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SMOOTH APPROXIMATION AND ITS APPLICATION TO SOME 1D PROBLEMS

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Abstract

In the contribution, we are concerned with the exact interpolation of the data at nodes given and also with the smoothness of the interpolating curve and its derivatives. This task is called the problem of smooth approximation of data. The interpolating curve or surface is defined as the solution of a variational problem with constraints. We discuss the proper choice of basis systems for this way of approximation and present the results of several 1D numerical examples that show the quality of smooth approximation.

1. Introduction

Measurements of the values of a continuous function of one, two, or three independent variables are carried out in many branches of science and technology. We always get a finite number of function values evaluated at a finite number of points but we are interested also in intermediate values corresponding to other points. This is the well-known problem of *interpolation*.

In this contribution, we are concerned only with the exact interpolation of data given at nodes but more complex problems are mentioned in Section 5, too. The history of interpolation has its roots in the pre-computer era. Moreover, approximation of data does not have a unique solution as our requirements on the smoothness of the approximating curve or surface may be very subjective. A possible criterion is to minimize the integral of the squared magnitude of the interpolating function. Since the minimization is carried out over a restricted set of smooth functions we cannot expect that the minimum equals zero. A more sophisticated criterion is to minimize, with some weights chosen, the integrals of the squared magnitude of some (or possibly all) derivatives of the interpolating function. The cubic spline interpolation is known to be the approximation of this kind.

We confine ourselves to the case of one independent variable. We briefly summarize the approach of Talmi and Gilat [3] in Section 2. Several basis systems of functions for 1D smooth approximation are shown in Section 3. In the next section, we present results of numerical experiments comparing the classical interpolation formulae and various versions of the smooth approximation. In Section 5 we finally sum up the results presented and give possible directions for further research.

2. Smooth approximation

Let us consider the linear vector space $\widetilde{W}$ of complex functions g continuous together with their derivatives of all orders on the possible infinite interval (a, b). For $g, h \in \widetilde{W}$ we construct the expression

$$(g, h) = \sum_{l=0}^{\infty} B_l \int_a^b [g^{(l)}(x)]^* h^{(l)}(x)\,\mathrm{d}x, \tag{1}$$

where * denotes the complex conjugate, $B_0 > 0$, and $\{B_l\}_{l=0}^{\infty}$ is a sequence of non-negative numbers. Let us further put

$$\|g\| = \sqrt{(g, g)}, \tag{2}$$

i.e.

$$\|g\|^2 = \sum_{l=0}^{\infty} B_l \int_a^b |g^{(l)}(x)|^2\,\mathrm{d}x. \tag{3}$$

If the value of $\|g\|$ exists and is finite we call it the norm of the function g. If the same is true for the function h then it can be proven that the expression (1) exists and is finite, too, and, moreover, it has the properties of the *inner product of functions g and h*. We can prove that the set of all such functions forms a Hilbert space W corresponding to the sequence $\{B_l\}$. The choice of this sequence defines weights of the individual derivatives in the expression (3).

It can be shown that in the case $B_0 = 0$ the expression (2) is only a seminorm. We consider this case later.

Let f be a (complex, in general) function continuous on the interval (a, b). Let the values $f_j = f(X_j)$ of this function f at the finite number of mutually distinct nodes $X_1, X_2, \ldots, X_N \in (a, b)$ be given, e.g. measured, where N is a fixed integer.

Following [3] we formulate the *problem of smooth approximation* of the above function f that is represented by its values at N nodes. Let us choose a sequence $\{B_l\}$. Further let us choose a system of functions $g_k \in W$, $k = 1, 2, \ldots$, that is complete and orthogonal (with respect to the inner product (1)), i.e.,

$$(g_k, g_n) = 0 \quad \text{for} \quad k \neq n, \qquad (g_k, g_k) = \|g_k\|^2 \neq 0. \tag{4}$$

Then the problem of smooth approximation is to find the coefficients A_k of the series

$$z(x) = \sum_{k=1}^{\infty} A_k g_k(x) \tag{5}$$

such that

$$z(X_j) = f_j, \quad j = 1, \dots, N, \tag{6}$$

and

$$\text{the quantity } \ \|z\| \ \text{ attains its minimum.} \tag{7}$$

Apparently,

$$\|z\|^2 = \sum_{k=1}^{\infty} A_k^* A_k \|g_k\|^2 \tag{8}$$

due to (4) and (5). The smooth approximation problem thus consists of the variational problem (7), i.e. minimizing the functional (8), with constraints (6). It is solved by the method of Lagrange multipliers in the proof of the following theorem.

Note that when minimizing (8), we not only minimize the integral of $|z|^2$ but also (with a weight B_l chosen) the integral of $|z^{(l)}|^2$, i.e. of the lth derivative. This can be of importance in processing such measurements where also a good approximation of the first derivative is needed.

Put

$$R(x, y) = \sum_{k=1}^{\infty} \frac{g_k(x) g_k^*(y)}{\|g_k\|^2}. \tag{9}$$

The principal result of [3] is the following theorem.

Theorem 1. *Let $X_i \neq X_j$ for all $i \neq j$. Assume that the series* (9) *converges for all $x, y \in (a, b)$. Then the problem* (6), (7) *of smooth approximation has the unique solution*

$$z(x) = \sum_{j=1}^{N} \lambda_j R(x, X_j), \tag{10}$$

where the coefficients λ_j, $j = 1, \dots, N$, are the unique solution of the linear algebraic system

$$\sum_{j=1}^{N} \lambda_j R(X_i, X_j) = f_i, \quad i = 1, \dots, N. \tag{11}$$

Proof. The proof can be put together from its pieces in Section 2 and Appendix C of [3]. Nevertheless, we present the proof briefly here. We use the Lagrange method, i.e. introduce the multipliers λ_j, $j = 1, \dots, N$, and subtract the constraint (6) with these multipliers from the functional $\|z\|$ to obtain the functional

$$\sum_{k=1}^{\infty} A_k^* A_k \|g_k\|^2 - \sum_{j=1}^{N} \lambda_j^* \left(\sum_{k=1}^{\infty} A_k g_k(X_j) - f_j \right),$$

where we have used (5) and (8). Differentiating with respect to A_n and λ_i to obtain the conditions necessary for extrema, we get

$$A_n^* \|g_n\|^2 - \sum_{i=1}^{N} \lambda_i^* g_n(X_i) = 0, \quad n = 1, 2, \dots,$$

from where we can compute

$$A_k = \frac{1}{\|g_k\|^2} \sum_{j=1}^{N} \lambda_j g_k^*(X_j), \quad k = 1, 2, \dots .$$

Substituting this into (5) and taking (9) into account, we obtain (10). The condition (6) becomes now (11), which is a system of N linear algebraic equations for the unknowns λ_j, $j = 1, \dots, N$. We finally show that the system (11) is nonsingular. Choosing μ_j arbitrary and putting

$$u(x) = \sum_{j=1}^{N} \mu_j R(x, X_j),$$

we calculate that

$$\|u\|^2 = (u, u) = \sum_{i=1}^{N} \sum_{j=1}^{N} \mu_i \mu_j^* (R(x, X_i), R(x, X_j)) = \sum_{i=1}^{N} \sum_{j=1}^{N} \mu_i \mu_j^* R(X_j, X_i) \geq 0 \quad (12)$$

for arbitrary μ_j, $j = 1, \dots, N$. On our assumptions that the system g_k is complete and $B_0 \neq 0$ we have $\|u\| = 0$ if and only if all μ_j are zero. Therefore, if not all μ_j are zero then $\|u\| > 0$ and the positive definiteness (and nonsingularity as well) of the matrix $[R(X_j, X_i)]$ follows directly from (12). The system (11) thus has a unique solution. □

For particular cases, some error estimates are given in Appendix B of [3].

To get a more general smooth approximation, we can choose a positive integer L and put $B_l = 0$ for $l = 0, 1, \dots, L-1$ (cf. [1]). As a consequence, the expression in (1) does not contain the first L terms and we denote it by $(\cdot, \cdot)_L$, the quantity $\|\cdot\|$ defined in (2) is a seminorm and we denote it by $|\cdot|_L$. Instead of (5) we can assume

$$z(x) = t(x) + \sum_{k=1}^{\infty} A_k g_k(x), \quad |g_k|_L \neq 0, \quad t(x) = \sum_{p=0}^{L-1} a_p \varphi_p(x), \qquad (13)$$

where $\{\varphi_p\}$, $p = 0, 1, \dots, L-1$, is a set of mutually orthogonal functions such that

$$(\varphi_p, \varphi_q)_L = 0, \quad p, q = 0, 1, \dots, L-1.$$

Then we put

$$|z|_L^2 = \sum_{k=1}^{\infty} A_k^* A_k |g_k|_L^2, \quad R_L(x, y) = \sum_{k=1}^{\infty} \frac{g_k(x) g_k^*(y)}{|g_k|_L^2}.$$

A statement analogous to that of Theorem 1. then holds. It is possible to prove that the solution of the problem of smooth approximation, consisting of the system (6) and the condition

$$\text{the quantity } \ |z|_L \ \text{ attains its minimum,}$$

has the unique solution

$$z(x) = \sum_{p=0}^{L-1} a_p \varphi_p(x) + \sum_{j=1}^{N} \lambda_j R_L(x, X_j),$$

where the coefficients a_p and λ_j are the solution of the system of $N+L$ linear algebraic equations

$$\sum_{j=1}^{N} \lambda_j \varphi_p(X_j) = 0, \quad p = 0, 1, \ldots, L-1,$$

$$\sum_{p=0}^{L-1} a_p \varphi_p(X_i) + \sum_{j=1}^{N} \lambda_j R_L(X_i, X_j) = f_i, \quad i = 1, \ldots, N.$$

As $B_l = 0$, $l = 0, 1, \ldots, L-1$, we minimize only the seminorm $|z|_L$ and the integrals of $|z^{(l)}|^2$, $l = 0, 1, \ldots, L-1$, cannot be minimized. On the other hand, it does not cause difficulties to put $B_l = 0$ for some $l > M$, where $M \geq 0$ and $B_M \neq 0$. As we have mentioned, the effect of this choice is only that the integral of $|z^{(l)}|^2$ is not minimized. In this way, we can put $B_l = 0$ for infinitely many indices l and make the sum in (1) as well as (3) finite.

In [3], the authors present a typical example, interpolating piecewise cubic splines from $C_2(a, b)$, that are known to minimize the integral of $|z''|^2$ over (a, b), see, e.g., [4]. The smooth approximation procedure gives splines of degree $2L-1$ if we put $B_l = 0$ for $l \neq L$, $B_L \neq 0$, i.e. $L = 2$ and $B_2 \neq 0$ in the cubic case. We use this cubic spline approximation in Section 4 to compute some numerical results.

3. Examples of basis systems of functions for smooth approximation

In [3], the authors present explicitly three types of functions f to be approximated, propose some proper basis systems of functions g_k, and compute the corresponding functions $R(x, y)$. The three types are

(a) f periodic, e.g. $f(x) = f(x + 2\pi)$.

(b) f nonperiodic, defined in $(-\infty, \infty)$, $f^{(l)}(\pm\infty) = 0$ for all $l \geq 0$.

(c) f nonperiodic, defined on a finite interval, e.g. $(-1, 1)$.

According to [3], the recommendations of basis systems for the individual types of f are as follows.

(a) The natural basis system for this case is

$$g_k(x) = \exp(\,\mathrm{i}kx), \quad k = \ldots, -2, -1, 0, 1, 2, \ldots. \tag{14}$$

This range of k requires a slight change in the above formulae. It is easy to show that the system (14) is complete and orthogonal with respect to the inner product (1),

$$\|g_k\|^2 = 2\pi \sum_{l=0}^{\infty} B_l k^{2l}, \quad \text{and} \quad R(x,y) = \sum_{k=-\infty}^{\infty} \frac{\exp(\,\mathrm{i}k(x-y))}{\|g_k\|^2}. \tag{15}$$

In Table II of [3] the authors present the values of $\|g_k\|$ for some particular choices of the sequence $\{B_l\}$.

(b) If the interval is $(-\infty, \infty)$ and functions f are nonperiodic, the authors in [1, 3] derive the proper basis system in such a way that they start with the system (14) on a finite interval (a, b) and carry out the passage of a and b to the infinity. At the same time, the sum in the definition (15) becomes the integral

$$R(x,y) = \int_{k=-\infty}^{\infty} \frac{\exp(\,\mathrm{i}k(x-y))}{\|g_k\|^2}\,\mathrm{d}k.$$

Integrals are often calculated analytically more easily than the corresponding sums. In Table II of [3] the authors present formulae for some choices of $\{B_l\}$. For instance, let $0 < D < 1$ and $B_l = D^{2l}/(2l)!$. Put

$$r = |x - y|. \tag{16}$$

Then

$$R(x,y) = \frac{1}{2D\cosh(\pi r/(2D))}. \tag{17}$$

We use the above basis system in the next section to show some numerical results.

(c) If f is defined on the interval $(-1, 1)$ and nonperiodic, a possible choice of basis system starts with the monomials

$$h_k(x) = x^k, \quad k = 0, 1, 2, \ldots. \tag{18}$$

This system is not orthogonal but we can get a complete and orthonormal system $\{g_k\}$ from $\{h_k\}$ by the Gram-Schmidt orthonormalization procedure (see, e.g., [4]) with respect to the inner product (1). All computations, including the substitution in the series (9) for $R(x, y)$, are carried out numerically. We perform this computation and use this basis system in the next section to show some numerical results.

4. Numerical experiments

In this section, we present results of some numerical examples. The solid line is used to depict the exact function f (case 0) in the graphs that follow. We employ three ways of smooth approximation:

I (dashed line) The procedure described in (b). Basis system (14) transformed to $(-\infty, \infty)$ with $B_l = D^{2l}/(2l)!$, $0 < D < 1$, and $R(x, y)$ given by (16), (17). We put $D = 1/3$.

II (dotted line) The procedure described in (c). Basis system $\{g_k\}$ obtained from (18) by orthonormalization with $B_l = D^{2l}/(2l)!$, $D = 1/3$, and $R(x, y)$ given by the general formula (9).

III (dashed line) Cubic spline interpolation obtained as a particular case of (b). Basis system (14) transformed to $(-\infty, \infty)$ with all $B_l = 0$ except for $B_2 = 1$. Further, $R_2(x, y) = |x - y|^3$ and (13) has the form

$$t(x) = a_0 + a_1 x.$$

Cubic splines are, at the same time, considered to belong to classical interpolation methods.

Further, we employ also two ways of classical interpolation (see, e.g., [2]):

IV (dotted line) Polynomial interpolation.

V (dash-dot line) Rational function interpolation.

The software for the classical interpolation is from the book [2], too.

Problem. The function to be approximated is

$$f(x) = \frac{1}{1 + 16(x + 0.5)^2} + \frac{1}{1 + 16(x - 0.25)^2}, \quad x \in [-1, 1],$$

and belongs to type (c). The function has two "almost poles" at $x = -0.5$ and $x = 0.25$. We constructed the smooth approximation and computed the classical interpolation in equidistant and nonequidistant grids. The results for the equidistant grid with $N = 9$ are presented in Fig. 1. The curves 0 and V are identical as f is a sum of two rational functions, and the curves I, II, and III are almost identical. Figure 2 shows the error of the solutions. The error of the polynomial approximation IV is omitted in Fig. 2 since, as expected, it is very large. Moreover, the errors of I, II, and III are similar. The largest L_∞ error in Fig. 2 is the error 0.027 of the smooth approximation II.

Further, we carried out the same computation in some nonequidistant grids. The results for $N = 9$ with the grid

$$\{-1.00, -0.80, -0.70, -0.60, 0.00, 0.30, 0.45, 0.75, 1.00\} \tag{19}$$

are presented in Fig. 3. The curves 0 and V are identical. Figure 4 shows the error of the solutions. The error of the polynomial approximation IV is omitted in Fig. 4. The largest L_∞ error in Fig. 4 is the error 0.141 of the smooth approximation II.

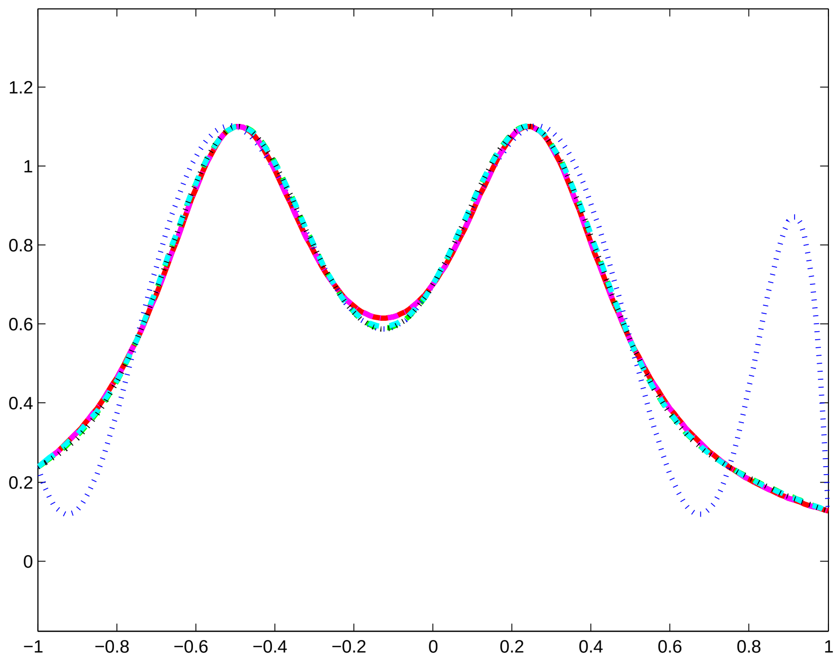

Figure 1: Interpolating functions for the problem, equidistant grid with $N = 9$. Curves at $x = 0.9$ from top to bottom: IV, all the rest of curves are almost identical.

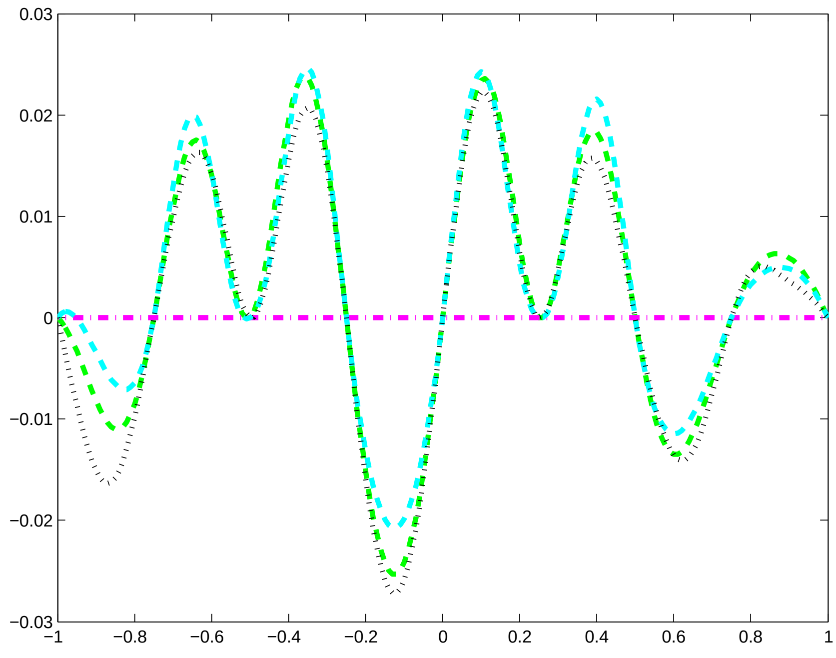

Figure 2: Error. The same equidistant grid as in Fig. 1. Different scaling on the vertical axis. Curves at $x = -0.1$ from top to bottom: V, III, I, II.

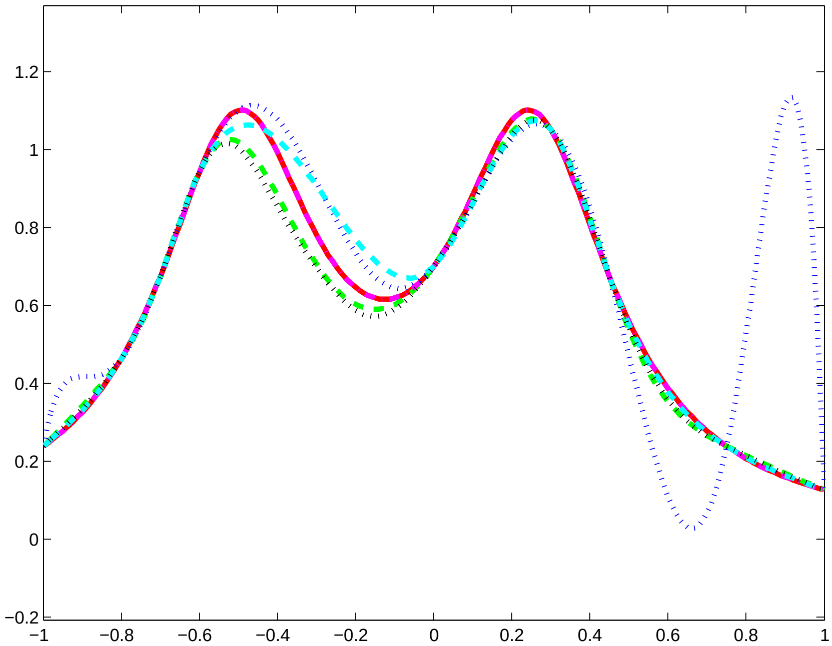

Figure 3: Interpolating functions for the problem, nonequidistant grid with $N = 9$ and nodes (19). Curves at $x = -0.2$ from top to bottom: III, IV, 0 identical to V, I, II.

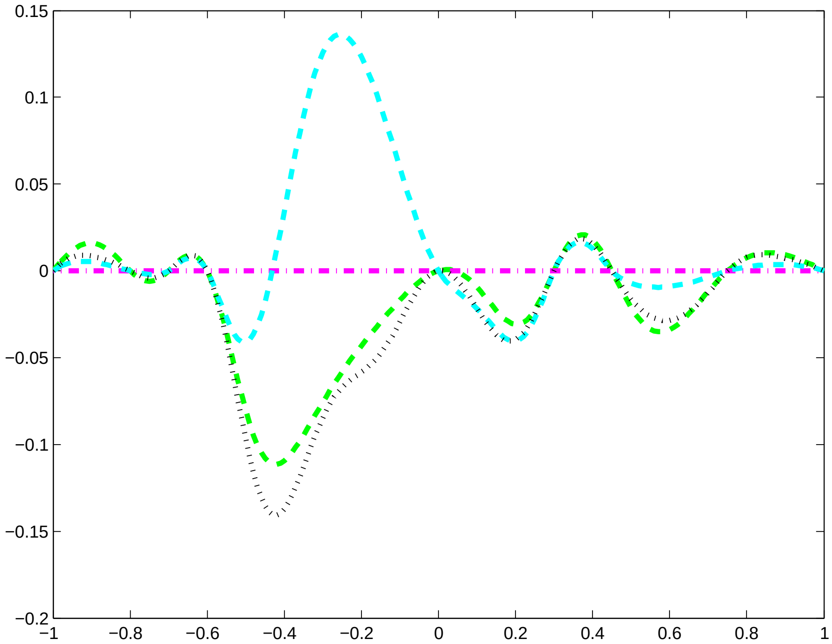

Figure 4: Error. The same nonequidistant grid as in Fig. 3. Different scaling on the vertical axis. Curves at $x = -0.2$ from top to bottom: III, V, I, II.

5. Conclusion

We have carried out some numerical experiments to compare the properties of smooth approximation and classical interpolation. They show that the smooth interpolation is a competitive method. The results shown in Section 4 are necessarily very inexact if $N < 9$. Except for the polynomial approximation IV, they are improving as N increases. The resulting curves fit the maxima at the points $x = -0.5$ and $x = 0.25$ quite well even if they are not the grid nodes.

The L_∞ error, except for the error of the polynomial interpolation, decreases as N increases. Nevertheless, we should keep in mind that the only exact conditions on the approximation are the values at nodes. We saw that the behavior of the interpolants between nodes (their smoothness) can be governed by some rules that add some, maybe subjective, information to the problem.

Since the extent of this paper is limited we present only a single example. We are aware that we can draw no principal conclusions from it.

We have been concerned only with the problem of smooth *exact interpolation of function values* at nodes (6). Moreover, the smooth approximation approach can be employed also in the *exact Hermite interpolation* (i.e. interpolation of function values as well as values of some derivatives at nodes) and in the *smoothing of data* when not the exact interpolation of data at nodes but a smooth interpolation curve (best fit curve) is required. These subjects are also covered in [3].

The 2D case is much more interesting and makes many important applications possible. The interpolation nodes can be arbitrarily placed in the plane. Particular physical use can lead to very specific requirements on the smoothness of the approximating surface. This is the direction we are going to continue this research.

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