Radek Kučera

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INTERPOLATING AND SMOOTHING BIQUADRATIC SPLINE

RADEK KUČERA, Ostrava

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Summary. The paper deals with the biquadratic splines and their use for the interpolation in two variables on the rectangular mesh. The possibilities are shown how to interpolate function values, values of the partial derivative or values of the mixed derivative. Further, the so-called smoothing biquadratic splines are defined and the algorithms for their computation are described. All of these biquadratic splines are derived by means of the tensor product of the linear spaces of the quadratic splines and their bases are given by the so-called fundamental splines.

Keywords: quadratic spline, biquadratic spline, derivative, interpolation, smoothing

AMS classification: 65D05, 65D07

1. INTRODUCTION

Let us have a closed rectangular domain $\Omega = [a, b] \times [c, d]$ in the (x, y)-plane with a mesh given by sets of knots in each of the variables

$$(\Delta xy) = (\Delta x) \times (\Delta y), \tag{1}$$

$$\begin{aligned}
&(\Delta x) = \{x_i\,;\, i \in \mathcal{I}\}, \quad (\Delta y) = \{y_j\,;\, j \in \mathcal{J}\},\\
&\mathcal{I} = \{0, 1, \ldots, n+1\}, \quad \mathcal{J} = \{0, 1, \ldots, m+1\},\\
&a = x_0 < x_1 < x_2 < \ldots < x_n < x_{n+1} = b,\\
&c = y_0 < y_1 < y_2 < \ldots < y_m < y_{m+1} = d.
\end{aligned}$$

For an interpolation on such a mesh (of cartesian product type), the tensor product technique is used which can be practically realized by means of polynomials. However, this possibility is not used very often because the common polynomial interpolation has certain bad features (nonuniform convergence, no shape preserving properties). Therefore the tensor product technique and splines are combined in [B62], [B78], [ZKM80], [N89].

The main results of this paper are stated in Sections 5 and 6 where the problems interpolation of, respectively, partial and the mixed derivatives are solved. The biquadratic splines are used because they have the extremal property which makes it possible to define smoothing splines. Similar construction for bicubic splines (interpolating function values) is shown in [I75], [ZKM80]. For the first time, an incorrect form of the minimized functional was stated for the bicubic case in [ANW67].

The possibility to use biquadratic splines for interpolation of function values is discussed in Section 4. Section 2 contains the basic knowledge about quadratic splines from [K92], [KK93]. The last Section 6 shows some examples.

2. Quadratic spline

2.1 Definition. Continuity conditions. We consider an interval $[a, b]$ and a set of knots (Δx). A function $s(x) = s_2^1(x)$ is called *a quadratic spline on the set of knots* (Δx) if it has the following properties:

a) $s(x)$ is a quadratic polynomial on every interval $[x_i, x_{i+1}]$, $i = 0(1)n$;
b) $s(x) \in C^1[a, b]$.

The set of all quadratic splines on the mesh (Δx) forms a linear space, we denote it $S(\Delta x) = S_2^1(\Delta x)$. It is also known that $\dim S(\Delta x) = n + 3$, see [B78], [ZKM80].

Denote $h_i = x_{i+1} - x_i$, $s_i = s(x_i)$, $s'_i = s'(x_i)$. The spline $s(x)$ can be written on the interval $[x_i, x_{i+1}]$ as

$$s(x) = s_i + s'_i(x - x_i) + (s'_{i+1} - s'_i)(x - x_i)^2/(2h_i). \tag{2}$$

The continuity conditions at the knots x_i, $i = 1(1)n + 1$ yield the relations between the parameters s_i, s'_i :

$$(s'_{i-1} + s'_i)/2 = (s_i - s_{i-1})/h_{i-1}, \; i = 1(1)n + 1. \tag{3}$$

2.2 F-fundamental splines. Let us have real numbers m'_0, m_i, $i \in \mathcal{I}$, and consider a spline $s(x) \in S(\Delta x)$ which interpolates the given function values:

$$s'_0 = m'_0, \; s_i = m_i, \; i \in \mathcal{I}. \tag{4}$$

The computation of the values of this spline can be done by means of the relations (3) and the formula (2). It is useful to express the solution of the problem (4) in the form

$$s(x) = m_0'\bar{h}(x) + \sum_{k=0}^{n+1} m_k h_k(x), \tag{5}$$

where $\bar{h}(x)$, $h_k(x) \in S(\Delta x)$, $k \in \mathcal{I}$, are the so-called *F-fundamental quadratic splines* which are defined by the conditions

$$\begin{aligned} h_k'(x_0) &= 0, \qquad h_k(x_i) = \delta_{ki}, \qquad i \in \mathcal{I}, \\ \bar{h}'(x_0) &= 1, \qquad \bar{h}(x_i) = 0, \qquad i \in \mathcal{I}. \end{aligned}$$

It is proved in [KK93] that the F-fundamental splines form a basis of the linear space $S(\Delta x)$.

2.3 Df-fundamental splines. Let us have real numbers m_0, m_i', $i \in \mathcal{I}$, and consider a spline $s(x) \in S(\Delta x)$ which interpolates the given values of the first derivative:

$$s_0 = m_0, \ s_i' = m_i', \ i \in \mathcal{I}. \tag{6}$$

The computation of the values of this spline can be done by means of the relations (3) and the formula (2)—similar as in Subsection 2.2. It is useful to express the solution of the problem (6) in the form

$$s(x) = m_0\bar{f}(x) + \sum_{k=0}^{n+1} m_k' f_k(x), \tag{7}$$

where $\bar{f}(x)$, $f_k(x) \in S(\Delta x)$, $k \in \mathcal{I}$, are the so-called *Df-fundamental quadratic splines* which are defined by the conditions

$$\begin{aligned} f_k(x_0) = 0, \quad f_k'(x_i) &= \delta_{ki}, \ i \in \mathcal{I}, \\ \bar{f}(x) \equiv 1 \quad &\text{on } [a, b]. \end{aligned}$$

It is proved in [KK93] that the Df-fundamental splines form a basis of the linear space $S(\Delta x)$.

2.4 Extremal properties. Smoothing spline. Let us have an interval $[a, b]$ with a mesh (Δx) and prescribed values of the first derivative m_i', $i \in \mathcal{I}$. Introduce the space of functions

$$V = \{f \in W_2^2[a, b];\ f'(x_i) = m_i', \ i \in \mathcal{I}\}$$

and the functional

$$J_1(f) = \int_a^b [f''(x)]^2 \, \mathrm{d}x. \tag{8}$$

Theorem 1. *The minimal value of $J_1(f)$ on the set V is attained for every quadratic spline $s(x) \in S(\Delta x)$ with $s_i' = m_i'$, $i \in \mathcal{I}$.* [K92]

The spline from this theorem is not unique; we can prescribe some function value for the unique determination, e.g. an initial condition $s_0 = m_0$ as in (6).

Further we will consider real numbers $\alpha > 0$ and $w_i > 0$, $i \in \mathcal{I}$, and introduce the functional

$$J_2(f) = \alpha \int_a^b [f''(x)]^2 \, \mathrm{d}x + \sum_{i=0}^{n+1} w_i [f'(x_i) - m_i']^2. \tag{9}$$

Theorem 2. *The functional $J_2(f)$ attains its minimum on $W_2^2[a,b]$ for some quadratic spline $s_\alpha(x) \in S(\Delta x)$.* [K92]

A spline $s_\alpha(x) \in S(\Delta x)$ from Theorem 2 is called *a smoothing quadratic spline.* The parameters $s_i' = s_\alpha'(x_i)$, $i \in \mathcal{I}$, of the smoothing spline can be computed from the system of linear equations derived in [K92] with tri-diagonal, symmetric and diagonally dominant matrix:

$$\begin{aligned}
(w_0 + p_0)s_0' - p_0 s_1' &= w_0 m_0', \\
-p_{i-1}s_{i-1}' + (w_i + p_{i-1} + p_i)s_i' - p_i s_{i+1}' &= w_i m_i', \ i = 1(1)n, \\
-p_n s_n' + (w_{n+1} + p_n)s_{n+1}' &= w_{n+1} m_{n+1}',
\end{aligned} \tag{10}$$

where $p_i = \alpha / h_i$.

The smoothing spline is not unique; we can prescribe some function value for the unique determination, e.g again an initial condition $s_\alpha(x_0) = m_0$.

2.5 $\mathbf{S}_\alpha$-fundamental splines. It is possible to express the smoothing quadratic spline by means of a certain basis of the linear space $S(\Delta x)$ where the prescribed values m_0, m_i', $i \in \mathcal{I}$, are used as the coefficients of the linear combination. The following lemma is needed for the construction of such a basis (see [KK93]).

Lemma 1. *Let us have a mesh (Δx), $\alpha > 0$, $w_i > 0$, m_i', $i \in \mathcal{I}$. A quadratic spline $s_\alpha(x) \in S(\Delta x)$ minimizes $J_2(f)$ on $W_2^2[a,b]$ if and only if*

$$s_i' + \alpha[s_\alpha''(x_i-) - s_\alpha''(x_i+)]/w_i = m_i', \quad i \in \mathcal{I}, \tag{11}$$

where $s_\alpha''(x_0-) = s_\alpha''(x_{n+1}+) = 0$.

We have used the notation $f(a+) = \lim\limits_{x \to a+} f(x)$, $f(a-) = \lim\limits_{x \to a-} f(x)$.

Definition 1. Let us have a mesh (Δx), $\alpha > 0$, $w_i > 0$, $i \in \mathcal{I}$. Quadratic splines $\bar{\varphi}(x) = \bar{\varphi}_\alpha(x)$, $\varphi_k(x) = \varphi_{\alpha k}(x) \in S(\Delta x)$, $k \in \mathcal{I}$, are called the S_α-fundamental splines if they have the following properties:

$$\varphi_k(x_0) = 0, \quad \varphi_k'(x_i) + \alpha[\varphi_k''(x_i-) - \varphi_k''(x_i+)]/w_i = \delta_{ki}, \quad i \in \mathcal{I},$$
$$\bar{\varphi}(x) \equiv 1 \quad on\ [a,b].$$

It is proved in [KK93] that the S_α-fundamental splines form a basis of the linear space $S(\Delta x)$. The smoothing spline from Theorem 2 can be written for arbitrary values m_k' and m_0 as

$$s_\alpha(x) = m_0 + \sum_{k=0}^{n+1} m_k' \varphi_k(x). \tag{12}$$

This formula is not suitable for computations but we will use it for construction of biquadratic splines. Of course the derivatives $s_i' = s_\alpha'(x_i)$ of this spline are computed from the system of linear equations (10) and then we use the relations (3) and the formula (2) together with some other function value (e.g. initial condition $s_0 = m_0$) for computation of the values of the smoothing spline.

3. Biquadratic spline

3.1 Definition. Representation on rectangle. Let us have a closed rectangular domain $\Omega = [a,b] \times [c,d]$ with a set of knots (Δxy) (see (1)) and let us denote the subrectangles $\Omega_{ij} = [x_i, x_{i+1}] \times [y_j, y_{j+1}]$. A function $s(x,y) = s_{22}^{11}(x,y)$ is called a *biquadratic spline on the set of knots* (Δxy) if it has the following properties:

a) $s(x,y)$ is a biquadratic polynomial on every Ω_{ij}, $i = 0(1)n$, $j = 0(1)m$;

b) $s(x,y) \in C^{11}(\Omega)$ (continuous the first derivatives $\frac{\partial s}{\partial x}$, $\frac{\partial s}{\partial y}$ and consequently the mixed derivative $\frac{\partial^2 s}{\partial x \partial y}$).

On each of the rectangles Ω_{ij} we may use for $s(x,y)$ the piecewise polynomial representation $s(x,y) = \sum_{k=0}^{2} \sum_{l=0}^{2} a_{ij}^{kl} x^k y^l$ with nine coefficients a_{ij}^{kl}, $k,l = 0(1)2$, which are generally different on different Ω_{ij}. In [K87] another representations of $s(x,y)$ on a rectangle Ω_{ij} were studied.

Denote

$$D^{kl} f(x,y) = \frac{\partial^{k+l} f}{\partial x^k \partial y^l}(x,y), \quad s_{ij}^{kl} = D^{kl} s(x_i, y_j) \tag{13}$$

where $f(x,y)$ is a function and $s(x,y)$ is a biquadratic spline. We will represent the biquadratic spline $s(x,y)$ on Ω_{ij} by means of parameters s_{ij}^{00}, s_{ij}^{10}, s_{ij}^{01}, s_{ij}^{11}, $s_{i,j+1}^{01}$, $s_{i,j+1}^{11}$, $s_{i+1,j}^{10}$, $s_{i+1,j}^{11}$, $s_{i+1,j+1}^{11}$ (see Figure 1). So we must know four parameters at each knot (x_i, y_j) (except some boundary knots). This representation is suitable for us because the one-dimensional algorithm based on the formula (2) can be used and because algorithms in the next sections will give parameters for this representation.

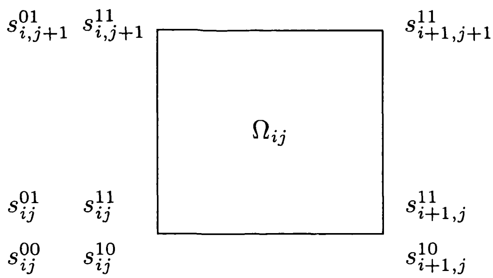

Figure 1.

(Δy) (Δx)	$h_j(y)$	$f_j(y)$	$\varphi_j(y)$
$h_i(x)$	$\mathbf{f}^{00}$	$\mathbf{f}^{01}$	$\mathbf{s}^{01}$
$f_i(x)$	$\mathbf{f}^{10}$	$\mathbf{f}^{11}$	$\mathbf{s}^{11\mathbf{y}}$
$\varphi_i(x)$	$\mathbf{s}^{10}$	$\mathbf{s}^{11\mathbf{x}}$	$\mathbf{s}^{11}$

Table 1.

3.2 Tensor product. Denote by $S(\Delta xy) = S_{22}^{11}(\Delta xy)$ the linear space of all biquadratic splines on the set of knots (Δxy). We can obtain it as the tensor product of the quadratic splines spaces in one variable $S(\Delta x)$, $S(\Delta y)$:

$$\begin{aligned} &S(\Delta xy) = S(\Delta x) \otimes S(\Delta y), \\ &\dim S(\Delta xy) = \dim S(\Delta x) \dim S(\Delta y) = (n+3)(m+3). \end{aligned} \tag{14}$$

Similar and still more general tensor product constructions are done in [B78], [ZKM80], [N89], [EMM89]. Since we constructed three various bases of the linear space of the quadratic splines in the previous sections we obtain nine various tensor product bases of the space $S(\Delta xy)$. Each of them is suitable for the solution of some problems (notation from Table 1 is used):

- $\mathbf{f}^{00}$ – interpolation of the given function values $s_{ij}^{00} = m_{ij}^{00}$;
- $\mathbf{f}^{10}$ – interpolation of the given values of the partial derivative $s_{ij}^{10} = m_{ij}^{10}$;
- $\mathbf{f}^{11}$ – interpolation of the given values of the mixed derivative $s_{ij}^{11} = m_{ij}^{11}$;
- $\mathbf{s}^{10}$ – smoothing spline for the given values of the partial derivative $s_{ij}^{10} = m_{ij}^{10}$;
- $\mathbf{s}^{11}$ – smoothing spline for the given values of the mixed derivative $s_{ij}^{11} = m_{ij}^{11}$;
- $\mathbf{s}^{11\mathbf{x}}$ – smoothing spline for the given values of the mixed derivative $s_{ij}^{11} = m_{ij}^{11}$, where the smoothing is done in the x-variable;

the cases $\mathbf{f}^{01}$, $\mathbf{s}^{01}$, $\mathbf{s}^{11\mathbf{y}}$ are analogous.

We have to prescribe further $n+m+5$ parameters for the solution of each such problem because $\dim S(\Delta xy)$ is greater than the number of the knots (x_i, y_j) (see (14)).

4. Interpolation of the given function values

Let us have values m_{ij}^{00}, $i \in \mathcal{I}$, $j \in \mathcal{J}$. We search for a spline $s(x,y) \in S(\Delta xy)$ such that

$$s_{ij}^{00} = m_{ij}^{00}, \ i \in \mathcal{I}, \ j \in \mathcal{J}. \tag{15}$$

For uniqueness we must prescribe other $n+m+5$ parameters, e.g.

$$s_{00}^{11} = m_{00}^{11} \ \ s_{0j}^{10} = m_{0j}^{10}, \ \ s_{i0}^{01} = m_{i0}^{01}, \ \ j \in \mathcal{J}, \ i \in \mathcal{I}. \tag{16}$$

Theorem 3. *There exists a unique solution $s(x,y) \in S(\Delta xy)$ of the problem* (15), (16).

Proof. The linear space $S(\Delta xy)$ has the tensor product basis $\mathbf{f}^{00}$:

$$\bar{h}(x)\bar{h}(y), \ \bar{h}(x)h_j(y), \ h_i(x)\bar{h}(y), \ h_i(x)h_j(y), \ \ i \in \mathcal{I}, \ j \in \mathcal{J},$$

where $\bar{h}(x)$, $h_i(x)$ (or $\bar{h}(y)$, $h_j(y)$) are the F-fundamental splines on the mesh (Δx) (or (Δy), respectively). It follows from their construction that the spline

$$\begin{aligned} s(x,y) = m_{00}^{11}\bar{h}(x)\bar{h}(y) &+ \sum_{i=0}^{n+1} m_{i0}^{01} h_i(x)\bar{h}(y) \\ &+ \sum_{j=0}^{m+1} m_{0j}^{10}\bar{h}(x)h_j(y) + \sum_{i=0}^{n+1}\sum_{j=0}^{m+1} m_{ij}^{00} h_i(x)h_j(y) \end{aligned}$$

solves the problem (15), (16). □

From the last formula we have

$$\begin{cases} s(x_i,y) = m_{i0}^{01}\bar{h}(y) + \displaystyle\sum_{j=0}^{m+1} m_{ij}^{00} h_j(y), \quad i \in \mathcal{I}, \\ s(x,y_j) = m_{0j}^{10}\bar{h}(x) + \displaystyle\sum_{i=0}^{n+1} m_{ij}^{00} h_i(x), \quad j \in \mathcal{J}, \\ D^{01}s(x,y_0) = m_{00}^{11}\bar{h}(x) + \displaystyle\sum_{i=0}^{n+1} m_{i0}^{01} h_i(x), \\ D^{10}s(x_i,y) = s_{i0}^{11}\bar{h}(y) + \displaystyle\sum_{j=0}^{m+1} s_{ij}^{10} h_j(y), \quad i \in \mathcal{I}. \end{cases} \tag{17}$$

The first formula (17) shows for fixed $i \in \mathcal{I}$ that $s(x_i, y)$ is the quadratic spline which interpolates the function values $s_j = m_{ij}^{00}$, $j \in \mathcal{J}$, on the mesh (Δy) and complies with the initial condition $s'_0 = m_{i0}^{01}$ (compare with (5)). Therefore we can use the relations (3) for the computation of the values $s_{ij}^{01} = s'_j$, $j \in \mathcal{J}$—this is the first step of the following algorithm. A similar consideration for the other formulas (17) gives the other steps of the algorithm.

Algorithm 1.

1° Compute s_{ij}^{01}, $j \in \mathcal{J}$, from the values m_{i0}^{01}, m_{ij}^{00}, $j \in \mathcal{J}$, on the vertical lines $x = x_i$, $i \in \mathcal{I}$;

2° compute s_{ij}^{10}, $i \in \mathcal{I}$, from the values m_{0j}^{10}, m_{ij}^{00}, $i \in \mathcal{I}$, on the horizontal lines $y = y_j$, $j \in \mathcal{J}$;

3° compute s_{i0}^{11}, $i \in \mathcal{I}$, from the values m_{00}^{11}, m_{i0}^{01}, $i \in \mathcal{I}$, on the horizontal line $y = y_0$;

4° compute s_{ij}^{11}, $j \in \mathcal{J}$, from the values s_{i0}^{11}, s_{ij}^{10}, $j \in \mathcal{J}$, on the vertical lines $x = x_i$, $i \in \mathcal{I}$.

We know the values s_{ij}^{00}, s_{ij}^{10}, s_{ij}^{01}, s_{ij}^{11} at all knots (x_i, y_j) after using this algorithm.

5. Interpolation and smoothing of the partial derivatives

5.1 Formulation and solution of the problem. Let us have values m_{ij}^{10}, $i \in \mathcal{I}$, $j \in \mathcal{J}$. We search for a spline $s(x,y) \in S(\Delta xy)$ such that

$$s_{ij}^{10} = m_{ij}^{10}, \quad i \in \mathcal{I},\ j \in \mathcal{J}. \tag{18}$$

For uniqueness we must prescribe other $n + m + 5$ parameters, e.g.

$$s_{00}^{01} = m_{00}^{01}, \quad s_{0j}^{00} = m_{0j}^{00}, \quad s_{i0}^{11} = m_{i0}^{11}, \quad j \in \mathcal{J},\ i \in \mathcal{I}. \tag{19}$$

Theorem 4. *There exists a unique solution $s(x,y) \in S(\Delta xy)$ of the problem* (18), (19).

Proof. The linear space $S(\Delta xy)$ has the tensor product basis $\mathbf{f}^{10}$:

$$\bar{f}(x)\bar{h}(y),\ \bar{f}(x)h_j(y),\ f_i(x)\bar{h}(y),\ f_i(x)h_j(y),\quad i \in \mathcal{I}, j \in \mathcal{J},$$

where $\bar{f}(x)$, $f_i(x)$ are the Df-fundamental splines on the mesh (Δx) and $\bar{h}(y)$, $h_j(y)$ are the F-fundamental splines on the mesh (Δy). It follows from their construction that the spline

$$\begin{aligned} s(x,y) = m_{00}^{01}\bar{h}(y) &+ \sum_{i=0}^{n+1} m_{i0}^{11} f_i(x)\bar{h}(y) \\ &+ \sum_{j=0}^{m+1} m_{0j}^{00} h_j(y) + \sum_{i=0}^{n+1}\sum_{j=0}^{m+1} m_{ij}^{10} f_i(x) h_j(y) \end{aligned}$$

solves the problem (18), (19). $\square$

From the last formula we have

$$
(20) \qquad \begin{cases} s(x,y_j) = m_{0j}^{00} + \sum_{i=0}^{n+1} m_{ij}^{10} f_i(x), \quad j \in \mathcal{J}, \\ D^{10}s(x_i,y) = m_{i0}^{11}\bar{h}(y) + \sum_{j=0}^{m+1} m_{ij}^{10} h_j(y), \quad i \in \mathcal{I}, \\ s(x_0,y) = m_{00}^{01}\bar{h}(y) + \sum_{j=0}^{m+1} m_{0j}^{00} h_j(y), \\ D^{01}s(x,y_j) = s_{0j}^{01} + \sum_{i=0}^{n+1} s_{ij}^{11} f_i(x), \quad j \in \mathcal{J}. \end{cases}
$$

From the formulas (20), we obtain the following algorithm for the computation of the parameters s_{ij}^{00}, s_{ij}^{01}, s_{ij}^{11}, $i \in \mathcal{I}$, $j \in \mathcal{J}$, by means of a similar argument as we have obtained Algorithm 1.

Algorithm 2.

1° Compute s_{ij}^{00}, $i \in \mathcal{I}$, from the values m_{0j}^{00}, m_{ij}^{10}, $i \in \mathcal{I}$, on the horizontal lines $y = y_j$, $j \in \mathcal{J}$;

2° compute s_{ij}^{11}, $j \in \mathcal{J}$, from the values m_{i0}^{11}, m_{ij}^{10}, $j \in \mathcal{J}$, on the vertical lines $x = x_i$, $i \in \mathcal{I}$;

3° compute s_{0j}^{01}, $j \in \mathcal{J}$, from the values m_{00}^{01}, m_{0j}^{00}, $j \in \mathcal{J}$, on the vertical line $x = x_0$;

4° compute s_{ij}^{01}, $i \in \mathcal{I}$, from the values s_{0j}^{01}, s_{ij}^{11}, $i \in \mathcal{I}$, on the horizontal lines $y = y_j$, $j \in \mathcal{J}$.

5.2 Extremal properties. On the rectangle $\Omega = [a,b] \times [c,d]$ let us have a mesh (Δxy) and prescribed values of the partial derivative with respect to the x-variable m_{ij}^{10}, $i \in \mathcal{I}$, $j \in \mathcal{J}$. Introduce the set of functions

$$
V_1 = \{f \in W_2^{22}(\Omega);\, D^{10}f(x_i,y_j) = m_{ij}^{10}, i \in \mathcal{I}, j \in \mathcal{J}\}
$$

and the functional

$$
J_3(f) = \sum_{j=0}^{m+1} \int_a^b [D^{20}f(x,y_j)]^2 \,\mathrm{d}x.
$$

Theorem 5. *The minimal value of $J_3(f)$ on the set V_1 is attained for every biquadratic spline $s(x,y) \in S(\Delta xy)$ with $s_{ij}^{10} = m_{ij}^{10}$, $i \in \mathcal{I}$, $j \in \mathcal{J}$.*

Proof. Let us have $f \in V_1$, $s \in V_1 \cap S(\Delta xy)$, then

$$J_3(f-s) = J_3(f) - J_3(s) - 2\sum_{j=0}^{m+1} I_j,$$

where

$$\begin{aligned} I_j &= \int_a^b [D^{20}f(x,y_j) - D^{20}s(x,y_j)]D^{20}s(x,y_j)\,\mathrm{d}x \\ &= \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} [D^{20}f(x,y_j) - D^{20}s(x,y_j)]D^{20}s(x,y_j)\,\mathrm{d}x. \end{aligned} \tag{21}$$

Using integration by parts and the identity $D^{30}s(x,y_j) \equiv 0$ on $[x_i, x_{i+1}]$ we obtain

$$\begin{aligned} &\int_{x_i}^{x_{i+1}} [D^{20}f(x,y_j) - D^{20}s(x,y_j)]D^{20}s(x,y_j)\,\mathrm{d}x \\ &\quad = [D^{10}f(x_{i+1},y_j) - D^{10}s(x_{i+1},y_j)]D^{20}s(x_{i+1}-,y_j) - \\ &\quad\quad - [D^{10}f(x_i,y_j) - D^{10}s(x_i,y_j)]D^{20}s(x_i+,y_j) = 0. \end{aligned}$$

Therefore $0 \leqslant J_3(f-s) = J_3(f) - J_3(s)$, which implies $J_3(s) \leqslant J_3(f)$. □

The spline from this theorem is not unique; we must prescribe other parameters for its unique determination, for example (19).

5.3 Smoothing spline. We will use the notation from Subsection 5.2. Further let us have $\alpha > 0$ and $v_i > 0$, $i \in \mathcal{I}$. Denote

$$J_4(f) = \alpha J_3(f) + \sum_{i=0}^{n+1}\sum_{j=0}^{m+1} v_i[D^{10}f(x_i,y_j) - m_{ij}^{10}]^2.$$

Lemma 2. *The spline $s(x,y) \in S(\Delta xy)$ minimizes $J_4(f)$ on $W_2^{22}(\Omega)$ if and only if*

$$s_{ij}^{10} + \alpha d_{ij}/v_i = m_{ij}^{10}, \quad i \in \mathcal{I}, j \in \mathcal{J}, \tag{22}$$

where $d_{ij} = D^{20}s(x_i-,y_j) - D^{20}s(x_i+,y_j)$ and $D^{20}s(x_0-,y_j) = D^{20}s(x_{n+1}+,y_j) = 0$.

Proof. a) First let us prove that the conditions (22) are necessary. Let us consider a biquadratic spline $s(x,y) \in S(\Delta xy)$ which minimizes the functional $J_4(f)$.

Introduce for $t \in R$ the spline $s_1(x,y) = s(x,y) + tf_k(x)h_l(y)$, where $f_k(x)$ or $h_l(y)$ is a Df-fundamental or an F-fundamental spline, respectively. Then

$$J_4(s_1) - J_4(s) = t^2 a_{kl} + 2tb_{kl}$$

with

$$a_{kl} = \alpha \int_a^b [f_k''(x)]^2 \, \mathrm{d}x + v_k > 0,$$

$$b_{kl} = \alpha \int_a^b f_k''(x) D^{20} s(x, y_l) \, \mathrm{d}x + v_k [D^{10} s(x_k, y_l) - m_{kl}^{10}].$$

If $b_{kl} \neq 0$ then we have a contradiction because the real number t can be chosen such that $|t| < 2|b_{kl}|/a_{kl}$, $\operatorname{sgn}(t) = \operatorname{sgn}(b_{kl})$ and we obtain $J_4(s_1) < J_4(s)$. Therefore

$$(23) \qquad 0 = b_{kl} = \alpha \sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} f_k''(x) D^{20} s(x, y_l) \, \mathrm{d}x + v_k [D^{10} s(x_k, y_l) - m_{kl}^{10}].$$

Using integration by parts and the identity $D^{30} s(x, y_l) \equiv 0$ on $[x_i, x_{i+1}]$ for the integrals in formula (23) we obtain

$$\sum_{i=0}^{n} \int_{x_i}^{x_{i+1}} f_k''(x) D^{20} s(x, y_l) \, \mathrm{d}x = D^{20} s(x_k-, y_l) - D^{20} s(x_k+, y_l).$$

Substituting this result into (23) we obtain (22).

b) We shall prove that the conditions (22) are sufficient. Let us have $f(x,y) \in W_2^{22}(\Omega)$ and let the spline $s(x,y) \in S(\Delta xy)$ comply with (22). Denote

$$\bar{J}_4(f - s) = \alpha J_3(f - s) + \sum_{i=0}^{n+1} \sum_{j=0}^{m+1} v_i [D^{10} f(x_i, y_j) - D^{10} s(x_i, y_j)]^2 \geqslant 0.$$

This functional can be rewritten also as

$$\bar{J}_4(f - s) = J_4(f) - J_4(s) - 2\left(\alpha \sum_{j=0}^{m+1} I_j + M\right),$$

where I_j are defined by (21) and

$$M = \sum_{i=0}^{n+1} \sum_{j=0}^{m+1} v_i [D^{10} f(x_i, y_j) - D^{10} s(x_i, y_j)][D^{10} s(x_i, y_j) - m_{ij}^{10}].$$

By the same computation as in the proof of Theorem 5 and using conditions (22) we now obtain

$$\sum_{j=0}^{m+1} I_j = -M/\alpha.$$

So it follows that $J_4(f) - J_4(s) = \bar{J}_4(f - s) \geqslant 0$, which proves the lemma. □

Theorem 6. *The functional $J_4(f)$ attains its minimum on $W_2^{22}(\Omega)$ for some biquadratic spline $s_\alpha(x,y) \in S(\Delta xy)$. Its derivatives s_{ij}^{10}, $i \in \mathcal{I}$, $j \in \mathcal{J}$, are defined uniquely.*

Proof. a) The linear space $S(\Delta xy)$ has the tensor product basis $\mathbf{s}^{10}$:

$$\bar{\varphi}(x)\bar{h}(y),\ \bar{\varphi}(x)h_j(y),\ \varphi_i(x)\bar{h}(y),\ \varphi_i(x)h_j(y),\quad i \in \mathcal{I}, j \in \mathcal{J},$$

where $\bar{h}(y)$, $h_j(y)$ are the F-fundamental splines on the mesh (Δy) and $\bar{\varphi}(x)$, $\varphi_i(x)$ are the S_α-fundamental splines on the mesh (Δx) with the parameters $w_i = u_i$. It is easy to verify that the spline

$$\begin{aligned} s_\alpha(x,y) = {} & m_{00}^{01}\bar{h}(y) + \sum_{i=0}^{n+1} m_{i0}^{11}\varphi_i(x)\bar{h}(y) + \\ & + \sum_{j=0}^{m+1} m_{0j}^{00} h_j(y) + \sum_{i=0}^{n+1}\sum_{j=0}^{m+1} m_{ij}^{10}\varphi_i(x)h_j(y) \end{aligned} \tag{24}$$

fulfils the conditions (22) for arbitrary values m_{00}^{01}, m_{i0}^{11}, $m_{0j}^{00} \in R$.

b) Suppose that in addition to the spline (24) there exists another biquadratic spline $\bar{s}(x,y) \in S(\Delta xy)$ with $D^{10}s_1(x_k,y_l) \neq D^{10}s_\alpha(x_k,y_l)$ for certain indices k, l which minimizes $J_4(f)$. It can be also expressed in terms of the basis $\mathbf{s}^{10}$ with some coefficients n_{00}^{01}, n_{i0}^{11}, n_{0j}^{00}, n_{ij}^{10} as

$$\bar{s}(x,y) = n_{00}^{01}\bar{h}(y) + \sum_{i=0}^{n+1} n_{i0}^{11}\varphi_i(x)\bar{h}(y) + \sum_{j=0}^{m+1} n_{0j}^{00}h_j(y) + \sum_{i=0}^{n+1}\sum_{j=0}^{m+1} n_{ij}^{10}\varphi_i(x)h_j(y).$$

For certain indices p, q, $n_{pq}^{10} \neq m_{pq}^{10}$ and we obtain a contradiction because the condition (22) cannot be fulfilled for the spline $\bar{s}(x,y)$ at the knot (x_p,y_q). □

A spline $s_\alpha(x,y) \in S(\Delta xy)$ from the last theorem is called a *smoothing biquadratic spline for the partial derivatives with respect to the x-variable.*

From (24) we obtain

$$D^{10}s_\alpha(x,y_j) = \sum_{i=0}^{n+1} m_{ij}^{10}\varphi_i'(x),\ j \in \mathcal{J}.$$

This formula shows how to compute the values s_{ij}^{10} of the smoothing spline because for a fixed j the expression on the right-hand side is the derivative of a one-dimensional smoothing spline on the mesh (Δx) which smoothes the first derivatives $m_i' = m_{ij}^{10}$, $i \in \mathcal{I}$. Compare with (12).

Algorithm 3.

1° Compute $s_{ij}^{10} = s_i'$, $i \in \mathcal{I}$, from the system of linear equations (10) where $w_i = v_i$, $m_i' = m_{ij}^{10}$ and $p_i = \alpha/(x_{i+1} - x_i)$, $i \in \mathcal{I}$, on each horizontal line $y = y_j$, $j \in \mathcal{J}$.

The values s_{ij}^{10}, $i \in \mathcal{I}$, $j \in \mathcal{J}$, do not determine the smoothing spline uniquely, therefore we must give other $n + m + 5$ suitable parameters. If we prescribe the values (19) we can use Algorithm 2 for the subsequent computation.

6. Interpolation and smoothing of the mixed derivatives

6.1 Formulation and solution of the problem. Let us have values m_{ij}^{11}, $i \in \mathcal{I}$, $j \in \mathcal{J}$. We search for a spline $s(x,y) \in S(\Delta xy)$ such that

$$s_{ij}^{11} = m_{ij}^{11}, \quad i \in \mathcal{I}, j \in \mathcal{J}. \tag{25}$$

For uniqueness we must prescribe other $n + m + 5$ parameters, for example

$$s_{00}^{00} = m_{00}^{00}, \quad s_{i0}^{10} = m_{i0}^{10}, \quad s_{0j}^{01} = m_{0j}^{01}, \quad i \in \mathcal{I}, j \in \mathcal{J}. \tag{26}$$

Theorem 7. *There exists a unique solution $s(x,y) \in S(\Delta xy)$ of the problem* (25), (26).

The proof is analogous to that of Theorem 4 or Theorem 3. The spline which solves the problem (25), (26) can be written by means of the tensor product basis $\mathbf{f}^{11}$ as

$$s(x,y) = m_{00}^{00} + \sum_{i=0}^{n+1} m_{i0}^{10} f_i(x) + \sum_{j=0}^{m+1} m_{0j}^{01} f_j(y) + \sum_{i=0}^{n+1} \sum_{j=0}^{m+1} m_{ij}^{11} f_i(x) f_j(y)$$

where $f_i(x)$ and $f_j(y)$ are the Df-fundamental splines on the mesh (Δx) and (Δy), respectively. From this formula we have

$$\begin{cases} D^{10}s(x_i,y) = m_{i0}^{10} + \sum_{j=0}^{m+1} m_{ij}^{11} f_j(y), \quad i \in \mathcal{I}, \\ D^{01}s(x,y_j) = m_{0j}^{01} + \sum_{i=0}^{n+1} m_{ij}^{11} f_i(x), \quad j \in \mathcal{J}, \\ s(x,y_0) = m_{00}^{00} + \sum_{i=0}^{n+1} m_{i0}^{10} f_i(x), \\ s(x_i,y) = s_{i0}^{00} + \sum_{j=0}^{m+1} s_{ij}^{01} f_j(y), \quad i \in \mathcal{I}. \end{cases} \tag{27}$$

From the formulas (27) we obtain the following algorithm for the computation of the values s_{ij}^{00}, s_{ij}^{10}, s_{ij}^{01}, $i \in \mathcal{I}$, $j \in \mathcal{J}$, by means of similar argument as Algorithm 1 was obtained.

Algorithm 4.

1° Compute s_{ij}^{10}, $j \in \mathcal{J}$, from the values m_{i0}^{10}, m_{ij}^{11}, $j \in \mathcal{J}$, on the vertical lines $x = x_i$, $i \in \mathcal{I}$;

2° compute s_{ij}^{01}, $i \in \mathcal{I}$, from the values m_{0j}^{01}, m_{ij}^{11}, $i \in \mathcal{I}$, on the horizontal lines $y = y_j$, $j \in \mathcal{J}$;

3° compute s_{i0}^{00}, $i \in \mathcal{I}$, from the values m_{00}^{00}, m_{i0}^{10}, $i \in \mathcal{I}$, on the horizontal line $y = y_0$;

4° compute s_{ij}^{00}, $j \in \mathcal{J}$, from the values s_{i0}^{00}, s_{ij}^{01}, $j \in \mathcal{J}$, on the vertical lines $x = x_i$, $i \in \mathcal{I}$.

6.2 Extremal properties. Let us have rectangle $\Omega = [a,b] \times [c,d]$ with a mesh (Δxy), prescribed values of the mixed derivative m_{ij}^{11} and parameters $u_i > 0$, $v_j > 0$, $i \in \mathcal{I}$, $j \in \mathcal{J}$, $\alpha > 0$. Introduce the set of functions

$$V_2 = \{f \in W_2^{22}(\Omega); D^{11} f(x_i, y_j) = m_{ij}^{11}, i \in \mathcal{I}, j \in \mathcal{J}\}$$

and the functional

$$\begin{aligned} J_5(f) = & \int_a^b \int_c^d [D^{22} f(x,y)]^2 \, \mathrm{d}y \, \mathrm{d}x \\ & + \frac{1}{\alpha} \Big\{ \sum_{i=0}^{n+1} u_i \int_c^d [D^{12} f(x_i, y)]^2 \, \mathrm{d}y + \sum_{j=0}^{m+1} v_j \int_a^b [D^{21} f(x, y_j)]^2 \, \mathrm{d}x \Big\}. \end{aligned}$$

The parameter α could be included into the parameters u_i, v_j at the integrals. We write it separately because it is suitable for the construction of the smoothing spline.

Theorem 8. *The minimal value of $J_5(f)$ on the set V_2 is attained for every biquadratic spline $s(x,y) \in S(\Delta xy)$ with $s_{ij}^{11} = m_{ij}^{11}$, $i \in \mathcal{I}$, $j \in \mathcal{J}$.*

The proof is analogous to that of Theorem 5, only some adjustments must be done in both variables. The spline from this theorem is again not unique; we must prescribe other parameters for its unique determination, for example (26).

6.3 Smoothing spline. This section is analogous to Section 5.3, similar constructions are also done for bicubic splines in [ZKM80], [EMM89]. Now we are using notation from Section 6.2 and further denote

$$J_6(f) = \alpha^2 J_5(f) + \sum_{i=0}^{n+1} \sum_{j=0}^{m+1} u_i v_j [D^{11} f(x_i, y_j) - m_{ij}^{11}]^2.$$

Lemma 3. *The spline $s(x,y) \in S(\Delta xy)$ minimizes $J_6(f)$ on $W_2^{22}(\Omega)$ if and only if*

$$s_{ij}^{11} + \alpha^2 d_{ij}/(u_i v_j) = m_{ij}^{11}, \quad i \in \mathcal{I},\ j \in \mathcal{J}, \tag{28}$$

where

$$d_{ij} = \left[[D^{22}s(x,y)]_{x_i+}^{x_i-}\right]_{y_j+}^{y_j-} + \frac{1}{\alpha}\{u_i[D^{12}s(x_i,y)]_{y_j+}^{y_j-} + v_j[D^{21}s(x,y_j)]_{x_i+}^{x_i-}\}$$

and $D^{12}(x_i,y_0-) = D^{12}(x_i,y_{m+1}+) = D^{21}s(x_0-,y_j) = D^{21}s(x_{n+1},y_j) = 0$.

This lemma can be used to prove the following theorem.

Theorem 9. *The functional $J_6(f)$ attains its minimum on $W_2^{22}(\Omega)$ for some biquadratic spline $s_\alpha(x,y) \in S(\Delta xy)$. Its mixed derivatives s_{ij}^{11}, $i \in \mathcal{I}$, $j \in \mathcal{J}$, are defined uniquely.*

A spline from Theorem 9 is called a *smoothing spline for the mixed derivatives* and can be expressed in terms of the tensor product basis $\mathbf{s}^{11}$ as

$$s_\alpha(x,y) = m_{00}^{00} + \sum_{i=0}^{n+1} m_{i0}^{10}\varphi_i(x) + \sum_{j=0}^{m+1} m_{0j}^{01}\varphi_j(y) + \sum_{i=0}^{n+1}\sum_{j=0}^{m+1} m_{ij}^{11}\varphi_i(x)\varphi_j(y)$$

with arbitrary $m_{00}^{00}, m_{i0}^{10}, m_{0j}^{01} \in R$ where $\varphi_i(x)$ and $\varphi_j(y)$ are the S_α-fundamental splines on the mesh (Δx) with parameters $w_i = u_i$ and on the mesh (Δy) with the parameters $w_j = v_j$, respectively . This formula gives

$$D^{11}s_\alpha(x,y) = \sum_{i=0}^{n+1}\sum_{j=0}^{m+1} m_{ij}^{11}\varphi_i'(x)\varphi_j'(y).$$

If we denote

$$s_j'(x) = \sum_{i=0}^{n+1} m_{ij}^{11}\varphi_i'(x), \quad j \in \mathcal{J}, \tag{29}$$

then the mixed derivatives of the spline $s_\alpha(x,y)$ on the lines $x = x_i$ can be rewritten in the form

$$D^{11}s_\alpha(x_i,y) = \sum_{j=0}^{m+1} s_j'(x_i)\varphi_j'(y), \quad i \in \mathcal{I}. \tag{30}$$

The formula (29) can be interpreted for fixed j as the derivative of a one-dimensional smoothing quadratic spline which smoothes the first derivatives $m_i' = m_{ij}^{11}$, $i \in \mathcal{I}$ on the mesh (Δx), see (12). Similarly, the formula (30) can be interpreted for fixed i as the derivative of a quadratic spline which smoothes the first derivatives $m_j' = s_j'(x_i)$, $j \in \mathcal{J}$, on the mesh (Δy).

Algorithm 5.

1° Compute $s'_j(x_i) = s'_i$, $i \in \mathcal{I}$, from the system of linear equations (10) where $w_i = u_i$, $m'_i = m^{11}_{ij}$ and $p_i = \alpha/(x_{i+1} - x_i)$, $i \in \mathcal{I}$, on each horizontal line $y = y_j$, $j \in \mathcal{J}$;

2° compute $s^{11}_{ij} = s'_j$, $j \in \mathcal{J}$, from the system of linear equations (10) where $w_j = v_j$, $m'_j = s'_j(x_i)$ and $p_j = \alpha/(y_{j+1} - y_j)$, $j \in \mathcal{J}$, on each horizontal line $x = x_i$, $i \in \mathcal{I}$.

The values s^{11}_{ij}, $i \in \mathcal{I}$, $j \in \mathcal{J}$, do not determine the smoothing spline uniquely, therefore we must give other $m + n + 5$ suitable parameters. If we prescribe the parameters (26) we can use Algorithm 4 for the subsequent computation.

7. Examples

We interpolate the function

$$f(x, y) = \mathrm{e}^{\sin x \sin y} \quad \text{on} \quad \Omega = [0, 5] \times [0, 5]$$

with the mesh of equidistant knots $(\Delta xy) = \{(5i/7, 5j/7),\ i = 0(1)7,\ j = 0(1)7\}$. All parameters for the computations are taken exactly from the function or its derivatives except for the example drawn in Figure 5. In this figure the biquadratic spline is constructed by means of Algorithm 4 but the necessary derivatives were computed by formulas for the numerical derivative from the function values.

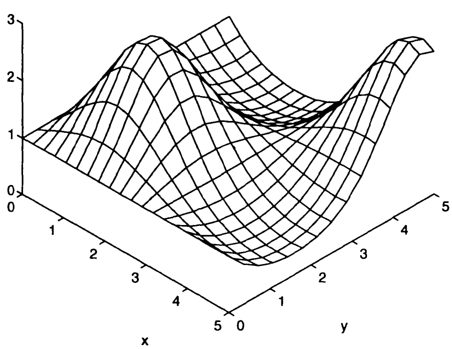

Figure 2 – graph of the function $f(x, y)$;

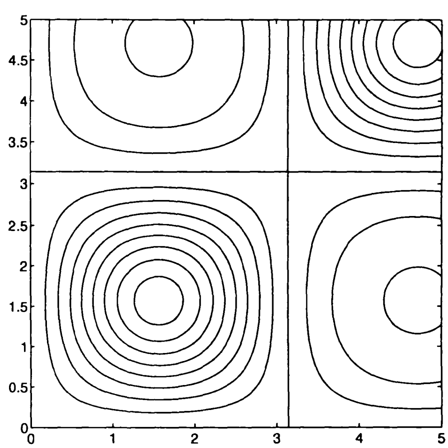

Figure 3 – isolines of the function $f(x, y)$;

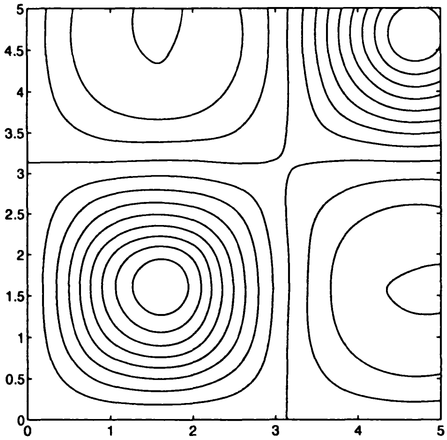

Figure 4 – interpolation of the function values (Alg. 1);

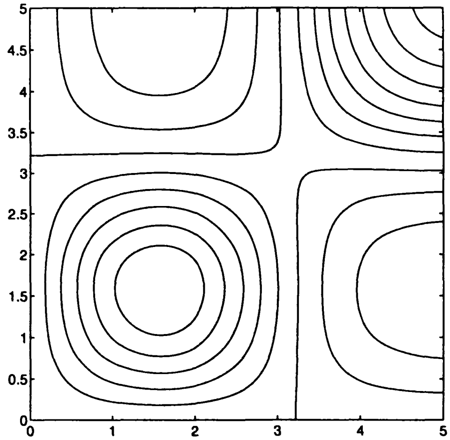

Figure 5 – interpolation of the values of the mixed derivative (Alg. 4) given by formulas of the numerical derivative from the function values;

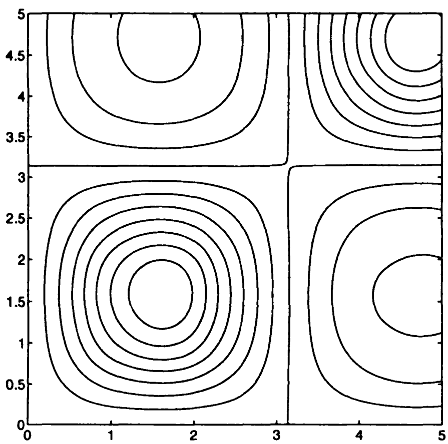

Figure 6 – interpolation of the values of the partial derivative with respect to the x-variable (Alg. 2);

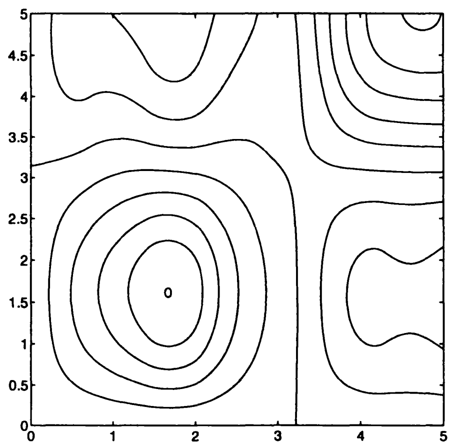

Figure 7 – smoothing spline for the values of the partial derivative (Alg. 3), $v_i = 1$, $\alpha = 1$;

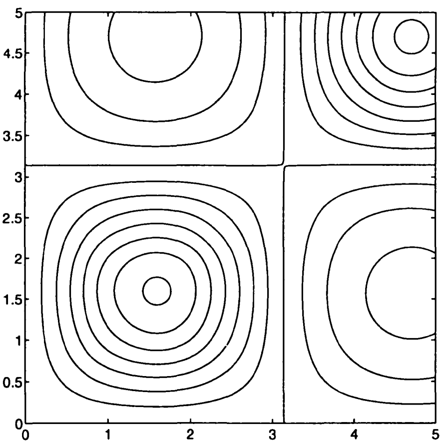

Figure 8 – interpolation of the values of the mixed derivative (Alg. 4);

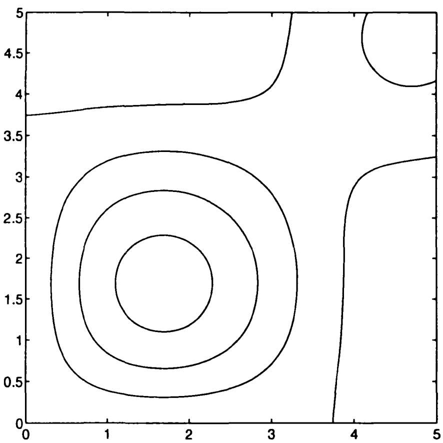

Figure 9 – smoothing spline for the values of the mixed derivative (Alg. 5), $u_i = v_j = 1$, $\alpha = 0.2$.

Differences between the isolines are 0.2.

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Author's address: *Radek Kučera*, Technical University in Ostrava, Institut of Mathematics, třída 17. listopadu 33, 708 33 Ostrava-Poruba, Czech Republic.