

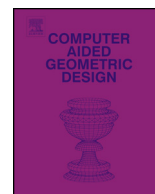


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On shape-preserving capability of cubic L^1 spline fits[☆]Ziteng Wang^{a,*}, Shu-Cherng Fang^a, John E. Lavery^{a,b}^a Edward P. Fitts Department of Industrial and Systems Engineering, North Carolina State University, Raleigh, NC 27695-7906, USA^b Mathematical Sciences Division and Computing Sciences Division, Army Research Office, Army Research Laboratory, P.O. Box 12211, Research Triangle Park, NC 27709-2211, USA

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ABSTRACT

Cubic L^1 spline fits have shown some favorable shape-preserving property for geometric data. To quantify the shape-preserving capability, we consider the basic shape of two parallel line segments in a given window. When one line segment is sufficiently longer than the other, the spline fit can preserve its linear shape in at least half of the window. We propose to use the minimum of such length difference as a shape-preserving metric because it represents the extra information that the spline fits need to preserve the shape. We analytically calculate this metric in a 3-node window for second-derivative-based, first-derivative-based and function-value-based spline fits. In a 5-node window, we compute this metric numerically. In both cases, the shape-preserving metric is rather small, which explains the observed strong shape-preserving capability of spline fits. Moreover, the function-value-based spline fits are indicated to preserve shape better than the other two types of spline fits. This study initiates a quantitative research on shape preservation of L^1 spline fits.

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1. Introduction

Shape preservation is an important objective in the interpolation and approximation of data with abrupt changes in magnitude and/or spacing, such as natural and urban terrain, geophysical features, robot paths, financial data and many other irregular phenomena. Over the past decade and more, L^1 splines have been developed for multiscale univariate (Auquiart et al., 2007a; Cheng et al., 2002; Lavery, 2000, 2002) and bivariate (Lavery, 2001; Wang et al., 2005; Zhang et al., 2006) data and have shown excellent performances in shape preservation, such as L^1 interpolating splines (Auquiart et al., 2007b; Cheng et al., 2005b; Jin et al., 2010; Nyiri et al., 2011; Yu et al., 2010), L^1 smoothing splines (Cheng et al., 2005a; Lavery, 2000) and L^1 spline fits (Lavery, 2004; Wang et al., 2014). Applications on urban terrain reconstruction can be seen, for example, in Bulatov and Lavery (2010) and Lin et al. (2006).

Cubic L^1 spline fits are defined by minimizing an L^1 data fitting functional over a manifold of L^1 interpolating splines. Such L^1 interpolating splines are calculated by minimizing an L^1 interpolating functional. Regarding the order of derivative that is involved in the L^1 interpolating functional, there are three types of spline fits which are second-derivative based, first-derivative based and function-value based, respectively (Jin et al., 2011; Lavery, 2006, 2009). Global algorithms and local moving-window approach have been designed and both produce spline fits that preserve shapes well (Lavery, 2004; Wang et al., 2014; Jin et al., 2010; Yu et al., 2010).

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* Corresponding author.

E-mail addresses: zwang23@ncsu.edu (Z. Wang), fang@ncsu.edu (S.-C. Fang), john.e.lavery4.civ@mail.mil (J.E. Lavery).

Nevertheless, to the best of our knowledge, no theoretic analysis on the shape-preserving capability of the L^1 spline fits is available while the demand for it is growing. Fundamentally, such a theory should define shape preservation in a mathematical form so that different data-approximating principles could be fairly compared. In particular, comparison of the three types of spline fits is of interest. Practically, it should enable us to explain or predict the approximating results of cubic L^1 spline fits in various circumstances. It could help users improve the spline nodes placement or acquire more data where needed. This study is the first step towards this direction. We propose a metric to assess the capability of spline fits in preserving a given linear shape. Then we compare second-derivative-based, first-derivative-based and function-value-based spline fits against this metric. Throughout this paper, by “spline fits” we refer to the univariate cubic L^1 spline fits. Bivariate splines, multivariate splines and polynomials of higher orders are beyond the scope of this paper.

One of the basic principles of shape preservation is that, if some portion of the data is aligned along a straight line segment, the spline fit should reconstruct that line segment. We consider two parallel horizontal line segments, which is a simple and often seen pattern in irregular and multiscale geometric data. For example, a building and its ground around may form such a pattern. This pattern is characterized by a Heaviside step function. Another practical significance of Heaviside step function is in G01 codes in CNC machining, where there is often data lying along a straight line and they need to be fitted by splines (Farouki and Shah, 1996). Spline fits, however, are designed to be C^1 -smooth and thus cannot perfectly recover the jump between the two parallel line segments. Additionally, the spline nodes in applied scenarios are usually fixed a priori. Then, the shape-preserving performance of a spline fit is highly dependent on the relative positions of spline nodes and data. In this study, we approximate the Heaviside step function by spline fits in a window of odd-number equally spaced spline nodes. Naturally, the definition of spline fits is generalized to handle not only discrete data but also functions. In this window, the two parallel line segments may have different lengths. Without loss of generality, we assume the line segment on the left is longer than the line segment on the right. When this length difference is large enough, the spline fit will preserve the linear shape of the longer line segment in at least the left half of the window. The shorter line segment is not necessarily preserved. The reason to this phenomenon is that the longer line segment provides sufficient extra information that leads the spline fit to preserve its linear shape. This extra information can be represented by the length difference between the line segments. Hence, we define the “shape-preserving metric” to be the minimum of such length difference that the linear shape of the longer line segment can be preserved. A smaller metric value indicates the stronger shape-preserving capability.

To calculate the shape-preserving metric, we develop an analytic approach in a 3-node window and a numerical procedure in a 5-node window. In the 3-node window, to keep the information contained in the Heaviside step function from being completely lost, we impose boundary conditions that the first and third spline node have the same function value and first derivative as the Heaviside step function. Then, we can solve the spline fit problem analytically and obtain the explicit relation between the length difference and the function value and first derivative at the middle spline node. Thus, the metric is the minimum length difference such that the middle spline node has the same function value and first derivative as the Heaviside step function. In the 5-node window, we keep increasing the length difference by a given precision and solve the spline fit problem numerically. The metric is the corresponding length difference when the linear shape is preserved for the first time. No boundary conditions are fixed in this case.

Results in 3-node and 5-node windows show that all three types of spline fits have relatively small shape-preserving metrics compared to the space between adjacent spline nodes. Furthermore, we find the second-derivative-based spline fits yield the biggest metric value and the function-value-based spline fits have the smallest. This suggests that the function-value-based spline fits may perform better in shape preservation than the other two types of spline fits.

The remaining of this paper is organized as follows. In Section 2, we extend the second-derivative-based cubic L^1 spline fits to function approximation and introduce first-derivative-based spline fits and function-value-based spline fits. In Section 3, we define the shape-preserving metric by approximating the Heaviside step function in a given window. In Section 4, we calculate the shape-preserving metrics for the three types of spline fits in a 3-node window with fixed boundary conditions. In Section 5, we numerically compute the shape-preserving metrics in a 5-node window. Section 6 summarizes the paper with some concluding remarks.

2. Spline fits for functions

Cubic L^1 spline fits are originally designed in Lavery (2004) to be used for approximating discrete data and they are based on second derivatives of the splines. In this section, we extend the use of spline fits to function approximation and introduce first-derivative and function-value-based spline fits. Suppose the function to be approximated is $f(x)$, $-\infty < x < \infty$. Let the monotonically increasing spline nodes be x_i , $i = 0, 1, \dots, I$. The function values and first derivatives of the spline fit at these nodes are denoted by z_i and b_i , respectively. Let $\mathbf{z} = (z_0, z_1, \dots, z_I)$ and $\mathbf{b} = (b_0, b_1, \dots, b_I)$. Also let $h_i = x_{i+1} - x_i$ and $\Delta z_i = \frac{z_{i+1} - z_i}{h_i}$. We consider C^1 -smooth piecewise cubic polynomials $z(x)$ with nodes x_i , $i = 0, 1, \dots, I$, of the form

$$z(x) = z_i + b_i(x - x_i) + \frac{1}{h_i} [-(2b_i + b_{i+1}) + 3\Delta z_i](x - x_i)^2 + \frac{1}{h_i^2} [b_i + b_{i+1} - 2\Delta z_i](x - x_i)^3 \quad (1)$$

in each interval $[x_i, x_{i+1}]$, $i = 0, 1, \dots, I - 1$. A cubic L^1 spline fit is a function $z(x)$ of form (1) that minimizes the L^1 fitting functional

$$F(\mathbf{z}, \mathbf{b}) := \int_{x_0}^{x_I} |z(x) - f(x)| dx$$

over a manifold of cubic L^1 interpolating splines. The free parameters in a cubic L^1 spline fit are the function values z_i , $i = 0, 1, \dots, I$, at the nodes. For each $\mathbf{z}$, the first derivatives b_i , $i = 0, 1, \dots, I$ of the corresponding interpolating spline are calculated by minimizing an L^1 interpolating functional as described below.

The second-derivative-based interpolating functional is

$$G(\mathbf{b}) := \int_{x_0}^{x_I} \left| \frac{d^2 z}{dx^2} \right| dx$$

with $\mathbf{z}$ fixed. Therefore, the second-derivative-based spline fit optimization problem is

$$\begin{aligned} \min_{\mathbf{z}} \quad & \int_{x_0}^{x_I} |z(x) - f(x)| dx \\ \text{s.t. } \quad & \mathbf{b} = \arg \min_{\mathbf{b}} \int_{x_0}^{x_I} \left| \frac{d^2 z}{dx^2} \right| dx. \end{aligned} \quad (2)$$

The lower-level problem is called the interpolating spline problem.

For the first-derivative-based interpolating spline, the interpolating functional is

$$G(\mathbf{b}) := \sum_{i=0}^{I-1} \int_{x_i}^{x_{i+1}} \frac{1}{h_i} \left| \frac{dz}{dx} - \frac{d\zeta}{dx} \right| dx$$

where $\zeta(x)$ is the piecewise linear function that connects (x_i, z_i) , $i = 0, 1, \dots, I$, i.e.,

$$\zeta(x) = z_i + \frac{\Delta z_i}{h_i}(x - x_i) \quad (3)$$

in each interval $[x_i, x_{i+1}]$. Consequently, the first-derivative-based spline fit optimization problem is

$$\begin{aligned} \min_{\mathbf{z}} \quad & \int_{x_0}^{x_I} |z(x) - f(x)| dx \\ \text{s.t. } \quad & \mathbf{b} = \arg \min_{\mathbf{b}} \sum_{i=0}^{I-1} \int_{x_i}^{x_{i+1}} \frac{1}{h_i} \left| \frac{dz}{dx} - \frac{d\zeta}{dx} \right| dx. \end{aligned}$$

The function-value-based interpolating functional is

$$G(\mathbf{b}) := \sum_{i=0}^{I-1} \int_{x_i}^{x_{i+1}} \frac{1}{h_i^2} |z(x) - \zeta(x)| dx$$

where $\zeta(x)$ is the same as in (3). The function-value-based spline fit optimization problem is

$$\begin{aligned} \min_{\mathbf{z}} \quad & \int_{x_0}^{x_I} |z(x) - f(x)| dx \\ \text{s.t. } \quad & \mathbf{b} = \arg \min_{\mathbf{b}} \sum_{i=0}^{I-1} \int_{x_i}^{x_{i+1}} \frac{1}{h_i^2} |z(x) - \zeta(x)| dx. \end{aligned}$$

For each given $\mathbf{z}$, we denote the optimal solution to the interpolating spline problem by $\mathbf{b}^*(\mathbf{z})$. The optimal solution to the spline fit problem is denoted by $\mathbf{z}^*$.

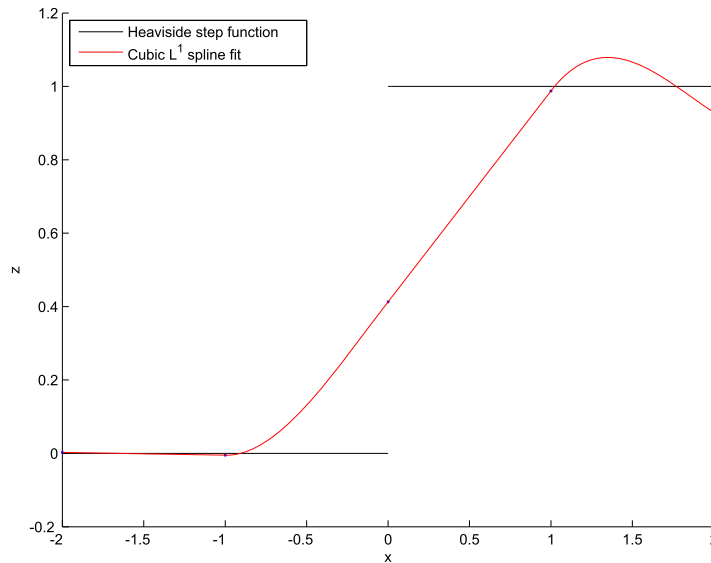


Fig. 1. Second-derivative-based spline fit fails to preserve linear shape of $H_0(x)$.

3. Shape-preserving metric

Consider the following Heaviside step function with a jump at $x = \epsilon \geq 0$:

$$H_\epsilon(x) = \begin{cases} 0, & \text{if } x \leq \epsilon, \\ 1, & \text{if } x > \epsilon. \end{cases}$$

$H_\epsilon(x)$ characterizes the geometric pattern of two parallel line segments, as shown in Fig. 1. W.l.o.g., the gap between two parallel line segments is set to be 1. We approximate $H_\epsilon(x)$ in a window of $I + 1$ equally spaced spline nodes $x_0 = -\frac{I}{2}, \dots, x_{I/2} = 0, \dots, x_I = \frac{I}{2}$ where $I \geq 2$ is an even number. For convenience, the splines nodes are set to be equally spaced and the space between each two adjacent nodes is 1. General spacing settings can be handled without difficulty. If the spline fit $z(x)$ satisfies $z(x) = H_\epsilon(x)$ for all $x_0 = -\frac{I}{2} \leq x \leq 0 = x_{I/2}$, we say the spline fit ϵ -preserves the linear shape. (If not specified otherwise, we use “preserve” instead of “ ϵ -preserve” for simplicity.) For example, it is easy to see that when $\epsilon = \frac{I}{2}$, we have $H_\epsilon(x) = 0$. The spline fit satisfies $z_i = b_i = 0$, $i = 0, \dots, I$ and preserves the linear shape.

The spline fit can preserve the linear shape when the longer line segment contains sufficient extra information over the shorter one. Such extra information is represented by the length difference of the two parallel line segments in $H_\epsilon(x)$, which is 2ϵ . For simplicity, we use ϵ to denote this length difference. We propose the shape-preserving metric as defined below.

Definition 1. The ϵ -shape-preserving metric ϵ^* of cubic L^1 spline fits for approximating $H_\epsilon(x)$ is defined as the minimum of such ϵ that the spline fit $z(x)$ satisfies $z(x) = H_\epsilon(x)$ for $x_0 \leq x \leq x_{I/2}$.

For simplicity, we use “shape-preserving metric” to refer to “ ϵ -shape-preserving metric” in the rest of this paper.

The existence of ϵ^* is guaranteed. Actually, $\epsilon^* \leq \frac{I}{2}$. As we will show in the later sections, when $\epsilon < \epsilon^*$, the spline fit fails to preserve the linear shape. When $\epsilon \geq \epsilon^*$, the spline fit preserves the linear shape. Fig. 1 illustrates that the second-derivative-based spline fit fails to preserve the linear shape of $H_0(x)$ in a 5-node window. Fig. 2 illustrates the second-derivative-based spline fit preserves the linear shape of $H_{0.5}(x)$ in a 5-node window.

4. Calculate ϵ^* in a 3-node window

In this section, we calculate ϵ^* for the three types of spline fits in a 3-node window, i.e., $I = 2$. Noting that a 3-node window is relatively small, we impose boundary conditions so that the information of $H_\epsilon(x)$ can be contained at the boundary. Specifically, we set

$$z_0 = 0, b_0 = 0, z_2 = 1 \text{ and } b_2 = 0. \quad (4)$$

That means that, the boundary nodes coincide with $H_\epsilon(x)$ in terms of function values and first derivatives. In this case, the linear shape will be preserved for $-1 \leq x \leq 0$ if $z_1 = 0$ and $b_1 = 0$.

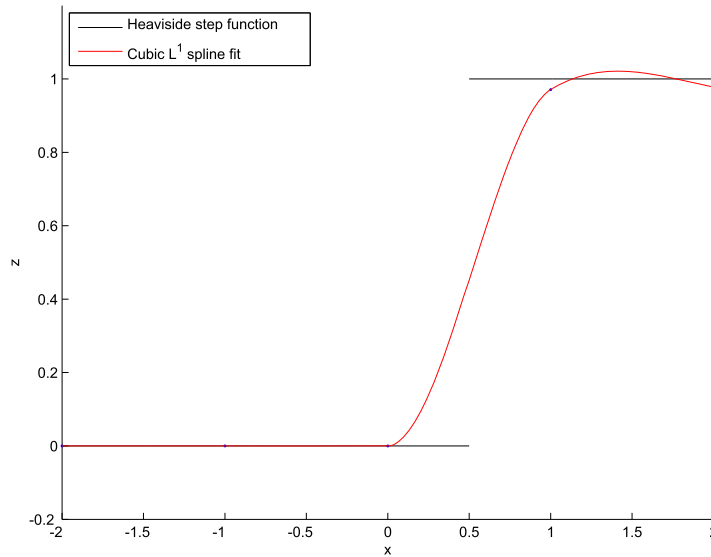


Fig. 2. Second-derivative-based spline fit preserves linear shape of $H_{0.5}(x)$.

We adopt an analytic approach. For second-derivative-based spline fits, we can solve the interpolating spline problem in (2) for the first derivative b_1 , which is a function in z_1 . Then we solve the spline fit problem (2) and analyze the relation between the optimal solution z_1^* and ϵ . We prove that there exists $\epsilon^* > 0$ such that $z_1^* = 0$ if and only if $\epsilon \geq \epsilon^*$. In this case, $b_1^*(z_1^*) = 0$ and thus spline fit preserves linear shape. The value of ϵ^* can be analytically calculated. Shape-preserving metrics of first-derivative-based and function-value-based spline fits are calculated by similar procedures.

4.1. Second-derivative-based spline fits

The solution to the interpolating spline problem is given by the following theorem:

Theorem 1. Given $z_0 = 0$, $b_0 = 0$, $z_2 = 1$ and $b_2 = 0$, the first derivative b_1^* that minimizes the second-derivative-based L^1 interpolating functional

$\int_{-1}^1 \left| \frac{d^2 z}{dx^2} \right| dx$ is a function of z_1 with the following explicit form:

$$b_1^*(z_1) = \begin{cases} 0, & \text{if } z_1 \leq 0, \\ 4z_1(1 - z_1), & \text{if } 0 < z_1 \leq \frac{1}{4}, \\ 1 - z_1, & \text{if } \frac{1}{4} < z_1 \leq \frac{2}{5}, \\ \text{smaller root of } z_1 = \frac{1}{12}(6 - \sqrt{2}\sqrt{21b_1^2 - \sqrt{b_1^2(81b_1^2 - 156b_1 + 76)} - 38b_1 + 18}), & \text{if } \frac{2}{5} < z_1 \leq \frac{1}{2}, \\ \text{smaller root of } z_1 = \frac{1}{12}(6 + \sqrt{2}\sqrt{21b_1^2 - \sqrt{b_1^2(81b_1^2 - 156b_1 + 76)} - 38b_1 + 18}), & \text{if } \frac{1}{2} < z_1 \leq \frac{3}{5}, \\ z_1, & \text{if } \frac{3}{5} < z_1 < \frac{3}{4}, \\ 4z_1(1 - z_1), & \text{if } \frac{3}{4} < z_1 \leq 1, \\ 0, & \text{if } z_1 > 1. \end{cases} \quad (5)$$

Proof. By direct calculation, we have

$$\begin{aligned} z''(-1) &= -2b_1 + 6z_1, & z''(0^-) &= 4b_1 - 6z_1, \\ z''(0^+) &= -4b_1 - 6z_1 + 6, & z''(1) &= 2b_1 + 6z_1 - 6. \end{aligned}$$

Note that $z''(x)$ is discontinuous at $x = 0$. The expression of $G(b_1)$ depends on the signs of $z''(-1)$, $z''(0^-)$, $z''(0^+)$ and $z''(1)$. Accordingly, there are 11 cases as shown in Table 1, along with their defining linear inequalities in terms of b_1 and z_1 . The second column denotes the signs of $(z''(-1), z''(0^-), z''(0^+), z''(1))$. Fig. 3 illustrates the 11 cases in a (z_1, b_1) plane. Within

Table 1

Cases in calculating $b_1^*(z_1)$ for second-derivative-based interpolating splines.

Case	$z''(x)$	$\bar{b}_1(z_1)$	$G'(\bar{b}_1)$
1	$(+, +, +, -)$	$\begin{cases} 3z_1, & \text{if } 0 \leq z_1 \leq \frac{1}{4}, \\ 1 - z_1, & \text{if } \frac{1}{4} \leq z_1 \leq \frac{2}{5}, \\ \frac{3}{2}z_1, & \text{if } \frac{2}{5} \leq z_1 \leq \frac{1}{2}. \end{cases}$	$\begin{cases} < 0, & \text{if } 0 \leq z_1 \leq \frac{1}{4}, \\ = 0, & \text{if } \frac{1}{4} \leq z_1 \leq \frac{2}{5}, \\ > 0, & \text{if } \frac{2}{5} \leq z_1 \leq \frac{1}{2}. \end{cases}$
2	$(+, +, -, +)$	$\max\{\frac{3}{2}z_1, 3(1 - z_1)\}$	> 0
3	$(+, +, -, -)$	$\max\{\frac{3}{2}z_1, \frac{3}{2}(1 - z_1)\}$	> 0
4	$(+, -, +, +)$	$\frac{3}{2}(1 - z_1)$	< 0
5	$(+, -, +, -)$	$\begin{cases} 3z_1, & \text{if } z_1 \leq 0, \\ \frac{3}{2}z_1, & \text{if } 0 \leq z_1 \leq \frac{2}{5}, \\ \text{smaller root of } z_1 = \frac{1}{12}(6 - \sqrt{2}\sqrt{21b_1^2 - \sqrt{b_1^2(81b_1^2 - 156b_1 + 76)} - 38b_1 + 18}), & \text{if } \frac{2}{5} \leq z_1 \leq \frac{1}{2}, \\ \text{smaller root of } z_1 = \frac{1}{12}(6 + \sqrt{2}\sqrt{21b_1^2 - \sqrt{b_1^2(81b_1^2 - 156b_1 + 76)} - 38b_1 + 18}), & \text{if } \frac{1}{2} \leq z_1 \leq \frac{3}{5}, \\ \frac{3}{2}(1 - z_1), & \text{if } \frac{3}{5} \leq z_1 \leq 1, \\ 3(1 - z_1), & \text{if } z_1 \geq 1. \end{cases}$	$\begin{cases} \leq 0, & \text{if } z_1 < \frac{2}{5}, \\ = 0, & \text{if } \frac{2}{5} \leq z_1 \leq \frac{3}{5}, \\ \leq 0, & \text{if } z_1 > \frac{3}{5}. \end{cases}$
6	$(+, -, -, +)$	$\begin{cases} 3(1 - z_1), & \text{if } \frac{2}{3} \leq z_1 \leq \frac{3}{4}, \\ 4z_1(1 - z_1), & \text{if } \frac{3}{4} \leq z_1 \leq 1, \\ 0, & \text{if } z_1 \geq 1. \end{cases}$	$\begin{cases} > 0, & \text{if } \frac{2}{3} \leq z_1 \leq \frac{3}{4}, \\ = 0, & \text{if } \frac{3}{4} \leq z_1 \leq 1, \\ = 0, & \text{if } z_1 \geq 1. \end{cases}$
7	$(+, -, -, -)$	$\begin{cases} \frac{3}{2}(1 - z_1), & \text{if } \frac{1}{2} \leq z_1 \leq \frac{3}{5}, \\ z_1, & \text{if } \frac{3}{5} \leq z_1 \leq \frac{3}{4}, \\ 3(1 - z_1), & \text{if } \frac{3}{4} \leq z_1 \leq 1. \end{cases}$	$\begin{cases} > 0, & \text{if } \frac{1}{2} \leq z_1 \leq \frac{3}{5}, \\ = 0, & \text{if } \frac{3}{5} \leq z_1 \leq \frac{3}{4}, \\ < 0, & \text{if } \frac{3}{4} \leq z_1 \leq 1. \end{cases}$
8	$(-, +, +, -)$	$\begin{cases} 0, & \text{if } z_1 \leq 0, \\ 4z_1(1 - z_1), & \text{if } 0 \leq z_1 \leq \frac{1}{4}, \\ 3z_1, & \text{if } \frac{1}{4} \leq z_1 \leq \frac{1}{3}. \end{cases}$	$\begin{cases} = 0, & \text{if } z_1 \leq 0, \\ = 0, & \text{if } 0 \leq z_1 \leq \frac{1}{4}, \\ > 0, & \text{if } \frac{1}{4} \leq z_1 \leq \frac{1}{3}. \end{cases}$
9	$(-, +, -, +)$	$\max\{3z_1, 3(1 - z_1)\}$	> 0
10	$(-, +, -, -)$	$\max\{3z_1, \frac{3}{2}(1 - z_1)\}$	> 0
11	$(-, -, +, -)$	$\frac{3}{2}z_1$	< 0

each case, we minimize $G(b_1)$ for any given z_1 and denote its minimizer by $\bar{b}_1(z_1)$. The results are listed in Table 1. We use Case 9 and Case 5 as examples to show how to find $\bar{b}_1(z_1)$.

In Case 9, $z''(-1) \leq 0$, $z''(0^-) \geq 0$, $z''(0^+) \leq 0$ and $z''(1) \geq 0$. The roots of $z''(x) = 0$ in $[-1, 0]$ and $[0, 1]$ are

$$u_1 = \frac{-2b_1 + 3z_1}{3(b_1 - 2z_1)} \text{ and } u_2 = \frac{2b_1 - 3(1 - z_1)}{3(b_1 - 2(1 - z_1))},$$

respectively. Hence, for any fixed z_1 ,

$$G(b_1) = \int_{-1}^{u_1} -\frac{d^2z}{dx^2} dx + \int_{u_1}^0 \frac{d^2z}{dx^2} dx + \int_0^{u_2} -\frac{d^2z}{dx^2} dx + \int_{u_2}^1 \frac{d^2z}{dx^2} dx = 2[b_1 - z'(u_1) - z'(u_2)].$$

The first derivative of $G(b_1)$ is

$$G'(b_1) = 2 \left[\frac{(b_1 + z_1 - 1)(b_1 + 3z_1 - 3)}{3(b_1 + 2z_1 - 2)^2} + \frac{(b_1 - z_1)(b_1 - 3z_1)}{3(b_1 - 2z_1)^2} + 1 \right].$$

Note that $b_1 \geq 3z_1$ and $b_1 \geq 3(1 - z_1)$. Then $G'(b_1) > 0$ for all $z_1 \in \mathbb{R}$. Therefore, the minimizer b_1 of $G(b_1)$ in this case is

$$\bar{b}_1(z_1) = \max\{3z_1, 3(1 - z_1)\}.$$

$G'(\bar{b}_1) > 0$ in this case.

In Case 5, $z''(-1) \geq 0$, $z''(0^-) \leq 0$, $z''(0^+) \geq 0$ and $z''(1) \leq 0$. We have

$$G(b_1) = \int_{-1}^{u_1} \frac{d^2z}{dx^2} dx + \int_{u_1}^0 -\frac{d^2z}{dx^2} dx + \int_0^{u_2} +\frac{d^2z}{dx^2} dx + \int_{u_2}^1 -\frac{d^2z}{dx^2} dx = 2[z'(u_1) + z'(u_2) - b_1]$$

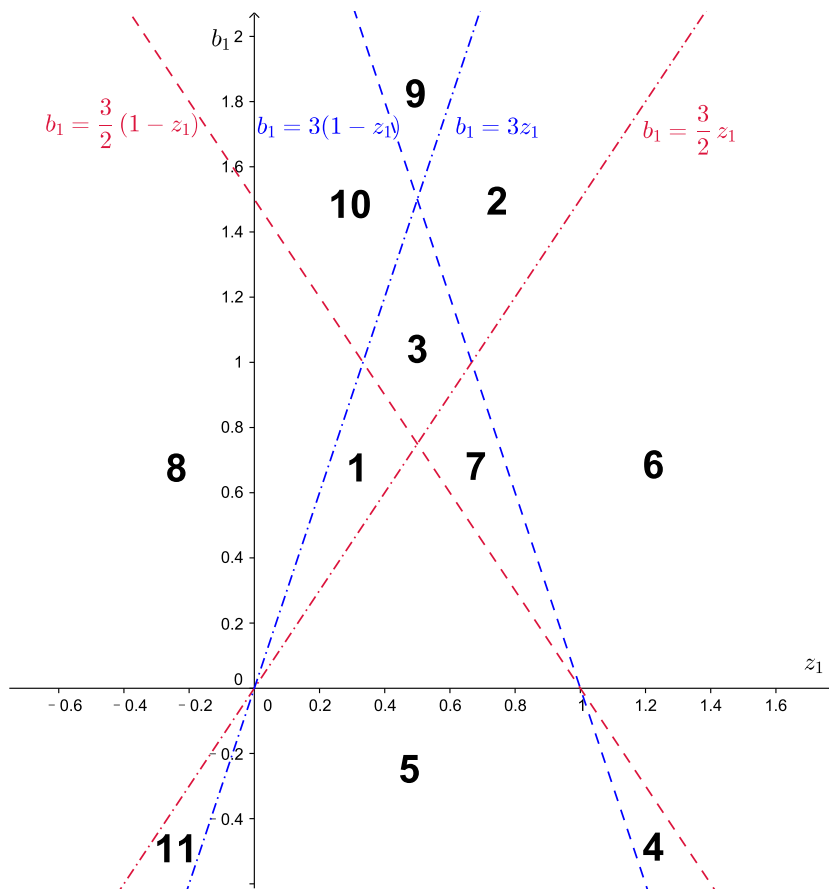


Fig. 3. The 11 cases in calculating $b_1^*(z_1)$ for second-derivative-based interpolating splines.

and

$$G'(b_1) = 2 \left[-\frac{(b_1 + z_1 - 1)(b_1 + 3z_1 - 3)}{3(b_1 + 2z_1 - 2)^2} - \frac{(b_1 - 3z_1)(b_1 - z_1)}{3(b_1 - 2z_1)^2} - 1 \right].$$

Within this case, for $z_1 \leq 0$, we have $G'(3z_1) = -\frac{2(3z_1-1)(11z_1-5)}{(5z_1-2)^2} \leq 0$. Consequently, $\bar{b}_1(z_1) = 3z_1$. We also have $\bar{b}_1(z_1) = \frac{3}{2}z_1$ for $0 \leq z_1 \leq \frac{2}{5}$, $\bar{b}_1(z_1) = \frac{3}{2}(1 - z_1)$ for $\frac{3}{5} \leq z_1 \leq 1$, and $\bar{b}_1(z_1) = 3(1 - z_1)$ for $z_1 \geq 1$.

For $\frac{2}{5} \leq z_1 \leq \frac{1}{2}$, we have $G'(\frac{3}{2}z_1) \geq 0$ and $G'(0) < 0$. Hence, $\bar{b}_1(z_1)$ solves the equation $G(b_1) = 0$. Fig. 4 shows the curve $G'(b_1) = 0$. We can see that in the region corresponding to Case 5, $\bar{b}_1(z_1)$ is the smaller root of the equation $G'(b_1) = 0$. Finding an explicit form of $\bar{b}_1(z_1)$ is a difficult task. (We tried in Mathematica and the obtained expression of $\bar{b}_1(z_1)$ is complicated and inaccurate.) Nevertheless, by simplifying $G'(b_1) = 0$, we have

$$z_1 = \frac{1}{12} (6 - \sqrt{2} \sqrt{21b_1^2 - \sqrt{b_1^2(81b_1^2 - 156b_1 + 76)} - 38b_1 + 18}). \quad (6)$$

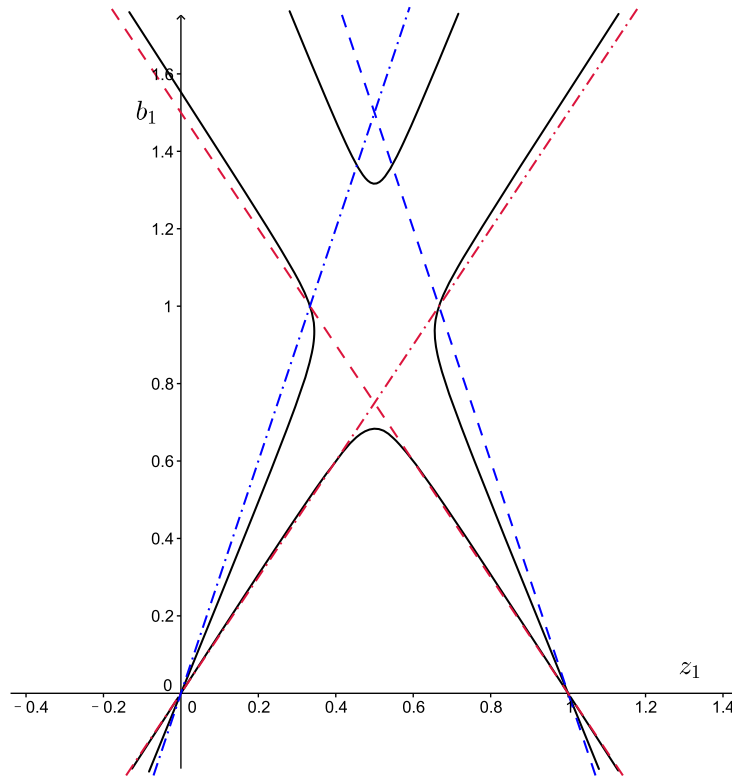
Therefore, for $\frac{2}{5} \leq z_1 \leq \frac{1}{2}$, $\bar{b}_1(z_1)$ is the smaller root of Equation (6).

For $\frac{1}{2} \leq z_1 \leq \frac{3}{5}$, $\bar{b}_1(z_1)$ is the smaller root of the equation

$$z_1 = \frac{1}{12} (6 + \sqrt{2} \sqrt{21b_1^2 - \sqrt{b_1^2(81b_1^2 - 156b_1 + 76)} - 38b_1 + 18}).$$

Similarly, we can calculate $\bar{b}_1(z_1)$ and the sign of $G'(\bar{b}_1)$ for all other cases. Note that $G(b_1)$ is continuous and convex in b_1 . Then $b_1^*(z_1)$ should be the $\bar{b}_1(z_1)$ that satisfies $G'(\bar{b}_1) = 0$. By observing Table 1, we have the expression as in Equation (5). Fig. 5 shows the graph of $b_1^*(z_1)$. □

Now we study the L^1 fitting functional and calculate the shape-preserving metric ϵ^* .

Fig. 4. Curve $G'(b_1) = 0$ in Case 5.

Lemma 1. For two splines $z(x)$ and $\tilde{z}(x)$ in the 3-node window with boundary conditions (4), if $b_1^*(z_1) = b_1^*(\tilde{z}_1)$, then $z(x) - \tilde{z}(x) = z(-x) - \tilde{z}(-x)$ for $-1 \leq x \leq 1$.

Proof. When $-1 \leq x \leq 0$, we have

$$z(x) - \tilde{z}(x) = \frac{1}{h_0}(x - x_0)^2(\Delta z_0 - \Delta \tilde{z}_0)[3 - \frac{2}{h_0}(x - x_0)] = (z_1 - \tilde{z}_1)(1 - 3x^2 - 2x^3)$$

and

$$z(-x) - \tilde{z}(-x) = z_1 - \tilde{z}_1 + \frac{1}{h_1}(-x - x_1)^2(\Delta z_1 - \Delta \tilde{z}_1)[3 - \frac{2}{h_1}(-x - x_1)] = (z_1 - \tilde{z}_1)(1 - 3x^2 - 2x^3).$$

Therefore, $z(x) - \tilde{z}(x) = z(-x) - \tilde{z}(-x)$ for $-1 \leq x \leq 0$. Similar proof applies to $0 \leq x \leq 1$. $\square$

Lemma 2. Given any $0 < \epsilon \leq 1$, $0 \leq z_1^* \leq \frac{1}{4}$ holds for the second-derivative-based spline fit for $H_\epsilon(x)$.

Proof. We prove this lemma by considering different ranges of z_1 according to the expression of $b_1^*(z_1)$.

First, we prove that $z_1^* \leq \frac{1}{2}$. Consider two splines $z(x)$ and $\tilde{z}(x)$ with $z_1 > \frac{1}{2}$ and $\tilde{z}_1 = 1 - z_1$. By symmetry, the first derivatives at node x_1 for both splines are equal, i.e., $b_1^*(z_1) = b_1^*(\tilde{z}_1)$. We have $z(x) = 1 - \tilde{z}(-x)$ and

$$z(x) - \tilde{z}(x) = \frac{1}{h_0}(x - x_0)^2(\Delta z_0 - \Delta \tilde{z}_0)[3 - \frac{2}{h_0}(x - x_0)] \geq 0$$

for all $-1 \leq x \leq 0$. By Lemma 1 we have $z(x) - \tilde{z}(x) \geq 0$ for $-1 \leq x \leq 1$. When $\epsilon = 0$, we know $F_0(z_1, b_1^*(z_1)) = F_0(\tilde{z}_1, b_1^*(\tilde{z}_1))$. When $0 < \epsilon \leq 1$, we consider

$$F_\epsilon(z_1, b_1^*(z_1)) - F_0(z_1, b_1^*(z_1)) = \int_0^\epsilon [|z(x) - 0| - |z(x) - 1|] dx = \int_0^\epsilon [z(x) - |z(x) - 1|] dx$$

and

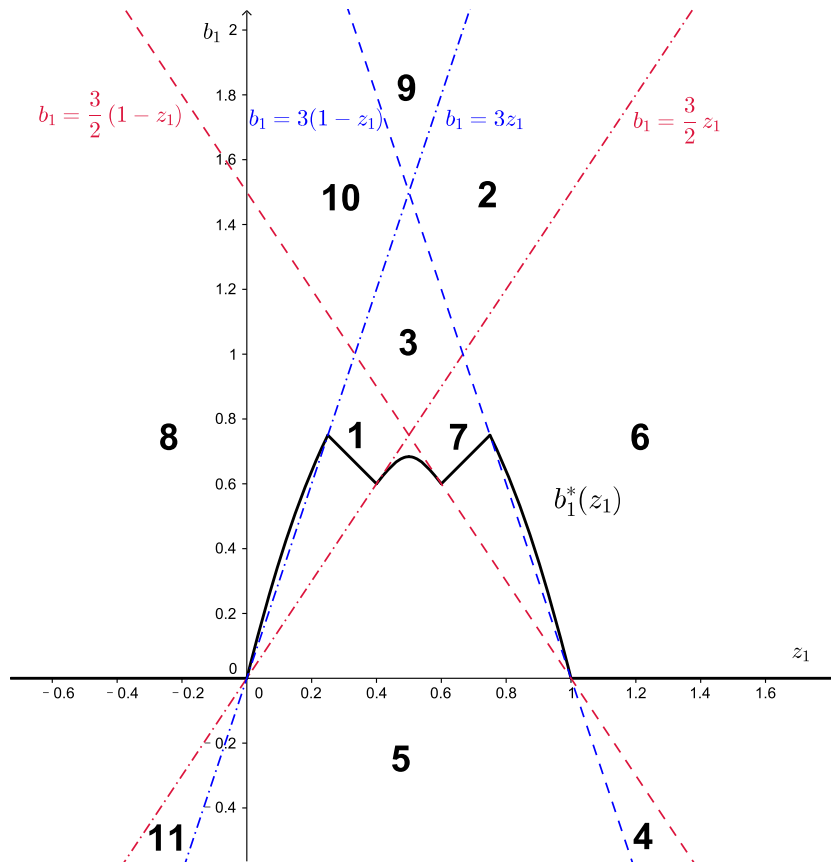


Fig. 5. $b_1^*(z_1)$ of second-derivative-based interpolating splines in a 3-node window with boundary conditions.

$$F_\epsilon(\tilde{z}_1, b_1^*(\tilde{z}_1)) - F_0(\tilde{z}_1, b_1^*(\tilde{z}_1)) = \int_0^\epsilon [|\tilde{z}(x) - 0| - |\tilde{z}(x) - 1|] dx = \int_0^\epsilon [|\tilde{z}(x)| - 1 + \tilde{z}(x)] dx.$$

(1) If $\frac{1}{2} < z_1 \leq \frac{3}{4}$, then $\frac{1}{2} < z(x) < 1$ and $0 < \tilde{z}(x) < z(x)$ for $0 \leq x \leq \epsilon$. Hence,

$$z(x) - |z(x) - 1| = 2z(x) - 1 > 2\tilde{z}(x) - 1 = |\tilde{z}(x)| - 1 + \tilde{z}(x).$$

(2) If $\frac{3}{4} < z_1 \leq 1$, then $0 < \tilde{z}(x) < \min\{z(x), 1\}$ for $0 \leq x \leq \epsilon$. Hence,

$$z(x) - |z(x) - 1| = \min\{2z(x) - 1, 1\} > 2\tilde{z}(x) - 1 = |\tilde{z}(x)| - 1 + \tilde{z}(x).$$

(3) If $z_1 > 1$, then $z(x) > 1$ and $\tilde{z}(x) < 1$ for $0 \leq x \leq \epsilon$. Hence,

$$z(x) - |z(x) - 1| = 1 > \max\{2\tilde{z}(x) - 1, -1\} = |\tilde{z}(x)| - 1 + \tilde{z}(x).$$

Therefore, for $0 < \epsilon \leq 1$, $F_\epsilon(z_1, b_1^*(z_1)) > F_\epsilon(\tilde{z}_1, b_1^*(\tilde{z}_1))$ with $z_1 > \frac{1}{2}$ and $\tilde{z}_1 = 1 - z_1$. The second-derivative-based spline fit has to satisfy $z_1^* \leq \frac{1}{2}$.

Second, we prove that $z_1^* \leq \frac{2}{5}$. Suppose that $\frac{2}{5} < z_1 \leq \frac{1}{2}$. It is easy to see there exists $\frac{1}{4} \leq \tilde{z}_1 \leq \frac{2}{5}$ such that $b_1^*(\tilde{z}_1) = b_1^*(z_1)$. Notice that $b_1^*(z_1) \leq 3z_1$, $b_1^*(z_1) \leq 3(1 - z_1)$, $b_1^*(\tilde{z}_1) \leq 3z_1$ and $b_1^*(\tilde{z}_1) \leq 3(1 - z_1)$. Thus, we have $0 \leq \tilde{z}(x) \leq z(x) \leq 1$ for all $-1 \leq x \leq 1$ and the equality holds only at $x = -1$ and 1 . By Lemma 1, we know $\int_{-1}^\epsilon |z(x) - 0| dx - \int_{-1}^\epsilon |\tilde{z}(x) - 0| dx = \int_\epsilon^1 |\tilde{z}(x) - 1| dx - \int_\epsilon^1 |z(x) - 1| dx$. Note $\int_{-\epsilon}^\epsilon |z(x) - 0| dx > \int_{-\epsilon}^\epsilon |\tilde{z}(x) - 0| dx$. Hence, $F_\epsilon(z_1, b_1^*(z_1)) > F_\epsilon(\tilde{z}_1, b_1^*(\tilde{z}_1))$. Consequently, $z_1^* \leq \frac{2}{5}$.

Third, we show that $z_1^* \leq \frac{1}{4}$. When $\frac{1}{4} \leq z_1 \leq \frac{2}{5}$, $b_1^*(z_1) = 1 - z_1$. Then, the fitting functional becomes

$$F_\epsilon(z_1, b_1^*(z_1)) = \frac{\epsilon^4 z_1}{2} - \frac{\epsilon^4}{2} - \frac{2\epsilon^3 z_1}{3} + \frac{2\epsilon^3}{3} - \epsilon^2 z_1 + \epsilon^2 + 2\epsilon z_1 - \epsilon + \frac{z_1}{6} + \frac{1}{3}.$$

The first derivative in z_1 is

$$\frac{dF_\epsilon(z_1, b_1^*(z_1))}{dz_1} = \frac{1}{6}(3\epsilon^4 - 4\epsilon^3 - 6\epsilon^2 + 12\epsilon + 1) = \frac{1}{6}[3\epsilon^4 + 4\epsilon(1 - \epsilon^2) + 6\epsilon(1 - \epsilon) + 2\epsilon + 1] > 0.$$

Therefore, the minimum z_1^* of $F_\epsilon(z_1, b_1^*(z_1))$ in $z_1 \leq \frac{2}{5}$ satisfies $z_1^* \leq \frac{1}{4}$.

Finally, we prove that $z_1^* \geq 0$. Suppose that $z_1 < 0$. Then we know $b_1^*(z_1) = 0$. For $-1 \leq x \leq 0$, $z(x) = z_1(1+x)^2(1-2x) \leq 0$. For $0 \leq x \leq 1$, $z(x) = 3x^2(1-z_1) - 2x^3(1-z_1) + z_1$. It is easy to verify that $z'(x) \geq 0$. Thus, $z(x) = 0$ has one root in $0 \leq x \leq 1$. Denote this root by $r(z_1)$. Using the implicit function theorem, we have

$$\frac{dr(z_1)}{dz_1} = -\frac{\frac{\partial z(x)}{\partial z_1}}{\frac{\partial z(x)}{\partial x}} = -\frac{-3x^2 + 2x^3 + 1}{6x(1-z_1)(1-x)} \leq 0.$$

Hence, $r(z_1)$ decreases as z_1 increases. For any $0 < \epsilon \leq 1$, there exists some node function value $z_1(\epsilon)$ such that $r(z_1(\epsilon)) = \epsilon$. When $z_1 < \tilde{z}_1 \leq z_1(\epsilon)$, we can easily see $z(x) \leq \tilde{z}(x)$ and, consequently, $F_\epsilon(z_1, b_1^*(z_1)) > F_\epsilon(\tilde{z}_1, b_1^*(\tilde{z}_1))$. When $z_1(\epsilon) < z_1 \leq 0$,

$$F_\epsilon(z_1, b_1^*(z_1)) = \int_{-1}^0 -z(x)dx + \int_0^{r(z_1)} -z(x)dx + \int_{r(z_1)}^\epsilon z(x)dx + \int_\epsilon^1 1 - z(x)dx.$$

Taking the derivative with respect to z_1 , we have

$$\frac{dF_\epsilon(z_1, b_1^*(z_1))}{dz_1} = \int_{-1}^0 -\frac{dz(x)}{dz_1}dx + \int_0^{r(z_1)} -\frac{dz(x)}{dz_1}dx + \int_{r(z_1)}^\epsilon \frac{dz(x)}{dz_1}dx + \int_\epsilon^1 -\frac{dz(x)}{dz_1}dx.$$

Notice that $\frac{dz(x)}{dz_1} \geq 0$ for $-1 \leq x \leq 1$. By direct calculation, we have $\int_{-1}^0 -\frac{dz(x)}{dz_1}dx + \int_0^1 \frac{dz(x)}{dz_1}dx = 0$. Hence, $\frac{dF_\epsilon(z_1, b_1^*(z_1))}{dz_1} \leq 0$ and $z_1^* \geq 0$.

Combining all arguments above, we have $0 \leq z_1^* \leq \frac{1}{4}$. $\square$

Theorem 2. Fix $z_0 = 0, b_0 = 0, z_2 = 1$ and $b_2 = 0$ in the 3-node window. The second-derivative-based spline fit for $H_\epsilon(x)$ preserves its linear shape in $-1 \leq x \leq 0$, i.e., $z_1^* = 0$ and $b_1^*(z_1^*) = 0$, if and only if $\epsilon \geq 0.250$. This means that the shape-preserving metric of second-derivative-based spline fits is 0.250.

Proof. To solve the spline fit problem, we only need to consider $0 \leq z_1 \leq \frac{1}{4}$. In this range of z_1 , $b_1 = 4z_1(1 - z_1) > 3z_1$. This means $z''(-1) \leq 0$ and the cubic L^1 spline fit intersects with $H_\epsilon(x)$ in the interval $-1 < x < 0$ at another point besides x_0 . Solve the equation $z(x) = 0$, we have this point $\bar{x} = \frac{1}{4z_1 - 2}$. The cubic L^1 spline fit has no other intersection with $H_\epsilon(x)$ than x_2 in the interval $0 \leq x \leq 1$ because $b_1^*(z_1) < 3(1 - z_1)$ when $0 \leq z_1 \leq \frac{1}{4}$.

The L^1 fitting functional then becomes

$$\begin{aligned} F_\epsilon(z_1, b_1^*(z_1)) &= \int_{-1}^{\bar{x}} [H_\epsilon(x) - z(x)]dx + \int_{\bar{x}}^0 [z(x) - H_\epsilon(x)]dx + \int_0^\epsilon [z(x) - H_\epsilon(x)]dx + \int_\epsilon^1 [H_\epsilon(x) - z(x)]dx \\ &= -2\epsilon^4 z_1^2 + 3\epsilon^4 z_1 - \epsilon^4 + \frac{16\epsilon^3 z_1^2}{3} - \frac{22\epsilon^3 z_1}{3} + 2\epsilon^3 - 4\epsilon^2 z_1^2 + 4\epsilon^2 z_1 + 2\epsilon z_1 - \epsilon \\ &\quad - \frac{8z_1^5}{3(2z_1 - 1)^3} + \frac{8z_1^4}{3(2z_1 - 1)^3} - \frac{2z_1^3}{(2z_1 - 1)^3} + \frac{z_1^2}{3} + \frac{z_1^2}{(2z_1 - 1)^3} - \frac{5z_1}{6} - \frac{3z_1}{16(2z_1 - 1)^3} + \frac{1}{2}. \end{aligned}$$

The first derivative in z_1 is

$$\begin{aligned} \frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1} &= \epsilon^4(3 - 4z_1) + \frac{2}{3}\epsilon^3(16z_1 - 11) + \epsilon^2(4 - 8z_1) + 2\epsilon + \frac{4z_1(73 - 64z_1(3(z_1 - 2)z_1 + 4)) - 31}{48(1 - 2z_1)^4}. \end{aligned}$$

Then we have

$$\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial \epsilon \partial z_1} = -2(\epsilon - 1)^2(\epsilon(8z_1 - 6) - 1)$$

and

$$\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1^2} = \frac{2(37 - 64z_1)z_1 - 11}{12(2z_1 - 1)^5} - \frac{4}{3}\epsilon^2(\epsilon(3\epsilon - 8) + 6).$$

It is easy to verify that $\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1^2} \geq \frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1^2} \Big|_{z_1=0}$ for $0 \leq z_1 \leq \frac{1}{4}$ and $0 \leq \epsilon \leq 1$. Notice that $\frac{\partial^2 F_{0.5}(z_1, b_1^*(z_1))}{\partial z_1^2} \Big|_{z_1=0} = 0$. Therefore, $\frac{\partial^2 F_{0.5}(z_1, b_1^*(z_1))}{\partial z_1^2} \geq 0$ for $0 \leq z_1 \leq \frac{1}{4}$. Then $\frac{\partial F_{0.5}(z_1, b_1^*(z_1))}{\partial z_1} \geq \frac{\partial F_{0.5}(z_1, b_1^*(z_1))}{\partial z_1} \Big|_{z_1=0} = \frac{15}{24} > 0$. On the other hand, $\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial \epsilon \partial z_1} \geq 0$ for $0 \leq z_1 \leq \frac{1}{4}$ and $0 \leq \epsilon \leq 1$. Hence, $\frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1} \geq 0$ for $0 \leq z_1 \leq \frac{1}{4}$ and $0.5 \leq \epsilon \leq 1$. This implies that $z_1^* = 0$ for $0.5 \leq \epsilon \leq 1$ and $\epsilon^* \leq 0.5$.

When $0 \leq z_1 \leq \frac{1}{4}$ and $0 \leq \epsilon \leq 0.5$, by noticing $\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1^2}$ is decreasing in ϵ , we have $\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1^2} \geq \frac{\partial^2 F_{0.5}(z_1, b_1^*(z_1))}{\partial z_1^2} \Big|_{z_1=0} = 0$. Consequently, $F_\epsilon(z_1, b_1^*(z_1))$ is convex in $0 \leq z_1 \leq \frac{1}{4}$ for $0 \leq \epsilon \leq 0.5$. Then $z_1 = 0$ minimizes $F_\epsilon(z_1, b_1^*(z_1))$ if $\frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1} \Big|_{z_1=0} \geq 0$. By direct calculation we have

$$\frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1} \Big|_{z_1=0} = 3\epsilon^4 - \frac{22\epsilon^3}{3} + 4\epsilon^2 + 2\epsilon - \frac{31}{48}.$$

Recall that $\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial \epsilon \partial z_1} \geq 0$. Solve the equation $\frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1} \Big|_{z_1=0} = 0$ and we have its unique solution

$$\begin{aligned} \epsilon^* &= \frac{11}{18} - \frac{1}{18} \sqrt{\frac{7}{2} \left(9\sqrt[3]{7 - \sqrt{22}} + 9\sqrt[3]{7 + \sqrt{22}} + 14 \right)} \\ &\quad + \frac{1}{18} \sqrt{\frac{7}{2} \left(-9\sqrt[3]{7 - \sqrt{22}} - 9\sqrt[3]{7 + \sqrt{22}} + 28 \sqrt{\frac{14}{9\sqrt[3]{7 - \sqrt{22}} + 9\sqrt[3]{7 + \sqrt{22}} + 14}} + 28 \right)} \\ &\simeq 0.250. \end{aligned}$$

Therefore, when $\epsilon \geq 0.250$, the second-derivative-based spline fit for $H_\epsilon(x)$ satisfies $z_1^* = 0$ and $b_1^*(z_1^*) = 0$. $\square$

4.2. First-derivative-based spline fits

Theorem 3. Given $z_0 = 0, b_0 = 0, z_2 = 1$ and $b_2 = 0$, the first derivative b_1^* that minimizes the first-derivative-based L^1 interpolating

functional $\int_{-1}^1 \left| \frac{dz}{dx} - \frac{d\zeta}{dx} \right| dx$ satisfies the following properties:

- (1) $b_1^*(z_1) = 0$, if $z_1 \leq 0$,
- (2) $z_1 \leq b_1^*(z_1) \leq 2z_1$, if $0 < z_1 \leq 0.255443$,
- (3) $0 < b_1^*(z_1) \leq z_1$, if $0.255443 < z_1 \leq \frac{1}{2}$,
- (4) $0 < b_1^*(z_1) \leq 1 - z_1$, if $\frac{1}{2} < z_1 \leq 0.755443$,
- (5) $1 - z_1 \leq b_1^*(z_1) \leq 2(1 - z_1)$, if $0.755443 < z_1 \leq 1$,
- (6) $b_1^*(z_1) = 0$, if $z_1 > 1$.

Proof. Note that the interpolating functional $\int_{-1}^1 \left| \frac{dz}{dx} - \frac{d\zeta}{dx} \right| dx$ is convex in z_1 and b_1 . Consequently, $G(b_1)$ is convex in b_1 for any given z_1 .

When $-1 \leq x \leq 0$, we have

$$z'(x) = 3(b_1 - 2z_1)(x + 1)^2 - 2(b_1 - 3z_1)(x + 1)$$

and $\zeta'(x) = z_1$.

When $z_1 \leq 0$ and $b_1 \geq z_1$, the equation $z'(x) - \zeta'(x) = 0$ has two roots in $-1 \leq x \leq 0$. Moreover,

$$w_1 = \frac{-\sqrt{b_1^2 - 3b_1z_1 + 3z_1^2} - 2b_1 + 3z_1}{3(b_1 - 2z_1)}, w_2 = \frac{\sqrt{b_1^2 - 3b_1z_1 + 3z_1^2} - 2b_1 + 3z_1}{3(b_1 - 2z_1)},$$

$$G_0(b_1) = \int_{-1}^{w_1} z'(x) - \zeta'(x) dx + \int_{w_1}^{w_2} \zeta'(x) - z'(x) dx + \int_{w_2}^0 z'(x) - \zeta'(x) dx,$$

and

$$\frac{dG_0}{db_1} = \int_{-1}^{w_1} \frac{\partial z'(x)}{\partial b_1} dx + \int_{w_1}^{w_2} -\frac{\partial z'(x)}{\partial b_1} dx + \int_{w_2}^0 \frac{\partial z'(x)}{\partial b_1} dx.$$

When $b_0 = 0$, we have

$$\frac{dG_0}{db_1} \Big|_{b_1=0} = -\frac{\sqrt{z_1^2}}{3\sqrt{3}z_1} = \frac{1}{3\sqrt{3}}.$$

Similarly, when $z_1 \leq 0$ and $b_1 \leq 1 - z_1$, we can calculate

$$\frac{dG_1}{db_1} \Big|_{b_1=0} = -\frac{\sqrt{(1-z_1)^2}}{3\sqrt{3}(1-z_1)} = -\frac{1}{3\sqrt{3}}.$$

Hence,

$$\frac{dG}{db_1} \Big|_{b_1=0} = \frac{dG_0}{db_1} \Big|_{b_1=0} + \frac{dG_1}{db_1} \Big|_{b_1=0} = 0.$$

Therefore, $b_1^*(z_1) = 0$ for $z_1 \leq 0$.

When $z_1 \geq 0$, $z_1 \leq b_1 \leq 2z_1$ and $b_1 \leq 1 - z_1$, the equation $z'(x) - \zeta'(x) = 0$ has one root w_2 in $-1 \leq x \leq 0$ and the following two roots w_3 and w_4 in $0 \leq x \leq 1$:

$$w_3 = \frac{-\sqrt{b_1^2 - 3b_1(1-z_1) + 3(1-z_1)^2} - 2b_1 + 3(1-z_1)}{3(b_1 - 2(1-z_1))},$$

$$w_4 = \frac{\sqrt{b_1^2 - 3b_1(1-z_1) + 3(1-z_1)^2} - 2b_1 + 3(1-z_1)}{3(b_1 - 2(1-z_1))}.$$

Then

$$G(b_1) = \int_{-1}^{w_2} \zeta'(x) - z'(x) dx + \int_{w_2}^0 z'(x) - \zeta'(x) dx + \int_0^{w_4} \zeta'(x) - z'(x) dx + \int_{w_4}^{w_3} z'(x) - \zeta'(x) dx + \int_{w_3}^1 \zeta'(x) - z'(x) dx.$$

We can verify that $G(b_1)|_{b_1 \rightarrow 2z_1} > 0$ for $0 \leq z_1 \leq \frac{1}{3}$ and $G(b_1)|_{b_1=1-z_1} > 0$ for $\frac{1}{3} \leq z_1 \leq \frac{1}{2}$. Furthermore, $G(b_1)|_{b_1=z_1}$ is increasing in $0 \leq z_1 \leq \frac{1}{2}$, $G(b_1)|_{b_1=z_1=0} < 0$ and $G(b_1)|_{b_1=z_1=\frac{1}{2}} > 0$. Denote the root of $G(b_1)|_{b_1=z_1} = 0$ by θ . We can compute $\theta \approx 0.255443$. Therefore, $z_1 \leq b_1^*(z_1) \leq 2z_1$, if $0 \leq z_1 \leq 0.255443$. Moreover, $b_1^*(z_1) \leq z_1$, if $0.255443 \leq z_1 \leq \frac{1}{2}$.

When $z_1 \geq 0$, $b_1 \leq z_1$ and $b_1 \leq 1 - z_1$, we can calculate

$$\frac{dG}{db_1} \Big|_{b_1=0} = -\frac{2}{3\sqrt{3}} < 0.$$

Then $0 < b_1^*(z_1) \leq z_1$, if $0.255443 \leq z_1 \leq \frac{1}{2}$. The remaining part of the theorem holds by symmetry. $\square$

Fig. 6 shows the graph of $b_1^*(z_1)$.

Lemma 3. Given any $0 < \epsilon \leq 1$, $0 \leq z_1^* \leq \frac{1}{2}$ holds for the first-derivative-based spline fit for $H_\epsilon(x)$.

Proof. Note that $0 \leq b_1^*(z_1) \leq 3(1-z_1)$ for $\frac{1}{2} \leq z_1 \leq 1$, $b_1^*(z_1) = 0$ for $z_1 \geq 1$, and $b_1^*(z_1) = 0$ for $z_1 \leq 0$. The proof of Lemma 2 can be applied. $\square$

Theorem 4. Fix $z_0 = 0$, $b_0 = 0$, $z_2 = 1$ and $b_2 = 0$ in the 3-node window. The first-derivative-based spline fit for $H_\epsilon(x)$ preserves its linear shape in $-1 \leq x \leq 0$, i.e., $z_1^* = 0$ and $b_1^*(z_1^*) = 0$, if and only if $\epsilon \geq 0.109$. This means that the shape-preserving metric of first-derivative-based spline fits is 0.109.

Proof. We only need to consider $0 \leq z_1 \leq \frac{1}{2}$. First, we prove that $z_1^* = 0$ minimizes $F_\epsilon(z_1, b_1^*(z_1))$ locally in $0 \leq z_1 \leq 0.255443$ only if $\epsilon \geq 0.109$. Second, that we prove when $\epsilon \geq 0.109$, $z_1^* = 0$ minimizes $F_\epsilon(z_1, b_1^*(z_1))$ globally in $0 \leq z_1 \leq \frac{1}{2}$.

We notice that $0 \leq z(x) \leq 1$ for $-1 \leq x \leq 1$ because $b_1^*(z_1) < \min\{3z_1, 3(1-z_1)\}$. Therefore,

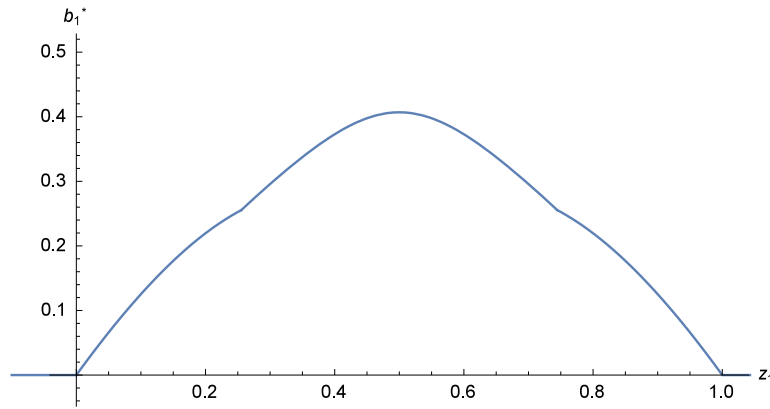


Fig. 6. $b_1^*(z_1)$ of first-derivative-based interpolating spline in a 3-node window with boundary conditions.

$$\begin{aligned} F_\epsilon(z_1, b_1^*(z_1)) &= \int_{-1}^0 [z(x) - H_\epsilon(x)] dx + \int_0^\epsilon [z(x) - H_\epsilon(x)] dx + \int_\epsilon^1 [H_\epsilon(x) - z(x)] dx \\ &= \left(\frac{\epsilon^4}{2} - \frac{4\epsilon^3}{3} + \epsilon^2 - \frac{1}{6} \right) b_1 + (\epsilon^4 - 2\epsilon^3 + 2\epsilon) z_1 - \epsilon^4 + 2\epsilon^3 - \epsilon + \frac{1}{2}. \end{aligned}$$

The first derivative in z_1 is

$$\frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1} = \left(\frac{\epsilon^4}{2} - \frac{4\epsilon^3}{3} + \epsilon^2 - \frac{1}{6} \right) \frac{db_1}{dz_1} + (\epsilon^4 - 2\epsilon^3 + 2\epsilon).$$

The second derivative in z_1 is

$$\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1^2} = \left(\frac{\epsilon^4}{2} - \frac{4\epsilon^3}{3} + \epsilon^2 - \frac{1}{6} \right) \frac{d^2 b_1}{dz_1^2}.$$

We observe from Fig. 6 that $b_1^*(z_1)$ is concave in $0 \leq z_1 \leq 0.255443$. Thus $\frac{d^2 b_1}{dz_1^2} \leq 0$. On the other hand, $(\frac{\epsilon^4}{2} - \frac{4\epsilon^3}{3} + \epsilon^2 - \frac{1}{6}) = \frac{1}{6}(\epsilon - 1)^3(3\epsilon + 1) \leq 0$ for $0 \leq \epsilon \leq 1$. Consequently, we have $\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1^2} \geq 0$ and then $F_\epsilon(z_1, b_1^*(z_1))$ is convex in z_1 . $z_1^* = 0$ minimizes $F_\epsilon(z_1, b_1^*(z_1))$ in $0 \leq z_1 \leq 0.255443$ if and only if $\frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1} \Big|_{z_1=0} \geq 0$. Notice that

$$\frac{\partial^2 F_\epsilon(z_1, b_1^*(z_1))}{\partial \epsilon \partial z_1} = 2(\epsilon - 1)^2 \epsilon \frac{db_1}{dz_1} + 2(\epsilon - 1)^2(2\epsilon + 1) \geq 0$$

for $0 \leq \epsilon \leq 1$. We need to solve the following equation for ϵ^* :

$$-\frac{\epsilon^4 - 2\epsilon^3 + 2\epsilon}{\frac{\epsilon^4}{2} - \frac{4\epsilon^3}{3} + \epsilon^2 - \frac{1}{6}} = \frac{db_1}{dz_1} \Big|_{z_1=0}. \quad (7)$$

Now we calculate $\frac{db_1}{dz_1} \Big|_{z_1=0}$. Suppose $\frac{db_1}{dz_1} \Big|_{z_1=0} = k$. Solve the equation

$$\lim_{z_1 \rightarrow 0} \frac{dG(b_1)}{db_1} \Big|_{b_1=kz_1} = 0$$

and we have $k = 1.37885$. Substituting $\frac{db_1}{dz_1} \Big|_{z_1=0} = 1.37885$ to Equation (7), we can obtain $\epsilon^* = 0.109$.

Now we prove that when $\epsilon \geq \epsilon^*$, $z_1^* = 0$ is the global minimum of $F_\epsilon(z_1, b_1^*(z_1))$ in $0 \leq z_1 \leq \frac{1}{2}$. We observe that $b_1^*(z_1)$ is concave in $0.255443 \leq z_1 \leq \frac{1}{2}$. Moreover, $\frac{db_1}{dz_1} \Big|_{z_1=0.255443} \leq 1$ because $b_1^*(0.255443) = 0.255443$ and $b_1 \leq z_1$ for $0.255443 \leq z_1 \leq \frac{1}{2}$. Hence, $\frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1} \geq 0$ in $0.255443 \leq z_1 \leq \frac{1}{2}$. Therefore, when $\epsilon \geq \epsilon^*$, $\frac{\partial F_\epsilon(z_1, b_1^*(z_1))}{\partial z_1}$ is monotonically increasing in $0 \leq z_1 \leq \frac{1}{2}$. The minimum is $z_1^* = 0$. $\square$

Remark 1. In the proof of Theorem 4, we used the concavity of function $b_1^*(z_1)$ in intervals $0 \leq z_1 \leq 0.255443$ and $0.255443 \leq z_1 \leq \frac{1}{2}$. This property of $b_1^*(z_1)$ is assumed without a mathematical proof because no analytic expression of $b_1^*(z_1)$ is available. Nevertheless, we can observe it in Fig. 6.

4.3. Function-value-based spline fits

Theorem 5. Given $z_0 = 0$, $b_0 = 0$, $z_2 = 1$ and $b_2 = 0$, the first derivative b_1^* that minimizes the function-value-based L^1 interpolating functional $\int_{-1}^1 |z(x) - \zeta(x)| dx$ satisfies the following properties:

- (1) $b_1^*(z_1) = 0$, if $z_1 \leq 0$,
- (2) $0 \leq b_1^*(z_1) \leq z_1$, if $0 \leq z_1 \leq \frac{1}{2}$,
- (3) $0 \leq b_1^*(z_1) \leq 1 - z_1$, if $\frac{1}{2} \leq z_1 \leq 1$,
- (4) $b_1^*(z_1) = 0$, if $z_1 \geq 1$.

Proof. Note that $G(b_1)$ is convex in b_1 for any given z_1 . When $-1 \leq x \leq 0$, we have

$$z(x) = (b_1 - 2z_1)(x+1)^3 - (b_1 - 3z_1)(x+1)^2$$

and $\zeta(x) = z_1(1+x)$.

When $z_1 \leq 0$ and $b_1 \geq z_1$, the equation $z(x) - \zeta(x) = 0$ has a root in $-1 < x < 0$ as $r_1 = \frac{z_1 - b_1}{b_1 - 2z_1}$. We have

$$G_0(b_1) = \int_{-1}^{r_1} z(x) - \zeta(x) dx + \int_{r_1}^0 \zeta(x) - z(x) dx$$

and

$$\frac{dG_0}{db_1} \Big|_{b_1=0} = \frac{1}{32}.$$

When $z_1 \leq 0$ and $b_1 \leq 1 - z_1$, the equation $z(x) - \zeta(x) = 0$ has a root in $0 < x < 1$ as $r_2 = \frac{b_1 + z_1 - 1}{b_1 + 2z_1 - 2}$. We have

$$G_1(b_1) = \int_0^{r_2} \zeta(x) - z(x) dx + \int_{r_2}^1 z(x) - \zeta(x) dx$$

and

$$\frac{dG_1}{db_1} \Big|_{b_1=0} = -\frac{1}{32}.$$

Hence,

$$\frac{dG(b_1)}{db_1} \Big|_{b_1=0} = 0$$

when $z_1 \leq 0$. Consequently, $b_1^*(z_1) = 0$ for $z_1 \leq 0$.

When $z_1 \geq 0$, $b_1 \leq z_1$ and $b_1 \leq 1 - z_1$, we have

$$G(b_1) = \int_{-1}^{r_1} \zeta(x) - z(x) dx + \int_{r_1}^0 z(x) - \zeta(x) dx + \int_0^{r_2} \zeta(x) - z(x) dx + \int_{r_2}^1 z(x) - \zeta(x) dx$$

and

$$\frac{dG}{db_1} \Big|_{b_1=0} = -\frac{1}{16} < 0.$$

Hence $b_1^*(z_1) > 0$ for $0 \leq z_1 \leq 1$.

When $0 \leq z_1 \leq \frac{1}{2}$, we have

$$\frac{dG}{db_1} \Big|_{b_1=z_1} = \frac{(z_1 - 1)^3(9z_1 - 5)}{6(2 - 3z_1)^4} > 0.$$

Hence $b_1^*(z_1) \leq z_1$ for $0 \leq z_1 \leq 1$. By symmetry we can prove the remaining of the theorem. $\square$

Fig. 7 shows the graph of $b_1^*(z_1)$.

Lemma 4. Given any $0 < \epsilon \leq 1$, $0 \leq z_1^* \leq \frac{1}{2}$ holds for the function-value-based spline fit for $H_\epsilon(x)$.

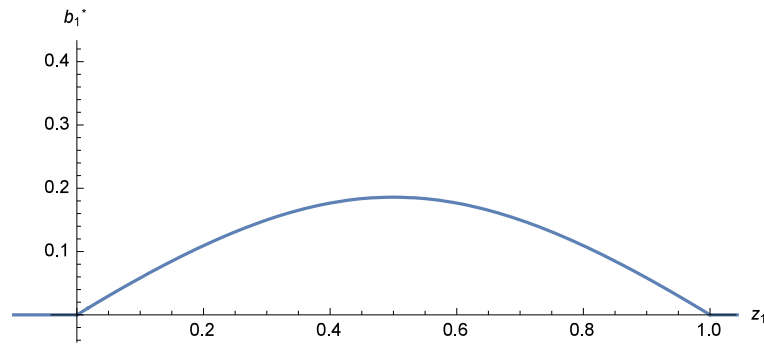


Fig. 7. $b_1^*(z_1)$ for function-value-based interpolating spline in a 3-node window with boundary conditions.

Table 2

Shape-preserving metrics calculated in a 3-node window.

	Second-derivative-based	First-derivative-based	Function-value-based
ϵ^*	0.250	0.109	0.050

Proof. Note that $0 \leq b_1^*(z_1) \leq 3(1 - z_1)$ for $\frac{1}{2} \leq z_1 \leq 1$, $b_1^*(z_1) = 0$ for $z_1 \geq 1$, and $b_1^*(z_1) = 0$ for $z_1 \leq 0$. The proof of Lemma 2 can be applied. $\square$

Theorem 6. Fix $z_0 = 0$, $b_0 = 0$, $z_2 = 1$ and $b_2 = 0$ in the 3-node window. The function-value-based spline fit for $H_\epsilon(x)$ preserves its linear shape in $-1 \leq x \leq 0$, i.e., $z_1^* = 0$ and $b_1^*(z_1^*) = 0$, if and only if $\epsilon \geq 0.050$. This means that the shape-preserving metric of function-value-based spline fits is 0.050.

Proof. Proof of Theorem 4 applies. For function-value-based spline fits, $\frac{db_1}{dz_1}|_{z_1=0} = 0.61191$ and $\epsilon^* = 0.050$. We also need the assumption of concavity of $b_1^*(z_1)$ here. This property can be observed in Fig. 7. $\square$

Table 2 shows the shape-preserving metrics of the three types of spline fits. The shape-preserving metrics are no more than 25% of the space between adjacent spline nodes. This implies the strong shape-preserving capability of spline fits. We can see that the shape-preserving metrics of the second-derivative-based, first-derivative-based and function-value-based spline fits decrease in sequence. This indicates that the function-value-based spline fits have the strongest shape-preserving capability among these three types of spline fits.

5. Compute ϵ^* in a 5-node window

In the local-calculation approaches for interpolating spline and spline fits, a window of 5 nodes is of the appropriate size for both accuracy and efficiency (Jin et al., 2010, 2011; Wang et al., 2014; Yu et al., 2010). To evaluate the shape-preserving performance of the local-calculation approach and provide further comparison of the three types of spline fits, we compute ϵ^* in a 5-node window. No boundary conditions are imposed in this case. Considering that a similar analysis as in Section 4 for the 5-node window case is extremely cumbersome, we compute ϵ^* numerically in this section. The numerically computational procedure is as follows.

Step 1 Set a precision increment of $0 < \Delta\epsilon < 1$. Let $\epsilon = 0$.

Step 2 Solve the spline fit problem numerically. If $z_0 = z_1 = z_2 = 0$ and $b_0 = b_1 = b_2 = 0$, go to Step 3. Otherwise, let $\epsilon = \epsilon + \Delta\epsilon$ and repeat Step 2.

Step 3 Output $\epsilon^* = \epsilon$. Stop.

In Step 2, we need to solve the interpolating spline problem for $\mathbf{b}^*(\mathbf{z})$. While analytic methods have been developed for second-derivative-based and first-derivative-based splines, no such method is available for function-value-based splines. To conduct a fair comparison of the three types of spline fits, we use the Lagrangian multiplier primal affine method as in Lavery (2004) and (2009). This algorithm is satisfyingly accurate for our purpose of comparing the metrics. We use the MATLAB function `fmincon` to numerically minimize the L^1 fitting functional, which is in general not analytically expressed. The starting point for `fmincon` is set as $\mathbf{z} = (0.5, 0.5, 0.5, 0.5, 0.5)$. The criterion of determining $z_0 = z_1 = z_2 = 0$ is that $|z_0| + |z_1| + |z_2| < 10^{-3}$. The criterion of determining $b_0 = b_1 = b_2 = 0$ is that $|b_0| + |b_1| + |b_2| < 10^{-3}$. We set $\Delta\epsilon = 0.001$.

The computational results are shown in Table 3. The strong capability of spline fits and superior performance of function-value-based spline fits are verified. Moreover, by comparing to Table 2, we note that the metrics in the 5-node window are

Table 3
Shape-preserving metrics computed in a 5-node window.

	Second-derivative-based	First-derivative-based	Function-value-based
ϵ^*	0.169	0.054	0.034

smaller than those in the 3-node window. This suggests that a 5-node window contains more information about the geometric pattern to be approximated. Hence, in the local-calculation approach for spline fits, the 5-node algorithm should be preferred to the 3-node algorithm.

Analysis and numerical study for windows of 7 or more nodes may provide additional comparison of the three types of splines. In Yu et al. (2010), numerical experiments for interpolating splines in 7-node windows and global windows are conducted respectively, and are compared with 5-node windows. Yu et al. (2010) claim that these experiments provide “a piece of evidence supporting the use of second-derivative-based 5-point-window L_1 splines.” For spline fits, we may also conduct experiments of different sizes. Since the numerical method would be very similar to that for 5-node windows, and the primary purpose of this paper is not calculating shape-preserving metrics of all kinds of windows, we leave the study of other window sizes to future research.

We close the section by giving the general form of minimum length difference needed for preserving linear shape of two parallel line segments. The next theorem shows that the minimum length difference is proportional to the node space and is independent of the gap between the parallel line segments.

Theorem 7. Let $l \geq 2$ be an even number, $\hat{\epsilon} > 0$, $D_1 > 0$ and $D_2 > 0$. The spline fit $\hat{z}(x)$ with nodes $\hat{x}_0 = -\frac{l}{2}D_1, \dots, \hat{x}_{l/2} = 0, \dots, \hat{x}_l = \frac{l}{2}D_1$ preserves the linear shape of the function

$$\hat{H}_{\hat{\epsilon}}(x) = \begin{cases} 0, & \text{if } x \leq \hat{\epsilon} \\ D_2, & \text{if } x > \hat{\epsilon} \end{cases}$$

in $\hat{x}_0 \leq x \leq \hat{x}_{l/2}$ if and only if $\hat{\epsilon} \geq D_1\epsilon^*$, where ϵ^* is the corresponding shape-preserving metric to the type of the spline fit.

Proof. Note that for any cubic spline $z(x)$ with first derivatives b_i at node x_i , $i = 0, \dots, l$ and $\hat{z}(x)$ with first derivatives $\hat{b}_i$ at node $\hat{x}_i$, $i = 0, \dots, l$, if $\hat{b}_i = \frac{D_2}{D_1}b_i$, $i = 0, \dots, l$, then $\hat{z}(x) = D_2z(\frac{x}{D_1})$ for all $\hat{x}_0 \leq x \leq \hat{x}_l$. Consequently, if $\mathbf{b}^*(\mathbf{z})$ minimizes the interpolating functional $G(\mathbf{b})$, then $\hat{\mathbf{b}}^*(\mathbf{z}) = \frac{D_2}{D_1}\mathbf{b}^*(\mathbf{z})$ will minimize $G(\hat{\mathbf{b}})$. For the fitting functional, we have $F(\mathbf{z}, \hat{\mathbf{b}}^*(\mathbf{z})) = D_1D_2F(\mathbf{z}, \mathbf{b}^*(\mathbf{z}))$. The spline fits for $\hat{H}_{\hat{\epsilon}}(x)$ and $H_{\epsilon}(x)$ will then have the same function values at nodes $\hat{x}_i$ and x_i , $i = 0, \dots, l$. Therefore, spline fit $\hat{z}(x)$ preserves linear shape of $\hat{H}_{\hat{\epsilon}}(x)$ if and only if $\frac{\hat{\epsilon}}{D_1} \geq \epsilon^*$, i.e., $\hat{\epsilon} \geq D_1\epsilon^*$. $\square$

6. Concluding remarks

We have defined a metric to quantitatively characterize the shape-preserving capability of three types of cubic L^1 spline fits. To calculate this metric, we have developed an analytic approach in a 3-node window and a numerical procedure in a 5-node window. In both cases, the spline fits are shown to have convincingly strong capability in preserving linear shape. The function-value-based spline fit yields the smallest metric, which suggests it is better in shape preservation than the other two types of spline fits. This paper is of the first theoretic study on shape-preserving property of cubic L^1 spline fits. Such a study may help explain phenomena in L^1 splines applications. It may also be used as a reference to improve spline node positions and collect data of better quality for shape preservation purposes.

Shape preservation deserves a more general and precise definition. We have discussed the principle of preserving linear shapes in given data. Another principle is to preserve convex shapes, such as corners and circles. To fully evaluate the shape-preserving capability, we need to investigate more shapes such as a triangular function or a circle. The shape-preserving metrics in these cases should be defined accordingly. Furthermore, an analytic approach for calculating the metric in a 5-node window is worth designing. The analysis in the 3-node window, as well as the analytic solution to the L^1 interpolating spline problem in a 5-node window (Jin et al., 2010, 2011; Yu et al., 2010), shows the potential in these regards.

As indicated, function-value-based spline fits may perform superiorly in shape preservation. Analytic methods for solving the function-value-based interpolating spline problem and spline fit problem become more necessary and appealing. Such computational development may also be used to better evaluate the shape-preserving capability.

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