\|s - f\|_\infty$ for $f(x) \equiv \sin(x)$ on $[\pi/4, 5\pi/4]$, irregular meshes.

# knots	6	12	24	48	96
NAT-spline	4.2e-2	1.2e-3	5.2e-4	1.7e-4	3.4e-4
NAK-spline	4.7e-2	1.2e-3	5.2e-4	1.4e-5	8.5e-7
Q-spline	4.6e-2	1.2e-3	5.2e-4	1.4e-5	8.5e-7
RNAK-spline	4.7e-2	1.2e-3	5.2e-4	1.4e-5	8.5e-7

Table 4
Errors $\|s - f\|_\infty$ for $f(x) \equiv 1/(1 + x^2)$ on $[-1, 3]$, irregular meshes.

# knots	6	12	24	48	96
NAT-spline	1.1e-1	1.5e-2	1.7e-3	1.8e-4	5.7e-5
NAK-spline	1.4e-1	6.2e-3	1.3e-3	1.8e-4	3.6e-5
Q-spline	2.7e-1	3.0e-2	1.3e-3	1.8e-4	3.6e-5
RNAK-spline	2.5e-1	2.1e-2	1.3e-3	1.8e-4	3.6e-5

values near x_0, the absolute value of $\rho = f_{(4)}$ in the definition of δ_1 is reduced and δ_1 is multiplied with $\max\{1 - \frac{5f_{(5)}(x_4-x_2)}{2f_{(4)}},\ 0\} \in [0, 1)$ moving the RNAK-spline closer to the NAK-spline.

Again, likewise for the right end point.

5. Numerical examples

In selected numerical examples the not-a-knot spline (NAK-spline) is compared with the natural spline (NAT-spline, $s''(a) = s''(b) = 0$), the Q-spline of Theorem 2, and the RNAK-spline (revised NAK-spline). The various splines were evaluated by computing (in parallel) the natural spline s_{nat} and two zero-interpolating splines s_1, s_2 with end conditions $s_1''(x_0) = 1,\ s_1''(x_n) = 0$, and $s_2''(x_0) = 0,\ s_2''(x_n) = 1$, and then determining α, β to form the final spline $s_{nat} + \alpha s_1 + \beta s_2$.

Tables 1 and 2 illustrate the result that the NAT-spline on an interval $[a, b]$ has an excellent approximation guarantee when $f''(a) = f''(b) = 0$ but only a second order approximation guarantee when $f''(a) \neq 0$ or $f''(b) \neq 0$ (as stated in Corollary 1). In comparison, for small h, the NAK-spline and the Q-spline display a low error independent of $f''(a)$ or $f''(b)$. To eliminate effects resulting from irregularities of the mesh, an equidistant mesh with 6,12,24,48, and 96 knots is considered first.

(In the last column of Table 1 the errors of all four splines coincided up to 15 digits; the maximum error was in the middle, where all splines coincide up to machine precision. Near the end points NAT was best followed by RNAK, Q, and NAK)

In Table 3 irregular meshes are considered with a random uniform distribution scaled such that the endpoints coincide with the end points of the given interval. For such irregular meshes, the observation that the natural spline results in a larger approximation error compared to the other three splines can be observed in Table 3 as well.

Table 3 illustrates the observation from several plots (not listed here) that the maximum error may occur in some sub-interval $[x_i, x_{i+1}]$ in the middle where $x_{i+1} - x_i$ is large and where several or all of the spline functions almost coincide.

The function f considered in Table 4 is due to Runge [4] who chose it as an example that polynomial interpolation may result in high error terms when f has poles in the complex plane (here at $\pm i$) near the domain of interpolation. For $n = 12$ the best approximation on the irregular mesh happened to be given by the NAK-spline illustrating the difficulty in identifying the cases where the NAK-spline

Table 5
Errors $\|s - f\|_\infty$ for $f(x) \equiv 1/(1 + exp(-x))$ on $[-1, 4]$, regular meshes.

# knots	6	12	24	48	96
NAT-spline	5.5e-3	9.6e-4	2.1e-4	5.1e-5	1.2e-5
NAK-spline	5.8e-4	1.3e-4	8.0e-6	4.6e-7	2.7e-8
Q-spline	2.3e-3	1.1e-4	8.2e-7	1.0e-7	6.6e-9
RNAK-spline	2.1e-3	1.0e-4	1.0e-6	4.4e-8	2.7e-9

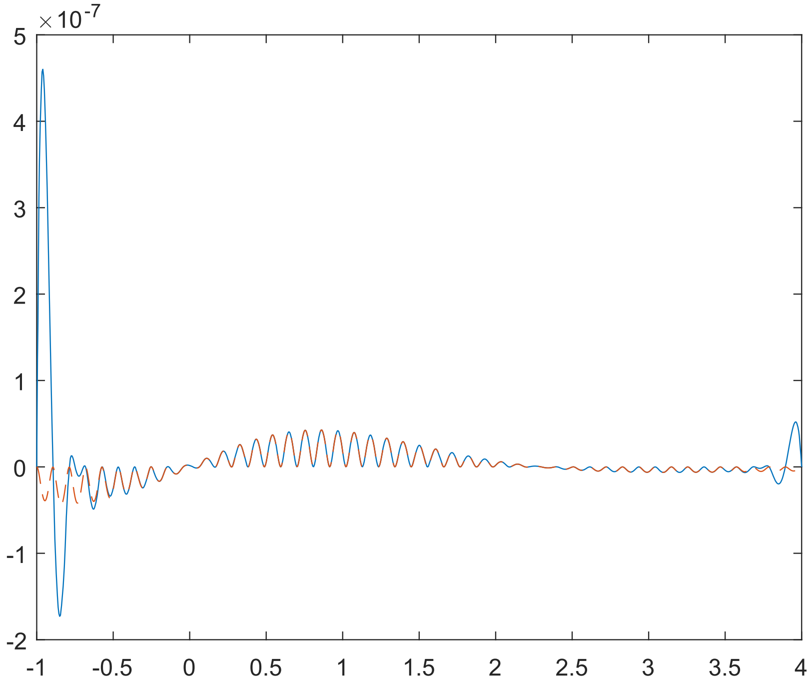

Fig. 4. Graph of $|s_{NAK} - f|$ (blue solid line) and of $|s_{RNAK} - f|$ (red dashed line) – for $f(x) \equiv 1/(1 + exp(-x))$ on $[-1, 4]$ and a regular mesh with 48 knots.

is best and adapting the RNAK-spline accordingly (without using further knowledge about f). The results of Table 4 also repeat the observation of Table 3 that irregular meshes may produce the maximum error terms somewhere in the middle where all splines coincide even though the splines do differ substantially near the end points. In this respect, random knots (of course, all four splines were always tested with the same random knots) are not a good choice for comparing different spline functions, and in a final table considering the logistic function, a regular mesh is used again.

Table 5 with the logistic function $x \mapsto 1/(1 + exp(-x))$ also is an example where the large mesh size in the case $n = 5$ (i.e. 6 knots) can lead to a lower approximation error of the not-a-knot-spline. Identifying such cases where the not-a-knot-spline is best remains an open question.

For illustration, Fig. 4 displays the difference $f(x) - s(x)$ of the logistic function and the NAK-spline (blue solid line) and the RNAK-spline (red dashed line) for the case $n = 48$.

Summarizing, the observation in the examples that were tested is that the NAK-spline and the Q-spline yield similar errors $\|s - f\|_\infty$ while the results of the NAT-spline may be much worse. The NAT-spline is somewhat better than the other splines if the second derivative at the end points happens to be zero or of small magnitude. In all examples, the approximation quality by the RNAK-spline is never much worse than by the NAK-spline and for smaller mesh sizes it is generally a bit better.

6. Conclusion

This work arose from an undergraduate class. It provides a convergence analysis for cubic spline interpolation at given data points without the use of derivative information. A near optimal result could be established when the mesh size is small and the underlying function is five times continuously differentiable. Selected numerical examples illustrate the theoretical results and suggest that the commonly used not-a-knot spline can be improved for small mesh sizes.

Acknowledgments

The author is indebted to an anonymous referee who helped to improve the presentation of the paper and to Melinda Hagedorn and Kevin Wischnewski for their critical comments.

Appendix. pseudo-codes

For the Q-spline a similar safeguard can be used as for the RNAK-spline to reduce the fourth order correction term for the computation of the cubic interpolant when the fifth finite difference is large and its sign indicates that the fourth order finite difference is an overestimate of $f^{(4)}/24$. This is implemented in Step 3. below. (The damping is slightly different from the damping in the RNAK-spline since the RNAK-spline uses a correction term for the intervals $[x_0, x_2]$ and $[x_{n-2}, x_n]$ while the Q-spline uses a correction on the intervals $[x_0, x_3]$ and $[x_{n-3}, x_n]$.)

Q-spline:

1. Input: $n + 1 \geq 6$ points $x_0 < \ldots < x_n$ with associated function values f_i for $0 \leq i \leq n$.
2. Compute the fourth and fifth order finite differences of f near the left end point,
   $\rho := f_{(4)}$ (based on the points $x_0, \ldots, x_4$) and $f_{(5)}$ (based on the points $x_0, \ldots, x_5$).
3. If $f_{(4)} \cdot f_{(5)} > 0$ % the estimate of $f^{(4)}/24$ may be too large
   $\rho := \rho \cdot \max\{0, 1 - \frac{5 \cdot (x_2 - x_1) f l_{(5)}}{2 f l_{(4)}}\}$ % damping based on fifth derivative
4. Compute the cubic interpolant to $\tilde{f}(x) := f(x) - \rho(x - x_0)^4$ at the points $x_0, \ldots, x_3$.
5. Evaluate the second derivative of the cubic interpolant at x_0.
6. Likewise near the right end point x_n, damping the fourth order correction term when $f_{(4)} \cdot f_{(5)} < 0$.
7. Compute the clamped natural spline based on the second derivatives of the cubic interpolants at x_0 and at x_n.

RNAK-spline:

1. Input: $n + 1 \geq 6$ points $x_0 < \ldots < x_n$ with associated function values f_i for $0 \leq i \leq n$.
2. Compute the natural interpolating spline s_{nat}.
3. Compute the spline s_1 interpolating the zero function with moments 1 and 0 at x_0 and x_n, and the spline s_2 interpolating the zero function with moments 0 and 1 at x_0 and x_n.
4. Compute the fourth and fifth order finite differences of f near the left end point,
   $\rho := f_{(4)}$ (based on the points $x_0, \ldots, x_4$) and $f_{(5)}$ (based on the points $x_0, \ldots, x_5$).
5. If $f_{(4)} \cdot f_{(5)} > 0$ % the estimate of $f^{(4)}/24$ may be too large
   $\rho := \rho \cdot \max\{0, 1 - \frac{5 \cdot (x_4 - x_2) f_{(5)}}{2 f_{(4)}}\}$ % damping based on fifth derivative
6. Set $\delta_1 := 12\rho(x_2 - x_0)$ the jump of s''' at x_1.
7. Likewise define the jump δ_2 at the right end point x_{n-1}, damping ρ when $f_{(4)} \cdot f_{(5)} < 0$.
8. Let $jump1(s) := s'''(x_1 + \epsilon) - s'''(x_1 - \epsilon)$ for small $\epsilon > 0$
   and $jump2(s) := s'''(x_{n-1} + \epsilon) - s'''(x_{n-1} - \epsilon)$.
   Solve

$$
\begin{aligned}
jump1(s_{nat}) + \alpha\; jump1(s_1) + \beta\; jump1(s_2) &= \delta_1 \\
jump2(s_{nat}) + \alpha\; jump1(s_2) + \beta\; jump2(s_2) &= \delta_2
\end{aligned}
$$

   for α and β and set $s = s_{nat} + \alpha s_1 + \beta s_2$.

Matlab codes for testing the above splines can be found at
https://github.com/florianjarre/Revised-not-a-knot-spline/tree/main

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