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High order interpolation and differentiation using B-splines

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Abstract

We present a methodology of high order accuracy that constructs in a systematic way functions which can be used for the accurate interpolation and differentiation of scattered data. The functions are based on linear combination of polynomials (herein B-splines are used). The technique is applied to one-dimensional datasets but can be extended as needed for multidimensional interpolation and differentiation. The methodology can also construct one-sided functions for high-order interpolation and differentiation. The constructed functions possess compact support. The penalty for the high order of accuracy is the need to solve a system of $L \times L$ equations where L is the order of the approximation. In order to have a robust solution of the $L \times L$ system the singular value decomposition technique was adopted. The proposed technique can also be applied in the context of other methods, in order to increase their accuracy. The main novel features of the technique are that no grid-based information (connectivity) is necessary and a minimum number of samples are required to achieve the desired order of approximation. The order of the approximation is not affected when more samples than the minimum necessary are added in the domain of influence.

1. Introduction

The reconstruction of continuous functions and/or their derivatives from a set of samples is a fundamental operation, with applications in many areas such as, signal processing [1], image analysis [1–4], visualization [5] and particle methods [6–8]. In most of the cases it is necessary to interpolate from discrete samples to intermediate values. Meijering [1] presented a thorough chronological overview of the developments in interpolation theory.

In most of the cases, the interpolation is based on the approximation of a sufficiently smooth function f through a kernel function W based on integral interpolant theory [9,10] or, more generally, on the approximation theory using convolution operators [11]. The kernel function is the essence of the interpolation algorithms and the trends in the interpolation techniques are focused on the improvement of the kernel

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function (better accuracy and/or reduction of the computational cost). In image and signal processing, interpolation is one of the fundamental tools. Extensive comparison and evaluation of the interpolation functions can be found in [2–4]. The particles methods [12] with best representatives particle-in-cell (PIC) [13–15], the vortex particle methods [8,16] and smooth particle hydrodynamics (SPH) [6,17,18] are using interpolation or differentiation based on the same principles. As examples of significant progresses of the interpolation functions we mention the fundamental set of interpolating kernels introduced by Schoenberg [9,10] and the construction of higher order kernels either by forcing the Taylor series of the sampled function to agree in as many terms as possible with the original signal [19], or by increasing the accuracy of the interpolation functions in a systematic way through extrapolation [20]. Both Keys [19] and Monaghan [20] derived the same kernel function W_4 (or M_4') or cubic convolution interpolation, which is one of the commonly and successfully used functions in particle methods [8,16] and image analysis [1–4]. Recent improvements are based on Taylor series expansion [21] or on design of functions close to the *sinc* function [22] or on linear combination of shifted versions of compactly-supported basis functions [23]. More extended review and references about the development of the interpolation methods can be found in [1].

Summarizing, we can conclude that there is an extended investigation and development for interpolation from uniform (equidistant) spaced samples. The interpolation is, most of the times, based on symmetric polynomial functions (usually splines) with compact support. The above characteristics (or assumptions) are often met in image and signal process. However, this is not the case in particle methods (like SPH). In addition, to the best of our knowledge, there is no significant body of work on non-symmetric or one-sided interpolation or differentiation functions, which can be useful for interpolation or differentiation near discontinuities or boundaries, with the exception of the first order nearest grid point (NGP) interpolation [7] and the second order biased ordinary interpolation shown in [24] (not a continuous function) and the recently proposed continuous function [25] (for staggered grids). In addition, during the proof stage of this paper a research report related to spline interpolation was brought to our attention by its author [26].

The aim of the present paper is to derive a technique that can reproduce kernel functions in a systematic way. The constructed kernels are characterized by high order of approximation, compact support, and can be applied to arbitrarily ordered samples. Additionally, the technique can produce centered or one-sided functions. The constructed functions presented herein are based on the centered B-splines introduced by Schoenberg [9,10]. Extension to different families of polynomial functions is also possible. The approximation optimization of the kernel function is based on the linear combination of functions with compact support (as in [20,23]) by matching terms in the Taylor series expansion (as in [19,21]). The proposed methodology can reproduce already existing functions for equidistant samples, which are based on B-splines like W_4 (or M_4') [20]. The penalty of the high order of accuracy for arbitrary sample is that one needs to solve, in the worst case scenario, a system of $L \times L$ equations, where L is the order of the approximation. The additional computational cost of the proposed methodology is deemed to be small compared to other relevant interpolation schemes. We believe that the present methodology is a significant step towards high order multidimensional interpolation and differentiation from arbitrarily sampled data.

The present paper is organized in two sections: In Section 2, we outline the basic mathematical framework in which the proposed technique is based. In Section 3, the interpolation and differentiation technique is evaluated for equidistant and non-equidistant samples using symmetric and one sided support.

2. Mathematical formulation

2.1. Integral interpolation – Taylor series expansion

Starting from integral interpolant theory, a linear interpolation operator, can be written in the form

$$\langle f(x)\rangle = \int_D f(x')\delta(x - x')\mathrm{d}x', \tag{1}$$

where x is a location vector, $f(x)$ is the interpolated function, D is the domain ($D = R^n$), δ is the delta function and the symbol $\langle\cdot\rangle$ denotes the approximated interpolation value. Instead of the delta function, a function W can be used

$$\langle f(x,h)\rangle = \int_D f(x')W(x - x', h)\mathrm{d}x', \tag{2}$$

where h is a scaling variable with dimensions of length and is termed the smoothing length, because it controls the degree to which the kernel W is spread in space. Note that it determines the domain of influence of the kernel and does not refer to any other separation distance. The function W is the key element the approximation and has the following properties:

$$\begin{aligned} &\int_D W(r - r', h)\mathrm{d}r' = 1, \\ &\langle f(r,h)\rangle \to f(r), \quad h \to 0. \end{aligned} \tag{3}$$

If we consider that the function f is known at a set of points $\{x_1, x_2, \ldots, x_N\}$ the operator (2) can approximated numerically using quadrature

$$\langle f(x,h)\rangle = \sum_{j=1}^{N} \frac{f_j}{n_j} W(x - x_j, h), \tag{4}$$

where $f_j \equiv f(x_j)$ and $n_j \equiv n(x_j)$ is the number density of the points at x. Note that in particle simulations the interpolation points are particles and the volume of the particles V_j is used instead of the number density.

$$\langle f(x,h)\rangle = \sum_{j=1}^{N} f_j V_j W(x - x_j, h). \tag{5}$$

The kernel function W should satisfy only Eq. (3) requirements, and it is clear that many functions can be used for interpolation. In [1–4,6,27,28] an extended survey can be found on interpolation functions. In the present work we will focus on the B-splines kernels introduced by Schoenberg [9,10].

Before proceeding further, we will define some parameters commonly used in B-splines terminology. The B-splines are piecewise polynomials functions. The degree of the polynomials defines the degree of the B-spline. The order of the B-spline (or order of approximation, L) gives a global estimate of how fast the error of the approximation decays when the sampling step become finer. The regularity of the B-spline (R) defines how many times the function is continuously differentiable. The support or cut-off distance of the B-splines defines the normalized distance that the function is non-zero. The computational cost of the interpolation is strongly related to the support of the B-spline. In practice, for multidimensional computations, the interpolating kernels are useful and usable only when their support is short.

In Appendix A representative B-splines are shown. Generally they can be written in symbolic form as

$$M_n^l(x,h) = n_d \sum_{i=0}^{n-1} a_{i,l} s^i, \quad s = \frac{|x|}{h}, \tag{A.9}$$

where n_d is a normalization constant $\left(n_d \propto \frac{1}{h^d}\right)$, d is the dimension space of the problem $(f : R^d \rightarrow R)$ and the index l represents every segment of the spline.

Increasing the degree of B-splines, improves the smoothness of the interpolation quantity from possibly scattered samples without the need for connectivity or grid based information. However, their accuracy is limited to second order due to be positive in the entire area of support. This is easy to prove it if we write the Taylor series expansion around each of the set of points $\{x_1, x_2, \ldots, x_N\}$.

$$\begin{aligned}
f_1 &= f(x) + f'(x)(x_1 - x) + f''(x)\frac{(x_1 - x)^2}{2!} + f'''(x)\frac{(x_1 - x)^3}{3!} + f''''(x)\frac{(x_1 - x)^4}{4!} + \mathrm{HOT}, \\
f_2 &= f(x) + f'(x)(x_2 - x) + f''(x)\frac{(x_2 - x)^2}{2!} + f'''(x)\frac{(x_2 - x)^3}{3!} + f''''(x)\frac{(x_2 - x)^4}{4!} + \mathrm{HOT}, \\
&\vdots \\
f_N &= f(x) + f'(x)(x_N - x) + f''(x)\frac{(x_N - x)^2}{2!} + f'''(x)\frac{(x_N - x)^3}{3!} + f''''(x)\frac{(x_N - x)^4}{4!} + \mathrm{HOT}.
\end{aligned} \tag{6}$$

Multiplying each equation with the volume of each point and with the kernel function W yields.

$$\begin{aligned}
f_1 V_1 W(x - x_1, h) &= f(x) V_1 W(x - x_1, h) + f'(x)(x_1 - x) V_1 W(x - x_1, h) + f''(x)\frac{(x_1 - x)^2}{2!} V_1 W(x - x_1, h) \\
&\quad + f'''(x)\frac{(x_1 - x)^3}{3!} V_1 W(x - x_1, h) + f''''(x)\frac{(x_1 - x)^4}{4!} V_1 W(x - x_1, h) + \mathrm{HOT}, \\
f_2 V_2 W(x - x_2, h) &= f(x) V_2 W(x - x_2, h) + f'(x)(x_2 - x) V_2 W(x - x_2, h) + f''(x)\frac{(x_2 - x)^2}{2!} V_2 W(x - x_2, h) \\
&\quad + f'''(x)\frac{(x_2 - x)^3}{3!} V_2 W(x - x_2, h) + f''''(x)\frac{(x_2 - x)^4}{4!} V_2 W(x - x_2, h) + \mathrm{HOT}, \\
&\vdots \\
f_N V_N W(x - x_N, h) &= f(x) V_N W(x - x_N, h) + f'(x)(x_N - x) V_N W(x - x_N, h) + f''(x)\frac{(x_N - x)^2}{2!} V_N W(x - x_N, h) \\
&\quad + f'''(x)\frac{(x_N - x)^3}{3!} V_N W(x - x_N, h) + f''''(x)\frac{(x_N - x)^4}{4!} V_N W(x - x_N, h) + \mathrm{HOT},
\end{aligned} \tag{7}$$

if we sum all the equations

$$\begin{aligned}
\sum_{j=1}^{N} f_j V_j W(x - x_j, h) &= f(x) \sum_{j=1}^{N} V_j W(x - x_j, h) + f'(x) \sum_{j=1}^{N} (x_j - x) V_j W(x - x_j, h) \\
&\quad + \frac{f''(x)}{2!} \sum_{j=1}^{N} (x_j - x)^2 V_j W(x - x_j, h) + \frac{f'''(x)}{3!} \sum_{j=1}^{N} (x_j - x)^3 V_j W(x - x_j, h) \\
&\quad + \frac{f''''(x)}{4!} \sum_{j=1}^{N} (x_j - x)^4 V_j W(x - x_j, h) + \mathrm{HOT}.
\end{aligned} \tag{8}$$

The summations in Eq. (8) can be written as integrals

$$\begin{aligned}\int_D f(x')W(x-x',h)\mathrm{d}x' = f(x)\int_D W(x-x',h)\mathrm{d}x' + f'(x)\int_D (x'-x)W(x-x',h)\mathrm{d}x' \\ + \frac{f''(x)}{2!}\int_D (x'-x)^2 W(x-x',h)\mathrm{d}x' + \frac{f'''(x)}{3!}\int_D (x'-x)^3 W(x-x',h)\mathrm{d}x' \\ + \frac{f''''(x)}{4!}\int_D (x'-x)^4 W(x-x',h)\mathrm{d}x' + \mathrm{HOT}.\end{aligned} \quad (9)$$

From Eq. (9) it is clear that the moments of the interpolation function are strongly related to the accuracy of the interpolation [7,8]. For interpolation of order L accuracy, it is necessary that the function W satisfies the following properties

$$\begin{aligned}&\int_D W(x,h)\mathrm{d}x = 1,\\ &\int_D xW(x,h)\mathrm{d}x = 0,\\ &\int_D x^2 W(x,h)\mathrm{d}x = 0,\\ &\vdots\\ &\int_D x^L W(x,h)\mathrm{d}x = 0,\\ &\int_D x^{L+1} W(x,h)\mathrm{d}x < \infty.\end{aligned} \quad (10)$$

It is also clear that a positive symmetric function (like the B-splines) is limited to second order accuracy. Many successful attempts to construct high-order ($L > 2$) interpolating functions are based on the realization of Eq. (10) [19,21].

One of the disadvantages of the improved (more accurate) interpolated formulas, for example of the W_4 (or M_4') or cubic convolution interpolation [19,20], compared to the B-splines [9,10] is that their accuracy drops significantly away from the optimal design area (this reduction of accuracy is however not more pronounced than in other B-spline kernels). The optimal design area is defined as equidistant samples with smoothing length being equal to the spacing of the samples ($h = \mathrm{d}x$) (in Section 3.1 we will show an error analysis of this function). We must note the assumptions of equidistant samples and the smoothing length being equal to the sampling distance are matched most of the times in signal and image process, but this is not the case in particle methods [6].

Our idea for high-order interpolation is related to the construction of a kernel function W which satisfies Eq. (10) until the desired order L using a linear combination of k compactly supported functions W_k, where W_0 is one of the B-splines M_n and $W_1, W_1, \ldots, W_{k-1}$ are functions based on the derivatives of M_n. In the Sections 2.2 and 2.3 we will show how the basis functions are constructed.

2.2. Approximation by convolution and linear independent functions

From the classical theory of mollified approximation of a sufficiently regular function f [29] with a convolution operator $*$ and a kernel function g, the approximation of the function $\langle f \rangle$ can be written:

$$\langle f \rangle = f * g, \quad (11)$$

and the spatial derivatives can be approximated as

$$\langle \nabla f \rangle = (\nabla f) * g = f * \nabla g. \tag{12}$$

Eq. (2) is a convolution approximation and Eq. (12) is usually applied for the approximation of the derivatives [6,17,18]. The integral interpolant approximation of the derivatives equivalent to Eq. (2) is

$$\langle \nabla f(x,h) \rangle = \int_D \nabla f(x') W(x-x',h) \mathrm{d}x' = \int_D f(x') \nabla W(x-x',h) \mathrm{d}x', \tag{13}$$

which is valid for every continuous function f.

If a polynomial function is symmetric $f(x) = f(-x) = f^{\mathrm{s}}(x)$ or antisymmetric (with respect to $x = 0$) $f(x) = -f(-x) = f^{\mathrm{as}}(x)$ then it has the following forms, respectively:

$$f^{\mathrm{s}}(x) = \begin{cases} a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1} + a_n x^n & 0 \leqslant x, \\ a_0 - a_1 x + a_2 x^2 + \cdots + (-1)^{n-1} a_{n-1} x^{n-1} + (-1)^n a_n x^n & 0 > x, \end{cases} \tag{14}$$

$$f^{\mathrm{as}}(x) = \begin{cases} a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1} + a_n x^n & 0 \leqslant x, \\ -a_0 + a_1 x - a_2 x^2 + \cdots - (-1)^{n-1} a_{n-1} x^{n-1} - (-1)^n a_n x^n & 0 > x. \end{cases} \tag{15}$$

It is simple to show that when we differentiate a symmetric respective antisymmetric polynomial function the result is an antisymmetric respective symmetric function

$$\partial_x f^{\mathrm{s}}(x) = -\partial_x f^{\mathrm{s}}(-x) \qquad \partial_x f^{\mathrm{as}}(x) = \partial_x f^{\mathrm{as}}(-x). \tag{16}$$

The same holds when we multiply a function by x

$$x f^{\mathrm{s}}(x) = -x f^{\mathrm{s}}(-x) \qquad x f^{\mathrm{as}}(x) = x f^{\mathrm{as}}(-x). \tag{17}$$

The integral of an antisymmetric function around the axis $x = 0$ is zero

$$\int f^{\mathrm{as}}(x) \mathrm{d}x = 0. \tag{18}$$

If the interpolation function W is a symmetric polynomial function of degree n, we can show (using Eqs. (3), (13), (16)–(18) that

$$\int_D (x')^n \partial_x^n W(x-x',h) \mathrm{d}x' = (-1)^n n!, \tag{19}$$

which implies (from Eq. (3)) that the functions $\left\{ c_1 \frac{x \partial W}{\partial x}, c_2 \frac{x^2 \partial^2 W}{\partial x^2}, \ldots, c_n \frac{x^n \partial^n W}{\partial x^n} \right\}$ are also interpolation functions where $c_n = \frac{1}{(-1)^n n!}$.

The function W can be written as

$$W = a_0 + a_1 x + a_2 x^2 + \cdots + a_{n-1} x^{n-1} + a_n x^n = W_0. \tag{20}$$

The interpolation functions read

$$\begin{bmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 2 & 3 & \cdots & n \\ 0 & 0 & 1 \cdot 2 & 2 \cdot 3 & \cdots & (n-1) \cdot n \\ 0 & 0 & 0 & 1 \cdot 2 \cdot 3 & \cdots & (n-2) \cdot (n-1) \cdot n \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & n! \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 x \\ a_2 x^2 \\ a_3 x^3 \\ \vdots \\ a_n x^n \end{bmatrix} = \begin{bmatrix} W \\ x \partial W \\ x^2 \partial^2 W \\ x^3 \partial^3 W \\ \vdots \\ x^n \partial^n W \end{bmatrix} = \begin{bmatrix} W_0 \\ W_1/c_1 \\ W_2/c_2 \\ W_3/c_3 \\ \vdots \\ W_n/c_n \end{bmatrix}. \tag{21}$$

The determinant of the matrix in Eq. (21) is always non-zero

$$\begin{vmatrix} 1 & 1 & 1 & 1 & \cdots & 1 \\ 0 & 1 & 2 & 3 & \cdots & n \\ 0 & 0 & 1\cdot 2 & 2\cdot 3 & \cdots & (n-1)\cdot n \\ 0 & 0 & 0 & 1\cdot 2\cdot 3 & \cdots & (n-2)\cdot(n-1)\cdot n \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & n! \end{vmatrix} = 1!\cdot 2!\cdot 3!\cdots n! \neq 0 \tag{22}$$

and the functions $\{W_0, W_1, W_2, W_3, \ldots, W_n\}$ are linearly independent functions [30]. A linear combination of these functions W

$$W = C_0W_0 + C_1W_1 + C_2W_2 + C_3W_3 + \cdots + C_nW_n \tag{23}$$

can be used in order to construct a function that can satisfy Eq. (10) until the n moment.

$$\begin{aligned}
\begin{bmatrix} \int_D W\,\mathrm{d}x \\ \int_D xW\,\mathrm{d}x \\ \int_D x^2W\,\mathrm{d}x \\ \vdots \\ \int_D x^nW\,\mathrm{d}x' \end{bmatrix} &= \begin{bmatrix} \int_D (C_0W_0 + C_1W_1 + C_2W_2 + C_3W_3 + \cdots + C_nW_n)\mathrm{d}x \\ \int_D x(C_0W_0 + C_1W_1 + C_2W_2 + C_3W_3 + \cdots + C_nW_n)\mathrm{d}x \\ \int_D x^2(C_0W_0 + C_1W_1 + C_2W_2 + C_3W_3 + \cdots + C_nW_n)\mathrm{d}x \\ \vdots \\ \int_D x^n(C_0W_0 + C_1W_1 + C_2W_2 + C_3W_3 + \cdots + C_nW_n)\mathrm{d}x' \end{bmatrix} \\
&= \begin{bmatrix} \int_D W_0\,\mathrm{d}x & \int_D W_1\,\mathrm{d}x & \int_D W_2\,\mathrm{d}x & \int_D W_3\,\mathrm{d}x & \cdots & \int_D W_n\,\mathrm{d}x \\ \int_D xW_0\,\mathrm{d}x & \int_D xW_1\,\mathrm{d}x & \int_D xW_2\,\mathrm{d}x & \int_D xW_3\,\mathrm{d}x & \cdots & \int_D xW_n\,\mathrm{d}x \\ \int_D x^2W_0\,\mathrm{d}x & \int_D x^2W_1\,\mathrm{d}x & \int_D x^2W_2\,\mathrm{d}x & \int_D x^2W_3\,\mathrm{d}x & \cdots & \int_D x^2W_n\,\mathrm{d}x \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ \int_D x^nW_0\,\mathrm{d}x & \int_D x^nW_1\,\mathrm{d}x & \int_D x^nW_2\,\mathrm{d}x & \int_D x^nW_3\,\mathrm{d}x & \cdots & \int_D x^nW_n\,\mathrm{d}x \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ \vdots \\ C_n \end{bmatrix} \\
&= \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.
\end{aligned} \tag{24}$$

The construction the system of Eq. (24) does not guarantee that there exist no singularities. This is not considered however as disadvantage, since we can achieve a specified accuracy when solving a smaller subsystem of (24). For example for 3rd order accuracy the 3×3 subsystem of (24) is sufficient. For the solution of a system that might be singular the singular value decomposition [31,32] (SVD) technique can be used.

2.3. B-splines and high-order interpolation

Until now we formed a system of Eq. (24) which can construct a interpolation function that guarantees a desired order interpolation. The basic assumption made, is that the initial function W_0 is a symmetric polynomial interpolation function. Typical functions that satisfy these assumption are the B-splines M_n [9,10]. Because the B-splines are constructed by polynomial segments, the regularity of the functions W_k decreases every time we use a higher derivative of the function. The interpolation function can be written as

$$W(x,h) = \sum_{k=0}^{L} C_k x^k \frac{\partial^k}{\partial x^k} M_n(x,h). \tag{25}$$

As we noted before, the system (24) may be singular. This is always the case when the samples are symmetric and the odd moments are zero by definition $\left(\int_D x^k \frac{\partial^k}{\partial x^k} W = 0,\ k = 1, 3, \ldots, n\right)$. In Fig. 1 the representative functions based on M_6 and its derivatives are shown. In order to have an interpolation function W with regularity R and order of approximation L it is necessary to use B-splines of degree n where

$$n = L + R. \tag{26}$$

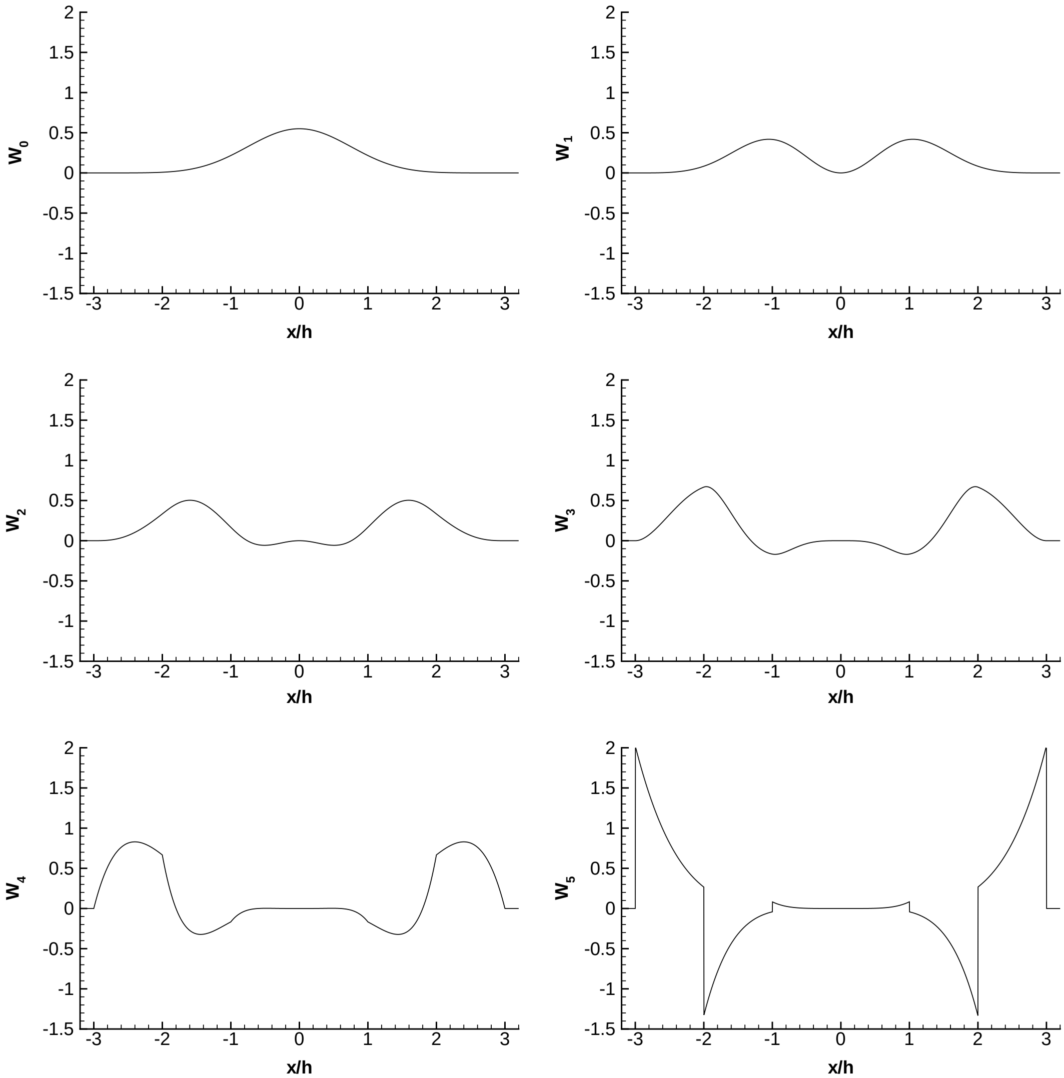

Fig. 1. The six linear independent functions based on the quintic spline (M_6).

We must note that the function shown in (25) is generating a family of interpolation functions which is different than the maximum order minimum support (MOMS) functions [23]. The latter functions are based on the general formula $W(x,h) = \sum_{k=0}^{L} C_k \frac{\partial^k}{\partial x^k} M_n(x,h)$ and in order to have symmetric interpolating function only the even derivatives are used. The functions based on Eq. (25) have higher regularity for the same order of approximation.

2.4. One-sided interpolation

The methodology we presented herein for high-order interpolation is based on the linear combination of interpolation functions in order to construct a function W which satisfies Eq. (24) to a desired order of approximation. We must note that any linear combination of non-interpolating functions that construct a function W which satisfies Eqs. (3) and (24) to a desired order of approximation, can also be used for interpolation.

Under this consideration it is clear that we can apply the methodology presented above for a polynomial function, without the need of having symmetric samples. This idea can construct one-sided functions that can achieve high-order interpolation. One-sided interpolation can be very useful in the presence of discontinuities [33,34] and sharp gradients (as in boundary layers).

In the present paper we will investigate numerically the one-sided interpolation based on the B-splines. We recognize that for one-sided interpolation it is possible that B-splines may not provide the optimum solution. Our aim, however, is to present a methodology that it is able to construct functions that reach high-order of approximation and is not restricted to a specific family of functions.

2.5. High-order differentiation

One fundamental property of the system of Eq. (24) is that it can provide also a function for the approximation of the derivatives if we a apply a different right-hand-side matrix. For example, the solution of the system

$$\begin{bmatrix} \int_D W_0\,\mathrm{d}x & \int_D W_1\,\mathrm{d}x & \int_D W_2\,\mathrm{d}x & \int_D W_3\,\mathrm{d}x & \cdots & \int_D W_n\,\mathrm{d}x \\ \int_D xW_0\,\mathrm{d}x & \int_D xW_1\,\mathrm{d}x & \int_D xW_2\,\mathrm{d}x & \int_D xW_3\,\mathrm{d}x & \cdots & \int_D xW_n\,\mathrm{d}x \\ \int_D x^2W_0\,\mathrm{d}x & \int_D x^2W_1\,\mathrm{d}x & \int_D x^2W_2\,\mathrm{d}x & \int_D x^2W_3\,\mathrm{d}x & \cdots & \int_D x^2W_n\,\mathrm{d}x \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ \int_D x^nW_0\,\mathrm{d}x & \int_D x^nW_1\,\mathrm{d}x & \int_D x^nW_2\,\mathrm{d}x & \int_D x^nW_3\,\mathrm{d}x & \cdots & \int_D x^nW_n\,\mathrm{d}x \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ \vdots \\ C_n \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{27}$$

yields a function W that can approximate the first order derivative. In general, the system (27) may not be solved when the function W is symmetric since the second equation may have no solution (Appendix B). To this end, the form of the second equation might be:

$$0 \cdot C_0 + 0 \cdot C_1 + 0 \cdot C_2 + 0 \cdot C_3 + \cdots + 0 \cdot C_n = 1. \tag{28}$$

To have a system that it is possible to solve, we need to use different basis functions. One idea is to use the derivatives of our interpolating functions $\{W_0, W_1, W_2, W_3, \ldots, W_n\}$. The differentiation function can be written as

$$\partial_x W = C_0\,\partial_x W_0 + C_1\,\partial_x W_1 + C_2\,\partial_x W_2 + C_3\,\partial_x W_3 + \cdots + C_{n-1}\,\partial_x W_{n-1}. \tag{29}$$

The corresponding algebraic system has the form

$$\begin{bmatrix} \int_D \partial_x W_0\,\mathrm{d}x & \int_D \partial_x W_1\,\mathrm{d}x & \int_D \partial_x W_2\,\mathrm{d}x & \int_D \partial_x W_3\,\mathrm{d}x & \cdots & \int_D \partial_x W_n\,\mathrm{d}x \\ \int_D x\,\partial_x W_0\,\mathrm{d}x & \int_D x\,\partial_x W_1\,\mathrm{d}x & \int_D x\,\partial_x W_2\,\mathrm{d}x & \int_D x\,\partial_x W_3\,\mathrm{d}x & \cdots & \int_D x\partial_x W_n\,\mathrm{d}x \\ \int_D x^2\,\partial_x W_0\,\mathrm{d}x & \int_D x^2\,\partial_x W_1\,\mathrm{d}x & \int_D x^2\,\partial_x W_2\,\mathrm{d}x & \int_D x^2\,\partial_x W_3\,\mathrm{d}x & \cdots & \int_D x^2\,\partial_x W_n\,\mathrm{d}x \\ \vdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ \int_D x^n\,\partial_x W_0\,\mathrm{d}x & \int_D x^n\,\partial_x W_1\,\mathrm{d}x & \int_D x^n\,\partial_x W_2\,\mathrm{d}x & \int_D x^n\,\partial_x W_3\,\mathrm{d}x & \cdots & \int_D x^n\partial_x W_n\,\mathrm{d}x \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ \vdots \\ C_n \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}. \tag{30}$$

Another possibility is to use an asymmetrical B-spline M_k^{as}, simply by changing the sign of a B-spline M_k according to the following formula

$$M_k^{\mathrm{as}}(x,h) = \mathrm{sign}(x)M_k(x,h). \tag{31}$$

And as a result, when we use M_k^{as} the terms of the odd lines of the system (27) may be zero, but the system is now solvable.

Using the ideas presented in the previous section we can also construct one-sided differentiation functions, which are comparable to the upwind differentiation formulas in finite differences.

Kernels for higher-order derivatives can be derived by simply changing the right-hand-side matrix of the system (27).

3. Results and discussion

3.1. Interpolation

As we mentioned before, this paper presents a methodology in order to construct interpolation functions and not just an interpolation kernel. For the sake of brevity we will validate our methodology for a few families of functions based on M_4, M_6, M_7 and M_8.

Fig. 2 shows an error analysis for M_4 and M_4', with the smoothing length h equal to the sample distance dx ($h = \mathrm{d}x$). In Fig. 2(a) the sample and the interpolation locations are depicted. The function that it is interpolated reads

$$f(x) = \sin(3.5\pi x) \tag{32}$$

(Fig. 2(b)). The error analysis is based on the absolute error

$$\mathrm{Error} = |f(x) - \langle f(x,h)\rangle|. \tag{33}$$

The M_4 error is almost uniform for the entire area of interpolation (Fig. 2(c)). M_4' is more accurate compared to M_4 as shown in Fig. 2(d). This is expected since M_4' achieves 3rd order of approximation whereas M_4 is 2nd order. Near $x = 0.4$ and $x = 0.5$ the error is considerably smaller since it corresponds to sample locations. When the smoothing length and the sample spacing are not equal ($h \neq \mathrm{d}x$), M_4' cannot reach 3rd order of approximation. Fig. 3(a) shows the maximum norm of the absolute error L_∞ for the cubic spline (M_4).

$$L_\infty = \max\left(|f(x) - \langle f(x,h)\rangle|\right) \tag{34}$$

for different values of the ratio $\mathrm{d}x/h$ in the range 0.5–2.0. The ratio $\mathrm{d}x/h$ is directly related to the number of point that contribute to the interpolation, as shown in Fig. 3(b). Since that the computational time is proportional to the number of points involved in the interpolation, it is desired to keep this number small. In Fig. 3(a) it is clear that M_4 is second order when $\mathrm{d}x/h < 1.15$. M_4' (Fig. 3(c)) shows a 3rd order accuracy near $\mathrm{d}x/h = 1$ as expected, but deviates significant for the other values of the ratio $\mathrm{d}x/h$. The order of the

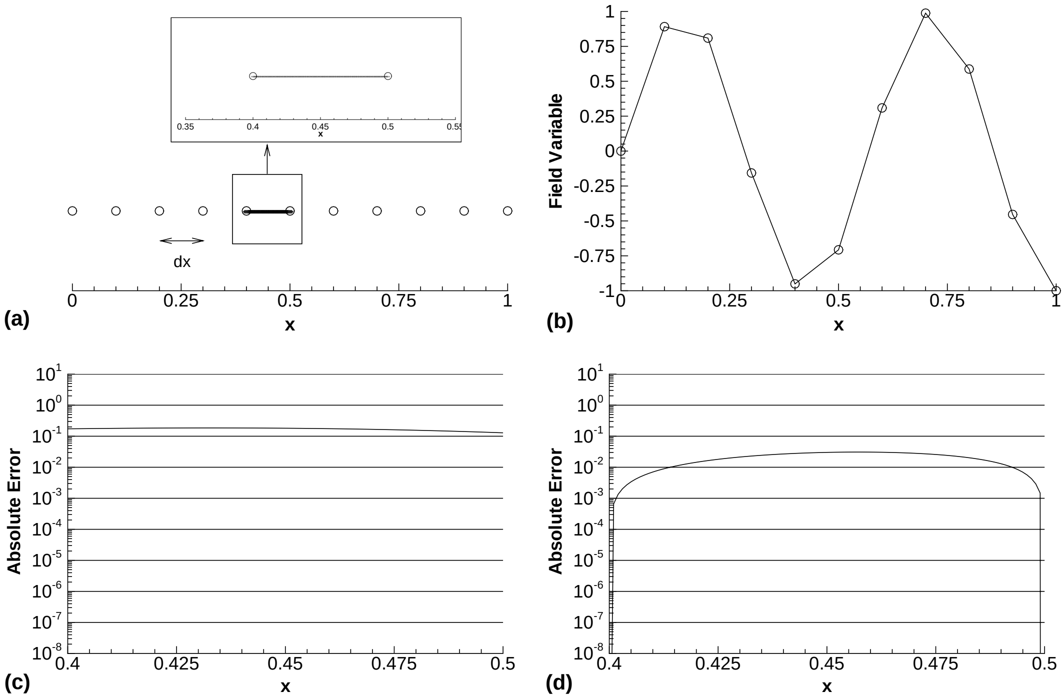

Fig. 2. Error analysis for M_4 and M_4'. (a) sample and interpolation locations, (b) field variable, (c) absolute error for M_4, (d) absolute error for M_4'.

interpolation is defined simply from the number of orders the error drops between the two cases using the standard formulation, $\left(\frac{\text{Error}_{\text{fine}}}{\text{Error}_{\text{coarse}}} = \left(\frac{\mathrm{d}x_{\text{fine}}}{\mathrm{d}x_{\text{coarse}}}\right)^{\text{Order}}\right)$. The error analysis of M_6 is shown in Fig. 3(d), where a 2nd order accuracy is achieved when $\mathrm{d}x/h < 1.35$.

Using the ideas outlined in 2.2 and 2.3 we can construct functions based on B-splines that can achieve higher order of approximation. In Fig. 4(b) the maximum absolute error for a 3rd order function based on M_6 using the three first basis functions $\{W_0, W_1, W_2\}$ is shown. In Appendix B we present the details for the solution of the system based on Eq. (24). The results indicate that the constructed function provides a 3rd order of approximation for $\mathrm{d}x/h < 2$. The overall behavior of the constructed functions is significantly better than the B-spline M_6 (shown in Fig. 4(a)). Similar results are observed when requesting 4th order accuracy using four basis functions $\{W_0, W_1, W_2, W_3\}$ (Fig. 4(c)) or 5th order accuracy using five basis functions $\{W_0, W_1, W_2, W_3, W_4\}$ (Fig. 4(d)). We note that in order to achieve a desired order of approximation a sufficient number of samples is required. This number of samples is equal to the order of approximation. From Fig. 3(b) for M_6 one expects a 3rd order of approximation for the entire range of $\mathrm{d}x/h$ $(0.5 < \mathrm{d}x/h < 2)$, 4th order for $\mathrm{d}x/h < 1.5$ and 5th for $\mathrm{d}x/h < 1.2$. The same limits are clear also in the error analysis plots of Fig. 4(c) and (d). Discrepancies can appear in the error plots and lead to much higher errors. This is due to the fact that the system of Eq. (24) is near singular (small determinant but not zero) and the technique presented in Appendix B is not appropriate. In order to avoid these discrepancies we are employing the SVD technique [35]. The basic idea is that we can solve a system based on Eq. (24) without imposing the condition that the number of equations and the number of unknowns are equal. Under this consideration when fewer equations than unknowns are used, we are not expecting a unique solution, and we can ignore the basis functions that can cause singularity. In Fig. 4(e) and (f) the error analysis of a 3rd and 4th order function based on M_6 is shown using a SVD algorithm. It is obvious that SVD removes the

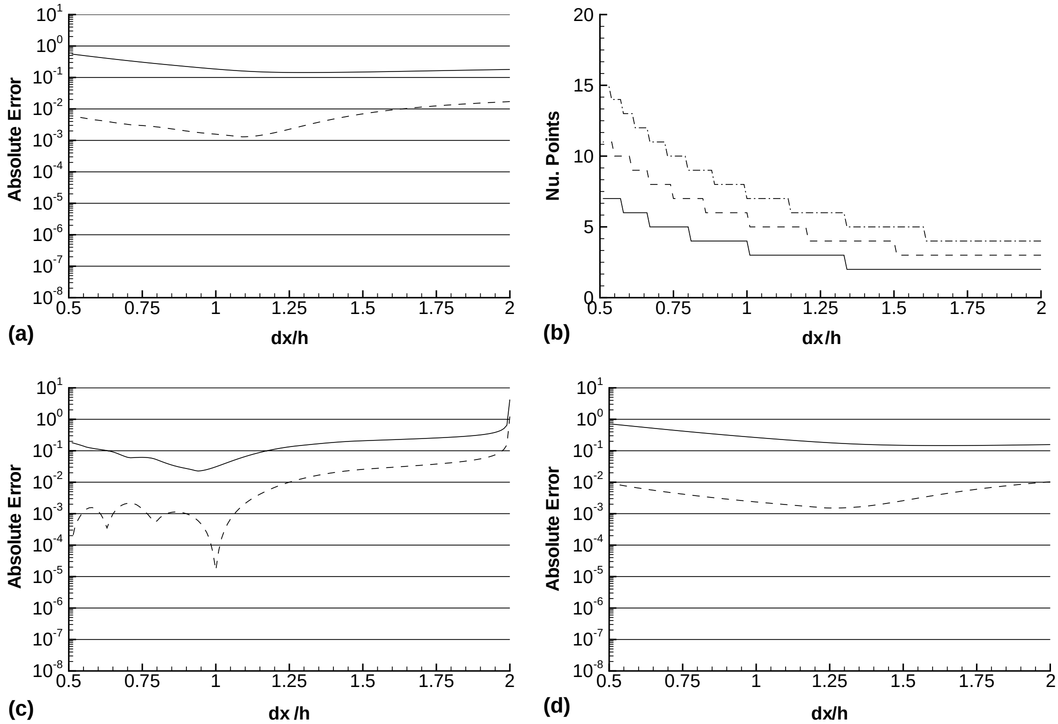

Fig. 3. Error analysis for M_4, M_4' and M_6. (a) L_∞ error of M_4 as a function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$, (b) number of corresponding particles as a function of smoothing length, (—) M_4 and M_4', (- - -) M_6, (-·-·-) M_8, (c) L_∞ error of M_4' as a function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$, (d) L_∞ error of M_6 as a function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$.

discrepancies compared to Fig. 4(b) and (c) and yields more uniform error distributions. The idea of using more basis functions than the desired order of approximations, strengths significantly the methodology and the additional degree of freedom makes the solution of the system more robust. The disadvantage is that the regularity R of the constructed function is smaller. Note that there is not a confirmation that the regularity and the order of approximation are coupled [21].

The interpolation technique presented in Sections 2.2 and 2.3 can be used to construct interpolation functions for non-equidistant samples. Fig. 5(a) shows the spacing between the samples, which is perturbed randomly around the average value. The standard B-splines M_6 and M_8 are producing a 2nd order approximation for a large part of the range of dx/h (Fig. 5(b)). Using the ideas presented in Sections 2.2 and 2.3 and an SVD algorithm we can construct 3rd and 4th order functions based on M_6 using four and five basis functions, respectively. The errors shown in Fig. 5(c) and (d) for the 3rd and 4th order functions demonstrate an approximation close to the desired order. Using M_8 we can achieve higher order of approximation than M_6 since more basis functions can constructed. In Fig. 5(e) and (f) a 5th and 6th order functions are shown based on six and seven basis functions, respectively. A high-order of interpolation is achieved with non-equidistant samples. The effectiveness of a SVD technique on the solution of the system, offers a robust and effective method to solve the system of Eq. (24).

As mentioned above in Section 2.4, we can apply the interpolation technique in order to construct one-sided interpolation functions. Fig. 6 shows results using M_4, M_6 and M_8 for interpolation from non-equidistant samples. The results indicate that we can construct high order one-sided interpolation functions

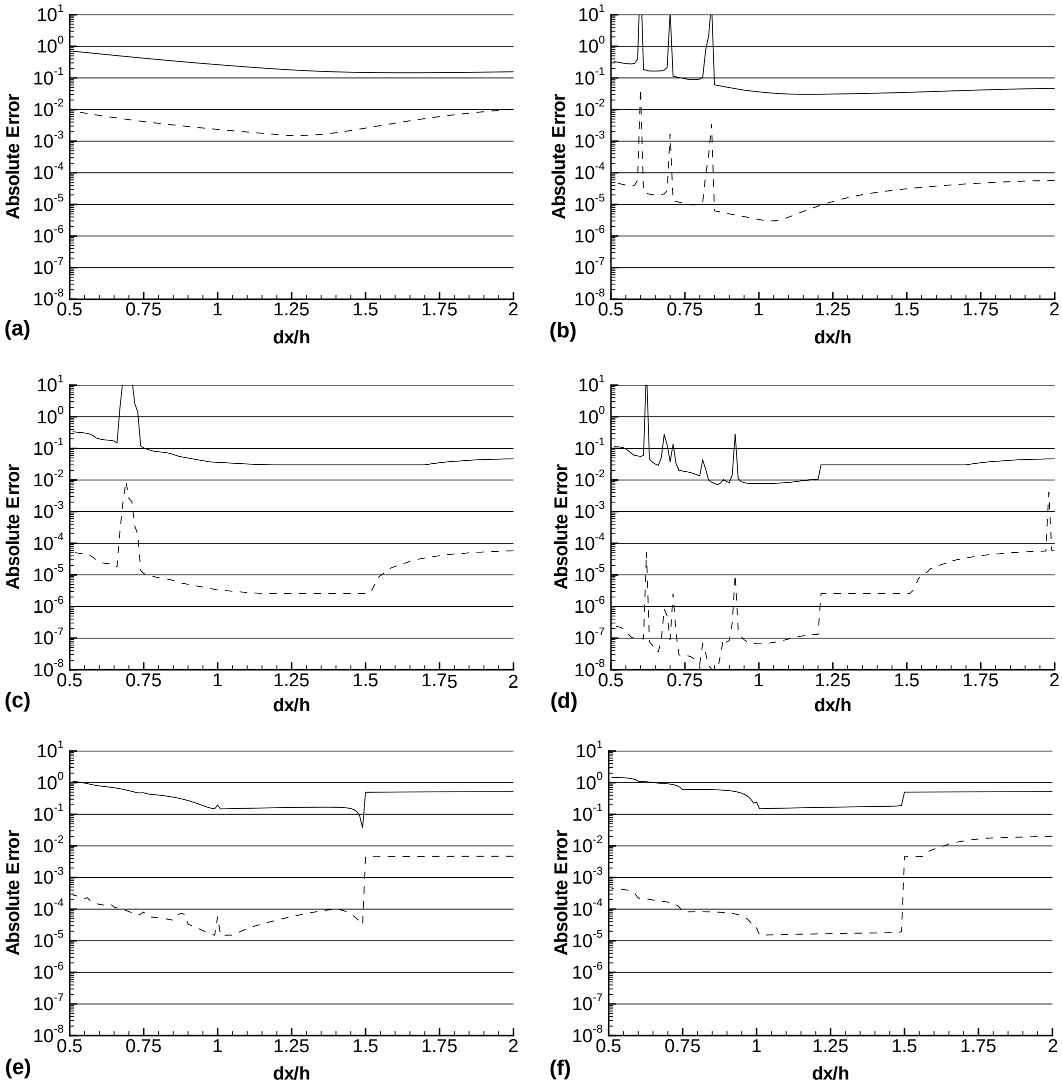

Fig. 4. Error analysis of 3rd, 4th and 5th order functions based on M_6. (a) L_∞ error of M_6 as a function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$, (b) L_∞ error of 3rd order function based on M_6 $\{W_0, W_1, W_2\}$ as function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$, (c) L_∞ error of 4th order function based on M_6 $\{W_0, W_1, W_2, W_3\}$ as function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$, (d) L_∞ error of 5th order function based on M_6 $\{W_0, W_1, W_2, W_3, W_4\}$ as function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$, (e) L_∞ error of 3rd order function based on M_6 $\{W_0, W_1, W_2, W_3\}$ using SVD as function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$, (f) L_∞ error of 4th order function based on M_6 $\{W_0, W_1, W_2, W_3, W_4\}$ using SVD as function of smoothing length (—) $dx = 0.1$, (- - -) $dx = 0.01$.

(2nd, 3rd and 4th order shown in Fig. 6(a)–(f)). The error is notably smooth, since the matrix of the system of Eq. (24) is generally not singular, and the system has solution. For this reason there is no need for more unknowns (basis functions) than equations in the system of Eq. (24).

Summarizing, the results demonstrate indeed that the present technique can construct interpolation functions that achieve high order of approximation from arbitrary data. The only requirement is a

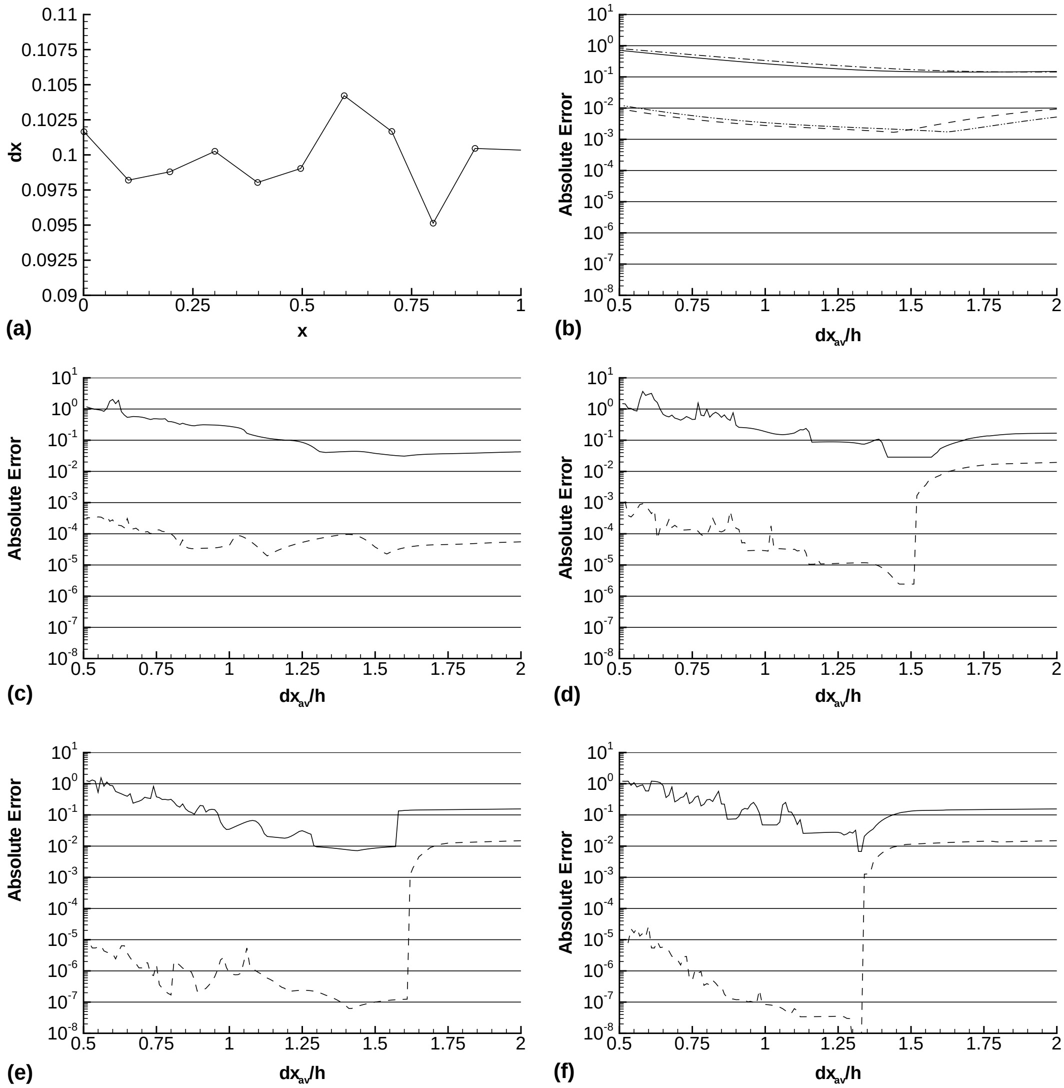

Fig. 5. Error analysis of functions based on M_6 and M_8 for non-equidistant samples. (a) Distance between the samples with average spacing $\mathrm{d}x_{\mathrm{av}} = 0.1$, (b) L_∞ error of M_6 and M_8 as a function of smoothing length (—) M_6 $\mathrm{d}x_{\mathrm{av}} = 0.1$, (- - -) M_6 $\mathrm{d}x_{\mathrm{av}} = 0.01$, (-·-·-) M_8 $\mathrm{d}x_{\mathrm{av}} = 0.01$, (-··-··-) M_8 $\mathrm{d}x_{\mathrm{av}} = 0.01$, (c) L_∞ error of 3rd order function based on M_6 $\{W_0, W_1, W_2, W_3\}$ using SVD as function of smoothing length (—) $\mathrm{d}x_{\mathrm{av}} = 0.1$, (- - -) $\mathrm{d}x_{\mathrm{av}} = 0.01$, (d) L_∞ error of 4th order function based on M_6 $\{W_0, W_1, W_2, W_3, W_4\}$ using SVD as function of smoothing length (—) $\mathrm{d}x_{\mathrm{av}} = 0.1$, (- - -) $\mathrm{d}x_{\mathrm{av}} = 0.01$, (e) L_∞ error of 5th order function based on M_8 $\{W_0, W_1, W_2, W_3, W_4, W_5\}$ using SVD as function of smoothing length (—) $\mathrm{d}x_{\mathrm{av}} = 0.1$, (- - -) $\mathrm{d}x_{\mathrm{av}} = 0.01$, (f) L_∞ error of 6th order function based on M_8 $\{W_0, W_1, W_2, W_3, W_4, W_5, W_6\}$ using SVD as function of smoothing length (—) $\mathrm{d}x_{\mathrm{av}} = 0.1$, (- - -) $\mathrm{d}x_{\mathrm{av}} = 0.01$.

minimum number of samples that is necessary to achieve the desired order of approximation. We have to note that when we apply the technique for interpolation on equidistant samples using $\mathrm{d}x = h$ the solution of the system of Eq. (24) returns functions that are already known in literature [20],

$$M_4' = 1.5M_4 - 0.5x\frac{\partial M_4}{\partial x}, \tag{35}$$

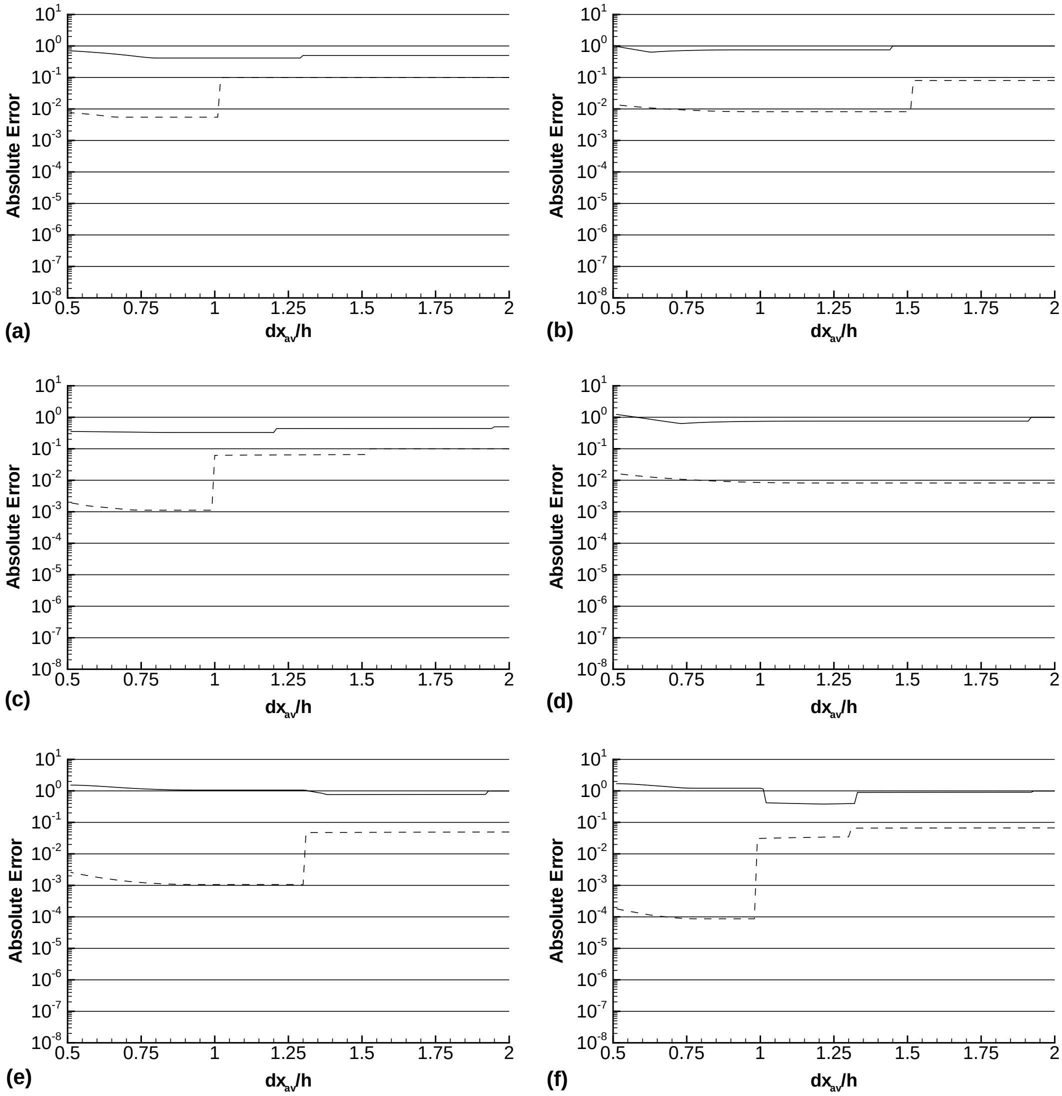

Fig. 6. Error analysis of one-sided interpolation using functions based on M_6 and M_8 using SVD for non-equidistant samples. (a) L_∞ error of 2nd order function based on M_4 $\{W_0, W_1\}$ as function of smoothing length (—) $\mathrm{d}x_{av} = 0.1$, (- - -) $\mathrm{d}x_{av} = 0.01$, (b) L_∞ error of 2nd order function based on M_6 $\{W_0, W_1\}$ as function of smoothing length (—) $\mathrm{d}x_{av} = 0.1$, (- - -) $\mathrm{d}x_{av} = 0.01$, (c) L_∞ error of 3rd order function based on M_6 $\{W_0, W_1, W_2\}$ as function of smoothing length (—) $\mathrm{d}x_{av} = 0.1$, (- - -) $\mathrm{d}x_{av} = 0.01$, (d) L_∞ error of 2nd order function based on M_8 $\{W_0, W_1\}$ as function of smoothing length (—) $\mathrm{d}x_{av} = 0.1$, (- - -) $\mathrm{d}x_{av} = 0.01$, (e) L_∞ error of 3rd order function based on M_8 $\{W_0, W_1, W_2\}$ as function of smoothing length (—) $\mathrm{d}x_{av} = 0.1$, (- - -) $\mathrm{d}x_{av} = 0.01$, (f) L_∞ error of 4th order function based on M_8 $\{W_0, W_1, W_2, W_3\}$ as function of smoothing length (—) $\mathrm{d}x_{av} = 0.1$, (- - -) $\mathrm{d}x_{av} = 0.01$.

$$M_5' = 1.5M_5 - 0.5x\frac{\partial M_5}{\partial x}, \tag{36}$$

which achieve 3rd and 4th orders of approximation. Using B-splines with higher support, we can achieve higher regularity with 4th order (W_6), or higher order of approximation (5th for W_7 and 6th for W_8)

$$M_6' = 1.5M_6 - 0.5x\frac{\partial M_6}{\partial x}, \tag{37}$$

$$M_7' = 18.75M_7 - 11.25x\frac{\partial M_7}{\partial x} + 2.5x^2\frac{\partial^2 M_7}{\partial x^2}, \tag{38}$$

$$M_8' = 18.75M_8 - 11.25x\frac{\partial M_8}{\partial x} + 2.5x^2\frac{\partial^2 M_8}{\partial x^2}. \tag{39}$$

All the above kernel functions Eqs. (35)–(39) are satisfying the one dimensional property

$$\sum_{i\in Z} M_n(x + ih, h) = \frac{1}{h}. \tag{40}$$

Representative one-sided interpolation functions based on M_4 and M_5

$$M_4^S = 1.125M_4 - 0.125x\frac{\partial M_4}{\partial x}, \tag{41}$$

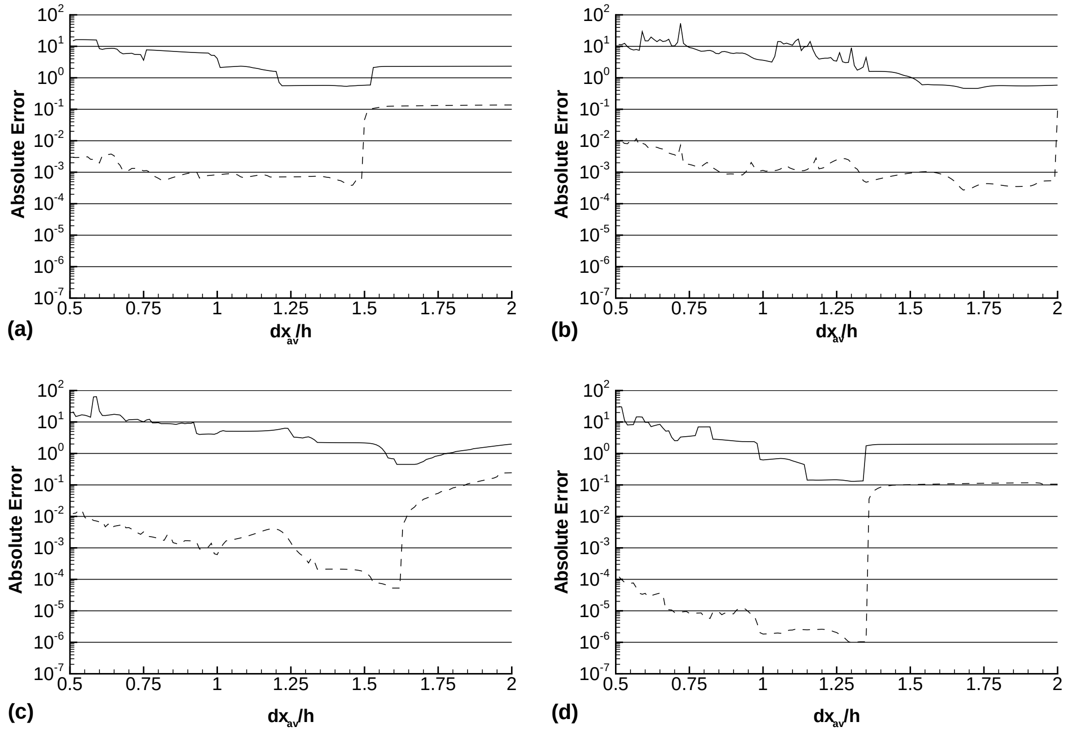

Fig. 7. Error analysis of differentiation using functions based on M_6 and M_8 using SVD for non-equidistant samples. (a) L_∞ error of 3rd order function based on M_6 $\{W_0, W_1, W_2, W_3, W_4\}$ as function of smoothing length (—) $dx_{av} = 0.1$, (- - -) $dx_{av} = 0.01$, (b) L_∞ error of 3rd order function based on M_8 $\{W_0, W_1, W_2, W_3, W_4\}$ as function of smoothing length (—) $dx_{av} = 0.1$, (- - -) $dx_{av} = 0.01$, (c) L_∞ error of 4th order function based on M_8 $\{W_0, W_1, W_2, W_3, W_4, W_5\}$ as function of smoothing length (—) $dx_{av} = 0.1$, (- - -) $dx_{av} = 0.01$, (d) L_∞ error of 5th order function based on M_8 $\{W_0, W_1, W_2, W_3, W_4, W_5, W_6\}$ as function of smoothing length (—) $dx_{av} = 0.1$, (- - -) $dx_{av} = 0.01$.

$$M_5^S = 1.2M_5 - 0.2x\frac{\partial M_5}{\partial x}. \tag{42}$$

The functions M_4^S and M_5^S achieve 2nd order accuracy.

3.2. *Differentiation*

As mentioned in Section 2.5, one can use the B-spline derivatives to construct functions that can be used for differentiation yielding high order of approximation. We will validate this methodology for two functions (M_6, M_8) herein, in the interest of brevity. However, the validity of the technique was tested successfully for a wealth of B-splines. The function to be differentiated is the same as in the case of interpolation (Eq. (32)) from which the exact values of the derivatives were calculated. The error analysis is performed using similar formulas to Eqs. (33) and (34).

The differentiation function is constructed from the derivatives of the basis functions (Eq. (30)). Fig. 7 shows the differentiation error based on functions constructed from M_6 and M_8 for non-equidistant samples. The results indicate that it is possible to construct functions that achieve high-order differentiation (3rd, 4th and 5th shown in Fig. 7(a)–(d)), if a sufficient number of samples is employed. Note that in order to have L order of approximation in differentiation, one needs to solve $L+1$ equations and at least $L+1$ samples are required.

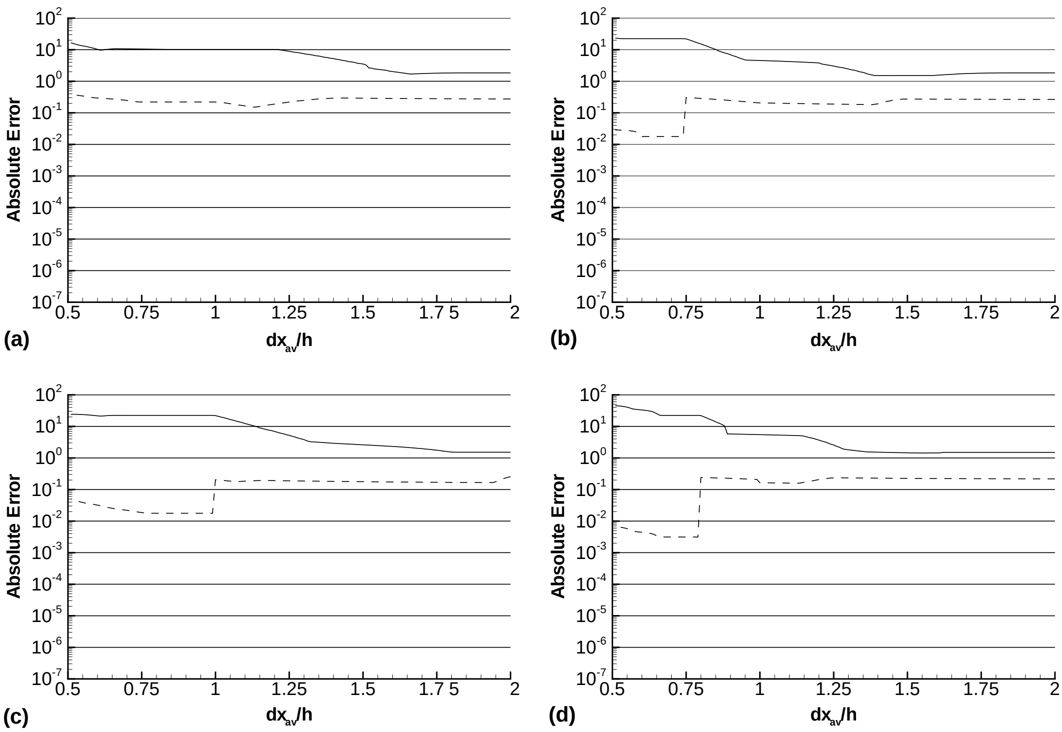

Fig. 8. Error analysis of one-sided differentiation using functions based on M_6 and M_8 using SVD for non-equidistant samples. (a) L_∞ error of 2nd order function based on M_6 $\{W_0, W_1, W_2\}$ as function of smoothing length (—) $dx_{av} = 0.1$, (- - -) $dx_{av} = 0.01$, (b) L_∞ error of 3rd order function based on M_6 $\{W_0, W_1, W_2, W_3\}$ as function of smoothing length (—) $dx_{av} = 0.1$, (- - -) $dx_{av} = 0.01$, (c) L_∞ error of 3rd order function based on M_8 $\{W_0, W_1, W_2, W_3\}$ as function of smoothing length (—) $dx_{av} = 0.1$, (- - -) $dx_{av} = 0.01$, (d) L_∞ error of 4th order function based on M_8 $\{W_0, W_1, W_2, W_3, W_4\}$ as function of smoothing length (—) $dx_{av} = 0.1$, (- - -) $dx_{av} = 0.01$.

The same basis functions (M_6, M_8) were employed for one-sided differentiation. Fig. 8 shows representatives results for 2nd, 3rd and 4th order for differentiation from non-equidistant samples. It is clear that it is possible to create functions that realize high order one-sided differentiation. The error is generally smooth, the system is generally non-singular and has a solution and there is no need for more basis functions than the equations in the system of Eq. (24).

With these results it is demonstrated that the technique we presented can construct functions that achieve high-order differentiation. The technique is robust, requiring only a minimum number of samples that is necessary in order to achieve the desired order of approximation. Similar results were obtained also when the asymmetrical splines (Eqs. (27) and (31)) were employed in order to construct the differentiation function (not shown here for brevity).

4. Conclusions

We presented a technique that can construct in a systematic manner interpolation and differentiation polynomial functions based on the linear combinations of linearly independent functions. The functions are constructed by matching terms in Taylor series expansions. This is identical to the conservation of high-order moments, where all the moments are defined as continuous integrals over the normalized coordinate space. The numerical implementation of these moments involves the approximation of the continuous integrals. The basis functions are based on the derivatives of spline functions (B-splines herein). For the solution of the algebraic equation system, a SVD technique was adopted. The constructed algorithm was tested against interpolation and differentiation for equidistant and non-equidistant samples and detailed error analysis was presented. Additionally, the technique was applied successfully to one-sided interpolation and differentiation. The additional computational cost of the methodology is considered to be small, since one solves small algebraic and local systems of size $L \times L$ in order to construct the appropriate weights for L order approximation. The computational cost can be more significant if the method is used for Lagrangian methods, like SPH, where the topology changes continuously and the constructed functions must be recomputed.

In the present work we applied the technique only for functions based on B-splines. In general, other polynomial functions can be used, for example higher order polynomials in order to achieve the highest possible order of approximation (equal to the support of the kernel) while controlling the regularity of the final function.

The presented technique can be used to construct functions or weights for high-order interpolation or differentiation. It can be applied to arbitrary samples without the need of connectivity or grid based information. The technique presented in this paper does not claim that it can produce unique high order kernels that are not dependent on the topology, but a robust methodology which can alter the accuracy according to the number of nodes involved. This is very important from a practical numerical-computational point of view, as it can couple accuracy and computational cost in an optimized manner. The technique is appropriate for multidimensional interpolation and differentiation of scattered samples either by constructing multidimensional functions, when matching multidimensional Taylor series expansions, or by constructing orthogonal projections in each dimension by matching one-dimensional Taylor series expansions in each dimension. The resulted functions increase the order of accuracy of already existing meshless methods like SPH [18]. The present technique is also relevant to grid based methodologies, to construct weights for stencils that achieve high-order interpolation or differentiation. It can also be employed to increase locally the accuracy of interpolation and differentiation simply by increasing the domain of influence of the kernel function and matching more terms in the Taylor expansions, as in p-adaptivity [36].

A future improvement of the present methodology could be the implementation of an algorithm that can automatically choose the maximum possible order of accuracy for a given function, for a random topology.

An extension to other families of functions presents also the possibility of future work. Our major efforts in the future will be dedicated to the application of the approach to different areas.

Acknowledgements

One of the authors (A.K.C.) is grateful to Julián Sagredo of the Seminar for Applied Mathematics at ETH Zurich for helpful discussions.

Appendix A

For completeness we are showing the first eight B-splines M_n $(W = M_n)$ $(n = 1.8)$ which correspond to the NGP interpolation formula

$$M_1(x,h) = n_d \begin{cases} 1 & 0 \leqslant s < \frac{1}{2}, \quad s = \frac{|x|}{h}, \\ 0 & s \geqslant \frac{1}{2}, \end{cases} \tag{A.1}$$

linear interpolation formula

$$M_2(x,h) = n_d \begin{cases} 1 - s & 0 \leqslant s < 1, \quad s = \frac{|x|}{h}, \\ 0 & s \geqslant 1, \end{cases} \tag{A.2}$$

quadratic spline

$$M_3(x,h) = n_d \begin{cases} \frac{3}{4} - s^2 & 0 \leqslant s < \frac{1}{2}, \quad s = \frac{|x|}{h}, \\ \frac{9}{8} - \frac{3}{2}s + \frac{s^2}{2} & \frac{1}{2} \leqslant s < \frac{3}{2}, \\ 0 & s \geqslant \frac{3}{2}, \end{cases} \tag{A.3}$$

cubic spline

$$M_4(x,h) = n_d \begin{cases} \frac{2}{3} - s^2 + \frac{s^3}{2} & 0 \leqslant s < 1, \quad s = \frac{|x|}{h}, \\ \frac{4}{3} - 2s + s^2 - \frac{s^3}{6} & 1 \leqslant s < 2, \\ 0 & s \geqslant 2, \end{cases} \tag{A.4}$$

quartic spline

$$M_5(x,h) = n_d \begin{cases} \frac{115}{192} - \frac{5s^2}{8} + \frac{s^4}{4} & 0 \leqslant s < \frac{1}{2}, \quad s = \frac{|x|}{h}, \\ \frac{55}{96} + \frac{5s}{24} - \frac{5s^2}{4} + \frac{5s^3}{6} - \frac{s^4}{6} & \frac{1}{2} \leqslant s < \frac{3}{2}, \\ \frac{625}{384} - \frac{125s}{48} + \frac{25s^2}{16} - \frac{5s^3}{12} + \frac{s^4}{24} & \frac{3}{2} \leqslant s < \frac{5}{2}, \\ 0 & s \geqslant \frac{5}{2}, \end{cases} \tag{A.5}$$

quintic spline

$$M_6(x,h) = n_d \begin{cases} \frac{11}{20} - \frac{s^2}{2} + \frac{s^4}{4} - \frac{s^5}{12} & 0 \leqslant s < 1, \quad s = \frac{|x|}{h}, \\ \frac{17}{40} + \frac{5s}{8} - \frac{7s^2}{4} + \frac{5s^3}{4} - \frac{3s^4}{8} + \frac{s^5}{24} & 1 \leqslant s < 2, \\ \frac{243}{120} - \frac{81s}{24} + \frac{9s^2}{4} - \frac{3s^3}{4} + \frac{s^4}{8} - \frac{s^5}{120} & 2 \leqslant s < 3, \\ 0 & s \geqslant 3, \end{cases} \tag{A.6}$$

sextic spline

$$M_7(x,h) = n_d \begin{cases} \frac{5887}{1920} - \frac{77s^2}{32} + \frac{7s^4}{8} - \frac{s^6}{6} & 0 \leqslant s < \frac{1}{2}, \quad s = \frac{|x|}{h}, \\ \frac{7861}{2560} - \frac{7s}{128} - \frac{273s^2}{128} - \frac{35s^3}{48} + \frac{63s^4}{32} - \frac{7s^5}{8} + \frac{s^6}{8} & \frac{1}{2} \leqslant s < \frac{3}{2}, \\ \frac{1379}{1280} + \frac{1267s}{160} - \frac{987s^2}{64} + \frac{133s^3}{12} - \frac{63s^4}{16} + \frac{7s^5}{10} - \frac{s^6}{20} & \frac{3}{2} \leqslant s < \frac{5}{2}, \\ \frac{117649}{7680} - \frac{16807s}{640} + \frac{2401s^2}{128} - \frac{343s^3}{48} + \frac{49s^4}{32} - \frac{7s^5}{40} + \frac{s^6}{120} & \frac{5}{2} \leqslant s < \frac{7}{2}, \\ 0 & s \geqslant \frac{7}{2}, \end{cases} \tag{A.7}$$

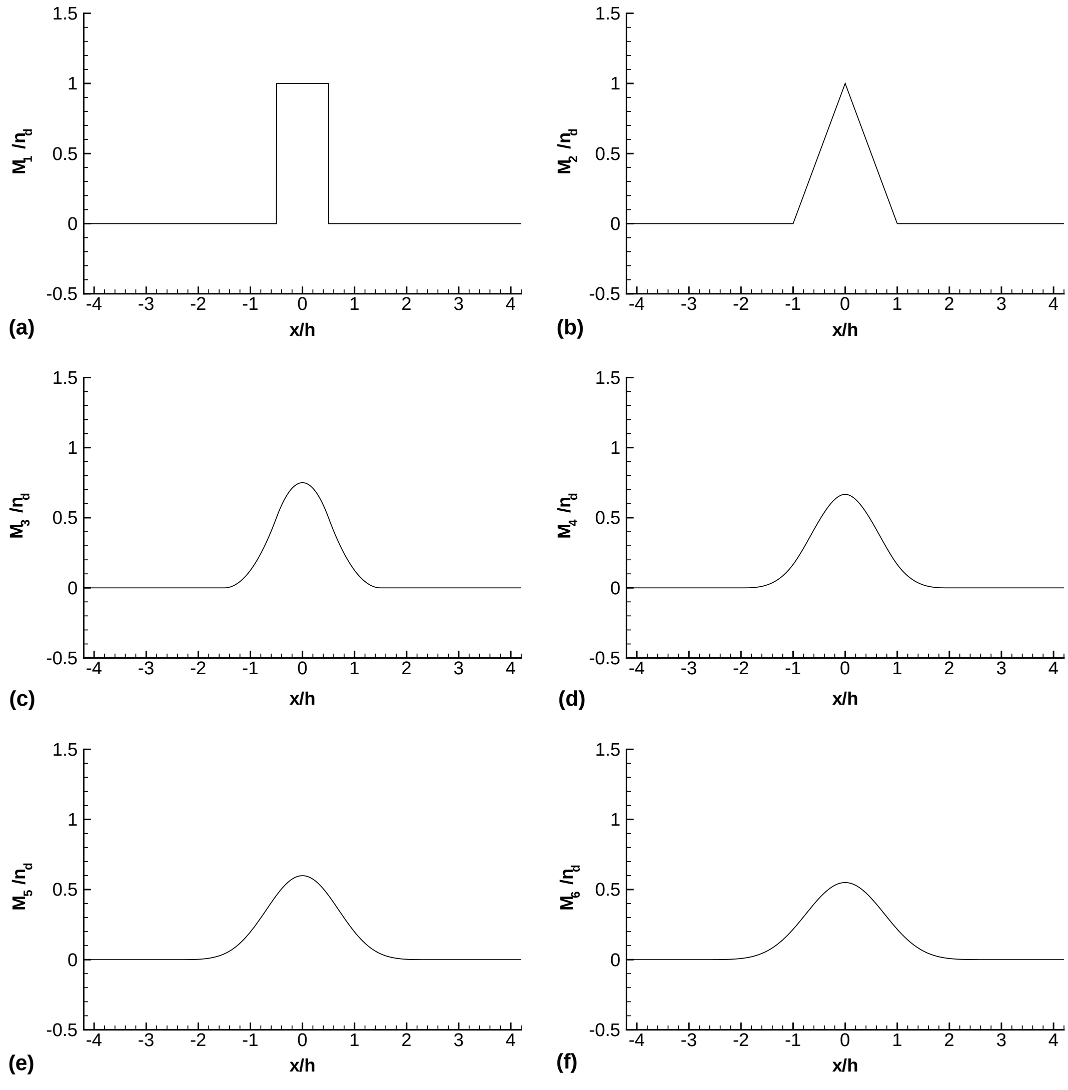

Fig. 9. The first six B-splines (M_1–M_6).

octic spline

$$M_8(x,h) = n_d \begin{cases} \frac{151}{315} - \frac{s^2}{3} + \frac{s^4}{9} - \frac{s^6}{36} + \frac{s^7}{144} & 0 \leqslant s < 1, \quad s = \frac{|x|}{h}, \\ \frac{103}{210} - \frac{7s}{90} - \frac{s^2}{10} - \frac{7s^3}{18} + \frac{s^4}{2} - \frac{7s^5}{30} + \frac{s^6}{20} - \frac{s^7}{240} & 1 \leqslant s < 2, \\ -\frac{139}{630} + \frac{217s}{90} - \frac{23s^2}{6} + \frac{49s^3}{18} - \frac{19s^4}{18} + \frac{7s^5}{30} - \frac{s^6}{36} + \frac{s^7}{20} & 2 \leqslant s < 3, \\ \frac{1024}{315} - \frac{256s}{45} + \frac{64s^2}{15} - \frac{16s^3}{9} + \frac{4s^4}{9} - \frac{s^5}{15} + \frac{s^6}{180} - \frac{s^7}{5040} & 3 \leqslant s < 4, \\ 0 & s \geqslant 4, \end{cases} \tag{A.8}$$

where n_d is a normalization constant that depends on the dimensionality of the problem and it is function of the smoothing length h ($n_d \propto \frac{1}{h^d}$), in order for the B-spline to satisfy Eq. (3). The first six B-splines are shown in Fig. 9.

In general the B-splines can written in symbolic form as

$$M_n^l(x,h) = n_d \sum_{i=0}^{n-1} a_{i,l} s^i, \quad s = \frac{|x|}{h}, \tag{A.9}$$

where the index l represents every segment of the spline.

Appendix B

The solution of the system of Eq. (24) can be singular or near singular. For a square matrix, if all elements of a row or column are zero, or if any row (or column) is equal to another row (or column), or if any row (or column) is a linear combination of other rows (or columns), then the matrix is singular. This can happen in the matrix of Eq. (24) and the determinant of a square sub-matrix is zero or close to zero. The inverse of the sub-matrix can not be calculated, but we must note that the singularity does not mean that the system has no solution. The existence of solution for such system depends on the right-hand-side matrix of Eq. (24). For example, for the equation

$$0 \cdot C_0 + 0 \cdot C_1 + 0 \cdot C_2 + 0 \cdot C_3 + \cdots + 0 \cdot C_n = \mathrm{RHS} \tag{B.1}$$

solution exists only when RHS = 0. This is the case many times for the even lines of the matrix of Eq. (24). Eq. (B.2) shows the system that needs to be solved to achieve 5th order of approximation.

$$\begin{bmatrix} \int_D W_0\,\mathrm{d}x & \int_D W_1\,\mathrm{d}x & \int_D W_2\,\mathrm{d}x & \int_D W_3\,\mathrm{d}x & \int_D W_4\,\mathrm{d}x \\ \int_D xW_0\,\mathrm{d}x \to 0 & \int_D xW_1\,\mathrm{d}x \to 0 & \int_D xW_2\,\mathrm{d}x \to 0 & \int_D xW_3\,\mathrm{d}x \to 0 & \int_D xW_4\,\mathrm{d}x \to 0 \\ \int_D x^2W_0\,\mathrm{d}x & \int_D x^2W_1\,\mathrm{d}x & \int_D x^2W_2\,\mathrm{d}x & \int_D x^2W_3\,\mathrm{d}x & \int_D x^2W_4\,\mathrm{d}x \\ \int_D x^3W_0\,\mathrm{d}x \to 0 & \int_D x^3W_1\,\mathrm{d}x \to 0 & \int_D x^3W_2\,\mathrm{d}x \to 0 & \int_D x^3W_3\,\mathrm{d}x \to 0 & \int_D x^3W_4\,\mathrm{d}x \to 0 \\ \int_D x^4W_0\,\mathrm{d}x & \int_D x^4W_1\,\mathrm{d}x & \int_D x^4W_2\,\mathrm{d}x & \int_D x^4W_3\,\mathrm{d}x & \int_D x^4W_4\,\mathrm{d}x \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}. \tag{B.2}$$

The even equations are satisfied automatically if the right hand side of the system is zero. For such cases instead of the system (B.2) a subsystem can be solved

$$\begin{bmatrix} \int_D W_0\,\mathrm{d}x & \int_D W_1\,\mathrm{d}x & \int_D W_2\,\mathrm{d}x \\ \int_D x^2W_0\,\mathrm{d}x & \int_D x^2W_1\,\mathrm{d}x & \int_D x^2W_2\,\mathrm{d}x \\ \int_D x^4W_0\,\mathrm{d}x & \int_D x^4W_1\,\mathrm{d}x & \int_D x^4W_2\,\mathrm{d}x \end{bmatrix} \begin{bmatrix} C_0 \\ C_1 \\ C_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \tag{B.3}$$

where for $C_3 = C_4 = 0$ is one solution of the system (B.2). There are also cases where the system under consideration has no solution. For example this happens when an equation with a zero right hand side can be written as a linear combination of other equations including the one that has a non-zero right hand side.

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