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(Article begins on next page)



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Differentiation Based on Optimal Local Spline Quasi-Interpolants with Applications

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Abstract. In this paper we propose a method for the approximation of the derivative of a function f based on discrete local optimal spline quasi-interpolants Q_k of degree $k = 3, 4, 5$. By differentiating $Q_k f$, we construct the approximation of the derivative at the quasi-interpolation nodes and the corresponding differentiation matrices. Some numerical results and applications to univariate boundary-value problems are given.

Keywords: Spline quasi-interpolants, Numerical differentiation, Spline collocation methods

PACS: 02.60.-x, 02.60.Jh, 02.70.Jn

INTRODUCTION

Local spline quasi-interpolation has been widely analysed in approximation theory (see e.g. [1, 3, 5, 7] and references therein), but only recently some studies have been devoted to its applications in the numerical differentiation [2, 4, 6]. In particular, in [2], the authors focus on approximations of first and second derivatives by those of local quadratic spline quasi-interpolants and their applications to collocation methods. The proposed formulas are very accurate at some points, thanks to the superconvergence properties of those operators and they give rise to good global approximations of derivatives on the whole domain of definition. In this paper, we propose differentiation formulas still based on discrete local spline quasi-interpolants, but of higher degree. We get differentiation matrices, that we use in collocation methods for the solution of some univariate boundary-value problems. We propose the same numerical tests of [2] and we show that spline quasi-interpolants of higher degree and smoothness provide very accurate results. Indeed, the results obtained with cubic splines are comparable to those given in [2] for quadratic case, as we expect from the theory, instead we obtain higher performances with quartic and quintic splines.

APPROXIMATION OF FIRST DERIVATIVES AND DIFFERENTIATION MATRICES

Let $I = [a, b]$ be a bounded interval endowed with a uniform knot partition $\Delta_n = \{x_i = a + ih, \ 0 \leq i \leq n\}$, with $h = (b - a)/n$ and k a non-negative integer. We define the spline space $\mathcal{S}_k^{k-1}(\Delta_n) = \{s \in C^{k-1}(I) : s|_{[x_i, x_{i+1}]} \in \mathbb{P}_k, i = 0, 1, \dots, n-1\}$ where \mathbb{P}_k denotes the space of polynomials in x of degree k .

We denote by $\{N_j^k(x)\}_{j=1}^{n+k}$ the basis of normalized B-splines defined on the extended knot partition $\{x_{-k} = \dots = x_{-1} = x_0 = a, \ x_i, \ 1 \leq i \leq n-1, \ b = x_n = x_{n+1} = \dots = x_{n+k}\}$ and spanning $\mathcal{S}_k^{k-1}(\Delta_n)$ [1]. With our notations the support of the B-spline N_j^k is $[x_{j-k-1}, x_j]$.

We define the following two sets of quasi-interpolation nodes:

- $\mathcal{T}_n^1 = \{t_i, i = 1, \dots, n+2\}$, where $t_1 = a, t_i = \frac{1}{2}(x_{i-2} + x_{i-1}),$ for $i = 2, \dots, n+1, t_{n+2} = b,$ in case k even;
- $\mathcal{T}_n^2 = \{t_i, i = 1, \dots, n+1\}$, where $t_1 = a, t_i = x_{i-1},$ for $i = 2, \dots, n, t_{n+1} = b,$ in case k odd.

Let f be a smooth function, we set $f_j = f(t_j)$ and we consider the spline quasi-interpolants (QI)

$$Q_k f(x) = \sum_{j=1}^{n+k} m_j(f) N_j^k(x) = \begin{cases} \sum_{j=1}^{n+2} f_j \tilde{N}_j^k(x) & k \text{ even} \\ \sum_{j=1}^{n+1} f_j \tilde{N}_j^k(x) & k \text{ odd,} \end{cases} \quad (1)$$

with

- $m_j(f) = \sum_i \lambda_{i,j} f(t_i), \lambda_{i,j} \in \mathbb{R},$ local linear functionals defined as combinations of discrete values of f at the points t_i lying in the support (or near the support) of $N_j^k,$ given in [6] for $k = 2, \dots, 5$ and constructed so that Q_k is exact

on \mathbb{P}_k , i.e. $Q_k p = p$, $p \in \mathbb{P}_k$. Consequently, $\|f - Q_k f\|_\infty = O(h^{k+1})$, for $f \in C^{k+1}(I)$;

- \tilde{N}_j^k the so-called fundamental functions associated with Q_k , given by linear combinations of B-splines N_j^k and obtained, after some algebra, from the expression of the functionals m_j .

We approximate the derivative of f by the derivative of $Q_k f$. We denote it by $Q'_k f$ and we remark that it belongs to $\mathcal{S}_{k-1}^{k-2}(\Delta_n)$, the spline space of degree $k-1$ defined on Δ_n . From (1), we obtain

$$Q'_k f(x) = \left(\sum_{j=1}^{n+k} m_j(f) N_j^k(x) \right)' = \begin{cases} \sum_{j=1}^{n+2} f_j \left(\tilde{N}_j^k \right)'(x) & k \text{ even} \\ \sum_{j=1}^{n+1} f_j \left(\tilde{N}_j^k \right)'(x) & k \text{ odd.} \end{cases} \quad (2)$$

If we approximate f' at the quasi-interpolation nodes we have to evaluate (2) at the points of \mathcal{T}_n^1 if k is even and \mathcal{T}_n^2 if k is odd. The values $\left(\tilde{N}_j^k \right)'(t_i)$, computed using the differentiation formula for the B-splines N_j^k (see [1]), can be stored in the differentiation matrix D_k , where $D_k \in \mathbb{R}^{(n+2) \times (n+2)}$ for k even and $D_k \in \mathbb{R}^{(n+1) \times (n+1)}$ for k odd.

Setting \mathbf{y} for the vector with components $y_j = f(t_j)$ and \mathbf{y}' for the vector with components $y'_j = Q'_k f(t_j)$, we get:

$$\mathbf{y}' = D_k \mathbf{y}, \quad (3)$$

where the matrix D_k has elements $d_{ij} = \left(\tilde{N}_j^k \right)'(t_i)$ and the following structure:

$$D_k = \frac{1}{h} \begin{pmatrix} D_k^{(1)} \\ D_k^{(2)} \\ D_k^{(3)} \end{pmatrix}, \quad \text{with} \quad D_k^{(1)}, D_k^{(3)} \in \begin{cases} \mathbb{R}^{(k+1) \times (n+2)} & \text{if } k \text{ even} \\ \mathbb{R}^{(k-1) \times (n+1)} & \text{if } k \text{ odd} \end{cases}, \quad D_k^{(2)} \in \begin{cases} \mathbb{R}^{(n-2k) \times (n+2)} & \text{if } k \text{ even} \\ \mathbb{R}^{(n-2k+3) \times (n+1)} & \text{if } k \text{ odd} \end{cases}$$

and

$$\begin{aligned} \bullet D_k^{(1)} = (d_{ij}) & \begin{cases} \neq 0 & 1 \leq i \leq k+1, 1 \leq j \leq i+k, & \text{if } k \text{ even} \\ \neq 0 & i=1, 1 \leq j \leq i+k; 2 \leq i \leq k-1, 1 \leq j \leq i+k-1, & \text{if } k \text{ odd} \\ = 0 & \text{otherwise} \end{cases} \\ \bullet D_k^{(2)} = (d_{ij}) & \begin{cases} \neq 0 & k+2 \leq i \leq n-k+1, i-k \leq j \leq i+k, j \neq i & \text{if } k \text{ even} \\ \neq 0 & k \leq i \leq n-k+2, i-k+1 \leq j \leq i+k-1, j \neq i & \text{if } k \text{ odd} \\ = 0 & \text{otherwise} \end{cases} \\ \bullet D_k^{(3)} = (d_{ij}) & \begin{cases} = -d_{n-i+3, n-j+3} & n-k+2 \leq i \leq n+2, i-k \leq j \leq n+2, & \text{if } k \text{ even} \\ = -d_{n-i+2, n-j+2} & n-k+3 \leq i \leq n, i-k+1 \leq j \leq n+1; i=n+1, i-k \leq j \leq n+1, & \text{if } k \text{ odd} \\ = 0 & \text{otherwise.} \end{cases} \end{aligned}$$

Now we report the nonzero elements of the differentiation matrices for quartic and quintic splines, i.e. $k=4$ and $k=5$, respectively:

- D_4

$$- D_4^{(1)} \in \mathbb{R}^{5 \times (n+2)}:$$

$$\begin{array}{ccccc} d_{11} = -352/105, & d_{12} = 35/8, & d_{13} = -35/24, & d_{14} = 21/40, & d_{15} = -5/56, \\ d_{21} = -13871/15120, & d_{22} = 357/2048, & d_{23} = 4561/4608, & d_{24} = -1489/5120, & d_{25} = 155/3584, \\ d_{26} = 47/55296, & & & & \\ d_{31} = 3767/15120, & d_{32} = -23887/27648, & d_{33} = -641/55296, & d_{34} = 26119/34560, & d_{35} = -27317/193536, \\ d_{36} = 101/9216, & d_{37} = 47/55296, & & & \\ d_{41} = -841/15120, & d_{42} = 1417/6912, & d_{43} = -7133/9216, & d_{44} = 1513/92160, & d_{45} = 35419/48384, \\ d_{46} = -3751/27648, & d_{47} = 101/9216, & d_{48} = 47/55296, & & \\ d_{51} = -47/15120, & d_{52} = -209/27648, & d_{53} = 463/3456, & d_{54} = -101521/138240, & d_{55} = -47/387072, \\ d_{56} = 20323/27648, & d_{57} = -3751/27648, & d_{58} = 101/9216, & d_{59} = 47/55296, & \end{array}$$

$$- D_4^{(2)} \in \mathbb{R}^{(n-8) \times (n+2)}:$$

$$\begin{aligned} d_{i,i-4} = -d_{i,i+4} = -47/55296, & \quad d_{i,i-3} = -d_{i,i+3} = -101/9216, & \quad d_{i,i-2} = -d_{i,i+2} = 3751/27648, \\ d_{i,i-1} = -d_{i,i+1} = -20323/27648, & \quad d_{i,i} = 0, \quad i = 6, \dots, n-3, \end{aligned}$$

$$- D_4^{(3)} \in \mathbb{R}^{5 \times (n+2)}, \text{ defined by the elements of } D_4^{(1)}.$$

• D_5

– $D_5^{(1)} \in \mathbb{R}^{4 \times (n+1)}$:

$$\begin{aligned} d_{11} &= -137/60, & d_{12} &= 5, & d_{13} &= -5, & d_{14} &= 10/3, & d_{15} &= -5/4, & d_{16} &= 1/5, \\ d_{21} &= -1/5, & d_{22} &= -13/12, & d_{23} &= 2, & d_{24} &= -1, & d_{25} &= 1/3, & d_{26} &= -1/20, \\ d_{31} &= 301/5760, & d_{32} &= -493/960, & d_{33} &= -115/384, & d_{34} &= 275/288, & d_{35} &= -83/384, & d_{36} &= 19/960, \\ d_{37} &= 13/5760, \\ d_{41} &= -1/60, & d_{42} &= 877/5760, & d_{43} &= -733/960, & d_{44} &= 13/384, & d_{45} &= 203/288, & d_{46} &= -223/1920, \\ d_{47} &= 1/320, & d_{48} &= 13/5760, \end{aligned}$$

– $D_5^{(2)} \in \mathbb{R}^{(n-7) \times (n+1)}$:

$$\begin{aligned} d_{i,i-4} &= -d_{i,i+4} = -13/5760, & d_{i,i-3} &= -d_{i,i+3} = -1/320, & d_{i,i-2} &= -d_{i,i+2} = 341/2880, \\ d_{i,i-1} &= -d_{i,i+1} = -2069/2880, & d_{i,i} &= 0, & i &= 5, \dots, n-3, \end{aligned}$$

– $D_5^{(3)} \in \mathbb{R}^{4 \times (n+1)}$, defined by the elements of $D_5^{(1)}$.

For the cubic case $k = 3$ see [6], where the matrix D_3 is given.

In order to analyse the error $(f - Q_k f)'$ at the quasi-interpolation nodes t_i , we consider (3) and we compute the Taylor expansion of f at these nodes. With the help of a computer algebra system, we get the following results.

Proposition 1 For sufficiently smooth functions f , the error at the quasi-interpolation nodes t_i is given by:

• for $k = 3$

$$\begin{aligned} |y'_i - f'_i| &= \frac{h^3}{4} |f_i^{(4)}| + O(h^4), \quad i = 1, n+1, & |y'_i - f'_i| &= \frac{h^3}{12} |f_i^{(4)}| + O(h^4), \quad i = 2, n, \\ |y'_i - f'_i| &= \frac{h^4}{30} |f_i^{(5)}| + O(h^6), \quad i = 3, \dots, n-1; \end{aligned}$$

• for $k = 4$

$$\begin{aligned} |y'_i - f'_i| &= \frac{7}{128} h^4 |f_i^{(5)}| + O(h^5), \quad i = 1, n+2, & |y'_i - f'_i| &= \frac{1583}{61440} h^4 |f_i^{(5)}| + O(h^5), \quad i = 2, n+1, \\ |y'_i - f'_i| &= \frac{1157}{110592} h^4 |f_i^{(5)}| + O(h^5), \quad i = 3, n, & |y'_i - f'_i| &= \frac{661}{184320} h^4 |f_i^{(5)}| + O(h^5), \quad i = 4, n-1, \\ |y'_i - f'_i| &= \frac{719}{552960} h^4 |f_i^{(5)}| + O(h^5), \quad i = 5, n-2, & |y'_i - f'_i| &= \frac{7}{5760} h^4 |f_i^{(5)}| + O(h^6), \quad i = 6, \dots, n-3. \end{aligned}$$

• for $k = 5$

$$\begin{aligned} |y'_i - f'_i| &= \frac{h^5}{6} |f_i^{(6)}| + O(h^6), \quad i = 1, n+1, & |y'_i - f'_i| &= \frac{h^5}{30} |f_i^{(6)}| + O(h^6), \quad i = 2, n, \\ |y'_i - f'_i| &= \frac{109}{5760} h^5 |f_i^{(6)}| + O(h^6), \quad i = 3, n-1, & |y'_i - f'_i| &= \frac{13}{5760} h^5 |f_i^{(6)}| + O(h^6), \quad i = 4, n-2, \\ |y'_i - f'_i| &= \frac{47}{4032} h^6 |f_i^{(7)}| + O(h^8), \quad i = 5, \dots, n-3. \end{aligned}$$

Since the global approximation error $(f - Q_k f)'$ is $O(h^k)$ [3], there appears a superconvergence phenomenon for the odd cases $k = 3, 5$ at the inner quasi-interpolation nodes.

Now we propose the following two examples of approximation of derivatives by the above formulas, in case $k = 3, 4, 5$ and we compare them with the results obtained in [2] by differentiation formulas based on quadratic quasi-interpolating splines. The test functions are $f = \phi_j$, $j = 1, 2$ on $I = [-1, 1]$, with $\phi_1(x) = \frac{1}{4}(1 - x^2)^2$ and $\phi_2(x) = \sin(\pi x) + \sin(5\pi x)$. We compute $\max_{v \in V} |f'(v) - Q'_k f(v)|$, where $V = \mathcal{T}_n^1$ for k even and $V = \mathcal{T}_n^2$ for k odd. These maximum absolute errors are reported in Table 1 for increasing values of n and they confirm the results of Proposition 1. As expected, we can notice that ϕ_1' is exactly reproduced using quartic and quintic splines.

COLLOCATION METHODS FOR UNIVARIATE BOUNDARY-VALUE PROBLEMS

We consider the following boundary-value problem

$$\begin{cases} \frac{d}{dx} \left(p(x) \frac{du(x)}{dx} \right) + r(x)u(x) = f(x), & \text{for } x \in I; \\ u(a) = u(b) = 0, \end{cases} \quad (4)$$

TABLE 1. Maximum absolute errors.

n		$k = 2$ [2]	$k = 3$	$k = 4$	$k = 5$		$k = 2$ [2]	$k = 3$	$k = 4$	$k = 5$
8	ϕ_1	6.5(-3)	2.3(-2)	5.6(-17)	5.5(-17)	ϕ_2	30.8	30.9	19.7	58.9
16		8.1(-4)	2.9(-3)	1.4(-16)	1.4(-16)		13.9	14.0	6.6	28.7
32		1.0(-4)	3.7(-4)	3.1(-16)	1.7(-16)		3.1	3.1	1.9(-1)	1.7
64		1.3(-5)	4.6(-5)	7.8(-16)	6.7(-16)		2.5(-1)	2.5(-1)	3.8(-2)	6.2(-2)
128		1.6(-6)	5.7(-6)	1.6(-15)	1.8(-15)		1.7(-2)	1.7(-2)	2.9(-3)	1.2(-3)

where $p \in C^1(I)$, $r \in C(I)$ and f is a piecewise continuous function on I . We can use the QIs previously considered and their differentiation matrices to solve this problem.

Let \mathbf{u} be the vector of unknown values of u at the points $\{t_i, i \in \mathcal{I}\}$, $\mathcal{I} = \{2, \dots, n+1\}$ if k is even and $\mathcal{I} = \{2, \dots, n\}$ if k is odd, and let $\tilde{\mathbf{u}}$ be the augmented vector with 0 as first and last elements. Considering $D_k \tilde{\mathbf{u}}$ we obtain an approximation of u' at the quasi-interpolation nodes. Then, we multiply this vector by the diagonal matrix P , with $P(i, i) = p(t_i)$ ($t_i \in \mathcal{T}_n^1$ if k is even, $t_i \in \mathcal{T}_n^2$ if k is odd) and we multiply again by D_k . Denoting by R the diagonal matrix defined by $R(i, i) = r(t_i)$ ($t_i \in \mathcal{T}_n^1$ if k is even, $t_i \in \mathcal{T}_n^2$ if k is odd), we see that the left-hand side of the differential equation (4) is approximated by the vector

$$\tilde{A}\tilde{\mathbf{u}} := (-D_k P D_k + R)\tilde{\mathbf{u}}.$$

Let A be the matrix deduced from \tilde{A} by deleting the first and last rows and columns, it is well-known ([8] Chap.7) that the problem is equivalent to solve the linear system $A\mathbf{u} = \mathbf{f}$, where \mathbf{f} is the vector of components $f(t_i)$, $i \in \mathcal{I}$.

We propose the following two test problems:

- Test 1: $-u''(x) + u(x) = (1 + \pi^2) \sin(\pi x)$, $u(-1) = u(1) = 0$, where $u(x) = \sin(\pi x)$.
 Test 2: $-u''(x) + u(x) = \exp\left(\frac{x}{2}\right) \left((100\pi^2 + \frac{3}{4}) \sin(10\pi x) - 10\pi \cos(10\pi x) \right) + (9\pi^2 + 1) \sin(3\pi x)$,
 $u(-1) = u(1) = 0$, where $u(x) = \exp\left(\frac{x}{2}\right) \sin(10\pi x) + \sin(3\pi x)$.

We compute $\max_{i \in \mathcal{I}} |u(t_i) - \mathbf{u}(i)|$, reporting our results in Table 2, for $k = 3, 4, 5$. If we compare them with those obtained in [2], in case $k = 2$ (also reported in Table 2), we can remark the good performances of the formulas based on high degree QIs.

TABLE 2. Maximum absolute errors.

n		$k = 2$ [2]	$k = 3$	$k = 4$	$k = 5$		$k = 2$ [2]	$k = 3$	$k = 4$	$k = 5$
8	Test 1	1.8(-2)	2.3(-2)	5.4(-3)	3.6(-3)	Test 2	39	41	34	38
16		1.2(-3)	1.3(-3)	2.1(-4)	1.0(-4)		22	22	16	19
32		7.6(-5)	8.2(-5)	7.6(-6)	1.6(-6)		2.9	3.4	1.5	2.8
64		4.8(-6)	5.3(-6)	3.3(-7)	2.2(-8)		1.2(-1)	2.4(-1)	2.3(-2)	5.3(-2)
128		3.0(-7)	3.4(-7)	1.7(-8)	3.2(-10)		6.3(-3)	1.4(-2)	1.2(-3)	9.7(-4)

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