Data Approximation by L^1 Spline Fits with Free Knots

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Abstract

L^1 spline fits are a class of spline models that have shown advantages in approximating irregular and multiscale data. This paper investigates the knot placement problem of L^1 spline fits under two scenarios. If the number of knots is given, we propose an augmented Lagrangian method to solve the bilevel L^1 spline fit problem and consequently, optimize the knot locations. In addition, if the knot number is also free, we propose a heuristic method to adaptively determine the knot number and locations. Numerical experiments show that L^1 spline fits with free knots can better approximate data than L^1 spline fits with pre-specified knots while requiring fewer knots and less input from the user. Comparison with state-of-the-art least square B-spline models shows that L^1 spline fits can approximate data with comparable squared error and significantly smaller absolute error.

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1. Introduction

L^1 splines refer to a collection of data interpolation and approximation models that are defined by minimization of various L^1-norm based functionals on spline functions. For example, L^1 interpolating splines minimize the L^1 energy functional which is the L^1-norm counterpart of the thin-plate energy functional commonly used in defining classical interpolating splines (Lavery, 2000b, 2001). L^1 smoothing splines and L^1 spline fits are two types of approximating splines that replace the squared error by the absolute

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deviation (l^1 norm) as the data-fitting metric (Lavery, 2000a, 2004). The use of these L^1-norm based minimization principles offers L^1 splines the advantages of being free from extraneous oscillation and better preserving linearity, convexity and other geometric shapes in data (Wang et al., 2015; Nie et al., 2017). Consequently, L^1 splines are highly capable of modeling noisy, irregular and multiscale data which has abrupt changes in magnitude, direction and/or spacing. Applications of L^1 splines and similar L^1-norm based spline models include scattered data interpolation and approximation (Lai and Wenston, 2004), urban and natural terrain reconstruction (Bulatov and Lavery, 2010; Lin et al., 2006), financial data modeling (Chiu et al., 2008), robot control (Olabi et al., 2010), and image processing (Dobrev et al., 2010; Nyiri et al., 2010; Gajny et al., 2014), among others.

Data approximation by L^1 splines can be carried out by using L^1 spline fits. An L^1 spline fit is defined by minimizing an L^1 data fitting functional over the set of L^1 interpolating splines (formal definition in Section 3). Dependent on the order of spline derivative 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 (Lavery, 2006, 2009). In this paper, we investigate second-derivative based univariate cubic L^1 spline fits, which will be referred to as L^1 spline fits hereafter unless otherwise specified. Other variants of L^1 spline fits are out of the scope and will be studied in the future.

We need three sets of parameters to specify a cubic spline: knots (including the number of knots and their locations), function values at the knots and first derivatives at the knots. Existing literature on L^1 spline fits treats knots as given and seeks the function values and associated first derivatives by solving a bilevel nonlinear programming problem. The upper level of the bilevel problem minimizes the L^1 data approximation error by choosing proper function values with associated first derivatives calculated by minimization of the L^1 interpolating functional in the lower level. Lavery (2004) develops an interior-point computational method with discretization of the objective functions. Wang et al. (2014) reformulate the bilevel problem as a nonlinear program by applying the recently developed 5-knot sliding window algorithm for minimizing the L^1 interpolating functional (Jin et al., 2010), and thus gradient methods can be used. However, not allowing knots to freely move limits the approximating power of L^1 spline fits.

In this paper, we treat the knots as free variables. That is, we approximate data by using L^1 spline fits with free knots. By freeing the knots we increase the modeling capability and flexibility of L^1 spline fits. Two scenarios in this regard are investigated. First, if the number of knots is pre-specified, we propose an augmented Lagrangian method to solve the L^1 spline fit problem with the knot locations being part of the decision variables. Second, if the number of knots is also free, we propose a heuristic method to adaptively decide the knot number and locations. In both scenarios, function values and the first derivatives of the L^1 spline fits are also optimized. Numerical experiments show that the L^1 spline fits with free knots produce smaller approximation error than that with pre-specified knots. Comparison with state-of-the-art knot placement methods shows that L^1 spline fits can approximate data with comparable squared error and significantly smaller absolute error than least square B-splines.

The main contributions of this paper are as follows. To the best of our knowledge, this research is the first to specifically address the knot placement problem of L^1 splines. With free knots being optimized to suit the data approximation needs, the L^1 spline fits can better capture the shapes and trends in data and consequently, can provide more insights for any subsequent data analysis and mining. Furthermore, this research increases the usability of L^1 splines. User input of knot number and locations will no longer required, which otherwise often demands problem-specific intelligence and experience.

The remainder of the paper is organized as follows. The next section reviews state-of-the-art methods of the knot placement problem for approximating splines. In Section 3, we provide the preliminaries about L^1 spline fits and define the L^1 spline fit optimization problem with free knots. In Section 4, we propose an augmented Lagrangian method for knot location optimization. In Section 5, we propose a heuristic method for determining the knot number. Numerical experiments are provided in Section 6. Section 7 concludes the paper.

2. Related Literature

To the best of our knowledge, this paper is the first study that specifically addresses the knot placement problem for L^1 splines. Nevertheless, there exists an extensive body of literature on knot placement methods for least square data approximation by B-splines. Despite the difference in definition from L^1 spline fits, the knot location selection methods for approximating B-splines are closely relevant and are therefore reviewed in this section.

A common strategy of knot placement is to choose knots from the data points. Plass and Stone (1983) use a dynamic programming scheme to reduce the complexity of enumerating all data points. Lyche and Mørken

(1988) assess the impact of each data point, if chosen as knot, on the overall approximation performance, and remove the unimportant ones. Some heuristic methods select knots from data points based on their geometric features. For example, Li et al. (2005) consider the discrete curvature of the data points and place knots with respect to the integration of the smoothed curvature to satisfy a heuristic rule. Park and Lee (2007) select knots from "dominant points" which are local curvature maximum points. Laube et al. (2018) develop support vector machine method which considers multiple features including curvature, angle and distance to neighbors. The limitation of this strategy is that knots must be data points and not completely free.

Another knot placement strategy is to generate a dense knot vector and then remove the redundant ones by certain criteria. Afterwards, the knots are often further adjusted and consolidated by some heuristic methods. Tjahjowidodo et al. (2015) iteratively bisect the data and use piecewise linear functions to fit the second derivatives. The break points of the piecewise linear functions are considered as candidates of knot locations. In a subsequent study, Dung and Tjahjowidodo (2017) adapt a similar bisecting method while directly fitting the subsets of data by B-splines to identify candidate knot locations. Noticing the discontinuity of the third derivative of cubic splines at the "active" knots, Van Loock et al. (2011) minimize the l^1 norm of the "jumps" of the third order derivative, and choose knot locations by the optimal sparse solution. Kang et al. (2015) further reduce the redundant knots without decreasing the approximation quality. Luo et al. (2019) propose additional criteria to keep knots with local maximum jumps and filter out knots with small jumps. Brandt et al. (2015) directly tackle the l^0 norm of the jumps and improve the knot selection quality. Yuan et al. (2013) form an extensive set of multi-resolution basis functions and use Lasso to select a sparse subset and their respective knots.

Optimization methods are among the first and current knot placement techniques. Jupp (1978) formulates the least square B-spline approximation problem with free knots as a nonlinear programming problem. The problem is then transformed to an unconstrained problem and is solved by Gauss-Newton method. Schwetlick and Schütze (1995) solve the linearly constrained nonlinear programming problem directly to avoid the quality loss due to back transformation in Jupp (1978). However, these optimization methods only find local optimum and do not guarantee global optimality. Beliakov (2004) employs the cutting angle method to find the global optimum. Metaheuristic optimization methods also have been applied to solve the knot placement optimization models. Examples include genetic algorithm (Yoshimoto et al., 1999), artificial immune system method (Ülker and

Arslan, 2009) and particle swarm optimization (Gálvez and Iglesias, 2011).

In this research, we propose an augmented Lagrangian method to optimize the knot locations when the number of knots is given a priori. This method directly solves the L^1 spline fits problem with knots being treated as variables and therefore, reducing the data approximation error remains the primary objective. Furthermore, the augmented Lagrangian method can incorporate the 5-knot sliding window algorithm which allows the bilevel L^1 spline fit problem to be reformulated as a nonlinear programming problem. Consequently, the subgradients of the L^1 data approximation error with respect to knots can be efficiently computed. Numerical experiments show that with carefully chosen initial knot locations and function values, the proposed method produces L^1 spline fits that can well approximate given data. Inspired by the success of the augmented Lagrangian, we propose an optimization-based heuristic method for determining knot number and locations.

3. L^1 Spline Fits with Free Knots

Let the data to be approximated be $\{(\hat{x}_m, \hat{z}_m)\}_{m=1}^M$ with $\hat{x}_1 \leq \hat{x}_2 \leq \ldots \leq \hat{x}_M$. We consider C^1-smooth piecewise cubic polynomials $z(x)$ as the data approximation model. To define $z(x)$, three sets of parameters are needed: knots $\mathbf{x} = (x_0, x_1, \ldots, x_I)$, $I \geq 1$, $x_0 < x_1 < \ldots < x_I$, function values $\mathbf{z} = (z_0, z_1, \ldots, z_I)$ and first derivatives $\mathbf{b} = (b_0, b_1, \ldots, b_I)$ at the knots. That is, $z_i = z(x_i)$ and $b_i = \frac{\mathrm{d}z}{\mathrm{d}x}(x_i)$, $i = 0, 1, \ldots, I$. We can easily derive that $z(x)$ takes the form

$$\begin{aligned} z(x) = \; & z_i + b_i(x - x_i) + \tfrac{1}{h_i}\left[-(2b_i + b_{i+1}) + 3\Delta z_i\right](x - x_i)^2 \\ & + \tfrac{1}{h_i^2}\left[b_i + b_{i+1} - 2\Delta z_i\right](x - x_i)^3 \end{aligned} \tag{1}$$

in each interval $[x_i, x_{i+1}]$, $i = 0, 1, \ldots, I-1$, where $h_i = x_{i+1} - x_i$ and $\Delta z_i = \frac{z_{i+1} - z_i}{h_i}$. To ensure that all data points are in the interval $[x_0, x_I]$, we set $x_0 = \hat{x}_1$ and $x_I = \hat{x}_M$ without loss of generality. Furthermore, to avoid unnecessary overshooting due to lack of data points in any interval $[x_i, x_{i+1}]$, we assume that $x_{i+1} - x_i \geq \delta, \forall i$, where $\delta = \min\{\hat{x}_{m+1} - \hat{x}_m, m = 1, \ldots, M-1\}$ denotes the minimal gap between x-parameter of two consecutive data points.

An L^1 spline fit is a function $z(x)$ of form (1) that minimizes the l^1-norm of the approximation error

$$f(\mathbf{x}, \mathbf{z}, \mathbf{b}) := \sum_{m=1}^{M} |z(\hat{x}_m) - \hat{z}_m|$$

over the set of L^1 interpolating splines. An L^1 interpolating spline with given knots $\mathbf{x}$ and function values $\mathbf{z}$ is defined to have such $\mathbf{b}$ that minimizes the (second-derivative based) L^1 interpolating functional

$$\int_{x_0}^{x_I} \left| \frac{\mathrm{d}^2 z}{\mathrm{d}x^2} \right| \mathrm{d}x.$$

Therefore, with $\mathbf{x}$ and $\mathbf{z}$ being free parameters and $\mathbf{b}$ dependent on $\mathbf{x}$ and $\mathbf{z}$, the L^1 spline fit problem with free knots can be formulated as the following bi-level optimization model:

$$\begin{aligned} \min_{\mathbf{x},\mathbf{z}} \quad & f(\mathbf{x}, \mathbf{z}, \mathbf{b}) \\ \text{s.t.} \quad & u_i(\mathbf{x}) := x_{i+1} - x_i - \delta \geq 0, \quad i = 0, 1, \ldots, I-1 \\ & \mathbf{b} = \arg\min_{\mathbf{b}} \int_{x_0}^{x_I} \left| \frac{\mathrm{d}^2 z}{\mathrm{d}x^2} \right| \mathrm{d}x. \end{aligned} \tag{2}$$

Note that the first knot x_0 and the last knot x_I are fixed to be $\hat{x}_1$ and $\hat{x}_M$, respectively. Instead of explicitly including $x_0 = \hat{x}_1$ and $x_I = \hat{x}_M$ as constraints, we continue to use $\mathbf{x}$ to denote the decision variables $(x_2, x_3, \ldots, x_{I-1})$ in model (2) with a slight abuse of notation. This model extends the one in Wang et al. (2014) which minimizes $\sum_{m=1}^{M} |z(\hat{x}_m) - \hat{z}_m|$ over $\mathbf{z}$ with given knot locations $\mathbf{x}$.

4. Knot Location Optimization Method

In this section we propose an augmented Lagrangian method to solve the L^1 spline fit with free knots problem (2) with the number of knots being given. The first key step is to convert the bilevel problem (2) to a (single level) nonlinear programming problem. For this purpose, we employ the analytic solution $\mathbf{b} = \mathbf{b}(\mathbf{x}, \mathbf{z})$ that minimizes $\int_{x_0}^{x_I} \left| \frac{\mathrm{d}^2 z}{\mathrm{d}x^2} \right| \mathrm{d}x$ that is derived in the 5-knot sliding window algorithm by Jin et al. (2010). The 5-knot sliding window algorithm is an analysis-based computational scheme for L^1 interpolating splines. The algorithm calculates the first derivative at each knot solely based on the knots and function values in the 5-knot local window to which the knot of interest is the center. This idea utilizes the piecewise nature of splines and excludes the complexity caused by less relevant regions, with negligible information loss. Consequently, a closed-form analytic solution $\mathbf{b} = \mathbf{b}(\mathbf{x}, \mathbf{z})$ can be derived, which drastically reduces computing time and enables parallel computation. Furthermore, the L^1 interpolating splines computed by the 5-knot sliding window algorithm have shown enhanced shape preservation results (Yu et al., 2010). By denoting $F(\mathbf{x},\mathbf{z}) := f(\mathbf{x},\mathbf{z},\mathbf{b}(\mathbf{x},\mathbf{z}))$ and adding slack variables $s_i, i = 0, 1, \dots, I-1$, we reformulate the model (2) as the following linearly constrained nonlinear programming problem

$$\begin{aligned} \min_{\mathbf{x},\mathbf{z}} \quad & F(\mathbf{x},\mathbf{z}) \\ \text{s.t.} \quad & v_i(\mathbf{x},\mathbf{s}) := u_i(\mathbf{x}) - s_i^2 = 0, \quad i = 0, 1, ..., I-1. \end{aligned} \tag{3}$$

The augmented Lagrangian function is defined as

$$\phi(\mathbf{x},\mathbf{z},\mathbf{s};\mathbf{w},\sigma) = F(\mathbf{x},\mathbf{z}) - \sum_{i=0}^{I-1} w_i v_i(\mathbf{x},\mathbf{s}) + \frac{\sigma}{2}\sum_{i=0}^{I-1} v_i(\mathbf{x},\mathbf{s})^2 \tag{4}$$

where $\mathbf{w} = (w_0, w_1, \dots, w_{I-1})$ are the multipliers and σ is the penalty factor. For any fixed σ , define the dual function in $\mathbf{w}$ as

$$\varphi(\mathbf{w};\sigma) = \min_{\mathbf{x},\mathbf{z},\mathbf{s}} \phi(\mathbf{x},\mathbf{z},\mathbf{s};\mathbf{w},\sigma).$$

Note that it is easy to find the closed-form

$$s_i^2 = \frac{1}{\sigma}\max\{0, \sigma u_i(\mathbf{x}) - w_i\}, i = 0, 1, \dots, I-1, \tag{5}$$

that minimizes $\phi(\mathbf{x},\mathbf{z},\mathbf{s};\mathbf{w},\sigma)$ with respect to $\mathbf{s}$ for given $\mathbf{x}$ and $\mathbf{z}$. Therefore, substituting (5) in (4), we have

$$\Phi(\mathbf{x},\mathbf{z};\mathbf{w},\sigma) = F(\mathbf{x},\mathbf{z}) + \frac{1}{2\sigma}\sum_{i=0}^{I-1}\{[\max\{0, w_i - \sigma u_i(\mathbf{x})\}]^2 - (w_i)^2\}$$

and

$$\varphi(\mathbf{w};\sigma) = \min_{\mathbf{x},\mathbf{z}} \Phi(\mathbf{x},\mathbf{z};\mathbf{w},\sigma).$$

By the theory of augmented Lagrangian method (e.g., Luenberger and Ye (2015)), for a sufficiently large σ, if $\mathbf{w}^*$ maximizes $\varphi(\mathbf{w};\sigma)$ and $(\mathbf{x}^*(\mathbf{w}^*), \mathbf{z}^*(\mathbf{w}^*))$ minimizes $\Phi(\mathbf{x},\mathbf{z};\mathbf{w}^*,\sigma)$, then $(\mathbf{x}^*(\mathbf{w}^*), \mathbf{z}^*(\mathbf{w}^*))$ is a local optimal solution to problem (3).

We use the subgradient method to minimize $\Phi(\mathbf{x},\mathbf{z};\mathbf{w},\sigma)$ due to the non-smoothness of $f(\mathbf{x},\mathbf{z},\mathbf{b})$, $\mathbf{b}(\mathbf{x},\mathbf{z})$ and the $\max\{\cdot\}$ operator. The subgradients are calculated by

$$\frac{\partial \Phi}{\partial x_i} = \frac{\partial f}{\partial x_i} + \sum_{i'=0}^{I} \frac{\partial f}{\partial b_{i'}} \frac{\partial b_{i'}}{\partial x_i} + \max\{0, w_i - \sigma u_i\} - \max\{0, w_{i-1} - \sigma u_{i-1}\}$$

and

$$\frac{\partial \Phi}{\partial z_i} = \frac{\partial f}{\partial z_i} + \sum_{i'=0}^{I} \frac{\partial f}{\partial b_{i'}} \frac{\partial b_{i'}}{\partial z_i}$$

for $i = 0, 1, \ldots, I$. For variants and implementation of subgradient methods please refer to Bazaraa et al. (2013) and references therein.

In each iteration of the augmented Lagrangian method, the multipliers $\mathbf{w}$ are updated in each iteration by the following gradient search step:

$$w_i^{(k+1)} = \max\left(0, w_i^{(k)} - \sigma u_i(\mathbf{x}^{(k)})\right).$$

For convergence purpose, we update σ by $\alpha\sigma$ if $\frac{||\mathbf{w}^{(k)} - \mathbf{w}^{(k-1)}||}{||\mathbf{w}^{(k-1)} - \mathbf{w}^{(k-2)}||} > \beta$ where $\alpha > 1$ and $\beta > 0$.

The proposed method is summarized in Algorithm 1.

5. Knot Number Heuristic Method

In this section, we propose a heuristic method to determine the number of knots and their locations. The method is inspired by the insight that the distance a given knot is moved by the knot location optimization method indicates its significance in reducing the approximation error. Therefore, we propose an iterative procedure by starting with equidistant knots $\mathbf{x}^{(0)} = \{x_0^{(0)}, x_1^{(0)}, \ldots, x_{I_0}^{(0)}\}$ with I_0 being a small integer, $x_0^{(0)} = \hat{x}_1$ and $x_{I_0}^{(0)} = \hat{x}_M$. Optimize $\mathbf{x}^{(0)}$ by Algorithm 1 and the new locations are denoted by $\mathbf{x}^{(*,0)}$. Calculate the location change of each knot $\Delta_i = |x_i^{(*,0)} - x_i^{(0)}|$ and find the knot with the largest change: $i_{\max} = \arg\max_i \Delta_i$. We construct $\mathbf{x}^{(1)}$ for next iteration by adding $x_{i_{\max}}^{(*,0)}$ as a new knot, redistributing $x_1^{(0)}, \ldots, x_{i_{\max}-1}^{(0)}$ equidistantly in $[\hat{x}_1, x_{i_{\max}}^{(*,0)})$ and redistributing $x_{i_{\max}+1}^{(0)}, \ldots, x_{I_0-1}^{(0)}$ equidistantly in $[x_{i_{\max}}^{(*,0)}, \hat{x}_M]$. Note that this iterative process does not guarantee that the L^1 approximation error strictly decreases in each iteration. Therefore, we keep record of the lowest approximation error ever achieved, and terminate the procedure if the lowest approximation error has remained constant for a certain number iterations.

Algorithm 1: Knot Location Optimization Method (KLOM)

Input: $\{(\hat{x}_m, \hat{z}_m)\}$

Output: $\mathbf{x}^*, \mathbf{z}^*, \mathbf{b}^*$

Initialization: $\mathbf{x}^{(0)}$, $\mathbf{z}^{(0)}$, $\mathbf{w}^{(0)}$, σ, $\alpha > 1$, $\beta > 0$, $\epsilon > 0$,;

Set $flag = 0$, $k = 0$;

while $flag < 1$ **do**

    Solve problem (3) by the subgradient method for $\mathbf{x}^{(k)}, \mathbf{z}^{(k)}, \mathbf{b}^{(k)}$;

    if $||\mathbf{v}(\mathbf{x}^{(k)}, \mathbf{s})|| < \epsilon$ **then**

        $flag = 1$;

        $(\mathbf{x}^*, \mathbf{z}^*, \mathbf{b}^*) = (\mathbf{x}^{(k)}, \mathbf{z}^{(k)}, \mathbf{b}^{(k)})$;

    else

        if $\frac{||\mathbf{w}^{(k)} - \mathbf{w}^{(k-1)}||}{||\mathbf{w}^{(k-1)} - \mathbf{w}^{(k-2)}||} > \beta$ **then**

            $\sigma = \alpha\sigma$;

        end

        $w_i^{(k+1)} = \max(0, w_i^{(k)} - \sigma u_i(\mathbf{x}^{(k)}))$;

        $k = k + 1$;

    end

end

6. Experiments

6.1. Benchmark data sets for L^1 splines

We approximate three benchmark data sets by the proposed L^1 spline fits with free knots and compare the results with that in Wang et al. (2014) which take knot locations as given. These data sets represent common shapes in multiscale data and have been used in multiple experiments of L^1 splines (Lavery, 2000a, 2004; Wang et al., 2014). Data set 1 represents a plateau with discontinuity between three linear segments. Data set 2 contains discontinuous flat portions, linear ramps and an outlier. Data set 3 is a cross section of 100-meter-posting terrain elevation data for Ft. Hood, Texas (Lavery, 2001). Abrupt changes in magnitude and spacing are found in all three data sets and consequently, often result in extraneous oscillation and loss of shape preservation if approximated by conventional L^2-norm based splines. However, L^1 spline fits can produce shape-preserving approximation of these data sets.

We feed the knot location optimization method (KLOM) with two settings of initial knot locations: $\mathbf{x}^1$ is the same as the given knots in Wang

Table 1: Comparison of L^1 spline fits by different methods

Data set	Experiment	No. of data points	No. of knots	MAE
1	Fixed knots $\mathbf{x}^1$	81	17	0.0494*
	KLOM + $\mathbf{x}^1$	81	17	<1e-4
	KLOM + $\mathbf{x}^2$	81	17	<1e-4
	KNHM	81	9	<1e-4
2	Fixed knots $\mathbf{x}^1$	117	17	0.123*
	KLOM + $\mathbf{x}^1$	117	17	0.0555
	KLOM + $\mathbf{x}^2$	117	17	0.0550
	KNHM	117	13	0.0442
3	Fixed knots $\mathbf{x}^1$	81	14	0.902*
	KLOM + $\mathbf{x}^1$	81	14	0.397
	KLOM + $\mathbf{x}^2$	81	14	0.349
	KNHM	81	19	0.151

* from Wang et al. (2014)

et al. (2014). $\mathbf{x}^2$ has the same knot number as $\mathbf{x}^1$ and better resembles the distribution of the data by having $x_0^2 = \hat{x}_1$, $x_i^2 = \hat{x}_{\lfloor \frac{M}{I} i \rfloor}, i = 1, \ldots, I-1$, and $x_I^2 = \hat{x}_M$. In the knot number heuristic method (KNHM), we set $I_0 = \lceil 0.05M \rceil$ and terminate if the lowest observed approximation remains unchanged for 2 iterations. To ensure solution quality and convergence speed of the subgradient routine, we use the implementation as suggested in Camerini et al. (1975).

Table 1 shows the mean l^1 approximation error, also called mean absolute error (MAE), which is defined as MAE $= \frac{\sum_{m=1}^{M} |z(\hat{x}_m) - \hat{z}_m|}{M}$. The number of knots determined by KNHM is also compared with the pre-specified knot number in Wang et al. (2014). The results clearly show that L^1 spline fits with free knots, computed by both methods proposed in this paper, can better approximate data than that with fixed knots. Furthermore, the heuristic method uses fewer knots to achieve better approximation results for data set 1 and 2. For data set 3, the heuristic method substantially improves the approximation performance by placing only a few more knots.

The L^1 spline fits are plotted in Figures 1, 2 and 3. The given data points are marked as circles and the knot locations are indicated by the triangles. We see that the L^1 spline fits with free knots better preserve

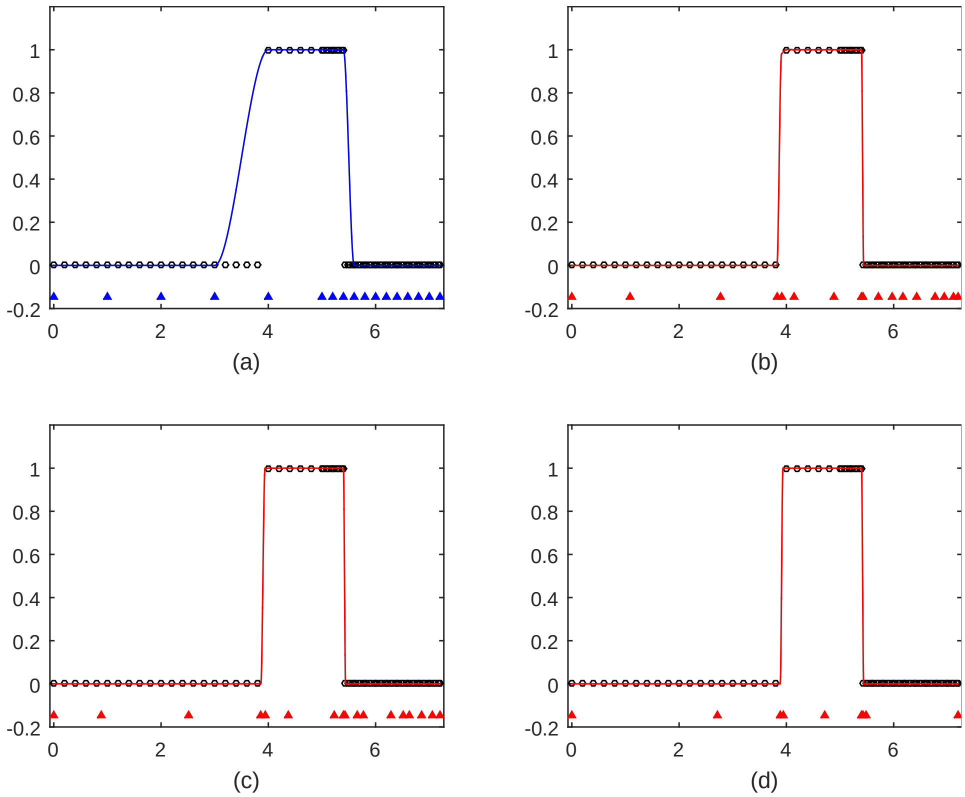

Figure 1: L^1 spline fits for data set 1: (a) fixed knots (Wang et al., 2014); (b) KLOM with $\mathbf{x}^1$; (c) KLOM with $\mathbf{x}^2$; (d) KNHM

shapes in data, for example, the linear shape in interval $[3, 4]$ of data set 1, the linear shapes in intervals $[4, 5]$, $[7, 8]$ and $[8, 9]$ of data set 2, and the stair-like shape in interval $[3000, 5000]$ of data set 3. We also point out that the heuristic method places three knots in each of the linear segments of data set 1 which has been proven to be the minimum number of knots needed for linear shape preservation (Wang et al., 2015).

6.2. Titanium heat data

Titanium heat data was used by De Boor and Rice (1968) for spline fitting and has since become a classical test data set. The difficulty to approximate Titanium heat data is due to its sharp peak as depicted in Figure 4. The data originally ranged from $[595, 1075]$ and for consistency with common practice in literature, are linearly scaled to $[0, 75]$ which has no effect on the optimal knot distribution.

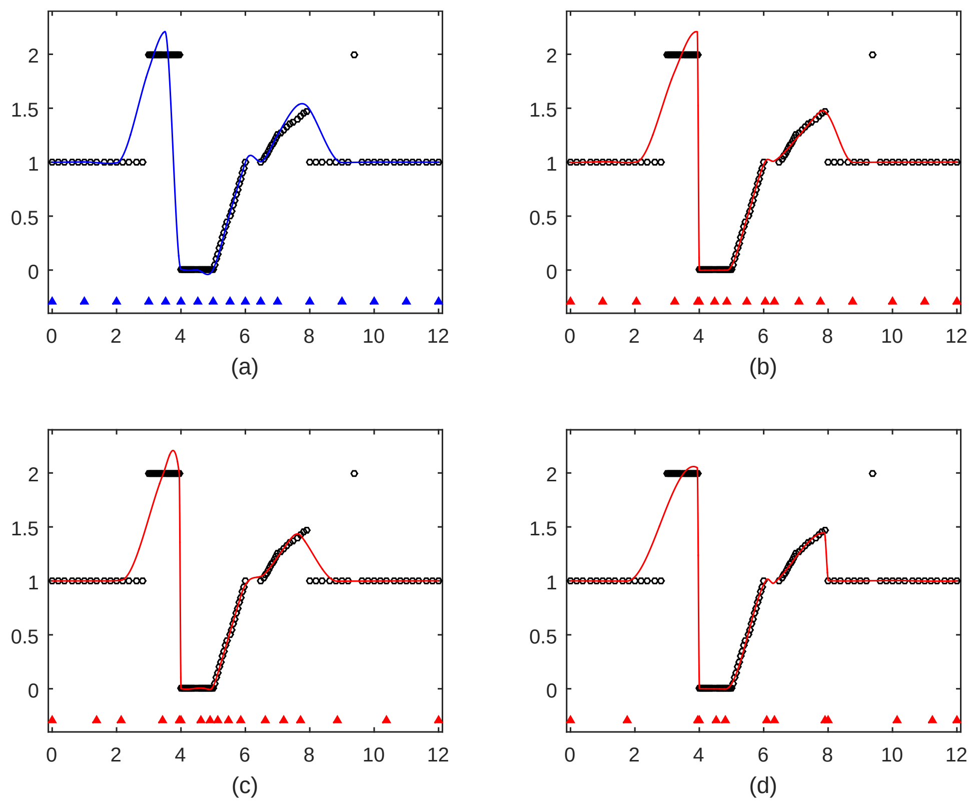

Figure 2: L^1 spline fits for data set 2: (a) fixed knots (Wang et al., 2014); (b) KLOM with $\mathbf{x}^1$; (c) KLOM with $\mathbf{x}^2$; (d) KNHM

We approximate the Titanium heat data by L^1 spline fits with the proposed knot number heuristic method (KNHM) and compare with other five studies other five studies, all of which address knot placement for least-square B-splines. Given knot number being five, De Boor and Rice (1968) and Jupp (1978) initialize their local optimization methods by a knot vector that is very close to the proved optimum, and Beliakov (2004) develops a global optimization method to find the same optimum as Jupp (1978). With knot number being free, the Lasso-based heuristic method by Yuan et al. (2013) chooses 6 interior knots from a 8-level multi-resolution B-spline basis function set, while the sparse optimization-based heuristic methods in Kang et al. (2015) and Luo et al. (2019) both select 5 knots from 100 equidistant ones. In contrast, the proposed knot number heuristic method in this paper requires no dense knot vector as input and adaptively places new knots where the local optimization subroutine suggests.

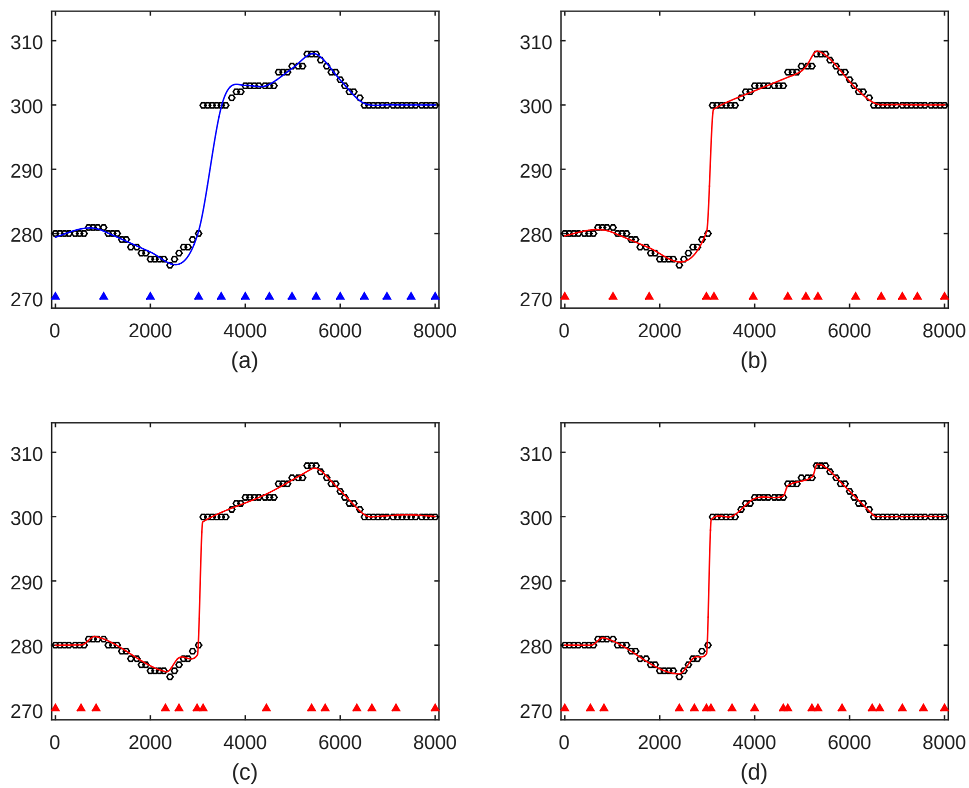

Figure 3: L^1 spline fits for data set 3: (a) fixed knots (Wang et al., 2014); (b) KLOM with $\mathbf{x}^1$; (c) KLOM with $\mathbf{x}^2$; (d) KNHM

Figure 5 shows that the L^1 spline fit accurately approximates the peak and other portions of the data. Table 2 lists the knot locations, the (l^2-norm based) residual error and the (l^1-norm based) mean absolute error of the approximating splines. The residual error (RE) has been used in literature on least square spline approximation of the Titanium heat data and is defined as:

$$\mathrm{RE} = \sqrt{\frac{\sum_{m=1}^{M} c_m (z(\hat{x}_m) - \hat{z}_m)^2}{M-1}}$$

where $c_1 = c_M = 0.5$ and $c_m = 1, m = 2, \ldots, M-1$. Note that the residual error of the L^1 spline fit (RE $= 0.0160$) is of the same magnitude as the other listed methods despite their fundamental difference in approximation metrics. More importantly, the L^1 spline fit has significantly smaller MAE than the other B-splines (97.8% reduction than MAE of Jupp (1978)). This

Table 2: Comparison of approximating splines for Titanium heat data

Method	Interior knots	RE	MAE
De Boor and Rice (1968)	$(37.55, 43.99, 48.04, 49.29, 59.82)$	0.0131	0.470
Jupp (1978)	$(37.65, 43.97, 47.37, 50.12, 59.20)$	0.0123	0.446
Beliakov (2004)	$(37.65, 43.97, 47.37, 50.12, 59.20)$	0.0123	0.446
Yuan et al. (2013)	$(18.00, 39.34, 44.82, 46.61, 50.13, 58.33)$	0.0177	0.588
Kang et al. (2015)	$(38.41, 43.50, 47.04, 51.00, 58.09)$	0.0141	0.507
Luo et al. (2019)	$(38.14, 43.71, 47.25, 50.50, 57.92)$	0.0133	0.503
KNHM	$(23.94, 42.01, 47.11, 53.71, 65.61)$	0.0160	0.00985

experiment not only proves the effectiveness of the proposed knot number heuristic method, but provides additional evidence that L^1 splines have advantages in shape-preserving data approximation over conventional spline models.

7. Concluding Remarks

This paper has addressed the important knot placement problem of L^1 spline fitting. We have formulated an optimization model for L^1 spline fits with free knots and have proposed an augmented Lagrangian method to optimize the knot locations. Despite the non-convexity of the problem, the proposed method can produce shape-preserving L^1 spline fits with reduced data approximation error. Furthermore, we have suggested a heuristic method for determining knot number and locations simultaneously. Results show that the heuristic method can adaptively place knots at proper locations. The experiment on the classic Titanium heat data reveals that data approximation using L^1 splines may produce better results than state-of-the-art least square B-splines. This research increases the flexibility of L^1 spline fits as a data approximating tool while requiring minimal input from the user.

This study provides preliminary but sufficient evidence that further investigation of the knot placement problem for L^1 splines may lead to significant advances in robust, shape-preserving and computationally efficient data approximation. The proposed methods and results are also a basis for bivariate and multivariate L^1 spline fits. Future development of global optimization methods will enhance the modeling capability of L^1 spline fits and more broadly, spline-based data models.

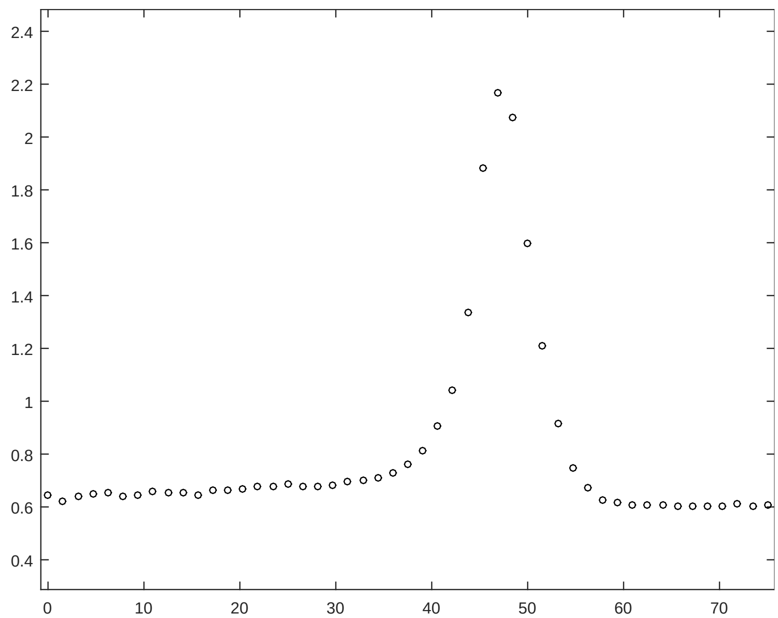

Figure 4: Titanium heat data (De Boor and Rice, 1968)

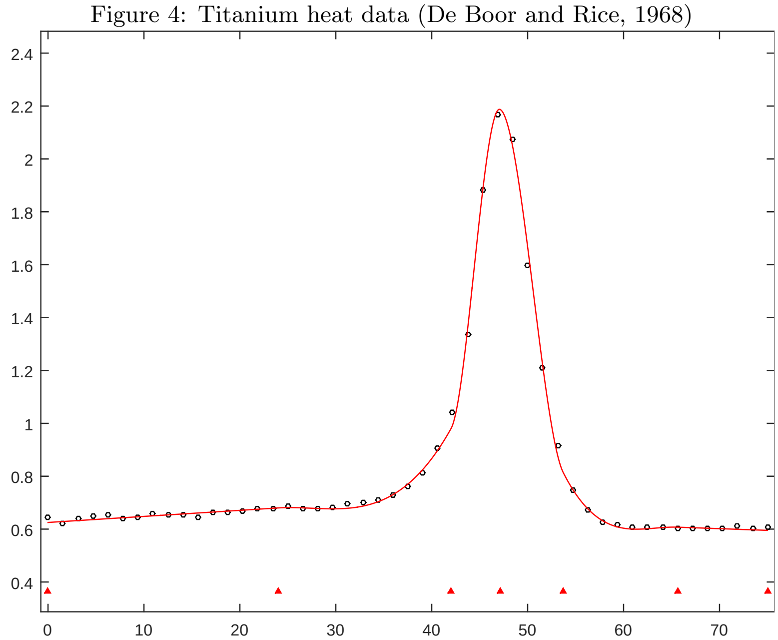

Figure 5: L^1 spline fit for Titanium heat data

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