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THE REGULARIZED SPLINE (R-SPLINE) METHOD FOR FUNCTION APPROXIMATION

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Many constructions of cubic splines are described in the literature. Most of the methods focus on cubic splines of defect 1, i.e., cubic splines that are continuous together with their first and second derivative. However, many applications do not require continuity of the second derivative. The Hermitian cubic spline is used for such problems. For the construction of a Hermitian spline we have to assume that both the values of the interpolant function and the values of its derivative on the grid are known. The derivative values are not always observable in practice, and they are accordingly replaced with difference derivatives, and so on. In the present article, we construct a C^1 cubic spline so that its derivative has a minimum norm in L_2. The evaluation of the first derivative on a grid thus reduces to the minimization of the first-derivative norm over the sought values.

Keywords: Hermitian cubic spline, interpolation, approximation, regularized spline, C^1 cubic spline

Introduction

Consider a C^1 cubic spline, i.e., a Hermitian spline. In the usual sense, a cubic spline is represented as a function continuous together with its first and second derivatives, i.e., a C^2 function. All the coefficients of a classical cubic spline are found from the smooth matching condition and the boundary conditions; such a spline has a minimum-norm second derivative [1]. Many authors have studied modified cubic splines [1–7]. In the construction of the Hermitian spline, the values of both the function and its derivative are assumed known on a grid. In practice, it is quite difficult to measure the derivative and its values are usually computed by various numerical methods. In the present article, we construct a C^1 cubic spline whose coefficients are all determined by minimizing the first-derivative norm on the entire numerical segment. This technique produces a so-called regularized spline (R-spline).

For the approximation problem we apply Tikhonov regularization [9], which preserves the stability of the spline over the entire segment regardless of the number of given values and the grid increment. The second derivative of the resulting spline is not continuous; only continuity of the first derivative is ensured.

Interpolating Regularized Spline

We construct a polynomial cubic spline on $[a,b]$ that interpolates the function $f(x)$ given N values f_n, $n \in [1,N]$, on a uniform grid $\{x_n\}_{n=1}^{N}$. On the numerical segment the first derivative of the spline is continuous and attains the minimum norm in L_2.

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Auxiliary functions are introduced for the construction of the spline at $x \in [x_n, x_{n+1}]$:

$$Q_n(x) = \frac{(x_{n+1}-x)^2}{h^2}\left(1+2\frac{x-x_n}{h}\right) \quad \text{and} \quad R_n(x) = \frac{(x_n-x)^2}{h^2}\left(1+2\frac{(x_{n+1}-x)}{h}\right),$$

$$\psi_n(x) = \frac{(x_{n+1}-x)^2(x-x_n)}{h^2} \quad \text{and} \quad \varphi_n(x) = \frac{(x-x_{n+1})(x-x_n)^2}{h^2},$$

where $h = x_{n+1} - x_n$, $n \in [1, N-1]$.

These functions have the following properties:

$$R_n(x_{n+1}) = 1, \quad R_n(x_n) = 0, \quad R'_n(x_n) = 0, \quad R'_n(x_{n+1}) = 0,$$

$$Q_n(x_{n+1}) = 0, \quad Q_n(x_n) = 1, \quad Q'_n(x_n) = 0, \quad Q'_n(x_{n+1}) = 0.$$

$$\varphi_n(x_{n+1}) = 0, \quad \varphi_n(x_n) = 0, \quad \varphi'_n(x_n) = 0, \quad \varphi'_n(x_{n+1}) = 1,$$

$$\psi_n(x_{n+1}) = 0, \quad \psi_n(x_n) = 0, \quad \psi'_n(x_n) = 1, \quad \psi'_n(x_{n+1}) = 0.$$

The spline is thus written in the form

$$S(x) = S_n(x), \quad x \in [x_n, x_{n+1}]$$

$$S_n(x) = f_n Q_n(x) + f_{n+1} R_n(x) + p_n \psi_n(x) + p_{n+1}\varphi_n(x), \tag{1}$$

where p_n, $n \in [1, N]$ are the first derivative values on the grid;

$$S_n(x_n) = f_n; \quad S_n(x_{n+1}) = f_{n+1}; \quad S'_n(x_n) = p_n; \quad S'_n(x_{n+1}) = p_{n+1};$$

here $S(x) \in C^1$.

To complete the definition of the spline, we need the derivative values on the grid. In the construction of a Hermitian spline, the derivative values are assumed known and the spline (1) thus fully interpolates the function from given values. However, in most problems, we only have approximate knowledge of the derivative. We therefore propose to choose the minimum-norm C^1 spline. To this end, the derivative values on the grid are obtained from the condition

$$\min_{\boldsymbol{p}} \int_a^b (S'(x))^2 \, dx \tag{2}$$

where $\boldsymbol{p} = (p_1, p_2, \ldots, p_N)$. We accordingly obtain a linear system in the unknowns p_n, $n \in [1, N]$:

$$\frac{\partial}{\partial p_i}\int_a^b (S'(x))^2 \, dx = \frac{\partial}{\partial p_i}\sum_{n=1}^{N-1}\int_{x_n}^{x_{n+1}} (S'_n(x))^2 \, dx = 2\sum_{n=1}^{N-1}\int_{x_n}^{x_{n+1}} S'_n(x)\frac{\partial S'_n(x)}{\partial p_i} dx = 0, \quad i \in [1, N].$$

Note that

$$\frac{\partial S_n'(x)}{\partial p_i} = \begin{cases} \psi_i'(x), & n = i, \\ \varphi_{i-1}'(x), & n = i-1, \\ 0, & n \neq i, \quad n \neq i-1. \end{cases}$$

We thus obtain the system of equations

$$\begin{cases} \dfrac{\partial}{\partial p_1}\displaystyle\int_a^b (S'(x))^2\,dx = 2\int_{x_1}^{x_2} S_1'(x)\psi_1'(x)\,dx = 0, \\ \dfrac{\partial}{\partial p_i}\displaystyle\int_a^b (S'(x))^2\,dx = 2\int_{x_{i-1}}^{x_i} S_{i-1}'(x)\varphi_{i-1}'(x)\,dx + 2\int_{x_i}^{x_{i+1}} S_i'(x)\psi_i'(x)\,dx = 0, \qquad i \in [2, N-1]. \\ \dfrac{\partial}{\partial p_N}\displaystyle\int_a^b (S'(x))^2\,dx = 2\int_{x_N}^{x_N} S_{N-1}'(x)\varphi_{N-1}'(x)\,dx = 0, \end{cases}$$

Hence

$$\begin{cases} 4p_1 - p_2 = \dfrac{3}{h}(f_2 - f_1), \\ -p_{i-1} + 8p_i - p_{i+1} = \dfrac{3}{h}(f_{i+1} - f_i), \\ -p_N + 4p_{N+1} = \dfrac{3}{h}(f_{N+1} - f_N). \end{cases}$$

We obtain a tridiagonal matrix with diagonal dominance. The system matrix is nonsingular and a unique solution $\boldsymbol{p} = (p_1, p_2, \ldots, p_N)$ exists. Evaluating $\boldsymbol{p} = (p_1, p_2, \ldots, p_N)$, we can apply (1) to find the value of the spline at every point $x \in [a, b]$.

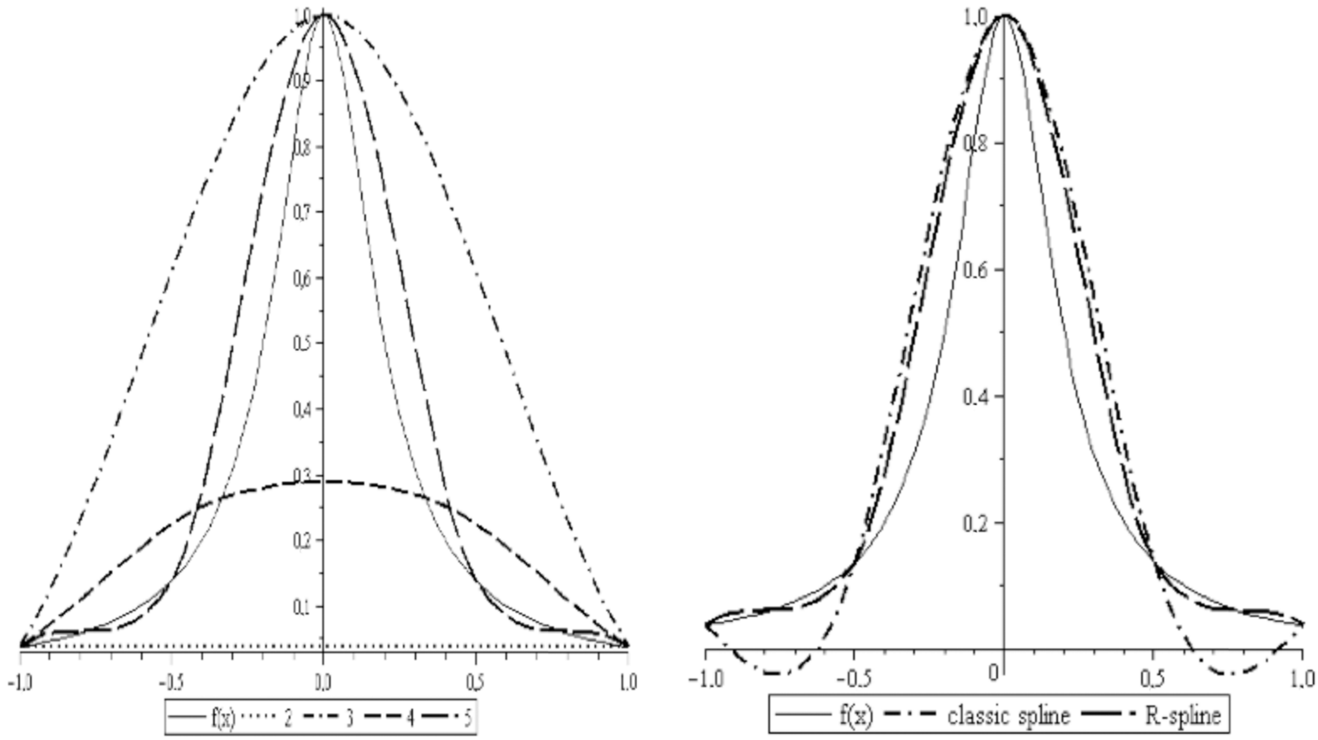
In the classical cubic spline we have an additional continuity condition for the second derivative $S''(x)$, which enables us to find p_n, $n \in [2, N-1]$, in terms of p_1 and p_N. The values $p_1 = f'(x_1)$ and $p_N = f'(x_N)$ are determined from the conditions of the problem [1–8] or are specified approximately.

Example 1

To assess the efficiency of the R-spline properties, we construct an interpolation of the Runge function

$$f(x) = \frac{1}{1 + 25x^2}$$

on the closed interval $x \in [-1, 1]$. Figure 1a shows the interpolation for a grid consisting of 2, 3, 4, and 5 values. With interpolation on 2 given values, the minimum-norm derivative is attained with a straight-line spline (the dotted line in Fig. 1). With 3 points, we have the dash-dotted curve; with 4 values, the R-spline is described



(a) **(b)**

Fig. 1. R-spline interpolation with 2, 3, 4, and 5 given values.

by the dashed curve. This is the minimum-derivative curve among all the C^1 cubic splines. Since none of the points is at the maximum, the R-spline is unable to describe the peak of the Runge function. With 5 points, the R-spline clearly begins to describe the behavior of the Runge function. The grid increment is obviously too big for us to say anything useful about the interpolant function.

Note that with 5 given values, the R-spline produces a better description of the interpolant function than the classical spline (Fig. 1b).

Interpolation of the Runge function on $x \in [-1,1]$ with more than 5 points, for instance, with 7 given values, produces a fairly good approximation, and starting with 9 values the result almost totally coincides with the Runge function (Fig. 2). No oscillations build up at the ends of the interval.

Figure 3 plots the absolute value of the difference between the R-spline and the Runge function (solid curve) and between the classical C^2 cubic spline and the Runge function (dotted curve). The interpolation has been constructed using 9 given values.

The advantage of the R-spline over the classical spline depends on the class of problems being solved. The minimum-norm property of the derivative is particularly advantageous when dealing with functions that have abrupt peaks or rapidly growing (varying) derivative values.

Approximating Regularized Spline

Applied problems basically involve empirical data, which are obtained in the course of an experiment or are observed under natural conditions. Such data include various errors, such as instrumental errors, environmental

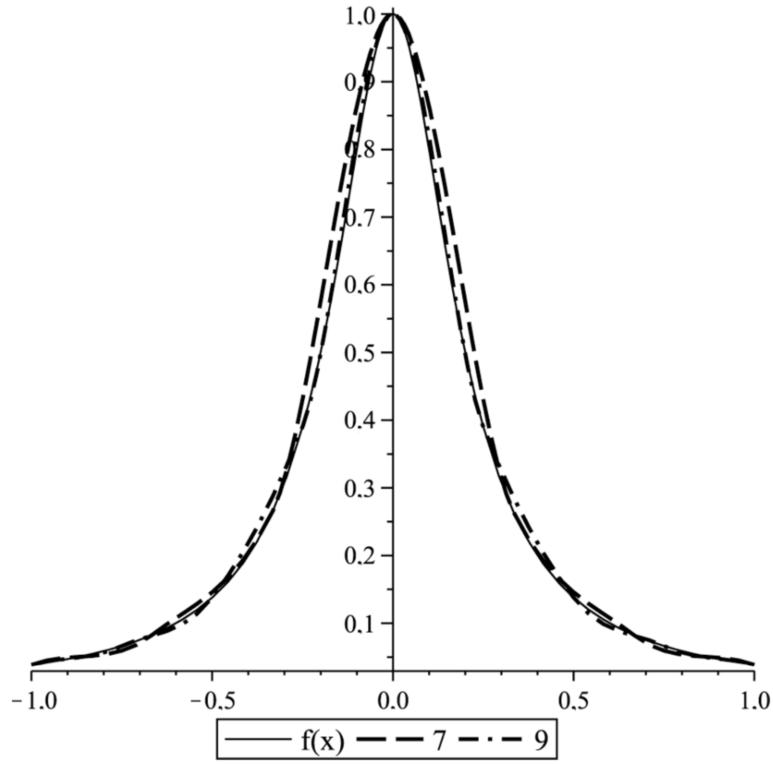


Fig. 2. R-spline interpolation with 7 and 9 given values.

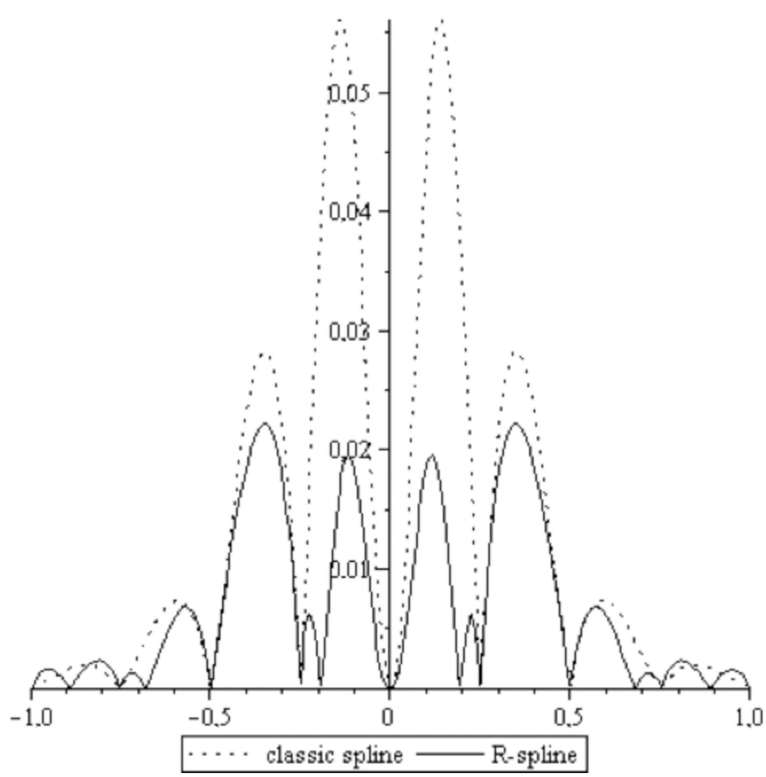


Fig. 3. Absolute difference between the Runge function and the spline.

effects, natural forces, and other factors unrelated to the experiment. Various data smoothing algorithms have been accordingly developed [8, 10, 11]. Data approximation is required to produce a smooth curve from a given class of solutions dictated by the relevant mathematical model. Given that the R-spline has a minimum-norm first derivative, we construct a data-approximation algorithm that produces a solution from the class of C^1 cubic splines, ensuring a minimum-norm first derivative.

Consider the approximation of the function $f(x)$ given on the grid $\{x_k^*\}_{k=1}^K$ with some error δ^* by a regularized spline. In this case, both the derivative values p_n and the function values f_n are unknown on the spline grid $\{x_n\}_{n=1}^N$. For simplicity, we take $K = N$ so that the grids $\{x_k^*\}_{k=1}^K$ and $\{x_n\}_{n=1}^N$ are identical. Thus, to find all the unknowns, we must satisfy condition (2) including the unknowns f_n, $n \in [1, N]$, i.e.,

$$\min_{\overline{p},\overline{f}} \|S'(x)\|_{L_2}^2, \qquad \overline{p} = (p_1, p_2, \ldots, p_N), \qquad \overline{f} = (f_1, f_2, \ldots, f_N) \tag{3}$$

with the additional condition

$$\left\| \overline{S(x^*)} - \overline{f(x^*)} \right\|_{R^N}^2 \le \delta^2, \tag{4}$$

where $\overline{S(x^*)} = \left(S(x_1^*), S(x_2^*), \ldots, S(x_N^*) \right)$ and $\overline{f(x^*)} = \left(\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_N \right)$ are known with an error δ^*; δ is the known mean-square error of the function $f(x)$.

By Tikhonov's regularization theory, problem (3)–(4) reduces to the unconstrained minimum problem [9]

$$\min_{\overline{p},\overline{f}} \left\{ \left\| \overline{S(x^*)} - \overline{f(x^*)} \right\|_{R^N}^2 + \alpha \|S'(x)\|_{L_2}^2 \right\}, \tag{5}$$

where the regularization parameter α is determined by the discrepancy method [9]. Problem (5) reduces to the problem

$$\min_{\overline{p},\overline{f}} \sum_{i=1}^{N} \left(S(x_i) - \tilde{f}_i \right)^2 + \alpha \int_a^b \left(S'(x) \right)^2 dx .$$

We have thus obtained a system of $2N$ equations in $2N$ unknowns:

$$\begin{cases} \dfrac{\partial}{\partial p_k} \displaystyle\sum_{i=1}^{N} \left(S(x_i) - \tilde{f}_i \right)^2 + \alpha \int_a^b \left(S'(x) \right)^2 dx = 0, & k = 1, 2, \ldots, N, \\[2ex] \dfrac{\partial}{\partial f_k} \displaystyle\sum_{i=1}^{N} \left(S(x_i) - \tilde{f}_i \right)^2 + \alpha \int_a^b \left(S'(x) \right)^2 dx = 0, & k = 1, 2, \ldots, N. \end{cases}$$

The solution of problem (5) produces a unique regularized spline given the parameters $\overline{p} = (p_1, p_2, \ldots, p_N)$ and $\overline{f} = (f_1, f_2, \ldots, f_N)$.

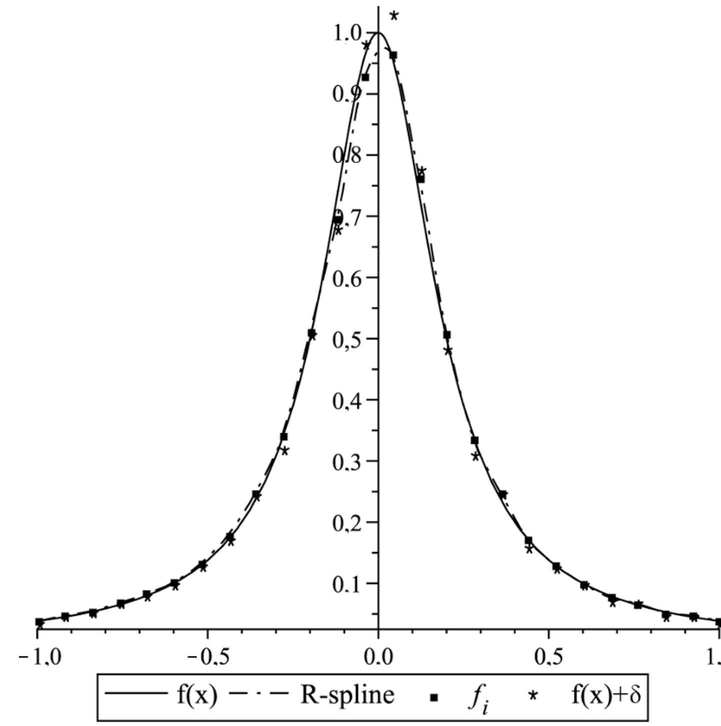


Fig. 4. Approximation with 26 values.

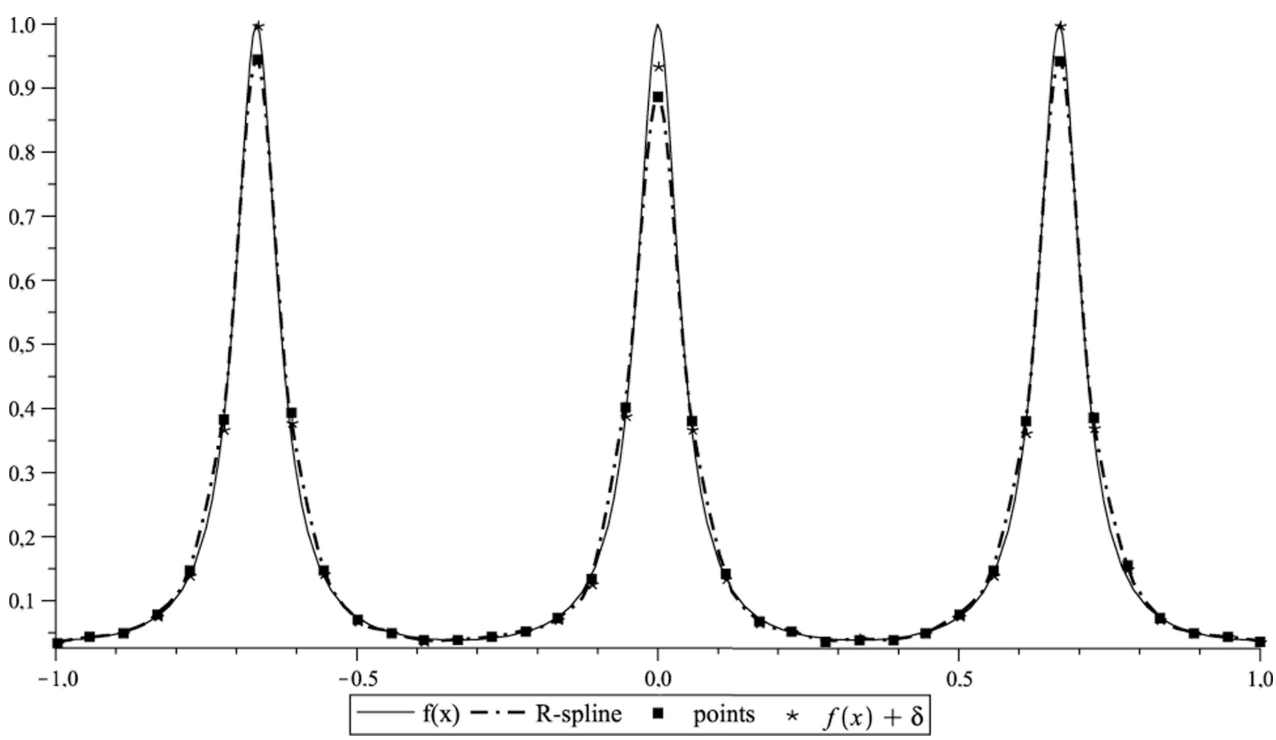


Fig. 5. Approximation of the function $f(x) = \dfrac{1}{1 + 25\left(\sin\left(\dfrac{3}{2}\pi x\right)\right)^2}$.

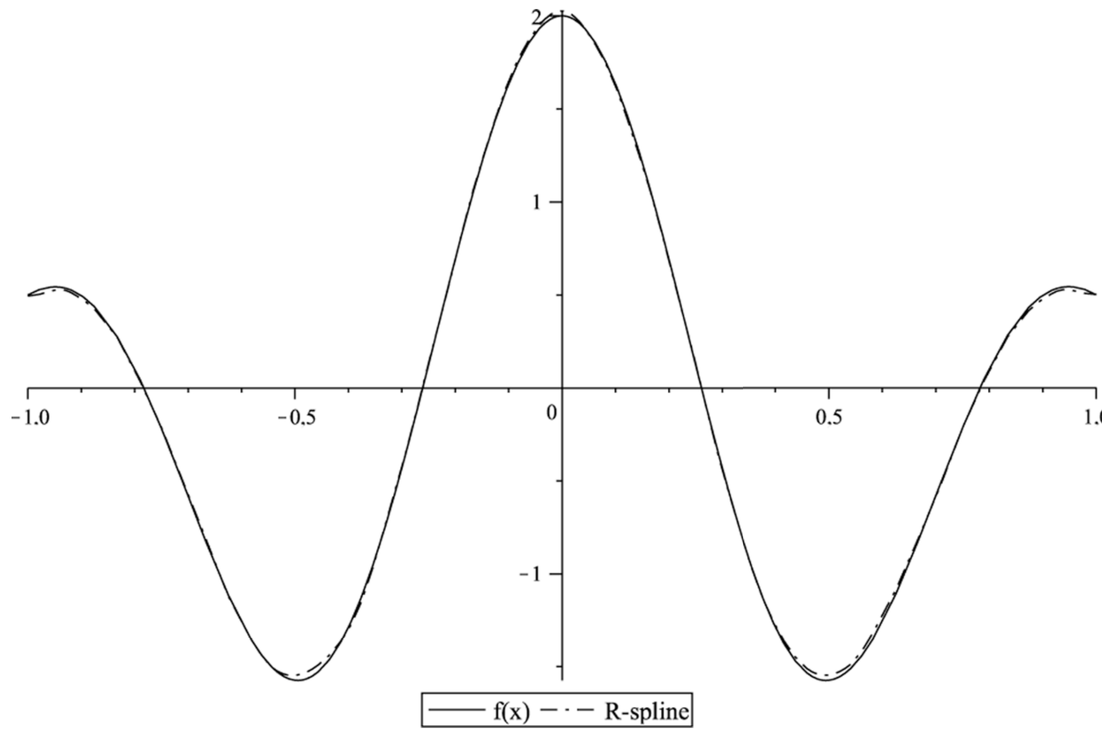


Fig. 6. Approximation of the function $f(x) = \cos\left(\frac{3}{2}\pi x\right) + \cos\left(\frac{7}{3}\pi x\right)$.

Example 2

We now consider an example of approximating a Runge function defined in a tabular form with an error on the closed interval $x \in [-1,1]$. Figure 4 is an example based on 26 values with 10% relative error. Despite the large injected error, the R-spline smooths the results and efficiently approximates the Runge function.

Figure 5 is the R-spline approximation of the function

$$f(x) = \frac{1}{1 + 25\left(\sin\left(\frac{3}{2}\pi x\right)\right)^2} \qquad \text{on} \quad x \in [-1,1].$$

This function has several peaks in the given interval. The S-spline is free from oscillations between the peaks, a common effect in approximation. The function $f(x) = \frac{1}{1 + 25\left(\sin\left(\frac{3}{2}\pi x\right)\right)^2}$ is specified with 10% relative error on a grid of 37 values. The approximation is stable, despite the fairly large increment. The condition of minimum-norm first derivative suppresses the oscillations of the R-spline.

Figure 6 shows the R-spline approximation of the smoothly varying function

$$f(x) = \cos\left(\frac{3}{2}\pi x\right) + \cos\left(\frac{7}{3}\pi x\right) \qquad \text{on} \quad x \in [-1,1].$$

The function is defined with 3% error on a grid of 25 values. Despite the large grid increment, it is difficult to distinguish the R-spline from the exact function in the diagram.

The proposed smoothing method with R-splines efficiently constructs an approximation from a tabular definition of a function with an error.

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